

ПРИМЉЕНО:		04.02.2020	
Рад.јед.	б р о ј	Арх.шифра	Прилог
ФР01	138/1		

Научном већу Института за физику у Београду

Београд, 4. фебруар 2020. године

Предмет: Молба за покретање поступка за избор у звање научни сарадник

М О Л Б А

С обзиром да испуњавам критеријуме прописане од стране Министарства просвете, науке и технолошког развоја за избор у звање научни сарадник, молим Научно веће Института за физику у Београду да покрене поступак за мој избор у звање научни сарадник.

У прилогу достављам:

1. мишљење руководиоца лабораторије са предлогом комисије за избор у звање;
2. стручну биографију;
3. преглед научне активности;
4. елементе за квалитативну и квантитативну оцену научног доприноса са доказима;
5. списак и копије објављених радова и других публикација;
6. податке о цитираности;
7. уверење о одбрањеној докторској дисертацији.

С поштовањем,


др Душан Вудраговић

ПРИМЉЕНО: 04.02.2020			
Рад.јед.	б р о	Арх.шифра	Прилог
0901	138/2		

Научном већу Института за физику у Београду

Предмет: Мишљење руководиоца Центра о избору др Душана Вудраговића у звање научни сарадник

Др Душан Вудраговић је запослен у Лабораторији за примену рачунара у науци, у оквиру Националног центра изузетних вредности за изучавање комплексних система Института за физику у Београду. У истраживачком раду бави се физиком ултрахладних диполних Бозе гасова, као и развојем паралелних нумеричких алгоритама за проучавање оваквих система. С обзиром да испуњава све предвиђене услове у складу са Правилником о поступку, начину вредновања и квантитативном исказивању научноистраживачких резултата истраживача МПНТР, сагласан сам са покретањем поступка за избор др Душана Вудраговића у звање научни сарадник.

За састав комисије за избор др Душана Вудраговића у звање научни сарадник предлажем:

- (1) др Антун Балаж, научни саветник, Институт за физику у Београду,
- (2) др Ивана Васић, виши научни сарадник, Институт за физику у Београду,
- (3) проф. др Милан Дамњановић, редовни професор Физичког факултета Универзитета у Београду.

др Антун Балаж
научни саветник
руководилац Центра за изучавање
комплексних система

Стручна биографија Душана Вудраговића

Душан Вудраговић је рођен 3. маја 1980. године у Сремској Митровици. Основну школу Доситеј Обрадовић завршио је у Путинцима, а Гимназију Стеван Пузић у Руми. Основне студије је похађао на Физичком факултету Универзитета у Београду на смеру Примењена физика и информатика у периоду од 1999. до 2005. године. Током студија добио је стипендије Министарства науке Републике Србије и Владе Републике Србије, као и награду 1000 најбољих студената у Србији Норвешке амбасаде у Београду. Дипломирао је 2005. године са просечном оценом 9.62. Дипломски рад под називом Мерење ефективне трансверзалне емитансе јонског снопа урадио је под руководством проф. др Ивана Аничина.

У периоду од 2006. до 2008. године боравио је у ЦЕРН-у (Женева) као сарадник на ФП6 пројектима SEE-GRID-2 (SEE-GRID eInfrastructure for regional eScience) и EGEE-II (Enabling Grids for E-science).

Докторске студије на Физичком факултету Универзитета у Београду уписао је 2012. године. Докторску дисертацију под насловом Faraday waves in ultracold dipolar Bose gases (Фарадејеви таласи у ултрахладним диполним Бозе гасовима) урађену под менторством др Антуна Балажа, одбранио је 24. децембра 2019. године.

Душан Вудраговић је запослен у Институту за физику у Београду као истраживач сарадник у Лабораторији за примену рачунара у науци Националног центра изузетних вредности за изучавање комплексних система. У оквиру међународне сарадње, тренутно је ангажован на Хоризонт 2020 пројектима NI4OS-Europe (*National Initiatives for Open Science in Europe*) и SMARTCHAIN (*Towards Innovation - driven and smart solutions in short food supply chains*).

До сада је Душан Вудраговић објавио 23 рада у међународним часописима и више саопштења са међународних скупова штампаних у изводу.

Преглед научне активности Душана Вудраговића

Душан Вудраговић је започео свој истраживачки рад на АТЛАС колаборацији 2008. године. Ангажованост на АТЛАС колаборацији прекида 2012. године, након чега, под менторством др Антуна Балажа, ради у Лабораторији за примену рачунара у науци на Институту за физику у Београду. У свом научном раду бави се проблемима ултрахладних бозонских гасова у присуству дипол-дипол интеракције, као и развојем паралелних нумеричких алгоритама и програма за нумеричке симулације ових физичких система.

Кандидат је успешно развио и имплементирао нумерички метод подељеног корака за решавање Грос-Питаевски једначине са контактним и диполним интеракционим чланом. Метод је прво развијен за ултрахладне Бозе гасове чије се интеракције могу описати помоћу контактне интеракционог потенцијала, а затим је уопштен на системе у којима се, поред контактне, у обзир мора узети и дипол-дипол интеракција. Развијени метод омогућава разматрање анизотропних тродимензионалних система, али је проширен и на специјалне ниже-димензионалне случајеве који узимају у обзир различите симетрије замке у којој је смештен Бозе-Ајнштајн кондензат: тродимензионалне аксијално- и радијално-симетричне замке, дводимензионалне цилиндрично-симетричне замке, изотропне сферно-симетричне и анизотропне једнодимензионалне и дводимензионалне замке. Рачунарски кодови су паралелизовани и прилагођени за коришћење на графичким картицама. Резултати су представљени у следећим међународним часописима:

- **D. Vudragović**, I. Vidanović, A. Balaž, P. Muruganandam, and S. K. Adhikari, *C Programs for Solving the Time-dependent Gross-Pitaevskii Equation in a Fully Anisotropic Trap*, Comput. Phys. Commun. **183**, 2021 (2012), M21a; DOI: 10.1016/j.cpc.2009.04.015; IF(2012) = 3.078;
- R. Kishor Kumar, L. Young-S., **D. Vudragović**, A. Balaž, P. Muruganandam, and S. K. Adhikari, *Fortran and C Programs for the Time-dependent Dipolar Gross-Pitaevskii Equation in an Anisotropic Trap*, Comput. Phys. Commun. **195**, 117 (2015), M21a; DOI: 10.1016/j.cpc.2015.03.024; IF(2015) = 3.635;
- L. Young-S., **D. Vudragović**, P. Muruganandam, S. K. Adhikari, and A. Balaž, *OpenMP Fortran and C Programs for Solving the Time-dependent Gross-Pitaevskii Equation in an Anisotropic Trap*, Comput. Phys. Commun. **204**, 209 (2016), M21a; DOI: 10.1016/j.cpc.2016.03.015; IF(2016) = 3.936;
- L. Young-S., P. Muruganandam, S. K. Adhikari, V. Loncar, **D. Vudragović**, and A. Balaž, *OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross-Pitaevskii equation*, Comput. Phys. Commun. **220**, 503 (2017), M21a; DOI: 10.1016/j.cpc.2017.07.013; IF(2017) = 3.748.

У свом истраживању Душан Вудраговић је проучавао феномене Фарадејевих и резонантних таласа густине у ултрахладним бозонским системима са контактном и

дипол-дипол интеракцијом. Овакви таласи настају као резултат хармонијске модулације система и представљају нелинеарне екситације система услед присуства интеракција, спрезањем колективних осцилација и параметарских резонанци. У оквиру теорије средњег поља развио је варијациони приступ за опис динамике Фарадејевих и резонантних таласа у диполним кондензатима. Овај приступ је заснован на Гаусовом варијационом анзацу који за параметре има ширине кондензата, конјуговане фазе, а укључује и модулације густине како би описао динамику таласа густине.

Користећи развијени варијациони приступ, као и пун нумерички приступ, детаљно је проучавао особине таласа густине у диполним кондензатима на нултој температури, где дипол-дипол интеракција игра важну улогу због нарушења симетрије услед анизотропије система. Извео је једначине кретања које описују динамику модулисаног диполног бозонског система и идентификовао најнестабилније моде које одговарају Фарадејевим и резонантним таласима. Даље, на основу тога, извео је аналитичке изразе за просторне периоде оба типа таласа густине, као и њихову зависност од јачине контактне и дипол-дипол интеракције. Добијене варијационе резултате упоредио је са резултатима детаљних нумеричких симулација које решавају диполну Грос-Питаевски једначину у три просторне димензије и добио веома добро слагање.

Душан Вудраговић је проучавао и утицај контактне и дипол-дипол интеракције на својства основног стања и колективних осцилација диполних кондензата. Док повећање јачине контактне интеракције увек доводи до ширења кондензата, ситуација је сложенија када се мења јачина дипол-дипол интеракције. За замку у облику цигаре у којој су диполи оријентисани у радијалном смеру, показао је да повећање јачине дипол-дипол интеракције доводи до ширења кондензата у лонгитудиналном правцу и у правцу поларизације, док се ширина у трећем правцу смањује. Поред тога, проучавао је и фреквенције колективних мода, где су ефекти интеракција мање изражени. Ово се посебно односи на монополну (дишућу) и квадруполну моду, чије вредности практично остају константне у целом распону експериментално релевантних вредности јачина интеракција. Са друге стране, фреквенција радијалне квадруполне моде је осетљивија на промену јачине интеракције, посебно јачине контактне интеракције, док при промени јачине дипол-дипол интеракције показује немонотон понашање. Резултати су представљени у следећем међународном часопису:

- **D. Vudragović** and A. Balaž, *Faraday and Resonant Waves in Dipolar Cigar-Shaped Bose-Einstein Condensates*, *Symmetry* **11**, 1090 (2019)
M22; DOI: 10.3390/sym11091090; IF(2018) = 2.143.

Елементи за квалитативну оцену научног доприноса др Душана Вудраговића

1 Квалитет научних резултата

1.1 Значај научних резултата

Најзначајнији радови др Душана Вудраговића су:

- **D. Vudragović** and A. Balaž, *Faraday and Resonant Waves in Dipolar Cigar-Shaped Bose-Einstein Condensates*, *Symmetry* **11**, 1090 (2019)
M22; DOI: 10.3390/sym11091090; IF(2018) = 2.143;
- **D. Vudragović**, I. Vidanović, A. Balaž, P. Muruganandam, and S. K. Adhikari, *C Programs for Solving the Time-dependent Gross-Pitaevskii Equation in a Fully Anisotropic Trap*, *Comput. Phys. Commun.* **183**, 2021 (2012)
M21a; DOI: 10.1016/j.cpc.2009.04.015; IF(2012) = 3.078.

У првом раду кандидат је развио варијациони и нумерички приступ за проучавање особина таласа густине у диполним кондензатима на нултој температури, где дипол-дипол интеракција игра важну улогу због нарушења симетрије услед анизотропије система. Користећи ове приступе, проучио је:

- колективне осцилације и динамику Фарадејевих таласа у ултрахладним бозонским системима са контактном и дипол-дипол интеракцијом;
- појаву резонантних таласа и утицај дипол-дипол интеракције на њихове особине у диполним Бозе-Ајнштајн-кондензованим системима.

Утицај контактне и дипол-дипол интеракције на фреквенције колективних мода и особине Фарадејевих таласа у диполним Бозе-Ајнштајн кондензатима испитао је детаљним нумеричким симулацијама и варијационим приступом. Посебно је проучавао зависност просторног и временског периода Фарадејевих таласа од јачине дипол-дипол интеракције. Сви прорачуни су изведени за реалистичне физичке системе, као што су атомски гасови хрома, диспрозијума и ербијума.

Типично време развоја резонантних таласа је много мање од времена које је потребно за појаву Фарадејевих таласа. Кандидат је проучио утицај јачине диполне интеракције на ова карактеристична времена. Такође, испитао је раније уочени феномен појаве снажнијег резонантног одговора система за модулативну фреквенцију која је двоструко већа од радијалне фреквенције замке, иако би се очекивало да се најважнија резонанца добија када су ове фреквенције једнаке.

У другом раду кандидат је развио нумеричку методу за решавање Грос-Питаевски једначине за ултрахладне бозонске системе са диполном интеракцијом, која представља резултат теорије средњег поља. Временски зависна диполна Грос-Питаевски једначина је парцијална диференцијална једначина по просторним координатама и времену и има структуру нелинеарне Шредингерове једначине, тако да садржи први

извод таласне функције по времену и друге изводе по просторним координатама. Диполни интеракциони члан је описан помоћу просторног интеграла, пошто је у питању дугодоментна интеракција. Развијени метод подељеног корака за решавање Грос-Питаевски једначине укључује дискретизацију по простору и времену, појединачну интеграцију по просторним координатама и временску пропагацију дискретизоване једначине. С обзиром на велику нумеричку захтевност тродимензионалних симулација за проучавање реалних физичких система, сви алгоритми су паралелизовани и прилагођени за коришћење на графичким картицама.

1.2 Параметри квалитета часописа

Кандидат др Душан Вудраговић је објавио укупно 8 радова у међународним часописима и то:

- 4 рада у међународним часописима изузетних вредности *Computer Physics Communications* следећих импакт фактора $IF(2017) = 3.748$, $IF(2016) = 3.936$, $IF(2015) = 3.635$, $IF(2012) = 3.078$, односно $SNIP(2017) = 1.92$, $SNIP(2016) = 2.00$, $SNIP(2015) = 1.87$, $SNIP(2012) = 2.12$.
- 3 рада у врхунским међународним часописима *Journal of Grid Computing, Communications in Computational Physics* и *Nuclear Instruments and Methods in Physics Research Section B* следећих импакт фактора $IF(2011) = 1.310$, $IF(2012) = 1.863$, $IF(2015) = 1.389$, односно $SNIP(2011) = 1.89$, $SNIP(2012) = 1.32$, $SNIP(2015) = 1.00$, redom;
- 1 рад у истакнутом међународном часопису *Symmetry* импакт фактора $IF(2018) = 2.143$, односно $SNIP(2018) = 1.05$.

Библиометријски показатељи су сумирани у следећој табели.

	IF	M	SNIP
Укупно	21.102	69.0	13.17
Усредњено по чланку	2.638	8.6	1.65
Усредњено по аутору	4.318	12.9	2.53

1.3 Позитивна цитираност научних радова

Према подацима из базе Web of Science, радови Душана Вудраговића (не укључујући радове АТЛАС колаборације) цитирани су укупно 300 пута, од чега 290 пута изузимајући аутоцитате. Хиршов индекс је 6. Уколико се узму у обзир и радови АТЛАС колаборације, Душан Вудраговић је цитиран 1,953 пута, од чега 1,931 пута изузимајући аутоцитате. У овом случају Хиршов индекс је 15.

1.4 Међународна сарадња

Кандидат има изражену међународну сарадњу. Активно сарађује са групама др Садхана Кумара Адхикарија са Државног универзитета у Сао Паулу (Бразил), др Александру Николина са Универзитета у Букурешту (Румунија) и др Аксела Пелстера са Техничког универзитета у Кајзерслаутерну (Немачка). Поред тога, др Душан Вудраговић је учествовао на 3 билатерална пројекта између Србије и Немачке и на 15 пројеката Европске комисије у програмима FP6, FP7 и Horizon 2020. На већини ових пројеката био је руководиолац радних пакета или радних задатака.

2 Нормирање броја коауторских радова, патената и техничких решења

Окосница свих радова кандидата је развој нумеричких метода за проучавање особина диполних кондензата у којима дипол-дипол интеракција игра важну улогу због нарушења симетрије услед анизотропије система. Радови кандидата категорије M21a имају 5 или 6 аутора, па ови радови не мењају значајно нормиран број бодова. Рад категорије M22 има 2 аутора и рачуна се са пуном тежином. На радовима из категорије M21 број аутора је нешто виши и ово доприноси разлици између укупног ненормираног 90.0 и нормираног 77.1 броја бодова. Просечан број аутора на радовима категорије M21 је 8.3, па је ова разлика занемарљива.

3 Учешће у пројектима, потпројектима и пројектним задацима

Кандидат је учествовао на следећим националним пројектима:

- пројекат Министарства просвете, науке и технолошког развоја Републике Србије ОН171017 Моделирање и нумеричке симулације сложених вишечестичних система;
- пројекат Министарства просвете, науке и технолошког развоја Републике Србије ИИИИ43007 Истраживање климатских промена и њиховог утицаја на животну средину - праћење утицаја, адаптација и ублажавање.

Кандидат је учествовао на билатералним пројектима Србије и Немачке (QDDB, IBES, BES-L) у периоду од 2013. до 2020. године.

Кандидат је учествовао на следећим међународним пројектима као руководиоца радног пакета:

- NI4OS-Europe (2019-2022), National Initiatives for Open Science in Europe; European Commission, Horizon 2020, Implementing the European Open Science Cloud;
- VI-SEEM (2015-2018), Virtual Research Environment (VRE) in Southeast Europe and the Eastern Mediterranean (SEEM); European Commission, Horizon 2020, Research and innovation programme;
- SemaGrow (2012-2015), Data intensive techniques to boost the real-time performance of global agricultural data infrastructures; European Commission, FP7, Research infrastructures project;
- agINFRA (2011-2014), A data infrastructure to support agricultural scientific communities Promoting data sharing and development of trust in agricultural sciences; European Commission, FP7, Research infrastructures project;
- HP-SEE (2010-2012), High-Performance Computing Infrastructure for South East Europe's Research Communities; European Commission, FP7, Research infrastructures project.

Кандидат је учествовао на следећим међународним пројектима као руководиоца радног задатка:

- SMARTCHAIN (2018-2021), Towards Innovation - driven and smart solutions in short food supply chains; European Commission, Horizon 2020, Research and innovation programme;
- SEE-GRID-SCI (2008-2010), European Commission, FP7 project;
- LA@CERN (2008-2010), European Commission, Lifelong Learning Programme.

Кандидат је учествовао на следећим међународним пројектима као члан пројектог тима:

- PRACE-3IP (2012-2014), Partnership for Advanced Computing in Europe - Third Implementation Phase Project; European Commission, FP7, Research infrastructures project;
- PRACE-2IP (2011-2013), Partnership for Advanced Computing in Europe AISBL - Second Implementation Phase Project; European Commission, FP7, Research infrastructures project;
- PRACE-1IP (2010-2012), Partnership for Advanced Computing in Europe AISBL - First Implementation Phase Project; European Commission, FP7, Research infrastructures project;
- EGI-InSPIRE (2010-2014), Integrated Sustainable Pan-European Infrastructure for Researchers in Europe; European Commission, FP7, Research infrastructures project;
- EGEE-III (2008-2010), European Commission, FP7 project;
- EGEE-II (2006-2008), Enabling Grids for E-sciencE; European Commission, FP6, eInfrastructure project;
- SEE-GRID-2 (2006-2008), South Eastern European Grid-enabled eInfrastructure Development; European Commission, FP-6, regional eInfrastructure project.

4 Активност у научним и научно-стручним друштвима

4.1 Рецензије научних радова

Др Душан Вудраговић је био рецензент:

- 4 рада у часопису Data Technologies and Applications;
- 2 рада у часопису Physics Letters A;
- 1 рада у часопису Simulation: Transactions of the Society for Modeling and Simulation International.

4.2 Организација научних скупова

Др Душан Вудраговић био је члан организационог одбора конференције HP-SEE User Forum 2012, која је одржана од 17. до 19. октобра 2012. године у Народној библиотеци Србије у Београду.

4.3 Педагошки рад

Др Душан Вудраговић је организовао више уводних и напредних High-performance и High-throughput компјутинг регионалних тренинга који су у просеку трајали два дана и на којима је у просеку по тренингу учествовало 30 људи. Овде су наведени само неки од њих:

- High performance computing in function of business enhancement, 14-15 June 2018, Belgrade, Serbia;
- VI-SEEM regional climate training event, 11-13 October 2017, Belgrade, Serbia;
- VI-SEEM life sciences regional training, 19-21 October 2016, Belgrade, Serbia;
- Introduction to Parallel Programming with CUDA, 18 February, Belgrade, Serbia;
- Tuning and optimization of HPC application, 1 June, 2012, Belgrade, Serbia;
- PARADOXical training, 14 October 2011, Belgrade, Serbia.

У периоду од 2015 до 2016. године објавио је серију чланака под називом Природа кода у часопису Млади физичар, а од 2014. године учествује као предавач на Научно-едукативном кампу Михајло Идворски Пупин у Идвору.

5 Утицај научних резултата

Утицај научних резултата се огледа у броју цитата који су наведени у тачки 1.3. овог одељка, а значај резултата је описан у тачки 1. Овде се може навести и чињеница да је један M21a рад, на ком је кандидат први аутор, високо цитиран (тренутни број цитата је 141) и да је омогућио објављивање низа других публикација.

6 Конкретан допринос кандидата у реализацији радова у научним центрима у земљи и иностранству

Кандидат је све своје истраживачке активности реализовао у Институту за физику у Београду. Кандидат је дао кључни допринос у свим објављеним радовима, а његов допринос се огледа у изради потребних нумеричких симулација, добијању, интерпретацији и презентацији нумеричких резултата, писању радова и комуникацији са уредницима и рецензентима часописа.

Елементи за квантитативну оцену научног доприноса др Душана Вудраговића

1 Остварени М-бодови по категоријама публикација

Категорија	М-бодова по публикацији	Број публикација	Укупно М-бодова (нормирано)
M13	7.0	1	7.0 (7.0)
M21a	10.0	4	40.0 (36.7)
M21	8.0	3	24.0 (15.3)
M22	5.0	1	5.0 (5.0)
M23	3.0	1	3.0 (2.5)
M33	1.0	2	2.0 (1.6)
M34	0.5	6	3.0 (3.0)
M70	6.0	1	6.0 (6.0)

2 Поређење оствареног броја М-бодова са минималним условима потребним за избор у звање научног сарадника

	Потребно	Остварено (нормирано)
Укупно	16.0	90.0 (77.1)
M10+M20+M31+M32+M33+M41+M42	10.0	84.0 (71.1)
M11+M12+M21+M22+M23	6.0	79.0 (66.5)

Списак објављених радова и других публикација који се бодују

Монографска студија/поглавље у књизи M11 или рад у тематском зборнику водећег међународног значаја (M13)

1. **D. Vudragović**, and A. Balaž, *Science gateway for the Serbian condensed matter physics community*, [Science gateways for distributed computing infrastructures](#), Ed. Peter Kacsuk, p. 209-220, Springer (2014), DOI: 10.1007/978-3-319-11268-8.

Радови у међународним часописима изузетних вредности (M21a)

1. Luis E. Young-S., P. Muruganandam, S. K. Adhikari, V. Lončar, **D. Vudragović**, and A. Balaž, *OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross-Pitaevskii equation*, [Comput. Phys. Commun.](#) **220**, 503 (2017), DOI: 10.1016/j.cpc.2017.07.013; IF(2017) = 3.748.
2. Luis E. Young-S., **D. Vudragović**, P. Muruganandam, S. K. Adhikari, and A. Balaž, *OpenMP Fortran and C programs for solving the time-dependent Gross-Pitaevskii equation in an anisotropic trap*, [Comput. Phys. Commun.](#) **204**, 209 (2016), DOI: 10.1016/j.cpc.2016.03.015; IF(2016) = 3.936.
3. R. K. Kumar, Luis E. Young-S., **D. Vudragović**, A. Balaž, P. Muruganandam, and S. K. Adhikari, *Fortran and C programs for the time-dependent dipolar Gross-Pitaevskii equation in an anisotropic trap*, [Comput. Phys. Commun.](#) **195**, 117 (2015), DOI: 10.1016/j.cpc.2015.03.024; IF(2015) = 3.635.
4. **D. Vudragović**, I. Vidanović, A. Balaž, P. Muruganandam, and S. K. Adhikari, *C Programs for solving the time-dependent Gross-Pitaevskii equation in a fully anisotropic trap*, [Comput. Phys. Commun.](#) **183**, 2021 (2012), DOI: 10.1016/j.cpc.2009.04.015; IF(2012) = 3.078.

Радови у врхунским међународним часописима (M21)

1. B. P. Marinković, V. Vujčić, G. Sushko, **D. Vudragović**, S. Đorđević, S. Ivanović, M. Nešić, D. Jevremović, A. V. Solov'yov, and N. J. Mason, *Development of collisional data base for elementary processes of electron scattering by atoms and molecules*, [Nucl. Instrum. Meth. B](#) **354**, 90 (2015), DOI: 10.1016/j.nimb.2014.12.039, IF(2015) = 1.389.
2. A. Balaž, I. Vidanović, D. Stojiljković, **D. Vudragović**, A. Belić, and A. Bogojević, *SPEEDUP code for calculation of transition amplitudes via the effective action approach*, [Commun. Comput. Phys.](#) **11**, 739 (2012), DOI: 10.4208/cicp.131210.180411a, IF(2012) = 1.863.
3. A. Balaž, O. Prnjat, **D. Vudragović**, V. Slavnić, I. Liabotis, E. Atanassov, B. Jakimovski, and M. Savić, *Development of Grid e-Infrastructure in South-Eastern Europe*, [J. Grid Comput.](#) **9**, 135 (2011), DOI: 10.1007/s10723-011-9185-0, IF(2011) = 1.310.

Радови у истакнутим међународним часописима (M22)

1. **D. Vudragović**, and A. Balaž, *Faraday and Resonant Waves in Dipolar Cigar-Shaped Bose-Einstein Condensates*, [Symmetry](#) **11**, 1090 (2019), DOI: 10.3390/sym11091090; IF(2018) = 2.143.

Радови у међународним часописима (M23)

1. **D. Vudragović**, L. Ilić, P. Jovanović, S. Ničković, A. Bogojević, and A. Balaž, *VI-SEEM DREAMCLIMATE Service*, [Scal. Comput. Pract. Exp.](#) **19**, 215 (2018), DOI: 10.12694/scpe.v19i2.1396.

Саопштења са међународних скупова штампана у целини (M33)

1. **D. Vudragović**, P. Jovanović, and A. Balaž, *VI-SEEM virtual research environment*, [The 10th RO-LCG Conference](#), Sinaia, Romania, 26-28 October 2017.
2. J. Lappalainen, **D. Vudragović**, A. Balaž, F. Ruggieri, R. Barbera, R. Lovas, G. Stoitsis, and K. Kastrantas, *Federating computation and storage resources to support agricultural science communities*, [EFITA-WCCA-CIGR conference](#), Turin, Italy, 24-27 June 2013.

Саопштења са међународних скупова штампана у изводу (M34)

1. **D. Vudragović**, V. Veljić, I. Vasić, and A. Balaž, *Ground state and collective modes of dipolar BECs*, [The 7th International School and Conference on Photonics](#), Belgrade, Serbia, 26-30 August 2019.
2. V. Lončar, **D. Vudragović**, S. K. Adhikari, and A. Balaž, *Parallel solvers for dipolar Gross-Pitaevskii equation*, [The 6th International School and Conference on Photonics](#), Belgrade, Serbia, 28 August - 1 September 2017.
3. V. Lončar, **D. Vudragović**, A. Balaž, and A. Pelster, *Rosensweig instability due to three-body interaction or quantum fluctuations?*, [DPG Spring Meeting 2016](#), Hannover, Germany, 29 February - 4 March 2016.
4. **D. Vudragović**, and A. Balaž, *Faraday waves in dipolar Bose-Einstein condensates*, [The 19th Symposium on Condensed Matter Physics - SFKM 2015](#), Belgrade, Serbia, 7-11 September 2015.
5. **D. Vudragović**, and A. Balaž, *Faraday waves in dipolar Bose-Einstein condensates*, [The 5th International School and Conference on Photonics](#), Belgrade, Serbia, 24-28 August 2015.
6. V. Lončar, **D. Vudragović**, A. Balaž, and A. Pelster, *Faraday waves in dipolar Bose-Einstein condensates*, [DPG Spring Meeting 2015](#), Heidelberg, Germany, 23-27 March 2015.

Списак објављених радова на АТЛАС колаборацији и други радови који нису узети у обзир приликом бодовања квантитативних резултата кандидата

Монографска студија/поглавље у књизи M11 или рад у тематском зборнику водећег међународног значаја (M13)

1. O. Prnjat, A. Balaž, **D. Vudragović**, I. Liabotis, C. Sener, B. Marović, M. Kozlovsky, and G. Neagu, *SEE-GRID eInfrastructure for regional eScience*, [Data driven e-Science](#), Eds. S. C. Lin and E. Yen, p. 91, Springer (2011), DOI: 10.1007/978-1-4419-8014-4_7.

Монографска студија/поглавље у књизи M12 или рад у тематском зборнику водећег међународног значаја (M14)

1. D. Stanković, P. Jovanović, A. Jović, V. Slavnić, **D. Vudragović**, and A. Balaž, *Implementation and Benchmarking of New FFT Libraries in Quantum ESPRESSO*, [High-performance computing infrastructure for South East Europe's research communities](#), p. 155-162, Springer (2014).

Радови у међународним часописима изузетних вредности (M21a)

1. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Charged-particle multiplicities in pp interactions at $\sqrt{s}=900$ GeV measured with the ATLAS detector at the LHC*, [Phys. Lett. B](#) **688**, 21 (2010).
2. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Search for new particles in two-jet final states in 7 TeV proton-proton collisions with the ATLAS detector at the LHC*, [Phys. Rev. Lett.](#) **105**, 161801 (2010).

Радови у врхунским међународним часописима (M21)

1. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Search for quark contact interactions in dijet angular distributions in pp collisions at $\sqrt{s}=7$ TeV measured with the ATLAS detector*, [Phys. Lett. B](#) **694**, 327 (2011).
2. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Performance of the ATLAS detector using first collision data*, [J. High Energy Phys.](#) **9**, 056 (2010).

Радови у истакнутим међународним часописима (M22)

1. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Studies of the performance of the ATLAS detector using cosmic-ray muons*, [Eur. Phys. J. C](#) **71**, 1593 (2011).
2. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Measurement of inclusive jet and dijet cross sections in proton-proton collisions at 7 TeV centre-of-mass energy with the ATLAS detector*, [Eur. Phys. J. C](#) **71**, 1512 (2011).
3. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Readiness of the ATLAS liquid argon calorimeter for LHC collisions*, [Eur. Phys. J. C](#) **70**, 723 (2010).

4. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Drift time measurement in the ATLAS liquid argon electromagnetic calorimeter using cosmic muons*, [Eur. Phys. J. C **70**, 755 \(2010\)](#).
5. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *The ATLAS inner detector commissioning and calibration*, [Eur. Phys. J. C **70**, 787 \(2010\)](#).
6. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *The ATLAS simulation infrastructure*, [Eur. Phys. J. C **70**, 823 \(2010\)](#).
7. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Commissioning of the ATLAS muon spectrometer with cosmic rays*, [Eur. Phys. J. C **70**, 875 \(2010\)](#).
8. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *Readiness of the ATLAS tile calorimeter for LHC collisions*, [Eur. Phys. J. C **70**, 1193 \(2010\)](#).

Радови у међународним часописима (M23)

1. G. Aad, B. Abbott, J. Abdallah, ... **D. Vudragović**, and et al., *The ATLAS experiment at the CERN large hadron collider*, [J. Instrum. **3**, S08003 \(2008\)](#).
2. Lj. Simić, N. Vranješ, D. Reljić, **D. Vudragović**, and D. S. Popović, *WW production and triple gauge boson couplings at ATLAS*, [Acta Phys. Pol. B **38**, 525 \(2007\)](#).

Саопштења са међународних скупова штампана у целини (M33)

1. V. Slavnić, B. Acković, **D. Vudragović**, A. Balaž, A. Belić, and M. Savić, *Grid site monitoring tools developed and used at SCL*, [SEE-GRID-SCI User Forum 2009](#), Istanbul, Turkey, 9-10 December 2009.
2. V. Slavnić, B. Acković, **D. Vudragović**, A. Balaž, and A. Belić, *Operational Grid tools developed at SCL*, [SEE-GRID-SCI User Forum 2009](#), Istanbul, Turkey, 9-10 December 2009.
3. **D. Vudragović**, A. Balaž, V. Slavnić, and A. Belić, *Serbian participation in Grid computing projects*, [NEC 2009](#), Varna, Bulgaria, 7-14 September 2009.
4. O. Prnjat, A. Balaž, T. Gurov, M. Kon-Popovska, I. Liabotis, G. Neagu, B. Ortakaya, C. Sener, and **D. Vudragović**, *National Grid initiatives set-up and monitoring guidelines*, [The first EELA-2 conference](#), Bogota, Colombia, 25-27 February 2009.
5. N. Vranješ, Lj. Simić, D. Reljić, **D. Vudragović**, and D. S. Popović, *WW Production at the LHC in NLO Simulations*, [6th international conference of the Balkan physical union](#), Istanbul, Turkey, 22-26 August 2006.

Саопштења са међународних скупова штампана у изводу (M34)

1. **D. Vudragović**, V. Slavnić, I. Spasojević, V. Nedović, and A. Balaž, *AgINFRA - a data infrastructure to support agricultural scientific communities: promoting data sharing and development of trust in agricultural sciences*, [12th Congress of Nutrition](#), Belgrade, Serbia, 31 October 2012.

2. N. Manouselis, C. Thanopoulos, A. Balaž, **D. Vudragović**, V. Nedović, and I. Spasojević, *AgINFRA - a data infrastructure to support agricultural scientific communities: promoting data sharing and development of trust in agricultural sciences*, [6th Central European Congress on Food](#), Novi Sad, Serbia, 23-26 May 2012.

Саопштења са скупова националног значаја штампана у целини (M63)

1. **D. Vudragović**, A. Balaž, A. Belić, C. Kourkoumelis, D. Fassouliotis, and S. Vourakis, *Hybrid Pupil's Analysis Tool for Interactions in ATLAS*, [MIPRO 2010](#), Opatia, Croatia, 24-28 May 2010.
2. **D. Vudragović**, A. Balaž, A. Belić, and A. Bogojević, *QSPEEDUP: Quasi-MC Implementation of the SPEEDUP Path Integral Code*, [INFOTEH 2010](#), Jahorina, Bosnia and Herzegovina, 17-19 March 2010.
3. **D. Vudragović**, V. Slavnić, A. Balaž, and A. Belić, *WMSMON - GLite WMS Monitoring Tool*, [MIPRO 2009](#), Opatia, Croatia, 25-29 May 2009.
4. **D. Vudragović**, A. Balaž, V. Slavnić, and A. Belić, *Dwarf - the Framework for Authorized YUM/APT Repositories Management*, [INFOTEH 2009](#), Jahorina, Bosnia and Herzegovina, 18-20 March 2009.



OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross–Pitaevskii equation



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Partial differential equation

ABSTRACT

We present Open Multi-Processing (OpenMP) version of Fortran 90 programs for solving the Gross–Pitaevskii (GP) equation for a Bose–Einstein condensate in one, two, and three spatial dimensions, optimized for use with GNU and Intel compilers. We use the split-step Crank–Nicolson algorithm for imaginary- and real-time propagation, which enables efficient calculation of stationary and non-stationary solutions, respectively. The present OpenMP programs are designed for computers with multi-core processors and optimized for compiling with both commercially-licensed Intel Fortran and popular free open-source GNU Fortran compiler. The programs are easy to use and are elaborated with helpful comments for the users. All input parameters are listed at the beginning of each program. Different output files provide physical quantities such as energy, chemical potential, root-mean-square sizes, densities, etc. We also present speedup test results for new versions of the programs.

New version program summary

Program title: BEC-GP-OMP-FOR software package, consisting of: (i) imag1d-th, (ii) imag2d-th, (iii) imag3d-th, (iv) imagaxi-th, (v) imagcir-th, (vi) imagsph-th, (vii) real1d-th, (viii) real2d-th, (ix) real3d-th, (x) realaxi-th, (xi) realcir-th, (xii) realsph-th.

Program files doi: <http://dx.doi.org/10.17632/y8zk3jgn84.2>

Licensing provisions: Apache License 2.0

Programming language: OpenMP GNU and Intel Fortran 90.

Computer: Any multi-core personal computer or workstation with the appropriate OpenMP-capable Fortran compiler installed.

Number of processors used: All available CPU cores on the executing computer.

Journal reference of previous version: Comput. Phys. Commun. **180** (2009) 1888; *ibid.* **204** (2016) 209.

Does the new version supersede the previous version?: Not completely. It does supersede previous Fortran programs from both references above, but not OpenMP C programs from Comput. Phys. Commun. **204** (2016) 209.

Nature of problem: The present Open Multi-Processing (OpenMP) Fortran programs, optimized for use with commercially-licensed Intel Fortran and free open-source GNU Fortran compilers, solve the time-dependent nonlinear partial differential (GP) equation for a trapped Bose–Einstein condensate in one (1d), two (2d), and three (3d) spatial dimensions for six different trap symmetries: axially and radially symmetric traps in 3d, circularly symmetric traps in 2d, fully isotropic (spherically symmetric) and fully anisotropic traps in 2d and 3d, as well as 1d traps, where no spatial symmetry is considered.

Solution method: We employ the split-step Crank–Nicolson algorithm to discretize the time-dependent GP equation in space and time. The discretized equation is then solved by imaginary- or real-time propagation, employing adequately small space and time steps, to yield the solution of stationary and non-stationary problems, respectively.

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Reasons for the new version: Previously published Fortran programs [1,2] have now become popular tools [3] for solving the GP equation. These programs have been translated to the C programming language [4] and later extended to the more complex scenario of dipolar atoms [5]. Now virtually all computers have multi-core processors and some have motherboards with more than one physical computer processing unit (CPU), which may increase the number of available CPU cores on a single computer to several tens. The C programs have been adopted to be very fast on such multi-core modern computers using general-purpose graphic processing units (GPGPU) with Nvidia CUDA and computer clusters using Message Passing Interface (MPI) [6]. Nevertheless, previously developed Fortran programs are also commonly used for scientific computation and most of them use a single CPU core at a time in modern multi-core laptops, desktops, and workstations. Unless the Fortran programs are made aware and capable of making efficient use of the available CPU cores, the solution of even a realistic dynamical 1d problem, not to mention the more complicated 2d and 3d problems, could be time consuming using the Fortran programs. Previously, we published auto-parallel Fortran programs [2] suitable for Intel (but not GNU) compiler for solving the GP equation. Hence, a need for the full OpenMP version of the Fortran programs to reduce the execution time cannot be overemphasized. To address this issue, we provide here such OpenMP Fortran programs, optimized for both Intel and GNU Fortran compilers and capable of using all available CPU cores, which can significantly reduce the execution time.

Summary of revisions: Previous Fortran programs [1] for solving the time-dependent GP equation in 1d, 2d, and 3d with different trap symmetries have been parallelized using the OpenMP interface to reduce the execution time on multi-core processors. There are six different trap symmetries considered, resulting in six programs for imaginary-time propagation and six for real-time propagation, totaling to 12 programs included in BEC-GP-OMP-FOR software package.

All input data (number of atoms, scattering length, harmonic oscillator trap length, trap anisotropy, etc.) are conveniently placed at the beginning of each program, as before [2]. Present programs introduce a new input parameter, which is designated by `Number_of_Threads` and defines the number of CPU cores of the processor to be used in the calculation. If one sets the value 0 for this parameter, all available CPU cores will be used. For the most efficient calculation it is advisable to leave one CPU core unused for the background system's jobs. For example, on a machine with 20 CPU cores such that we used for testing, it is advisable to use up to 19 CPU cores. However, the total number of used CPU cores can be divided into more than one job. For instance, one can run three simulations simultaneously using 10, 4, and 5 CPU cores, respectively, thus totaling to 19 used CPU cores on a 20-core computer.

The Fortran source programs are located in the directory `src`, and can be compiled by the `make` command using the `makefile` in the root directory `BEC-GP-OMP-FOR` of the software package. The examples of produced output files can be found in the directory `output`, although some large density files are omitted, to save space. The programs calculate the values of actually used dimensionless nonlinearities from the physical input parameters, where the input parameters correspond to the identical nonlinearity values as in the previously published programs [1], so that the output files of the old and new programs can be directly compared. The output files are conveniently named such that their contents can be easily identified, following the naming convention introduced in Ref. [2]. For example, a file named `<code>-out.txt`, where `<code>` is a name of the individual program, represents the general output file containing input data, time and space steps, nonlinearity, energy and chemical potential, and was named `fort.7` in the old Fortran version of programs [1]. A file named `<code>-den.txt` is the output file with the condensate density, which had the names `fort.3` and `fort.4` in the old Fortran version [1] for imaginary- and real-time propagation programs, respectively. Other possible density outputs, such as the initial density, are commented out in the programs to have a simpler set of output files, but users can uncomment and re-enable them, if needed. In addition, there are output files for reduced (integrated) 1d and 2d densities for different programs. In the real-time programs there is also an output file reporting the dynamics of evolution of root-mean-square sizes after a perturbation is introduced. The supplied real-time programs solve the stationary GP equation, and then calculate the dynamics. As the imaginary-time programs are more accurate than the real-time programs for the solution of a stationary problem, one can first solve the stationary problem using the imaginary-time programs, adapt the real-time programs to read the pre-calculated wave function and then study the dynamics. In that case the parameter `NSTP` in the real-time programs should be set to zero and the space mesh and nonlinearity parameters should be identical in both programs. The reader is advised to consult our previous publication where a complete description of the output files is given [2]. A `readme.txt` file, included in the root directory, explains the procedure to compile and run the programs.

We tested our programs on a workstation with two 10-core Intel Xeon E5-2650 v3 CPUs. The parameters used for testing are given in sample input files, provided in the corresponding directory together with the programs. In Table 1 we present wall-clock execution times for runs on 1, 6, and 19 CPU cores for programs compiled using Intel and GNU Fortran compilers. The corresponding columns "Intel speedup" and "GNU speedup" give the ratio of wall-clock execution times of runs on 1 and 19 CPU cores, and denote the actual measured speedup for 19 CPU cores. In all cases and for all numbers of CPU cores, although the GNU Fortran compiler gives excellent results, the Intel Fortran compiler turns out to be slightly faster. Note that during these tests we always ran only a single simulation on a workstation at a time, to avoid any possible interference issues. Therefore, the obtained wall-clock times are more reliable than the ones that could be measured with two or more jobs running simultaneously. We also studied the speedup of the programs as a function of the number of CPU cores used. The performance of the Intel and GNU Fortran compilers is illustrated in Fig. 1, where we plot the speedup and actual wall-clock times as functions of the number of CPU cores for 2d and 3d programs. We see that the speedup increases monotonically with the number of CPU cores in all cases and has large values (between 10 and 14 for 3d

programs) for the maximal number of cores. This fully justifies the development of OpenMP programs, which enable much faster and more efficient solving of the GP equation. However, a slow saturation in the speedup with the further increase in the number of CPU cores is observed in all cases, as expected.

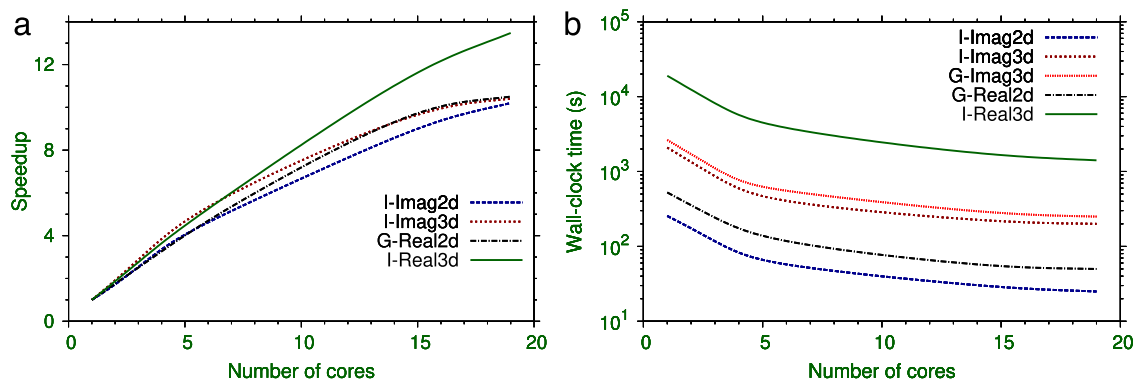


Fig. 1. (a) Speedup for 2d and 3d programs compiled with the Intel (I) and GNU (G) Fortran compilers as a function of the number of CPU cores, measured on a workstation with two Intel Xeon E5-2650 v3 CPUs. (b) Wall-clock execution time (in seconds) of 2d and 3d programs compiled with the Intel (I) and GNU (G) Fortran compilers as a function of the number of CPU cores.

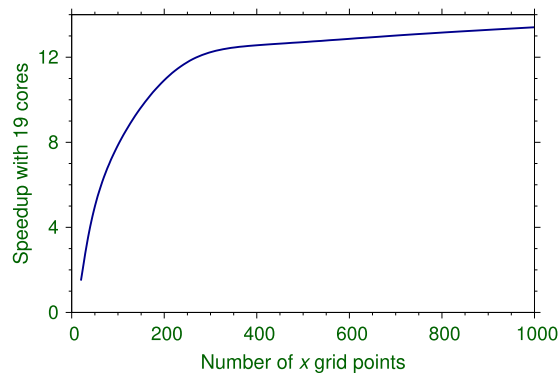


Fig. 2. Speedup of real2d-th program, compiled with the Intel Fortran 90 compiler and executed on 19 CPU cores on a workstation with two Intel Xeon E5-2650 v3 CPUs, as a function of the number of spatial discretization points $NX=NY$.

Table 1

Wall-clock execution times (in seconds) for runs with 1, 6, and 19 CPU cores of different programs using the Intel Fortran (`ifort`) and GNU Fortran (`gfortran`) compilers on a workstation with two Intel Xeon E5-2650 v3 CPUs, with a total of 20 CPU cores, and the obtained speedups for 19 CPU cores.

# of cores	1	1	6	6	19	19	19	19
Fortran	Intel time	GNU time	Intel time	GNU time	Intel time	GNU time	Intel speedup	GNU speedup
imag1d	52	60	22	22	20	22	2.6	2.7
imagcir	22	30	14	15	14	15	1.6	2.0
imagsph	24	30	12	15	12	14	2.4	2.1
real1d	205	345	76	108	62	86	3.3	4.0
realcir	145	220	55	73	48	59	3.0	3.7
realsph	155	250	57	76	46	61	3.4	2.7
imag2d	255	415	52	84	27	40	9.4	10.4
imagaxi	260	435	62	105	30	55	8.7	7.9
real2d	325	525	74	107	32	50	10.1	10.5
realaxi	160	265	35	49	16	24	10.0	11.0
imag3d	2080	2630	370	550	200	250	10.4	10.5
real3d	19500	26000	3650	5600	1410	2250	13.8	11.6

The speedup tends to increase for programs in higher dimensions, as they become more complex and have to process more data. This is why the speedups of the supplied 2d and 3d programs are larger than those of 1d programs. Also, for a single program the speedup increases with the size of the spatial grid, i.e., with the number of spatial discretization points, since this increases the amount of calculations performed by the program. To demonstrate this, we tested the supplied real2d-th program and varied the number of spatial discretization points $NX=NY$ from 20 to 1000. The measured speedup obtained when running this program on 19 CPU cores as a function of the number of discretization points is shown in Fig. 2. The speedup first increases rapidly with the number of discretization points and eventually saturates.

Additional comments: Example inputs provided with the programs take less than 30 minutes to run on a workstation with two Intel Xeon E5-2650 v3 processors (2 QPI links, 10 CPU cores, 25 MB cache, 2.3 GHz).
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OpenMP Fortran and C programs for solving the time-dependent Gross–Pitaevskii equation in an anisotropic trap



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ABSTRACT

We present new version of previously published Fortran and C programs for solving the Gross–Pitaevskii equation for a Bose–Einstein condensate with contact interaction in one, two and three spatial dimensions in imaginary and real time, yielding both stationary and non-stationary solutions. To reduce the execution time on multicore processors, new versions of parallelized programs are developed using Open Multi-Processing (OpenMP) interface. The input in the previous versions of programs was the mathematical quantity nonlinearity for dimensionless form of Gross–Pitaevskii equation, whereas in the present programs the inputs are quantities of experimental interest, such as, number of atoms, scattering length, oscillator length for the trap, etc. New output files for some integrated one- and two-dimensional densities of experimental interest are given. We also present speedup test results for the new programs.

New version program summary

Program title: BEC-GP-OMP package, consisting of: (i) imag1d, (ii) imag2d, (iii) imag3d, (iv) imagaxi, (v) imagcir, (vi) imagsph, (vii) real1d, (viii) real2d, (ix) real3d, (x) realaxi, (xi) realcir, (xii) realsph.

Catalogue identifier: AEDU_v4_0.

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/AEDU_v4_0.html

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland.

Licensing provisions: Apache License 2.0

No. of lines in distributed program, including test data, etc.: 130308.

No. of bytes in distributed program, including test data, etc.: 929062.

Distribution format: tar.gz.

Programming language: OpenMP C; OpenMP Fortran.

Computer: Any multi-core personal computer or workstation.

Operating system: Linux and Windows.

RAM: 1 GB.

Number of processors used: All available CPU cores on the executing computer.

Classification: 2.9, 4.3, 4.12.

Catalogue identifier of previous version: AEDU_v1_0, AEDU_v2_0.

Journal reference of previous version: Comput. Phys. Commun. 180 (2009) 1888; *ibid.* 183 (2012) 2021.

Does the new version supersede the previous version?: No. It does supersede versions AEDU_v1_0 and AEDU_v2_0, but not AEDU_v3_0, which is MPI-parallelized version.

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Nature of problem: The present OpenMP Fortran and C programs solve the time-dependent nonlinear partial differential Gross–Pitaevskii (GP) equation for a Bose–Einstein condensate in one (1D), two (2D), and three (3D) spatial dimensions in a harmonic trap with six different symmetries: axial- and radial-symmetry in 3D, circular-symmetry in 2D, and fully anisotropic in 2D and 3D.

Solution method: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation, in either imaginary or real time, over small time steps. The method yields the solution of stationary and/or non-stationary problems.

Reasons for the new version: Previously published Fortran and C programs [1,2] for solving the GP equation are recently enjoying frequent usage [3] and application to a more complex scenario of dipolar atoms [4]. They are also further extended to make use of general purpose graphics processing units (GPGPU) with Nvidia CUDA [5], as well as computer clusters using Message Passing Interface (MPI) [6]. However, a vast majority of users use single-computer programs, with which the solution of a realistic dynamical 1D problem, not to mention the more complicated 2D and 3D problems, could be time consuming. Now practically all computers have multicore processors, ranging from 2 up to 18 and more CPU cores. Some computers include motherboards with more than one physical CPU, further increasing the possible number of available CPU cores on a single computer to several tens. The present programs are parallelized using OpenMP over all the CPU cores and can significantly reduce the execution time. Furthermore, in the old version of the programs [1,2] the inputs were based on the mathematical quantity nonlinearity for the dimensionless form of the GP equation. The inputs for the present versions of programs are given in terms of phenomenological variables of experimental interest, as in Refs. [4,5], i.e., number of atoms, scattering length, harmonic oscillator length of the confining trap, etc. Also, the output files are given names which make identification of their contents easier, as in Refs. [4,5]. In addition, new output files for integrated densities of experimental interest are provided, and all programs were thoroughly revised to eliminate redundancies.

Summary of revisions: Previous Fortran [1] and C [2] programs for the solution of time-dependent GP equation in 1D, 2D, and 3D with different trap symmetries have been modified to achieve two goals. First, they are parallelized using OpenMP interface to reduce the execution time in multicore processors. Previous C programs [2] had OpenMP-parallelized versions of 2D and 3D programs, together with the serial versions, while here all programs are OpenMP-parallelized. Secondly, the programs now have input and output files with quantities of phenomenological interest. There are six trap symmetries and both in C and in Fortran there are twelve programs, six for imaginary-time propagation and six for real-time propagation, totaling to 24 programs. In 3D, we consider full radial symmetry, axial symmetry and full anisotropy. In 2D, we consider circular symmetry and full anisotropy. The structure of all programs is similar.

For the Fortran programs the input data (number of atoms, scattering length, harmonic oscillator trap length, trap anisotropy, etc.) are conveniently placed at the beginning of each program. For the C programs the input data are placed in separate input files, examples of which can be found in a directory named input. The examples of output files for both Fortran and C programs are placed in the corresponding directories called output. The programs then calculate the dimensionless nonlinearities actually used in the calculation. The provided programs use physical input parameters that give identical nonlinearity values as the previously published programs [1,2], so that the output files of the old and new programs can be directly compared. The output files are conveniently named so that their contents can be easily identified, following Refs. [4,5]. For example, file named <code>-out.txt, where <code> is a name of the individual program, is the general output file containing input data, time and space steps, nonlinearity, energy and chemical potential, and was named fort.7 in the old Fortran version. The file <code>-den.txt is the output file with the condensate density, which had the names fort.3 and fort.4 in the old Fortran version for imaginary- and real-time propagation, respectively. Other density outputs, such as the initial density, are commented out to have a simpler set of output files. The users can re-introduce those by taking out the comment symbols, if needed.

Table 1

Wall-clock execution times (in seconds) for runs with 1, 6 and 20 CPU cores with different programs using the Intel Fortran ifort (F-1, F-6 and F-20, respectively) and Intel C icc (C-1, C-6 and C-20, respectively) compilers using a workstation with two Intel Xeon E5-2650 v3 CPUs, with a total of 20 CPU cores, and obtained speedups (speedup-F = F-1/F-20, -speedup-C = C-1/C-20) for 20 CPU cores.

	F-1	F-6	F-20	speedup-F	C-1	C-6	C-20	speedup-C
imag1d	32	26	26	1.2	45	28	27	1.7
imagcir	15	15	15	1.0	21	15	15	1.4
imagsph	12	12	12	1.0	19	12	10	1.9
real1d	194	84	72	2.7	304	110	98	3.1
realcir	132	62	57	2.3	182	78	64	2.8
realsph	119	68	67	1.8	191	76	61	3.1
imag2d	190	66	52	3.7	394	77	33	11.9
imagaxi	240	74	56	4.3	499	113	55	9.1
real2d	269	70	47	5.7	483	96	35	13.8
realaxi	132	37	25	5.3	237	51	22	10.8
imag3d	1682	472	366	4.6	2490	545	202	12.3
real3d	15,479	3494	2082	7.4	22,228	4558	1438	15.5

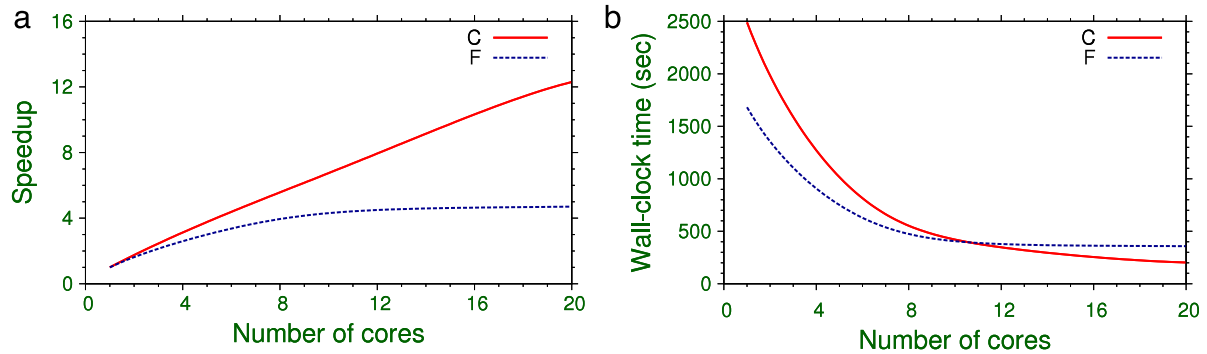


Fig. 1. (a) Speedup of the C and Fortran (F) imag3d programs as a function of the number of CPU cores, measured in a workstation with two Intel Xeon E5-2650 v3 CPUs. The speedup for the run with N CPU cores was calculated as the ratio between wall-clock execution times with one and N CPU cores. (b) Wall-clock time of the same runs as a function of the number of CPU cores.

Also, some new output files are introduced in this version of programs. The files `<code>-rms.txt` are the output files with values of root-mean-square (rms) sizes in the multi-variable cases. There are new files with integrated densities, such as `imag2d-den1d_x.txt`, where the first part (`imag2d`) denotes that the density was calculated with the 2D program `imag2d`, and the second part (`den1d_x`) stands for the 1D density in the x -direction, obtained after integrating out the 2D density $|\phi(x, y)|^2$ in the x - y plane over y -coordinate,

$$n_{1D}(x) = \int_{-\infty}^{\infty} dy |\phi(x, y)|^2. \quad (1)$$

Similarly, `imag3d-den1d_x.txt` and `real3d-den1d_x.txt` represent 1D densities from a 3D calculation obtained after integrating out the 3D density $|\phi(x, y, z)|^2$ over y - and z -coordinate. The files `imag3d-den2d_xy.txt` and `real3d-den2d_xy.txt` are the integrated 2D densities in the x - y plane from a 3D calculation obtained after integrating out the 3D density over the z -coordinate, and similarly for other output files. Again, calculation and saving of these integrated densities is commented out in the programs, and can be activated by the user, if needed.

In real-time propagation programs there are additional results for the dynamics saved in files, such as `real2d-dyna.txt`, where the first column denotes time, the second, third and fourth columns display rms sizes for the x -, y -, and r -coordinate, respectively. The dynamics is generated by multiplying the nonlinearity with a pre-defined factor during the NRUN iterations, and starting with the wave function calculated during the NPAS iterations. Such files were named `fort.8` in the old Fortran versions of programs. There are similar files in the 3D real-time programs as well.

Often it is needed to get a precise stationary state solution by imaginary-time propagation and then use it in the study of dynamics using real-time propagation. For that purpose, if the integer number NSTP is set to zero in real-time propagation, the density obtained in the imaginary-time simulation is used as initial wave function for real-time propagation, as in Refs. [4,5]. In addition, at the end of output files `<code>-out.txt`, we have introduced two new outputs, wall-clock execution time and CPU time for each run.

We tested our programs on a workstation with two 10-core Intel Xeon E5-2650 v3 CPUs, and present results for all programs compiled with the Intel compiler. In Table 1 we show different wall-clock execution times for runs on 1, 6 and 20 CPU cores for Fortran and C. The corresponding columns “speedup-F” and “speedup-C” give the ratio of wall-clock execution times of runs on 1 and 20 CPU cores, and denote the actual measured speedup for 20 CPU cores. For the programs with effectively one spatial variable, the Fortran programs turn out to be quicker for small number of cores, whereas for larger number of CPU cores and for the programs with three spatial variables the C programs are faster. We also studied the speedup of the programs as a function of the number of available CPU cores. The performance for the imag3d Fortran and C programs is illustrated in Fig. 1(a) and (b), where we plot the speedup and actual wall-clock time of the imag3d C and Fortran programs as a function of number of CPU cores in a workstation with two Intel Xeon E5-2650 v3 CPUs, with a total of 20 CPU cores. The plot in Fig. 1(a) shows that the C program parallelizes more efficiently than the Fortran program. However, as the wall-clock time in Fortran for a single CPU core is less than that in C, the wall-clock times in both cases are comparable, viz. Fig. 1(b). A saturation of the speedup with the increase of the number of CPU cores is expected in all cases. However, the saturation is attained quicker in Fortran than in C programs, and therefore the use of C programs could be recommended for larger number of CPU cores. For a small number of CPU cores the Fortran programs should be preferable. For example, from Table 1 we see that for 6 CPU cores the Fortran programs are faster than the C programs. In Fig. 1(a) the saturation of the speedup of the Fortran program is achieved for approximately 10 CPU cores, when the wall-clock time of the C program crosses that of the Fortran program.

Additional comments:

This package consists of 24 programs, see Program title above. For the particular purpose of each program, please see descriptions below.

Running time:

Example inputs provided with the programs take less than 30 min in a workstation with two Intel Xeon Processors E5-2650 v3, 2 QPI links, 10 CPU cores (25 MB cache, 2.3 GHz).

Program summary (i), (v), (vi), (vii), (xi), (xii)

Program title: imag1d, imagcir, imagsph, real1d, realcir, realsph.

Title of electronic files in C: (imag1d.c and imag1d.h), (imagcir.c and imagcir.h), (imagsph.c and imagsph.h), (real1d.c and real1d.h), (realcir.c and realcir.h), (realsph.c and realsph.h).

Title of electronic files in Fortran 90: imag1d.f90, imagcir.f90, imagsph.f90, real1d.f90, realcir.f90, realsph.f90.

Maximum RAM memory: 1 GB for the supplied programs.

Programming language used: OpenMP C and Fortran 90.

Typical running time: Minutes on a modern four-core PC.

Nature of physical problem: These programs are designed to solve the time-dependent nonlinear partial differential GP equation in one spatial variable.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields the solution of stationary problems.

Program summary (ii), (iv), (viii), (x)

Program title: imag2d, imagaxi, real2d, realaxi.

Title of electronic files in C: (imag2d.c and imag2d.h), (imagaxi.c and imagaxi.h), (real2d.c and real2d.h), (realaxi.c and realaxi.h).

Title of electronic files in Fortran 90: imag2d.f90, imagaxi.f90, real2d.f90, realaxi.f90.

Maximum RAM memory: 1 GB for the supplied programs.

Programming language used: OpenMP C and Fortran 90.

Typical running time: Hour on a modern four-core PC.

Nature of physical problem: These programs are designed to solve the time-dependent nonlinear partial differential GP equation in two spatial variables.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields the solution of stationary problems.

Program summary (iii), (ix)

Program title: imag3d, real3d.

Title of electronic files in C: (imag3d.c and imag3d.h), (real3d.c and real3d.h).

Title of electronic files in Fortran 90: imag3d.f90, real3d.f90.

Maximum RAM memory: 1 GB for the supplied programs.

Programming language used: OpenMP C and Fortran 90.

Typical running time: Few hours on a modern four-core PC.

Nature of physical problem: These programs are designed to solve the time-dependent nonlinear partial differential GP equation in three spatial variables.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields the solution of stationary problems.

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Fortran and C programs for the time-dependent dipolar Gross–Pitaevskii equation in an anisotropic trap[☆]



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ABSTRACT

Many of the static and dynamic properties of an atomic Bose–Einstein condensate (BEC) are usually studied by solving the mean-field Gross–Pitaevskii (GP) equation, which is a nonlinear partial differential equation for short-range atomic interaction. More recently, BEC of atoms with long-range dipolar atomic interaction are used in theoretical and experimental studies. For dipolar atomic interaction, the GP equation is a partial integro-differential equation, requiring complex algorithm for its numerical solution. Here we present numerical algorithms for both stationary and non-stationary solutions of the full three-dimensional (3D) GP equation for a dipolar BEC, including the contact interaction. We also consider the simplified one- (1D) and two-dimensional (2D) GP equations satisfied by cigar- and disk-shaped dipolar BECs. We employ the split-step Crank–Nicolson method with real- and imaginary-time propagations, respectively, for the numerical solution of the GP equation for dynamic and static properties of a dipolar BEC. The atoms are considered to be polarized along the z axis and we consider ten different cases, e.g., stationary and non-stationary solutions of the GP equation for a dipolar BEC in 1D (along x and z axes), 2D (in x – y and x – z planes), and 3D, and we provide working codes in Fortran 90/95 and C for these ten cases (twenty programs in all). We present numerical results for energy, chemical potential, root-mean-square sizes and density of the dipolar BECs and, where available, compare them with results of other authors and of variational and Thomas–Fermi approximations.

Program summary

Program title: (i) imag1dZ, (ii) imag1dX, (iii) imag2dXY, (iv) imag2dXZ, (v) imag3d, (vi) real1dZ, (vii) real1dX, (viii) real2dXY, (ix) real2dXZ, (x) real3d

Catalogue identifier: AEWL_v1_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEWL_v1_0.html

Program obtainable from: CPC Program Library, Queens University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>

No. of lines in distributed program, including test data, etc.: 111384

No. of bytes in distributed program, including test data, etc.: 604013

Distribution format: tar.gz

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[☆] This paper and its associated computer program are available via the Computer Physics Communication homepage on ScienceDirect (<http://www.sciencedirect.com/science/journal/00104655>).

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1. Introduction

After the experimental realization of atomic Bose–Einstein condensate (BEC) of alkali-metal and some other atoms, there has been a great deal of theoretical activity in studying the statics and dynamics of the condensate using the mean-field time-dependent Gross–Pitaevskii (GP) equation under different trap symmetries [1]. The GP equation in three dimensions (3D) is a

nonlinear partial differential equation in three space variables and a time variable and its numerical solution is indeed a difficult task specially for large nonlinearities encountered in realistic experimental situations [2]. Very special numerical algorithms are necessary for its precise numerical solution. In the case of alkali-metal atoms the atomic interaction in dilute BEC is essentially of short-range in nature and is approximated by a contact interaction and at zero temperature is parametrized by a single parameter in a dilute BEC – the *s*-wave atomic scattering length. Under this approximation the atomic interaction is represented by a cubic nonlinearity in the GP equation. Recently, we published the Fortran [3] and C [4] versions of useful programs for the numerical solution of the time-dependent GP equation with cubic nonlinearity under different trap symmetries using split-step Crank–Nicolson scheme and real- and imaginary-time propagations. Since then, these programs enjoyed widespread use [5].

More recently, there has been experimental observation of BEC of ^{52}Cr [6], ^{164}Dy [7] and ^{168}Er [8] atoms with large magnetic dipole moments. In this paper, for all trap symmetries the dipolar atoms are considered to be polarized along the *z* axis. In these cases the atomic interaction has a long-range dipolar counterpart in addition to the usual contact interaction. The *s*-wave contact interaction is local and spherically symmetric, whereas the dipolar interaction acting in all partial waves is nonlocal and asymmetric. The resulting GP equation in this case is a partial integro-differential equation and special algorithms are required for its numerical solution. Different approaches to the numerical solution of the dipolar GP equation have been suggested [9–14]. Yi and You [10] solve the dipolar GP equation for axially-symmetric trap while they perform the angular integral of the dipolar term, thus reducing it to one in axial (*z*, *z'*) and radial (ρ , ρ') variables involving standard Elliptical integrals. The dipolar term is regularized by a cut-off at small distances and then evaluated numerically. The dipolar GP equation is then solved by imaginary-time propagation. Goral and Santos [11] treat the dipolar term by a convolution theorem without approximation, thus transforming it to an inverse Fourier transformation (FT) of a product of the FT of the dipolar potential and the condensate density. The FT and inverse FT are then numerically evaluated by standard fast Fourier transformation (FFT) routines in Cartesian coordinates. The ground state of the system is obtained by employing a standard split-operator technique in imaginary time. This approach is used by some others [15]. Ronen et al. perform the angular integral in the dipolar term using axial symmetry. To evaluate it, in stead of FT in *x*, *y*, and *z* [11], they use Hankel transformation in the radial ρ variable and FT in the axial *z* variable. The ground state wave function is then obtained by imaginary-time propagation and dynamics by real-time propagation. This approach is also used by some others [16]. Bao et al. use Euler sine pseudospectral method for computing the ground states and a time-splitting sine pseudospectral method for computing the dynamics of dipolar BECs [9]. Blakie et al. solve the projected dipolar GP equation using a Hermite polynomial-based spectral representation [13]. Lahaye et al. use FT in *x*, *y*, and *z* to evaluate the dipolar term and employ imaginary- and real-time propagation after Crank–Nicolson discretization for stationary and nonstationary solution of the dipolar GP equation [14].

Here we provide Fortran and C versions of programs for the solution of the dipolar GP equation in a fully anisotropic 3D trap by real- and imaginary-time propagation. We use split-step Crank–Nicolson scheme for the nondipolar part as in Refs. [3,4] and the dipolar term is treated by FT in *x*, *y*, *z* variables. We also present the Fortran and C programs for reduced dipolar GP equation in one (1D) and two dimensions (2D) appropriate for a cigar- and disk-shaped BEC under tight radial (ρ) and axial (*z*) trapping, respectively [17]. In the 1D case, we consider two possibilities: the 1D BEC could be aligned along the polarization direction *z* or be aligned

perpendicular to the polarization direction along *x* axis. Similarly, in the 2D case, two possibilities are considered taking the 2D plane as *x*–*y*, perpendicular to polarization direction *z* or as *x*–*z* containing the polarization direction. This amounts to five different trapping possibilities – two in 1D and 2D each and one in 3D – and two solution schemes involving real- and imaginary-time propagation resulting in ten programs each in Fortran and C.

In Section 2 we present the 3D dipolar GP equation in an anisotropic trap. In addition to presenting the mean-field model and a general scheme for its numerical solution in Sections 2.1 and 2.2, we also present two approximate solution schemes in Sections 2.3 and 2.4 – Gaussian variational approximation and Thomas–Fermi (TF) approximation – in this case. The reduced 1D and 2D GP equations appropriate for a cigar- and a disk-shaped dipolar BEC are next presented in Sections 2.5 and 2.6, respectively. The details about the computer programs, and their input/output files, etc. are given in Section 3. The numerical method and results are given in Section 4. Finally, a brief summary is given in Section 5.

2. Gross–Pitaevskii (GP) equation for dipolar condensates in three dimensions

2.1. The mean-field Gross–Pitaevskii equation

At ultra-low temperatures the properties of a dipolar condensate of N_{at} atoms, each of mass *m*, can be described by the mean-field GP equation with nonlocal nonlinearity of the form: [10,18]

$$i\hbar \frac{\partial \phi(\mathbf{r}, t)}{\partial t} = \left[-\frac{\hbar^2}{2m} \nabla^2 + V_{\text{trap}}(\mathbf{r}) + \frac{4\pi \hbar^2 a N_{\text{at}}}{m} |\phi(\mathbf{r}, t)|^2 + N_{\text{at}} \int U_{\text{dd}}(\mathbf{r} - \mathbf{r}') |\phi(\mathbf{r}', t)|^2 d\mathbf{r}' \right] \phi(\mathbf{r}, t), \quad (1)$$

where $\int d\mathbf{r} |\phi(\mathbf{r}, t)|^2 = 1$. The trapping potential, V_{trap} is assumed to be fully asymmetric of the form

$$V_{\text{trap}}(\mathbf{r}) = \frac{1}{2} m (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

where ω_x , ω_y and ω_z are the trap frequencies, *a* the atomic scattering length. The dipolar interaction, for magnetic dipoles, is given by [11,16]

$$U_{\text{dd}}(\mathbf{R}) = \frac{\mu_0 \bar{\mu}^2}{4\pi} \frac{1 - 3 \cos^2 \theta}{|\mathbf{R}|^3}, \quad (2)$$

where $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ determines the relative position of dipoles and θ is the angle between \mathbf{R} and the direction of polarization *z*, μ_0 is the permeability of free space and $\bar{\mu}$ is the dipole moment of the condensate atom. To compare the contact and dipolar interactions, often it is useful to introduce the length scale $a_{\text{dd}} \equiv \mu_0 \bar{\mu}^2 m / (12\pi \hbar^2)$ [6].

Convenient dimensionless parameters can be defined in terms of a reference frequency $\bar{\omega}$ and the corresponding oscillator length $l = \sqrt{\hbar / (m\bar{\omega})}$. Using dimensionless variables $\bar{\mathbf{r}} = \mathbf{r}/l$, $\bar{\mathbf{R}} = \mathbf{R}/l$, $\bar{a} = a/l$, $\bar{a}_{\text{dd}} = a_{\text{dd}}/l$, $\bar{t} = t\bar{\omega}$, $\bar{x} = x/l$, $\bar{y} = y/l$, $\bar{z} = z/l$, $\bar{\phi} = l^{3/2} \phi$, Eq. (1) can be rewritten (after removing the overhead bar from all the variables) as

$$i \frac{\partial \bar{\phi}(\bar{\mathbf{r}}, \bar{t})}{\partial \bar{t}} = \left[-\frac{1}{2} \nabla^2 + \frac{1}{2} (\gamma^2 x^2 + \nu^2 y^2 + \lambda^2 z^2) + 4\pi a N_{\text{at}} |\bar{\phi}|^2 + 3N_{\text{at}} \bar{a}_{\text{dd}} \int V_{\text{dd}}^{3D}(\bar{\mathbf{R}}) |\bar{\phi}(\bar{\mathbf{r}}', \bar{t})|^2 d\bar{\mathbf{r}}' \right] \bar{\phi}(\bar{\mathbf{r}}, \bar{t}), \quad (3)$$

with

$$V_{\text{dd}}^{3D}(\bar{\mathbf{R}}) = \frac{1 - 3 \cos^2 \theta}{|\bar{\mathbf{R}}|^3}, \quad (4)$$

where $\gamma = \omega_x/\bar{\omega}$, $\nu = \omega_y/\bar{\omega}$, $\lambda = \omega_z/\bar{\omega}$. The reference frequency $\bar{\omega}$ can be taken as one of the frequencies ω_x , ω_y or ω_z or their geometric mean $(\omega_x\omega_y\omega_z)^{1/3}$. In the following we shall use Eq. (3) where we have removed the ‘bar’ from all variables.

Although we are mostly interested in the numerical solution of Eq. (3), in the following we describe two *analytical* approximation methods for its solution in the axially-symmetric case. These approximation methods – the Gaussian variational and TF approximations – provide reasonably accurate results under some limiting conditions and will be used for comparison with the numerical results. Also, we present reduced 1D and 2D mean-field GP equations appropriate for the description of a cigar and disk-shaped dipolar BEC under appropriate trapping condition. The numerical solution and variational approximation of these reduced equations will be discussed in this paper. A brief algebraic description of these topics are presented for the sake of completeness as appropriate for this study. For a full description of the same the reader is referred to the original publications.

2.2. Methodology

We perform numerical simulation of the 3D GP equation (3) using the split-step Crank–Nicolson method described in detail in Ref. [3]. Here we present the procedure to include the dipolar term in that algorithm. The inclusion of the dipolar integral term in the GP equation in coordinate space is not straightforward due to the singular behavior of the dipolar potential at short distances. It is interesting to note that this integral is well defined and finite. This problem has been tackled by evaluating the dipolar term in the momentum (k) space, where we do not face a singular behavior. The integral can be simplified in Fourier space by means of convolution as

$$\int d\mathbf{r}' V_{\text{dd}}^{3D}(\mathbf{r} - \mathbf{r}') n(\mathbf{r}', t) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{r}} \tilde{V}_{\text{dd}}^{3D}(\mathbf{k}) \tilde{n}(\mathbf{k}, t), \quad (5)$$

where $n(\mathbf{r}, t) = |\phi(\mathbf{r}, t)|^2$. The Fourier transformation (FT) and inverse FT, respectively, are defined by

$$\tilde{A}(\mathbf{k}) = \int d\mathbf{r} A(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad A(\mathbf{r}) = \frac{1}{(2\pi)^3} \int d\mathbf{k} \tilde{A}(\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (6)$$

The FT of the dipole potential can be obtained analytically [19]

$$\tilde{V}_{\text{dd}}^{3D}(\mathbf{k}) \equiv \frac{4\pi}{3} h_{3D}(\mathbf{k}) = \frac{4\pi}{3} \left(\frac{3k_z^2}{k^2} - 1 \right), \quad (7)$$

so that

$$\int d\mathbf{r}' V_{\text{dd}}^{3D}(\mathbf{r} - \mathbf{r}') n(\mathbf{r}', t) = \frac{4\pi}{3} \int \frac{d\mathbf{k}}{(2\pi)^3} e^{-i\mathbf{k}\cdot\mathbf{r}} h_{3D}(\mathbf{k}) \tilde{n}(\mathbf{k}, t). \quad (8)$$

To obtain Eq. (7), first the angular integration is performed. Then a cut-off at small r is introduced to perform the radial integration and eventually the zero cut-off limit is taken in the final result as shown in Appendix A of Ref. [19]. The FT of density $n(\mathbf{r})$ is evaluated numerically by means of a standard FFT algorithm. The dipolar integral in Eq. (3) involving the FT of density multiplied by FT of dipolar interaction is evaluated by the convolution theorem (5). The inverse FT is taken by means of the standard FFT algorithm. The FFT algorithm is carried out in Cartesian coordinates and the GP equation is solved in 3D irrespective of the symmetry of the trapping potential. The dipolar interaction integrals in 1D and 2D GP equations are also evaluated in momentum spaces. The solution algorithm of the GP equation by the split-step Crank–Nicolson method is adopted from Refs. [3,4].

The 3D GP equation (3) is numerically the most difficult to solve involving large RAM and CPU time. A requirement for the success

of the split-step Crank–Nicolson method using a FT continuous at the origin is that on the boundary of the space discretization region the wave function and the interaction term should vanish. For the long-range dipolar potential this is not true and the FT (7) is discontinuous at the origin. The space domain (from $-\infty$ to $+\infty$) cannot be restricted to a small region in space just covering the spatial extension of the BEC as the same domain is also used to calculate the FT and inverse FT used in treating the long-range dipolar potential. The use and success of FFT implies a set of noninteracting 3D periodic lattice of BECs in different unit cells. This is not true for long-range dipolar interaction which will lead to an interaction between BECs in different cells. Thus, boundary effects can play a role when finding the FT. Hence a sufficiently large space domain is to be used to have accurate values of the FT involving the long-range dipolar potential. It was suggested [12] that this could be avoided by truncating the dipolar interaction conveniently at large distances $r = R$ so that it does not affect the boundary, provided R is taken to be larger than the size of the condensate. Then the truncated dipolar potential will cover the whole condensate wave function and will have a continuous FT at the origin. This will improve the accuracy of a calculation using a small space domain. The FT of the dipolar potential truncated at $r = R$, as suggested in Ref. [12], is used in the numerical routines

$$\tilde{V}_{\text{dd}}^{3D}(\mathbf{k}) = \frac{4\pi}{3} \left(\frac{3k_z^2}{k^2} - 1 \right) \left[1 + 3 \frac{\cos(kR)}{k^2 R^2} - 3 \frac{\sin(kR)}{k^3 R^3} \right], \quad (9)$$

$$k = |\mathbf{k}|.$$

Needless to say, the difficulty in using a large space domain is the most severe in 3D. In 3D programs the cut-off R of Eq. (9) improves the accuracy of calculation and a smaller space region can be used in numerical treatment. In 1D and 2D, a larger space domain can be used relatively easily and no cut-off has been used. Also, no convenient and efficient analytic cut-off is known in 1D and 2D [12]. The truncated dipolar potential (9) has only been used in the numerical programs in 3D, e.g., *imag3d** and *real3d**. In all other numerical programs in 1D and 2D, and in all analytic results reported in the following the untruncated potential (7) has been used.

2.3. Gaussian variational approximation

In the axially-symmetric case ($\gamma = \nu$), convenient analytic Lagrangian variational approximation of Eq. (3) can be obtained with the following Gaussian ansatz for the wave function [20]

$$\phi(\mathbf{r}, t) = \frac{\pi^{-3/4}}{w_\rho(t)\sqrt{w_z(t)}} \times \exp \left[-\frac{\rho^2}{2w_\rho^2(t)} - \frac{z^2}{2w_z^2(t)} + i\alpha(t)\rho^2 + i\beta(t)z^2 \right] \quad (10)$$

where $\mathbf{r} = \{\rho, z\}$, $\rho = \{x, y\}$, $w_\rho(t)$ and $w_z(t)$ are widths and $\alpha(t)$ and $\beta(t)$ are chirps. The time dependence of the variational parameters $w_\rho(t)$, $w_z(t)$, $\alpha(t)$ and $\beta(t)$ will not be explicitly shown in the following.

The Lagrangian density corresponding to Eq. (3) is given by

$$\begin{aligned} \mathcal{L}(\mathbf{r}) = & \frac{i}{2} \left[\phi(\mathbf{r}) \frac{\phi^*(\mathbf{r})}{\partial t} - \phi^*(\mathbf{r}) \frac{\partial \phi(\mathbf{r})}{\partial t} \right] + \frac{|\nabla \phi(\mathbf{r})|^2}{2} \\ & + \frac{1}{2} (\gamma^2 \rho^2 + \lambda^2 z^2) |\phi(\mathbf{r})|^2 + 2\pi a N_{\text{at}} |\phi(\mathbf{r})|^4 \\ & + \frac{3a_{\text{dd}} N_{\text{at}}}{2} |\phi(\mathbf{r})|^2 \int V_{\text{dd}}(\mathbf{R}) |\phi(\mathbf{r}')|^2 d\mathbf{r}'. \end{aligned} \quad (11)$$

Consequently, the effective Lagrangian $L \equiv \int \mathcal{L}(\mathbf{r}) d\mathbf{r}$ (per particle) becomes [6,21]

$$L = \omega_\rho^2 \dot{\alpha} + \frac{\omega_z^2 \dot{\beta}}{2} + \frac{\gamma^2 \omega_\rho^2}{2} + \frac{\lambda^2 \omega_z^2}{4} + \frac{1}{2\omega_\rho^2} + \frac{1}{4\omega_z^2} + 2\omega_\rho^2 \alpha^2 + \omega_z^2 \beta^2 + \frac{N_{\text{at}}[a - a_{\text{ddf}}(\kappa)]}{\sqrt{2\pi} \omega_\rho^2 \omega_z}. \quad (12)$$

The Euler–Lagrangian equations with this Lagrangian leads to the following set of coupled ordinary differential equations (ODE) for the widths w_ρ and w_z [22]:

$$\ddot{w}_\rho + \gamma^2 w_\rho = \frac{1}{w_\rho^3} + \frac{N_{\text{at}}}{\sqrt{2\pi}} \frac{[2a - a_{\text{ddf}}(\kappa)]}{w_\rho^3 w_z}, \quad (13)$$

$$\ddot{w}_z + \lambda^2 w_z = \frac{1}{w_z^3} + \frac{2N_{\text{at}}}{\sqrt{2\pi}} \frac{[a - a_{\text{ddc}}(\kappa)]}{w_\rho^2 w_z^2}, \quad (14)$$

with $\kappa = w_\rho/w_z$ and

$$g(\kappa) = \frac{2 - 7\kappa^2 - 4\kappa^4 + 9\kappa^4 d(\kappa)}{(1 - \kappa^2)^2}, \quad (15)$$

$$c(\kappa) = \frac{1 + 10\kappa^2 - 2\kappa^4 - 9\kappa^2 d(\kappa)}{(1 - \kappa^2)^2}, \quad (16)$$

$$f(\kappa) = \frac{1 + 2\kappa^2 - 3\kappa^2 d(\kappa)}{1 - \kappa^2}, \quad d(\kappa) = \frac{\text{atanh}\sqrt{1 - \kappa^2}}{\sqrt{1 - \kappa^2}}. \quad (17)$$

The widths of a (time-independent) stationary state are obtained from Eqs. (13) and (14) by setting $\ddot{w}_\rho = \ddot{w}_z = 0$. The energy (per particle) of the stationary state is the Lagrangian (12) with $\alpha = \beta = 0$, e.g.,

$$\frac{E}{N_{\text{at}}} = \frac{1}{2w_\rho^2} + \frac{1}{4w_z^2} + \frac{N_{\text{at}}[a - a_{\text{ddf}}(\kappa)]}{\sqrt{2\pi} w_\rho w_z} + \frac{\gamma^2 w_\rho^2}{2} + \frac{\lambda^2 w_z^2}{4}. \quad (18)$$

The chemical potential $\mu = \partial E/\partial N_{\text{at}}$ of the stationary state is given by [22]

$$\mu = \frac{1}{2w_\rho^2} + \frac{1}{4w_z^2} + \frac{2N_{\text{at}}[a - a_{\text{ddf}}(\kappa)]}{\sqrt{2\pi} w_\rho w_z} + \frac{\gamma^2 w_\rho^2}{2} + \frac{\lambda^2 w_z^2}{4}. \quad (19)$$

2.4. Thomas–Fermi (TF) approximation

In the time-dependent axially-symmetric GP equation (3), when the atomic interaction term is large compared to the kinetic energy gradient term, the kinetic energy can be neglected and the useful TF approximation emerges. We assume the normalized density of the dipolar BEC of the form [1,23–25]

$$n(\mathbf{r}, t) \equiv |\phi(\mathbf{r}, t)|^2 = \frac{15}{8\pi R_\rho^2(t) R_z(t)} \left[1 - \frac{\rho^2}{R_\rho^2(t)} - \frac{z^2}{R_z^2(t)} \right], \quad (20)$$

where $R_\rho(t)$ and $R_z(t)$ are the radial and axial sizes. The time dependence of these sizes will not be explicitly shown in the following. Using the parabolic density (20), the energy functional E_{TF} may be written as [24]

$$E_{\text{TF}} \equiv E_{\text{trap}} + E_{\text{int}} = \left[\frac{N(2\gamma^2 R_\rho^2 + \lambda^2 R_z^2)}{14} \right] + \left[\frac{15}{28\pi} \frac{4\pi a N_{\text{at}}^2}{R_\rho^2 R_z} \left\{ 1 - \frac{a_{\text{ddf}}(\bar{\kappa})}{a} \right\} \right], \quad (21)$$

where $\bar{\kappa} = R_\rho/R_z$ is the ratio of the condensate sizes and $f(\bar{\kappa})$ is given by Eq. (17). In Eq. (21), E_{trap} is the energy in the trap and E_{int} is the interaction or release energy in the TF approximation. In the TF

regime one has the following set of coupled ODEs for the evolution of the condensate sizes [23]:

$$\ddot{R}_\rho = -R_\rho \gamma^2 + \frac{15aN_{\text{at}}}{R_\rho R_z} \left[\frac{1}{R_\rho^2} - \frac{a_{\text{dd}}}{a} \left(\frac{1}{R_\rho^2} + \frac{3}{2} \frac{f(\bar{\kappa})}{R_\rho^2 - R_z^2} \right) \right], \quad (22)$$

$$\ddot{R}_z = -\lambda^2 R_z + \frac{15aN_{\text{at}}}{R_\rho^2} \left[\frac{1}{R_z^2} + \frac{2a_{\text{dd}}}{a} \left(\frac{1}{R_z^2} + \frac{3}{2} \frac{f(\bar{\kappa})}{R_\rho^2 - R_z^2} \right) \right]. \quad (23)$$

The sizes of a stationary state can be calculated from Eqs. (22) and (23) by setting the time derivatives \ddot{R}_ρ and \ddot{R}_z to zero leading to the transcendental equation for $\bar{\kappa}$ [23]:

$$3\bar{\kappa}^2 \frac{a_{\text{dd}}}{a} \left[\left(1 + \frac{\lambda^2}{2\gamma^2} \right) \frac{f(\bar{\kappa})}{1 - \bar{\kappa}^2} - 1 \right] + \left(\frac{a_{\text{dd}}}{a} - 1 \right) \left(\bar{\kappa}^2 - \frac{\lambda^2}{\gamma^2} \right) = 0, \quad (24)$$

and

$$R_\rho = \left[\frac{15aN_{\text{at}}\bar{\kappa}}{\gamma^2} \left\{ 1 + \frac{a_{\text{dd}}}{a} \left(\frac{3}{2} \frac{\bar{\kappa}^2 f(\bar{\kappa})}{1 - \bar{\kappa}^2} - 1 \right) \right\} \right]^{1/5}, \quad (25)$$

with $R_z = R_\rho/\bar{\kappa}$. The chemical potential is given by [24]

$$\mu_{\text{TF}} \equiv E_{\text{trap}} + 2E_{\text{int}} = \frac{15}{8\pi} \frac{4\pi a N_{\text{at}}}{R_\rho^2 R_z} \left[1 - \frac{a_{\text{dd}}}{a} f(\bar{\kappa}) \right]. \quad (26)$$

We have the identities $E_{\text{TF}}/N_{\text{at}} = 5\mu_{\text{TF}}/7$, $E_{\text{int}}/N_{\text{at}} = 2\mu_{\text{TF}}/7$, $E_{\text{trap}}/N_{\text{at}} = 3\mu_{\text{TF}}/7$.

2.5. One-dimensional GP equation for a cigar-shaped dipolar BEC

2.5.1. z direction

For a cigar-shaped dipolar BEC with a strong axially-symmetric ($v = \gamma$) radial trap ($\lambda < v, \gamma$), we assume that the dynamics of the BEC in the radial direction is confined in the radial ground state [22,26,27]

$$\phi(\boldsymbol{\rho}) = \exp(-\rho^2/2d_\rho^2)/(d_\rho\sqrt{\pi}), \quad \gamma d_\rho^2 = 1, \quad \boldsymbol{\rho} \equiv (x, y), \quad (27)$$

of the transverse trap and the wave function $\phi(\mathbf{r})$ can be written as

$$\phi(\mathbf{r}, t) \equiv \phi_{1D}(z, t) \times \phi(\boldsymbol{\rho}) = \frac{1}{\sqrt{\pi} d_\rho^2} \exp\left[-\frac{\rho^2}{2d_\rho^2}\right] \phi_{1D}(z, t), \quad (28)$$

where $\phi_{1D}(z, t)$ is the effective 1D wave function for the axial dynamics and d_ρ is the radial harmonic oscillator length.

To derive the effective 1D equation for the cigar-shaped dipolar BEC, we substitute the ansatz (28) in Eq. (3), multiply by the ground-state wave function $\phi(\boldsymbol{\rho})$ and integrate over $\boldsymbol{\rho}$ to get the 1D equation [22,26]

$$i \frac{\partial \phi_{1D}(z, t)}{\partial t} = \left[-\frac{\partial_z^2}{2} + \frac{\lambda^2 z^2}{2} + \frac{2aN_{\text{at}}|\phi_{1D}|^2}{d_\rho^2} + 3a_{\text{dd}}N_{\text{at}} \int_{-\infty}^{\infty} V_{\text{dd}}^{1D}(|z - z'|) |\phi_{1D}(z', t)|^2 dz' \right] \phi_{1D}(z, t), \quad (29)$$

$$V_{\text{dd}}^{1D}(Z) = \frac{2\pi}{\sqrt{2}d_\rho} \left[\frac{4}{3} \delta(\sqrt{w}) + 2\sqrt{w} - \sqrt{\pi}(1 + 2w)e^w \{1 - \text{erf}(\sqrt{w})\} \right], \quad (30)$$

where $w = [Z/(\sqrt{2}d_\rho)]^2$, $Z = |z - z'|$. Here and in all reductions in Sections 2.5 and 2.6 we use the untruncated dipolar potential

(7) and not the truncated potential (9). The integral term in the 1D GP equation (29) is conveniently evaluated in momentum space using the following convolution identity [22]

$$\int_{-\infty}^{\infty} V_{\text{dd}}^{1D}(|z-z'|)|\phi_{1D}(z',t)|^2 dz' = \frac{4\pi}{3} \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} e^{-ik_z z} \tilde{n}(k_z, t) h_{1D}\left(\frac{k_z d_\rho}{\sqrt{2}}\right), \quad (31)$$

where

$$\tilde{n}(k_z, t) = \int_{-\infty}^{\infty} e^{ik_z z} |\phi_{1D}(z, t)|^2 dz, \quad (32)$$

$$\tilde{n}(\mathbf{k}_\rho) = \int e^{i\mathbf{k}_\rho \cdot \boldsymbol{\rho}} |\phi_{2D}(\boldsymbol{\rho})|^2 d\rho = e^{-k_\rho^2 d_\rho^2/4}, \quad k_\rho = \sqrt{k_x^2 + k_y^2} \quad (33)$$

$$h_{1D}(\zeta) \equiv \frac{1}{(2\pi)^2} \int d\mathbf{k}_\rho \left[\frac{3k_z^2}{\mathbf{k}^2} - 1 \right] |\tilde{n}(\mathbf{k}_\rho)|^2 = \frac{1}{2\pi d_\rho^2} \int_0^\infty du \left[\frac{3\zeta^2}{u + \zeta^2} - 1 \right] e^{-u}, \quad \zeta = \frac{k_z d_\rho}{\sqrt{2}}. \quad (34)$$

The 1D GP equation (29) can be solved analytically using the Lagrangian variational formalism with the following Gaussian ansatz for the wave function [22]:

$$\phi_{1D}(z, t) = \frac{\pi^{-1/4}}{\sqrt{w_z(t)}} \exp\left[-\frac{z^2}{2w_z^2(t)} + i\beta(t)z^2\right], \quad (35)$$

where $w_z(t)$ is the width and $\beta(t)$ is the chirp. The Lagrangian variational formalism leads to the following equation for the width $w_z(t)$ [22]:

$$\ddot{w}_z(t) + \lambda^2 w_z(t) = \frac{1}{w_z^3(t)} + \frac{2N_{\text{at}}}{\sqrt{2\pi}} \frac{[a - a_{\text{dd}}c(\hat{\kappa})]}{d_\rho^2 w_z^2(t)}, \quad \hat{\kappa} = \frac{d_\rho}{w_z(t)}. \quad (36)$$

The time-independent width of a stationary state can be obtained from Eq. (36) by setting $\ddot{w}_z(t) = 0$. The variational chemical potential for the stationary state is given by [22]

$$\mu = \frac{1}{4w_z^2} + \frac{2N_{\text{at}}[a - a_{\text{dd}}f(\hat{\kappa})]}{\sqrt{2\pi} w_z d_\rho^2} + \frac{\lambda^2 w_z^2}{4}. \quad (37)$$

The energy per particle is given by

$$\frac{E}{N_{\text{at}}} = \frac{1}{4w_z^2} + \frac{N_{\text{at}}[a - a_{\text{dd}}f(\hat{\kappa})]}{\sqrt{2\pi} w_z d_\rho^2} + \frac{\lambda^2 w_z^2}{4}. \quad (38)$$

2.5.2. x direction

For a cigar-shaped dipolar BEC with a strong axially-symmetric ($\nu = \lambda$) radial trap ($\gamma < \nu, \lambda$), we assume that the dynamics of the BEC in the radial direction is confined in the radial ground state [22,26,27]

$$\phi(\boldsymbol{\rho}) = \exp(-\rho^2/2d_\rho^2)/(d_\rho\sqrt{\pi}), \quad \nu d_\rho^2 = 1, \quad \boldsymbol{\rho} \equiv (y, z), \quad (39)$$

of the transverse trap and the wave function $\phi(\mathbf{r})$ can be written as

$$\phi(\mathbf{r}, t) \equiv \phi_{1D}(x, t) \times \phi(\boldsymbol{\rho}) = \frac{1}{\sqrt{\pi d_\rho^2}} \exp\left[-\frac{\rho^2}{2d_\rho^2}\right] \phi_{1D}(x, t), \quad (40)$$

where $\phi_{1D}(x, t)$ is the effective 1D wave function for the dynamics along x axis and d_ρ is the radial harmonic oscillator length.

To derive the effective 1D equation for the cigar-shaped dipolar BEC, we substitute the ansatz (40) in Eq. (3), multiply by the

ground-state wave function $\phi(\boldsymbol{\rho})$ and integrate over $\boldsymbol{\rho}$ to get the 1D equation

$$i \frac{\partial \phi_{1D}(x, t)}{\partial t} = \left[-\frac{\partial_x^2}{2} + \frac{\gamma^2 x^2}{2} + \frac{2aN_{\text{at}}|\phi_{1D}|^2}{d_\rho^2} + 4\pi a_{\text{dd}}N_{\text{at}} \int_{-\infty}^{\infty} \frac{dk_x}{2\pi} e^{-ik_x x} \tilde{n}(k_x, t) j_{1D}(\tau_x) \right] \phi_{1D}(x, t), \quad (41)$$

where $\tau_x = d_\rho k_x/\sqrt{2}$ and

$$j_{1D}(\tau_x) \equiv \frac{1}{(2\pi)^2} \int d\mathbf{k}_\rho \left[\frac{3k_z^2}{\mathbf{k}^2} - 1 \right] |\tilde{n}(\mathbf{k}_\rho)|^2 = \frac{\sqrt{2}}{2\pi d_\rho} \int_{-\infty}^{\infty} d\tau_y e^{-\tau_y^2} h_{2D}(\tau), \quad \tau_y = \frac{d_\rho k_y}{\sqrt{2}}, \quad \tau = \sqrt{\tau_x^2 + \tau_y^2}, \quad (42)$$

$$h_{2D}(\tau) = \frac{1}{\sqrt{2\pi} d_\rho} [2 - 3\sqrt{\pi} e^{\tau^2} \tau \{1 - \text{erf}(\tau)\}]. \quad (43)$$

To derive Eq. (41), the dipolar term in Eq. (3) is first written in momentum space using Eq. (8) and the integrations over k_y and k_z are performed in the dipolar term.

2.6. Two-dimensional GP equation for a disk-shaped dipolar BEC

2.6.1. x - y plane

For an axially-symmetric ($\nu = \gamma$) disk-shaped dipolar BEC with a strong axial trap ($\lambda > \nu, \gamma$), we assume that the dynamics of the BEC in the axial direction is confined in the axial ground state

$$\phi(z) = \exp(-z^2/2d_z^2)/(\pi d_z^2)^{1/4}, \quad d_z = \sqrt{1/(\lambda)}, \quad (44)$$

and we have for the wave function

$$\phi(\mathbf{r}) \equiv \phi(z) \times \phi_{2D}(\boldsymbol{\rho}, t) = \frac{1}{(\pi d_z^2)^{1/4}} \exp\left[-\frac{z^2}{2d_z^2}\right] \phi_{2D}(\boldsymbol{\rho}, t), \quad (45)$$

where $\boldsymbol{\rho} \equiv (x, y)$, $\phi_{2D}(\boldsymbol{\rho}, t)$ is the effective 2D wave function for the radial dynamics and d_z is the axial harmonic oscillator length. To derive the effective 2D equation for the disk-shaped dipolar BEC, we use ansatz (45) in Eq. (3), multiply by the ground-state wave function $\phi(z)$ and integrate over z to get the 2D equation [22,28]

$$i \frac{\partial \phi_{2D}(\boldsymbol{\rho}, t)}{\partial t} = \left[-\frac{\nabla_\rho^2}{2} + \frac{\gamma^2 x^2 + \nu^2 y^2}{2} + \frac{4\pi aN_{\text{at}}|\phi_{2D}|^2}{\sqrt{2\pi} d_z} + 4\pi a_{\text{dd}}N_{\text{at}} \int \frac{d\mathbf{k}_\rho}{(2\pi)^2} e^{-i\mathbf{k}_\rho \cdot \boldsymbol{\rho}} \tilde{n}(\mathbf{k}_\rho, t) h_{2D}\left(\frac{k_\rho d_z}{\sqrt{2}}\right) \right] \phi_{2D}(\boldsymbol{\rho}, t), \quad (46)$$

where $k_\rho = \sqrt{k_x^2 + k_y^2}$, and

$$\tilde{n}(\mathbf{k}_\rho, t) = \int d\boldsymbol{\rho} e^{i\mathbf{k}_\rho \cdot \boldsymbol{\rho}} |\phi_{2D}(\boldsymbol{\rho}, t)|^2, \quad (47)$$

$$\tilde{n}(k_z) = \int dz e^{ik_z z} |\phi(z)|^2 = e^{-k_z^2 d_z^2/4},$$

$$h_{2D}(\xi) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_z \left[\frac{3k_z^2}{\mathbf{k}^2} - 1 \right] |\tilde{n}(k_z)|^2 = \frac{1}{\sqrt{2\pi} d_z} [2 - 3\sqrt{\pi} \xi \exp(\xi^2) \{1 - \text{erf}(\xi)\}], \quad \xi = \frac{k_\rho d_z}{\sqrt{2}}. \quad (48)$$

To derive Eq. (46), the dipolar term in Eq. (3) is first written in momentum space using Eq. (8) and the integration over k_z is performed in the dipolar term.

The 2D GP equation (46) can be solved analytically using the Lagrangian variational formalism with the following Gaussian ansatz for the wave function [22]:

$$\phi_{2D}(\boldsymbol{\rho}, t) = \frac{\pi^{-1/2}}{w_\rho(t)} \exp \left[-\frac{\rho^2}{2w_\rho^2(t)} + i\alpha(t)\rho^2 \right], \quad (49)$$

where $w_\rho(t)$ is the width and $\alpha(t)$ is the chirp. The Lagrangian variational formalism leads to the following equation for the width w_ρ [22]:

$$\ddot{w}_\rho(t) + \gamma^2 w_\rho(t) = \frac{1}{w_\rho^3(t)} + \frac{N_{\text{at}}}{\sqrt{2\pi}} \frac{[2a - a_{\text{dd}}g(\bar{k})]}{w_\rho^3(t)d_z},$$

$$\bar{k} = \frac{w_\rho(t)}{d_z}. \quad (50)$$

The time-independent width of a stationary state can be obtained from Eq. (50) by setting $\ddot{w}_\rho(t) = 0$. The variational chemical potential for the stationary state is given by [22]

$$\mu = \frac{1}{2w_\rho^2} + \frac{2N_{\text{at}}[a - a_{\text{dd}}f(\bar{k})]}{\sqrt{2\pi}d_z w_\rho^2} + \frac{\gamma^2 w_\rho^2}{2}. \quad (51)$$

The energy per particle is given by

$$\frac{E}{N_{\text{at}}} = \frac{1}{2w_\rho^2} + \frac{N_{\text{at}}[a - a_{\text{dd}}f(\bar{k})]}{\sqrt{2\pi}d_z w_\rho^2} + \frac{\gamma^2 w_\rho^2}{2}. \quad (52)$$

2.6.2. x - z plane

For a disk-shaped dipolar BEC with a strong axial trap along y direction ($\nu > \lambda, \gamma$), we assume that the dynamics of the BEC in the y direction is confined in the ground state

$$\phi(y) = \exp(-y^2/2d_y^2)/(\pi d_y^2)^{1/4}, \quad d_y = \sqrt{1/\nu}, \quad (53)$$

and we have for the wave function

$$\phi(\mathbf{r}) \equiv \phi(y) \times \phi_{2D}(\boldsymbol{\rho}, t) = \frac{1}{(\pi d_y^2)^{1/4}} \exp \left[-\frac{y^2}{2d_y^2} \right] \phi_{2D}(\boldsymbol{\rho}, t), \quad (54)$$

where now $\boldsymbol{\rho} \equiv (x, z)$, and $\phi_{2D}(\boldsymbol{\rho}, t)$ is the circularly-asymmetric effective 2D wave function for the 2D dynamics and d_y is the harmonic oscillator length along y direction. To derive the effective 2D equation for the disk-shaped dipolar BEC, we use ansatz (54) in Eq. (3), multiply by the ground-state wave function $\phi(y)$ and integrate over y to get the 2D equation

$$i \frac{\partial \phi_{2D}(\boldsymbol{\rho}, t)}{\partial t} = \left[-\frac{\nabla_\rho^2}{2} + \frac{\gamma^2 x^2 + \lambda^2 z^2}{2} + \frac{4\pi a N_{\text{at}} |\phi_{2D}|^2}{\sqrt{2\pi} d_y} \right. \\ \left. + 4\pi a_{\text{dd}} N_{\text{at}} \int \frac{d\mathbf{k}_\rho}{(2\pi)^2} e^{-i\mathbf{k}_\rho \cdot \boldsymbol{\rho}} \tilde{n}(\mathbf{k}_\rho, t) j_{2D} \left(\frac{k_\rho d_y}{\sqrt{2}} \right) \right] \phi_{2D}(\boldsymbol{\rho}, t), \quad (55)$$

where $k_\rho = \sqrt{k_x^2 + k_z^2}$, and

$$j_{2D}(\xi) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk_y \left[\frac{3k_z^2}{k^2} - 1 \right] |\tilde{n}(k_y)|^2 \\ = \frac{1}{\sqrt{2\pi} d_y} \left[-1 + 3\sqrt{\pi} \frac{\xi^2}{\xi} \exp(\xi^2) \{1 - \text{erf}(\xi)\} \right], \\ \xi = \frac{k_\rho d_y}{\sqrt{2}}, \quad \xi_z = \frac{k_z d_y}{\sqrt{2}}. \quad (56)$$

To derive Eq. (55), the dipolar term in Eq. (3) is first written in momentum space using Eq. (8) and the integration over k_y is performed in the dipolar term.

3. Details about the programs

3.1. Description of the programs

In this subsection we describe the numerical codes for solving the dipolar GP equations (29) and (41) in 1D, Eqs. (46) and (55) in 2D, and Eq. (3) in 3D using real- and imaginary-time propagations. The real-time propagation yields the time-dependent dynamical results and the imaginary-time propagation yields the time-independent stationary solution for the lowest-energy state for a specific symmetry. We use the split-step Crank–Nicolson method for the solution of the equations described in Ref. [3]. The present programs have the same structure as in Ref. [3] with added subroutines to calculate the dipolar integrals. In the absence of dipolar interaction the present programs will be identical with the previously published ones [3]. A general instruction to use these programs in the nondipolar case can be found in Ref. [3] and we refer the interested reader to this article for the same.

The present Fortran programs named ('imag1dX.f90', 'imag1dZ.f90'), ('imag2dXY.f90', 'imag2dXZ.f90'), 'imag3d.f90', ('real1dX.f90', 'real1dZ.f90'), ('real2dXY.f90', 'real2dXZ.f90'), 'real3d.f90', deal with imaginary- and real-time propagations in 1D, 2D, and 3D and are to be contrasted with previously published programs [3] 'imagtime1d.F', 'imagtime2d.f90', 'imagtime3d.f90', 'realtime1d.F', 'realtime2d.f90', and 'realtime3d.f90', for the nondipolar case. The input parameters in Fortran programs are introduced in the beginning of each program. The corresponding C codes are called (imag1dX.c, imag1dX.h, imag1dZ.c, imag1dZ.h), (imag2dXY.c, imag2dXY.h, imag2dXZ.c, imag2dXZ.h), (imag3d.c, imag3d.h), (real1dX.c, real1dX.h, real1dZ.c, real1dZ.h), (real2dXY.c, real2dXY.h, real2dXZ.c, real2dXZ.h), (real3d.c, real3d.h), with respective input files ('imag1dX-input', 'imag1dZ-input'), ('imag2dXY-input', 'imag2dXZ-input'), 'imag3d-input', ('real1dX-input', 'real1dZ-input'), ('real2dXY-input', 'real1dXZ-input'), 'real3d-input', which perform identical executions as in the Fortran programs.

We present in the following a description of input parameters. The parameters NX, NY, and NZ in 3D (NX and NY in 2DXY, NX and NZ in 2DXZ), and N in 1D stand for total number of space points in x , y and z directions, where the respective space steps DX, DY, and DZ can be made equal or different; DT is the time step. The parameters NSTP, NPAS, and NRUN denote number of time iterations. The parameters GAMMA (γ), NU (ν), and LAMBDA (λ) denote the anisotropy of the trap. The number of atoms is denoted NATOMS (N_{at}), the scattering length is denoted AS (a) and dipolar length ADD (a_{dd}). The parameters G0 ($4\pi N_{\text{at}} a$) and GDD0 ($3a_{\text{dd}} N_{\text{at}}$) are the contact and dipolar nonlinearities. The parameter OPTION = 2 (default) defines the equations of the present paper with a factor of half before the kinetic energy and trap; OPTION = 1 defines a different set of GP equations without these factors, viz Ref. [3]. The parameter AHO is the unit of length and Bohr_a0 is the Bohr radius. In 1D the parameter DRHO is the radial harmonic oscillator d_ρ and in 2D the parameter D_Z or D_Y is the axial harmonic oscillator length d_z or d_y . The parameter CUTOFF is the cut-off R of Eq. (9) in the 3D programs. The parameters GPAR and GPAR are constants which multiply the nonlinearities G0 and GDD0 in realtime routines before NRUN time iterations to study the dynamics.

The programs, as supplied, solve the GP equations for specific values of dipolar and contact nonlinearities and write the wave function, chemical potential, energy, and root-mean-square (rms) size(s), etc. For solving a stationary problem, the imaginary-time programs are far more accurate and should be used. The real-time programs should be used for studying non-equilibrium problems reading an initial wave function calculated by the imaginary-time program with identical set of parameters (set NSTP = 0, for this

purpose, in the real-time programs). The real-time programs can also calculate stationary solutions in NSTP time steps (set NSTP \neq 0 in real-time programs), however, with less accuracy compared to the imaginary-time programs. The larger the value of NSTP in real-time programs, more accurate will be the result [3]. The nonzero integer parameter NSTP refers to the number of time iterations during which the nonlinear terms are slowly introduced during the time propagation for calculating the wave function. After introducing the nonlinearities in NSTP iterations the imaginary-time programs calculate the final result in NPAS plus NRUN time steps and write some of the results after NPAS steps to check convergence. The real-time programs run the dynamics during NPAS steps with unchanged initial parameters so as to check the stability and accuracy of the results. Some of the nonlinearities are then slightly modified after NPAS iterations and the small oscillation of the system is studied during NRUN iterations.

Each program is preset at fixed values of contact and dipolar nonlinearities as calculated from input scattering length(s), dipolar strength(s), and number of atom(s), correlated DX–DT values and NSTP, NPAS, and NRUN, etc. A study of the correlated DX and DT values in the nondipolar case can be found in Ref. [3]. Smaller the steps DX, DY, DZ and DT, more accurate will be the result, provided we integrate over a reasonably large space region by increasing NX, NY, and NZ, etc. Each supplied program produces result up to a desired precision consistent with the parameters employed – G0, GDD0, DX, DY, DZ, DT, NX, NY, NZ, NSTP, NPAS, and NRUN, etc.

3.2. Description of Output files

Programs ‘imagnd*’ ($n = 1, 2, 3, C$ and Fortran): They write final density in files ‘imagnd-den.txt’ after NRUN iterations. In addition, in 2D and 3D, integrated 1D densities ‘imagnd*-den1d_x.txt’, ‘imagnd*-den1d_y.txt’, ‘imagnd*-den1d_z.txt’, along $x, y,$ and $z,$ etc., are given. These densities are obtained by integrating the densities over eliminated space variables. In addition, in 3D integrated 2D densities ‘imag3d-den2d_xy.txt’, ‘imag3d-den2d_yz.txt’, ‘imag3d-den2d_zx.txt’, in $xy, yz,$ and zx planes can be written (commented out by default). The files ‘imagnd*-out.txt’ provide different initial input data, as well as chemical potential, energy, size, etc. at different stages (initial, after NSTP, NPAS, and after NRUN iterations), from which a convergence of the result can be inferred. The files ‘imagnd*-rms.txt’ provide the different rms sizes at different stages (initial, after NSTP, NPAS, and after NRUN iterations).

Programs ‘realnd*’ ($n = 1, 2, 3, C$ and Fortran): The same output files as in the imaginary-time programs are available in the real-time programs. The real-time densities are reported after NPAS iterations. In addition in the ‘realnd*-dyna.txt’ file the temporal evolution of the widths are given during NPAS and NRUN iterations. Before NRUN iterations the nonlinearities G0 and GDD0 are multiplied by parameters GPAR and GDPAR to start an oscillation dynamics.

3.3. Running the programs

In addition to installing the respective Fortran and C compilers one needs also to install the FFT routine FFTW in the computer. To run the Fortran programs the supplied routine fftw3.f03 should be included in compilation. The commands for running the Fortran programs using INTEL, GFortran, and Oracle Sun compilers are given inside the Fortran programs. The programs are submitted in directories with option to compile using the command ‘make’. There are two files with general information about the programs and FT for user named ‘readme.txt’ and ‘readme-fftw.txt’. The Fortran and C programs are in directories ./f_program and ./c_program. Inside these directories there are subdirectories such as ./input, ./output, ./src. The subdirectory ./output contains

output files the programs generate, ./input contains input files for C programs, and ./src contains the different programs. The command ‘make’ in the directory ./f_program or ./c_program compiles all the programs and generates the corresponding executable files to run. The command ‘make’ for INTEL, GFortran and OracleSun Fortran are given.

4. Numerical results

In this section we present results for energy, chemical potential and root-mean-square (rms) sizes for different stationary BECs in 1D, 2D, and 3D, and compare with those obtained by using Gaussian variational and TF approximations, wherever possible. We also compare with available results by other authors. For a fixed space and time step, sufficient number of space discretizing points and time iterations are to be allowed to get convergence.

First we present in Table 1 numerical results for the energy E , chemical potential μ , and rms size $\langle z \rangle$ calculated using the imaginary-time program for the 1D dipolar GP Eq. (29) for ^{52}Cr atoms with $a = 6 \text{ nm}$ ($\approx 113a_0$ with a_0 the Bohr radius), and $a_{dd} = 16a_0$ for $\lambda = 1, d_\rho = 1, l = 1 \mu\text{m}$ and for different number of atoms N_{at} and different space and time steps dz and dt . The Gaussian variational approximations obtained from Eqs. (36)–(38) are also given for comparison. The variational results provide better approximation to the numerical solution for a smaller number of atoms.

In Table 2 we present results for the energy E , chemical potential μ , and rms size $\langle \rho \rangle$ of the 2D GP Eq. (46) for $\gamma = \nu = 1, d_z = 1, l = 1 \mu\text{m}$. The numerical results are calculated using different space and time steps dx, dy and dt and different number N_{at} of ^{52}Cr atoms with $a_{dd} = 16a_0$ and $a = 6 \text{ nm}$. Axially-symmetric Gaussian variational approximations obtained from Eqs. (50)–(52) are also presented for comparison.

Now we present results of the solution of the 3D GP Eq. (3) with some axially-symmetric traps. In this case we take advantage of the cut-off introduced in Eq. (9) to improve the accuracy of the numerical calculation. The cut-off parameter R was taken larger than the condensate size and smaller than the discretization box. First we consider the model 3D GP equation with $a = 0$ and different $g_{dd} = 3a_{dd}N_{\text{at}} = 1, 2, 3, 4$ in an axially-symmetric trap with $\lambda = 1/2$ and $\nu = \gamma = 1$. The numerical results for different number of space and time steps together with Gaussian variational results obtained from Eqs. (18) and (19) are shown in Table 3. These results for energy E and chemical potential μ are compared with those calculated by Asad-uz-Zaman et al. [16,29]. The present calculation is performed in the Cartesian x, y, z coordinates and the dipolar term is evaluated by FT to momentum space. Asad-uz-Zaman et al. take advantage of the axial symmetry and perform the calculation in the axial ρ, z ($\rho \equiv x, y$) variables and evaluate the dipolar term by a combined Hankel–Fourier transformation to momentum space for ρ and z , respectively. The calculations of Asad-uz-Zaman et al. for stationary states involving two variables (ρ and z) thus could be more economic and accurate than the present calculation involving three Cartesian variables for the axially-symmetric configuration considered in Table 3. However, the present method, unlike that of Ref. [16], is readily applicable to the fully asymmetric configurations. Moreover, the present calculation for dynamics (non-stationary states) in 3D are more realistic than the calculations of Asad-uz-Zaman et al., where one degree of freedom is frozen. For example, a vortex could be unstable [30] in a full 3D calculation, whereas a 2D calculation could make the same vortex stable.

Next we consider the solution of the 3D GP Eq. (3) for a model condensate of ^{52}Cr atoms in a cigar-shaped axially-symmetric trap with $\gamma = \nu = 1, \lambda = 1/2$, first considered by Bao et al. [9]. The nonlinearities considered there ($4\pi a = 0.20716, 4\pi a_{dd} = 0.033146$) correspond to the following approximate values of

Table 1

The energy per particle E/N_{at} , chemical potential μ , and rms size $\langle z \rangle$ of the 1D GP Eq. (29) for $\lambda = 1$, $d_\rho = 1 \mu\text{m}$ for the ^{52}Cr BEC with $a = 6 \text{ nm}$, $a_{\text{dd}} = 16a_0$ and different number of atoms N_{at} . In Eqs. (3) and (29) the lengths are expressed in oscillator unit: $l = 1 \mu\text{m}$. Numerical results are calculated for parameters (A) $dx = dy = 0.1$, $dt = 0.0005$, $N = 2048$ (B) $dz = 0.1$, $dt = 0.001$, $N = 1024$ and compared with variational results obtained from Eqs. (36)–(38).

N_{at}	$\langle z \rangle$ var	$\langle z \rangle$ (B)	$\langle z \rangle$ (A)	E/N_{at} var	E/N_{at} (B)	E/N_{at} (A)	μ var	μ (B)	μ (A)
100	0.7939	0.7937	0.7937	0.7239	0.7222	0.7222	0.9344	0.9297	0.9297
500	1.0425	1.0381	1.0381	1.4371	1.4166	1.4166	2.2157	2.1691	2.1691
1000	1.2477	1.2375	1.2375	2.1376	2.0920	2.0920	3.4165	3.3234	3.3234
5000	2.0249	1.9939	1.9939	5.8739	5.6910	5.6910	9.6671	9.3488	9.3488
10,000	2.5233	2.4815	2.4815	9.2129	8.913	8.913	15.223	14.715	14.715
50,000	4.2451	4.1719	4.1719	26.505	25.622	25.622	43.993	42.527	42.527

Table 2

The energy per particle E/N_{at} , chemical potential μ , and rms size $\langle \rho \rangle$ of the 2D GP Eq. (46) for $\gamma = \nu = 1$, $d_z = 1 \mu\text{m}$ for the ^{52}Cr BEC with $a = 6 \text{ nm}$, $a_{\text{dd}} = 16a_0$ and different number of atoms N_{at} . In Eqs. (3) and (46) the lengths are expressed in oscillator unit: $l = 1 \mu\text{m}$. Numerical results are calculated for space and time steps (A) $dx = dy = 0.1$, $dt = 0.0005$, $NX = NY \equiv \mathcal{N} = 768$, (B) $dx = dy = 0.2$, $dt = 0.002$, $\mathcal{N} = 384$, and compared with variational results obtained from Eqs. (50), (51) and (52).

N_{at}	$\langle \rho \rangle$ var	$\langle \rho \rangle$ (B)	$\langle \rho \rangle$ (A)	E/N_{at} var	E/N_{at} (B)	E/N_{at} (A)	μ var	μ (B)	μ (A)
100	1.0985	1.097	1.097	1.2182	1.2156	1.2157	1.4187	1.4120	1.4119
500	1.3514	1.342	1.342	1.8653	1.8383	1.8383	2.5437	2.4840	2.4840
1000	1.5482	1.530	1.531	2.4571	2.3988	2.3988	3.5070	3.3901	3.3901
5000	2.2549	2.208	2.208	5.2206	4.9989	4.9989	7.8005	7.4249	7.4249
10,000	2.6824	2.619	2.619	7.3787	7.029	7.029	11.090	10.522	10.522
50,000	4.0420	3.934	3.934	16.680	15.793	15.793	25.161	23.789	23.789

Table 3

Energy per particle E/N_{at} and chemical potential μ from a solution of Eq. (3) for $\gamma = \nu = 1$, $\lambda^2 = 0.25$, $a = 0$ and different nonlinearity $g_{\text{dd}} \equiv 3a_{\text{dd}}N_{\text{at}}$. The present numerical results are compared with Gaussian variational results obtained from Eqs. (18) and (19) as well as numerical results of Asad-uz-Zaman et al. [16,29]. Numerical results are calculated for the following space and time steps and the following space discretizing points in the Crank–Nicolson discretization: (A) $dx = dy = dz = 0.05$, $dt = 0.0004$, ($NX = NY = NZ \equiv \mathcal{N} = 384$); (B) 0.1 , $dt = 0.002$, ($\mathcal{N} = 128$, $R = 6$); and (C) 0.2 , $dt = 0.007$, ($\mathcal{N} = 64$, $R = 6$).

g_{dd}	E/N_{at} var	E/N_{at} (C)	E/N_{at} (B)	E/N_{at} (A)	E/N_{at} [29]	μ var	μ (C)	μ (B)	μ (A)	μ [29]
0	1.2500	1.2498	1.2500	1.2500	1.2500	1.2500	1.2498	1.2500	1.2500	1.2500
1	1.2230	1.2220	1.2222	1.2222	1.2222	1.1934	1.1910	1.1912	1.1911	1.1911
2	1.1907	1.1872	1.1875	1.1874	1.1874	1.1203	1.1100	1.1100	1.1100	1.1100
3	1.1521	1.143	1.1439	1.1438	1.1437	1.0253	0.995	0.996	0.996	0.9955
4	1.1051	1.085	1.0857	1.0857	1.0856	0.8950	0.805	0.803	0.806	0.8062

Table 4

Energy per particle E/N_{at} , and chemical potential μ from a solution of Eq. (3) for $\gamma = \nu = 1$, $\lambda^2 = 0.25$, $4\pi a = 0.20716$, $4\pi a_{\text{dd}} = 0.033146$ and different number N_{at} of atoms. These nonlinearity parameters taken from Ref. [9] correspond to a ^{52}Cr dipolar BEC with $a \approx 100a_0$ and $a_{\text{dd}} \approx 16a_0$ and oscillator length $l \approx 0.321 \mu\text{m}$. Variational and TF results as well as numerical results of Bao et al. [9] are also shown. Numerical results are calculated using the following space and time steps and the following space discretizing points in the Crank–Nicolson discretization: (A) $dx = dy = dz = 0.15$, $dt = 0.002$; (B) $dx = dy = dz = 0.3$, $dt = 0.005$. In (A) we take $NX = NY = NZ \equiv \mathcal{N} = 128$, $R = 9$ for $N_{\text{at}} = 100, 500, 1000$ and $\mathcal{N} = 192$, $R = 14$, for $N_{\text{at}} = 5000, 10,000, 50,000$; and in (B) we take $\mathcal{N} = 64$, $R = 9$, for $N_{\text{at}} = 100, 500, 1000$ and $\mathcal{N} = 96$, $R = 14$, for $N_{\text{at}} = 5000, 10,000, 50,000$.

N_{at}	E/N_{at} var	E/N_{at} TF	E/N_{at} (B)	E/N_{at} (A)	E/N_{at} [9]	μ var	μ TF	μ (B)	μ (A)	μ [9]
100	1.579	0.945	1.567	1.567	1.567	1.840	1.322	1.813	1.813	1.813
500	2.287	1.798	2.224	2.224	2.225	2.951	2.518	2.835	2.835	2.837
1000	2.836	2.373	2.728	2.728	2.728	3.767	3.322	3.583	3.582	3.583
5000	5.036	4.517	4.744	4.744	4.745	6.935	6.324	6.485	6.486	6.488
10,000	6.563	5.960	6.146	6.146	6.147	9.100	8.344	8.475	8.475	8.479
50,000	12.34	11.35	11.46	11.46	11.47	17.23	15.89	15.96	15.97	15.98

Table 5

The rms sizes $\langle x \rangle$ and $\langle z \rangle$ for the same systems illustrated in Table 4 using the same cut-off parameter R .

N	$\langle z \rangle$ TF	$\langle z \rangle$ var	$\langle z \rangle$ (B)	$\langle z \rangle$ (A)	$\langle z \rangle$ [9]	$\langle x \rangle$ TF	$\langle x \rangle$ var	$\langle x \rangle$ (B)	$\langle x \rangle$ (A)	$\langle x \rangle$ [9]
100	1.285	1.316	1.305	1.303	1.299	0.600	0.799	0.794	0.795	0.796
500	1.773	1.797	1.752	1.752	1.745	0.828	0.952	0.938	0.939	0.940
1000	2.037	2.079	2.014	2.014	2.009	0.951	1.054	1.035	1.035	1.035
5000	2.810	2.904	2.795	2.795	2.790	1.313	1.392	1.353	1.353	1.354
10,000	3.228	3.345	3.217	3.216	3.212	1.508	1.586	1.537	1.537	1.538
50,000	4.454	4.629	4.450	4.450	4.441	2.080	2.171	2.093	2.093	2.095

a , a_{dd} and l : $a \approx 100a_0$, $a_{\text{dd}} \approx 16a_0$, and $l = 0.321 \mu\text{m}$. We present results for energy E and chemical potential μ in Table 4 and rms sizes $\langle z \rangle$ and $\langle x \rangle$ in Table 5. We also present

variational and Thomas–Fermi (TF) results in this case together with results of numerical calculation of Bao et al. [9]. The TF energy and chemical potential in Table 4 are calculated using Eqs. (21)

Table 6

Energy per particle E/N_{at} , chemical potential μ , and rms sizes from a solution of Eq. (3) for ^{52}Cr atoms with $\gamma = 1$, $\nu^2 = 1/2$, $\lambda^2 = 1/4$, $a = 110a_0$, $a_{\text{dd}} = 16a_0$, and harmonic oscillator length $l = 1 \mu\text{m}$ for different N_{at} . Numerical results are calculated using the following space and time steps and the following space discretizing points in the Crank–Nicolson discretization: (A) $dx = dy = dz = 0.1$, $dt = 0.001$; and (B) 0.2 , $dt = 0.003$. In (A) we take $NX = NY = NZ \equiv \mathcal{N} = 128$, $R = 6$ for $N_{\text{at}} = 100, 500, 1000$ and $\mathcal{N} = 256$, $R = 10.5$, for $N_{\text{at}} = 5000, 10,000, 50,000$; and in (B) we take $\mathcal{N} = 64$, $R = 6$, for $N_{\text{at}} = 100, 500, 1000$ and $\mathcal{N} = 128$, $R = 12$, for $N_{\text{at}} = 5000, 10,000, 50,000$.

N	E/N_{at} (B)	E/N_{at} (A)	μ (B)	μ (A)	$\langle x \rangle$ (B)	$\langle y \rangle$ (B)	$\langle z \rangle$ (B)	$\langle x \rangle$ (A)	$\langle y \rangle$ (A)	$\langle z \rangle$ (A)
100	1.219	1.219	1.321	1.321	0.742	0.901	1.120	0.742	0.901	1.119
500	1.525	1.525	1.830	1.830	0.818	1.032	1.379	0.818	1.032	1.379
1000	1.784	1.784	2.232	2.232	0.874	1.128	1.559	0.874	1.129	1.558
5000	2.885	2.885	3.857	3.858	1.079	1.463	2.132	1.079	1.463	2.132
10,000	3.673	3.673	4.992	4.992	1.206	1.660	2.450	1.206	1.660	2.449
50,000	6.713	6.713	9.306	9.306	1.609	2.260	3.383	1.609	2.260	3.383

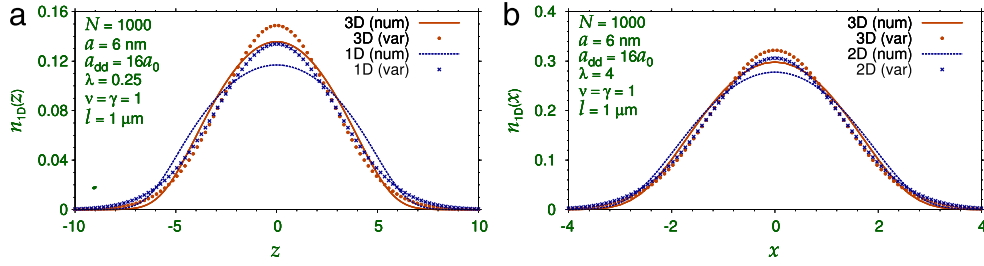


Fig. 1. (a) Numerical (num) and variational (var) results for the one-dimensional axial density $n_{1D}(z) = |\phi_{1D}(z)|^2$ along z axis for $\nu = \gamma = 1$, $\lambda = 0.25$ of a cigar-shaped BEC of $N_{\text{at}} = 1000$ atoms obtained using the 1D Eq. (29) and that obtained after integrating the 3D density from Eq. (3) over x and y : $n_{1D}(z) = \int |\phi(\mathbf{r})|^2 dx dy$. (b) Numerical (num) and variational (var) results for the 1D radial density $n_{1D}(x) = \int |\phi(\mathbf{r})|^2 dy dz$ along x axis for $\nu = \gamma = 1$, $\lambda = 4$ of a disk-shaped BEC of $N_{\text{at}} = 1000$ atoms obtained after integrating the 3D density from Eq. (3) over y and z and after integrating the 2D density from Eq. (46) over y as follows: $n_{1D}(x) = \int dy |\phi_{2D}(x, y)|^2$ and $n_{1D}(x) = \int dy dz |\phi_{3D}(x, y, z)|^2$. In all cases $a = 6 \text{ nm}$ and $a_{\text{dd}} = 16a_0$.

and (26), respectively. The TF sizes $\langle x \rangle$ and $\langle z \rangle$ in Table 5 are obtained from Eqs. (24) and (25) using the TF density (20). For small nonlinearities or small number of atoms, the Gaussian variational results obtained from Eqs. (13), (14), (18), and (19) are in good agreement with the numerical calculations as the wave function for small nonlinearities has a quasi-Gaussian shape. However, for large nonlinearities or large number of atoms, the wave function has an approximate TF shape (20), and the TF results provide better approximation to the numerical results, as can be seen from Tables 4 and 5.

After the consideration of 3D axially-symmetric trap now we consider a fully anisotropic trap in 3D. In Table 6 we present the results for energy E/N_{at} , chemical potential μ and rms sizes $\langle x \rangle$, $\langle y \rangle$, $\langle z \rangle$ of a ^{52}Cr BEC in a fully anisotropic trap with $\gamma = 1$, $\nu = 1/\sqrt{2}$, $\lambda = 1/2$ for different number of atoms. In this case we take $a = 110a_0$, $a_{\text{dd}} = 16a_0$ and $l = 1 \mu\text{m}$. The convergence of the calculation is studied by taking reduced space and time steps dx and dt and different number of space discretization points. Sufficient number of time iterations are to be allowed in each case to obtain convergence. In 3D the estimated numerical error in the calculation is less than 0.05%. The error is associated with the intrinsic accuracy of the FFT routine for long-range dipolar interaction.

The 1D and 2D GP Eqs. (29) and (46) are valid for cigar- and disk-shaped BECs, respectively. In case of cigar shape the 1D GP equation yields results for axial density and in this case it is appropriate to compare this density with the reduced axial density obtained by integrating the 3D density over radial coordinates: $n(z) \equiv |\varphi(z)|^2 = \int |\phi(x, y, z)|^2 dx dy$. In Fig. 1(a) we compare two axial densities obtained from the 1D and 3D GP equations. We also show the densities calculated from the Gaussian variational approximation in both cases. In the cigar case the trap parameters are $\nu = \gamma = 1$, $\lambda = 1/4$. Similarly, for the disk shape it is interesting to compare the density along the radial direction in the plane of the disk as obtained from the 3D Eq. (3) and the 2D Eq. (46). In this case it is appropriate to calculate the 1D radial density along, say, x direction by integrating 2D and 3D densities as follows: $n_{1D}(x) = \int dy |\phi_{2D}(x, y)|^2$ and $n_{1D}(x) = \int dy dz |\phi_{3D}(x, y, z)|^2$.

In Fig. 1(b) we compare two radial densities obtained from the 2D and 3D GP equations. We also show the densities calculated from the Gaussian variational approximation in both cases. For this illustration, we consider the trap parameters $\nu = \gamma = 1$, $\lambda = 4$. In both Figs. 1(a) and (b), the densities obtained from the solution of the 3D GP equation are in satisfactory agreement with those obtained from a solution of the reduced 1D and 2D equations. In Fig. 1, the numerical and variational densities are pretty close to each other, so are the results obtained from the 3D Eq. (3), on the one hand, and the ones obtained from the 1D and 2D Eqs. (29) and (46), on the other.

A dipolar BEC is stable for the number of atoms N_{at} below a critical value [31]. Independent of trap parameters, such a BEC collapses as N_{at} crosses the critical value. This can be studied by solving the 3D GP equation using imaginary-time propagation with a nonzero value of NSTP while the nonlinearities are slowly increased. In Fig. 2(a) we present the $N_{\text{at}} - a$ stability phase plot for a ^{164}Dy BEC with $a_{\text{dd}} = 130a_0$ in the disk-shaped trap with $\nu = \gamma = 1$, $\lambda = 5$ and 7. The oscillator length is taken to be $l = 1 \mu\text{m}$. The shaded area in these plots shows a metastable region where biconcave structure in 3D density appears. The metastable region corresponds to a local minimum in energy in contrast to a global minimum for a stable state. It has been established that this metastability is a manifestation of roton instability encountered by the system in the shaded region [31]. The biconcave structure in 3D density in a disk-shaped dipolar BEC is a direct consequence of dipolar interaction: the dipolar repulsion in the plane of the disk removes the atoms from the center to the peripheral region thus creating a biconcave shape in density. In Fig. 2(b) and (c) we plot the 3D isodensity contour of the condensate for $\lambda = 5$ with parameters in the shaded region corresponding to metastability. In Fig. 2(b) the density on the contour is 0.001 whereas in Fig. 2(c), it is 0.027. Only for a larger density on the contour the biconcave shape is visible. The biconcave shape predominates near the central region of the metastable dipolar BEC.

In Fig. 1 we critically tested the reduced 1D and 2D Eqs. (29) and (46) along the z axis and in the x - y plane, respectively, by

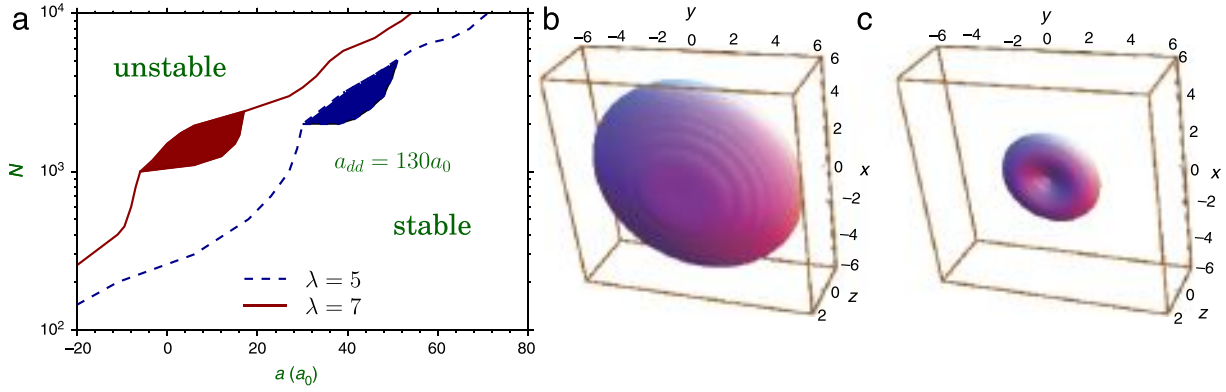


Fig. 2. (a) The $N_{\text{at}} - a$ stability phase plot for a ^{164}Dy BEC with $a_{\text{dd}} = 130a_0$ in a disk-shaped trap with $\nu = \gamma = 1$, $\lambda = 5$ and 7 and harmonic oscillator length $l = 1 \mu\text{m}$. The 3D isodensity contour plot of density of a disk-shaped ^{164}Dy BEC with $a_{\text{dd}} = 130a_0$ for $\nu = \gamma = 1$, $\lambda = 5$, $l = 1 \mu\text{m}$, $N_{\text{at}} = 3000$ and $a = 40a_0$ for densities $|\phi(x, y, z)|^2 =$ (b) 0.001 and (c) 0.027 on the contour.

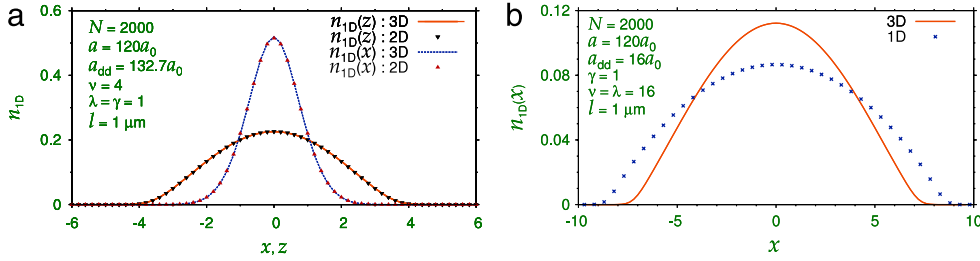


Fig. 3. (a) Numerical results for the 1D radial density $n_{1D}(x) = \int |\phi(\mathbf{r})|^2 dy dz$ along x axis and $n_{1D}(z) = \int |\phi(\mathbf{r})|^2 dx dy$ along z axis for $\lambda = \gamma = 1$, $\nu = 4$ of a disk-shaped BEC of $N_{\text{at}} = 2000$ ^{164}Dy atoms obtained after integrating the 3D density from Eq. (3) and the 2D density from Eq. (55) over the eliminated variables. (b) Numerical results for the 1D axial density $n_{1D}(x) = \int |\phi(\mathbf{r})|^2 dz dy$ along x axis for $\nu = \lambda = 16$, $\gamma = 1$ of a cigar-shaped BEC of $N_{\text{at}} = 2000$ ^{52}Cr atoms obtained using the 1D Eq. (41) and that obtained after integrating the 3D density from Eq. (3) over z and y : $n_{1D}(x) = \int |\phi(\mathbf{r})|^2 dz dy$. In all cases $a = 120a_0$ and (a) $a_{\text{dd}} = 132.7a_0$ (b) $a_{\text{dd}} = 16a_0$.

comparing the different 1D densities from these equations with those obtained from a solution of the 3D Eq. (3) as well as with the variational densities. Now we perform a similar test with the reduced 1D and 2D Eqs. (41) and (55) along the x axis and in the $x-z$ plane, respectively. We consider a BEC of 2000 atoms in a disk-shaped trap in the $x-z$ plane with $\lambda = \gamma = 1$ and $\nu = 4$. Because of the strong trap in the y direction, the resultant BEC is of quasi-2D shape in the $x-z$ plane without circular symmetry in that plane because of the anisotropic dipolar interaction. The integrated linear density along the x and z axes as calculated from the 2D GP Eq. (55) and the 3D GP Eq. (3) are illustrated in Fig. 3(a). Next we consider the BEC of 2000 atoms in a cigar-shaped trap along the x axis with $\nu = \lambda = 16$ and $\gamma = 1$. The integrated linear density along the x axis in this case calculated from the 3D Eq. (3) is compared with the same as calculate using the reduced 1D Eq. (41) in Fig. 3(b). In both cases the densities calculated from the 3D GP equation are in reasonable agreement with those calculated using the reduced Eqs. (55) and (41). Another interesting feature emerges from Figs. 1 and 3: the reduced 2D GP Eqs. (46) and (55) with appropriate disk-shaped traps yield results for densities in better agreement with the 3D GP Eq. (3) as compared to the 1D GP Eqs. (29) and (41) with appropriate cigar-shaped traps. This feature, also observed in non-dipolar BECs [17], is expected as the derivation of the reduced 1D equations involving two spatial integrations represent more drastic approximation compared to the same of the reduced 2D equations involving one spatial integration.

Now we report the dynamics of the dipolar BEC by real-time propagation using the stationary state calculated by imaginary-time propagation. In Fig. 4(a) we show the oscillation of the rms sizes $\langle z \rangle$ and $\langle \rho \rangle$ from the reduced 1D and 2D GP Eqs. (29) and (46), respectively. In Fig. 4(a) we consider $N_{\text{at}} = 10,000$, $a_{\text{dd}} = 16a_0$ (appropriate for ^{52}Cr), $a = 6 \text{ nm}$ ($\approx 113a_0$) and oscillator length $l = 1 \mu\text{m}$. In 1D, we take $dx = 0.025$, $dt = 0.0001$, $\lambda = 1$, $d_\rho = 1$,

number of space points $N = 2048$, and in 2D, we take $dx = dy = 0.2$, $dt = 0.001$, $\gamma = \nu = 1$, $d_z = 1$, $NX = NY = 512$. In real-time simulation the oscillation is started by multiplying the nonlinearities with the factor 1.05. To implement this, in real-time routine we take $\text{GPAR} = \text{GDPAR} = 1.1$ and also take $\text{NSTP} = 0$ to read the initial wave function. In 1D and 2D we also present results of the Gaussian variational approximations after a numerical solution of Eqs. (36) and (50), respectively. The frequency of the resultant oscillations agree well with the numerical 1D and 2D calculations. However, slight adjustment of the initial conditions, or initial values of width and its derivative, were necessary to get an agreement of the amplitude of oscillation obtained from variational approximation and numerical simulation. The initial values of width and its derivative are necessary to solve the variational equations (36) and (50). In Fig. 4(b) we illustrate the oscillation of the rms sizes $\langle x \rangle$, $\langle y \rangle$, and $\langle z \rangle$ in 3D using Eq. (3), where we perform real-time simulation using the bound state obtained by imaginary-time simulation as the initial state. The parameters used are $N_{\text{at}} = 1000$, $a = 110a_0$, $a_{\text{dd}} = 16a_0$, $\gamma = 1$, $\nu = 1/\sqrt{2}$, $\lambda = 1/2$, $l = 1 \mu\text{m}$, $NX = NY = NZ = 128$, $dx = dy = dz = 0.2$, $dt = 0.002$ in both real- and imaginary-time simulations. In addition, in real-time simulation the oscillation is started by multiplying the nonlinearities with the factor 1.1. To implement this, in real-time routine we take $\text{GPAR} = \text{GDPAR} = 1.1$ and also take $\text{NSTP} = 0$ to read the initial wave function.

5. Summary

We have presented useful numerical programs in Fortran and C for solving the dipolar GP equation including the contact interaction in 1D, 2D, 3D. Two sets of programs are provided. The imaginary-time programs are appropriate for solving the stationary problems, while the real-time codes can be used for

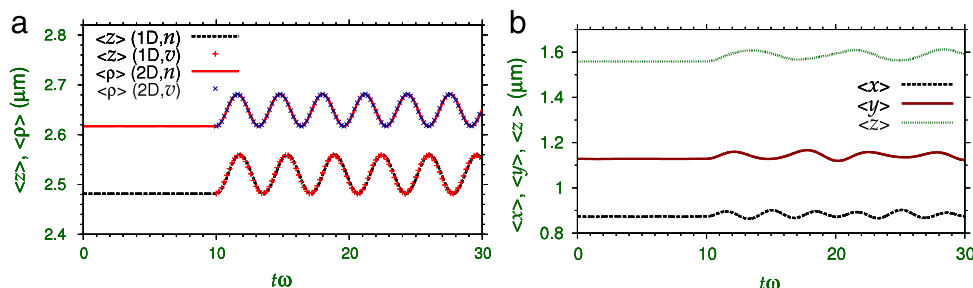


Fig. 4. (a) Numerical (n) and variational (v) results for oscillation of rms sizes (z) and (ρ) from the real-time simulation using Eq. (29) in 1D and Eq. (46) in 2D, respectively, for $N_{\text{at}} = 10,000$, $a = 6$ nm, $a_{\text{dd}} = 16a_0$, $l = 1$ μm , while a and a_{dd} were both multiplied by 1.05 after NPAS iterations at $t = 10$. The wave function was first calculated by imaginary-time routine with parameters $dx = 0.025$, $dt = 0.0001$, $\lambda = 1$, $d_\rho = 1$, NPAS = 10^5 , $N = 2048$ in 1D, and $dx = dy = 0.2$, $dt = 0.001$, $\gamma = 1$, $d_z = 1$ NPAS = 10^4 , $NX = NY = 512$ in 2D. The results of the variational approximations in 1D and 2D as obtained from a numerical solution of Eqs. (36) and (50) are also shown. (b) Numerical results for oscillation of rms sizes (x), (y) and (z) from the real-time simulation in 3D using Eq. (3), for $N_{\text{at}} = 1000$, $a = 110a_0$, $a_{\text{dd}} = 16a_0$, $l = 1$ μm , $\gamma = 1$, $v = 1/\sqrt{2}$, $\lambda = 1/2$, $NX = NY = NZ = 128$, $dx = dy = dz = 0.2$, and $dt = 0.002$ while a and a_{dd} were both multiplied by 1.1 after NPAS iterations. In all cases the real-time calculation was performed with NSTP = 0 reading the 3D density from the numerical solution of the imaginary-time program using the same parameters.

studying non-stationary dynamics. The programs are developed in Cartesian coordinates. We have compared the results of numerical calculations for statics and dynamics of dipolar BECs with those of Gaussian variational approximation, Thomas–Fermi approximation, and numerical calculations of other authors, where possible.

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C programs for solving the time-dependent Gross–Pitaevskii equation in a fully anisotropic trap[☆]

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ABSTRACT

We present C programming language versions of earlier published Fortran programs (Muruganandam and Adhikari (2009) [1]) for calculating both stationary and non-stationary solutions of the time-dependent Gross–Pitaevskii (GP) equation. The GP equation describes the properties of dilute Bose–Einstein condensates at ultra-cold temperatures. C versions of programs use the same algorithms as the Fortran ones, involving real- and imaginary-time propagation based on a split-step Crank–Nicolson method. In a one-space-variable form of the GP equation, we consider the one-dimensional, two-dimensional, circularly-symmetric, and the three-dimensional spherically-symmetric harmonic-oscillator traps. In the two-space-variable form, we consider the GP equation in two-dimensional anisotropic and three-dimensional axially-symmetric traps. The fully-anisotropic three-dimensional GP equation is also considered. In addition to these twelve programs, for six algorithms that involve two and three space variables, we have also developed threaded (OpenMP parallelized) programs, which allow numerical simulations to use all available CPU cores on a computer. All 18 programs are optimized and accompanied by makefiles for several popular C compilers. We present typical results for scalability of threaded codes and demonstrate almost linear speedup obtained with the new programs, allowing a decrease in execution times by an order of magnitude on modern multi-core computers.

New version program summary

Program title: GP-SCL package, consisting of: (i) imagtime1d, (ii) imagtime2d, (iii) imagtime2d-th, (iv) imagtimecir, (v) imagtime3d, (vi) imagtime3d-th, (vii) imagtimeaxial, (viii) imagtimeaxial-th, (ix) imagtimesph, (x) realtime1d, (xi) realtime2d, (xii) realtime2d-th, (xiii) realtimecir, (xiv) realtime3d, (xv) realtime3d-th, (xvi) realtimeaxial, (xvii) realtimeaxial-th, (xviii) realltimesph.

Catalogue identifier: AEDU_v2_0.

Program Summary URL: http://cpc.cs.qub.ac.uk/summaries/AEDU_v2_0.html.

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland.

Licensing provisions: Standard CPC licence, <http://cpc.cs.qub.ac.uk/licence/licence.html>.

No. of lines in distributed program, including test data, etc.: 180 583.

No. of bytes in distributed program, including test data, etc.: 1 188 688.

Distribution format: tar.gz.

Programming language: C and C/OpenMP.

Computer: Any modern computer with C language compiler installed.

Operating system: Linux, Unix, Mac OS, Windows.

RAM: Memory used with the supplied input files: 2–4 MB (i, iv, ix, x, xiii, xvi, xvii, xviii), 8 MB (xi, xii), 32 MB (vii, viii), 80 MB (ii, iii), 700 MB (xiv, xv), 1.2 GB (v, vi).

Number of processors used: For threaded (OpenMP parallelized) programs, all available CPU cores on the computer.

Classification: 2.9, 4.3, 4.12.

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Catalogue identifier of previous version: AEDU_v1_0.

Journal reference of previous version: Comput. Phys. Commun. 180 (2009) 1888.

Does the new version supersede the previous version?: No.

Nature of problem: These programs are designed to solve the time-dependent Gross–Pitaevskii (GP) nonlinear partial differential equation in one-, two- or three-space dimensions with a harmonic, circularly-symmetric, spherically-symmetric, axially-symmetric or fully anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Solution method: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation, in either imaginary or real time, over small time steps. The method yields solutions of stationary and/or non-stationary problems.

Reasons for the new version: Previous Fortran programs [1] are used within the ultra-cold atoms [2–11] and nonlinear optics [12,13] communities, as well as in various other fields [14–16]. This new version represents translation of all programs to the C programming language, which will make it accessible to the wider parts of the corresponding communities. It is well known that numerical simulations of the GP equation in highly experimentally relevant geometries with two or three space variables are computationally very demanding, which presents an obstacle in detailed numerical studies of such systems. For this reason, we have developed threaded (OpenMP parallelized) versions of programs `imagtime2d`, `imagtime3d`, `imagtimeaxial`, `realtime2d`, `realtime3d`, `realtimeaxial`, which are named `imagtime2d-th`, `imagtime3d-th`, `imagtimeaxial-th`, `realtime2d-th`, `realtime3d-th`, `realtimeaxial-th`, respectively. Fig. 1 shows the scalability results obtained for OpenMP versions of programs `realtime2d` and `realtime3d`. As we can see, the speedup is almost linear, and on a computer with the total of 8 CPU cores we observe in Fig. 1(a) a maximal speedup of around 7, or roughly 90% of the ideal speedup, while on a computer with 12 CPU cores we find in Fig. 1(b) that the maximal speedup is around 9.6, or 80% of the ideal speedup. Such a speedup represents significant improvement in the performance.

Summary of revisions: All Fortran programs from the previous version [1] are translated to C and named in the same way. The structure of all programs is identical. We have introduced the use of comprehensive input files, where all parameters are explained in detail and can be set by a user. We have also included makefiles with tested and verified settings for GNU's gcc compiler, Intel's icc compiler, IBM's xlc compiler, PGI's pgcc compiler, and Oracle's suncc (former Sun's) compiler. In addition to this, 6 new threaded (OpenMP parallelized) programs are supplied (`imagtime2d-th`, `imagtime3d-th`, `imagtimeaxial-th`, `realtime2d-th`, `realtime3d-th`, `realtimeaxial-th`) for algorithms involving two or three space variables. They are written by OpenMP-parallelizing the most computationally demanding loops in functions performing time evolution (`calcnu`, `calclux`, `calcluy`, `calcluz`), normalization (`calcnorm`), and calculation of physical quantities (`calcmuen`, `calcrms`). Since some of the dynamically allocated array variables are used within such loops, they had to be made private for each thread. This was done by allocating matrices instead of arrays, with the first index in all such matrices corresponding to a thread number.

Additional comments: This package consists of 18 programs, see Program title above, out of which 12 programs (i, ii, iv, v, vii, ix, x, xi, xiii, xiv, xvi, xviii) are serial, while 6 programs (iii, vi, viii, xii, xv, xvii) are threaded (OpenMP parallelized). For the particular purpose of each program, please see descriptions below.

Running time: All running times given in descriptions below refer to programs compiled with gcc on quad-core Intel Xeon X5460 at 3.16 GHz (CPU1), and programs compiled with icc on quad-core Intel Nehalem E5540 at 2.53 GHz (CPU2). With the supplied input files, running times on CPU1 are: 5 min (i, iv, ix, xii, xiii, xvii, xviii), 10 min (viii, xvi), 15 min (iii, x, xi), 30 min (ii, vi, vii), 2 h (v), 4 h (xv), 15 h (xiv). On CPU2, running times are: 5 min (i, iii, iv, viii, ix, xii, xiii, xvi, xvii, xviii), 10 min (vi, x, xi), 20 min (ii, vii), 1 h (v), 2 h (xv), 12 h (xiv).

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New version program summary (i)

Program title: `imagtime1d`.

Title of electronic files: `imagtime1d.c`, `imagtime1d.h`.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 4 MB.

Programming language used: C.

Typical running time: 2 min (CPU1), 1 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in one space dimension with a harmonic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (ii)

Program title: `imagtime2d`.

Title of electronic files: `imagtime2d.c`, `imagtime2d.h`.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 80 MB.

Programming language used: C.

Typical running time: 30 min (CPU1), 20 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (iii)

Program title: imagtime2d-th.

Title of electronic files: imagtime2d-th.c, imagtime2d-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 80 MB.

Programming language used: C/OpenMP.

Typical running time: 15 min (CPU1), 5 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (iv)

Program title: imagtimecir.

Title of electronic files: imagtimecir.c, imagtimecir.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 2 MB.

Programming language used: C.

Typical running time: 2 min (CPU1), 1 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with a circularly-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (v)

Program title: imagtime3d.

Title of electronic files: imagtime3d.c, imagtime3d.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 1.2 GB.

Programming language used: C.

Typical running time: 1.5 h (CPU1), 1 h (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (vi)

Program title: imagtime3d-th.

Title of electronic files: imagtime3d-th.c, imagtime3d-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 1.2 GB.

Programming language used: C/OpenMP.

Typical running time: 25 min (CPU1), 10 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation

in three space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (vii)

Program title: imagtimeaxial.

Title of electronic files: imagtimeaxial.c, imagtimeaxial.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 32 MB.

Programming language used: C.

Typical running time: 30 min (CPU1), 20 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an axially-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (viii)

Program title: imagtimeaxial-th.

Title of electronic files: imagtimeaxial-th.c, imagtimeaxial-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 32 MB.

Programming language used: C/OpenMP.

Typical running time: 10 min (CPU1), 5 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an axially-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (ix)

Program title: imagtimesph.

Title of electronic files: imagtimesph.c, imagtimesph.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 2.5 MB.

Programming language used: C.

Typical running time: 2 min (CPU1), 1 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with a spherically-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in imaginary time over small time steps. The method yields solutions of stationary problems.

New version program summary (x)

Program title: realtime1d.

Title of electronic files: realtime1d.c, realtime1d.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 4 MB.

Programming language used: C.

Typical running time: 15 min (CPU1), 10 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in one space dimension with a harmonic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xi)

Program title: realtime2d.

Title of electronic files: realtime2d.c, realtime2d.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 8 MB.

Programming language used: C.

Typical running time: 15 min (CPU1), 10 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xii)

Program title: realtime2d-th.

Title of electronic files: realtime2d-th.c, realtime2d-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 8 MB.

Programming language used: C/OpenMP.

Typical running time: 5 min (CPU1), 2 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xiii)

Program title: realtimecir.

Title of electronic files: realtimecir.c, realtimecir.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 3 MB.

Programming language used: C.

Typical running time: 5 min (CPU1), 5 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in two space dimensions with a circularly-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xiv)

Program title: realtime3d.

Title of electronic files: realtime3d.c, realtime3d.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 700 MB.

Programming language used: C.

Typical running time: 15 h (CPU1), 12 h (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xv)

Program title: realtime3d-th.

Title of electronic files: realtime3d-th.c, realtime3d-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 700 MB.

Programming language used: C/OpenMP.

Typical running time: 4 h (CPU1), 1.8 h (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an anisotropic trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xvi)

Program title: realtimeaxial.

Title of electronic files: realtimeaxial.c, realtimeaxial.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 4 MB.

Programming language used: C.

Typical running time: 10 min (CPU1), 5 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an axially-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

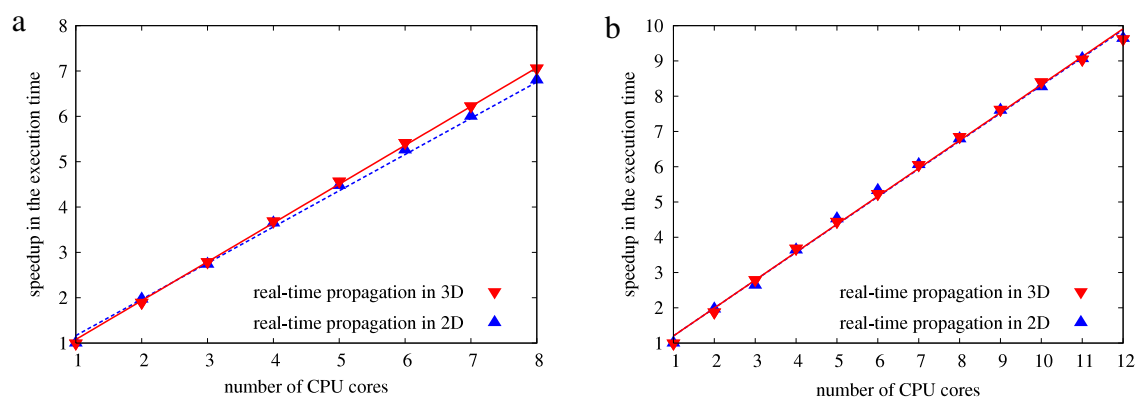


Fig. 1. (Colour online) Speedup in the execution time of realtime2d-th and realtime3d-th threaded (OpenMP parallelized) programs as a function of the number of CPU cores used. The results are obtained: (a) on an 8-core machine with $2 \times$ quad-core Intel Nehalem E5540 CPU at 2.53 GHz, using the icc compiler, (b) on a 12-core machine with $2 \times$ six-core Intel Nehalem X5650 CPU at 2.66 GHz, using the pgcc compiler. The spatial grid sizes used are 2000×2000 (realtime2d-th) and $1000 \times 1000 \times 300$ (realtime3d-th).

New version program summary (xvii)

Program title: realtimeaxial-th.

Title of electronic files: realtimeaxial-th.c, realtimeaxial-th.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 4 MB.

Programming language used: C/OpenMP.

Typical running time: 5 min (CPU1), 1 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with an axially-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

New version program summary (xviii)

Program title: reallimesph.

Title of electronic files: reallimesph.c, reallimesph.h.

Computer: Any modern computer with C language compiler installed.

Maximum RAM memory: 2.5 MB.

Programming language used: C.

Typical running time: 5 min (CPU1), 5 min (CPU2).

Nature of physical problem: This program is designed to solve the time-dependent GP nonlinear partial differential equation in three space dimensions with a spherically-symmetric trap. The GP equation describes the properties of a dilute trapped Bose–Einstein condensate.

Method of solution: The time-dependent GP equation is solved by the split-step Crank–Nicolson method by discretizing in space and time. The discretized equation is then solved by propagation in real time over small time steps. The method yields solutions of stationary and non-stationary problems.

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Development of collisional data base for elementary processes of electron scattering by atoms and molecules



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ABSTRACT

We present a progress report on the development of the Belgrade electron/molecule data base which is hosted by The Institute of Physics, University of Belgrade and The Astronomical Observatory Belgrade. The data base has been developed under the standards of Virtual Atomic Molecular Data Centre (VAMDC) project which provides a common portal for several European data bases that maintain atomic and molecular data. The Belgrade data base (BEAMDB) covers collisional data of electron interactions with atoms and molecules in the form of differential (DCS) and integrated cross sections as well as energy loss spectra. The final goal of BEAMDB becoming both a node within the VAMDC consortium and within the radiation damage RADAM data base has been achieved.

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1. Introduction

Curating, maintaining and distributing the large amounts of atomic and molecular (A&M) data that is produced from fundamental experiments and calculations is now widely recognised to be a necessity for the modern research community. There are many disparate communities which would benefit from such data collections including those engaged in astrophysical and atmospheric physics [1], plasma science and technology (with its applications to the plasma processing [2] or lighting [3] industries), biomedicine/biophysics and to other fundamental and applied research disciplines such as spectroscopy or surface science [4].

Such communities expect to be able to search for A&M data through a computerised and networked web-based infrastructure, e.g., a newly formed EU consortium (developed through a COST Action MP1002) is creating the RADAM (RADIATION DAMAGE) database [5] in order to provide A&M data to the radiation chemistry community. The idea of the RADAM database is to provide access to relevant data which spans from elementary processes through

to multi-scale and biological effect processes such that those developing models and radiotherapy tools can have access to current state of the art data. The importance of such data is highlighted by its use in the development of models of particle therapy that start from track structure and end by predicting cellular damage; such models are the basis of treatment planning [6]. In order to determine such track structures and to model the role of low energy electrons and positrons in biologically relevant media it is necessary to have a full set of cross sections that govern the elementary interactions along the track [7]. In addition, there is a necessity for predicting radiation induced DNA damage due to multi-scale processes or thermo-mechanical effects caused by the passage of charged particles such as heavy ions that are propagating through the tissue [8]. The present Belgrade data base (BEAMDB) is addressing a part of these needs being centred on electron collisions by molecular species and more specifically on biomolecules or molecules of biological relevance. Thus the newly created Belgrade database is oriented towards those researchers searching for state of the art collisional data.

Current data bases that cover the field of atomic and molecular physics can be distinguished between those that maintain mainly bibliographic data about the published work on atomic processes

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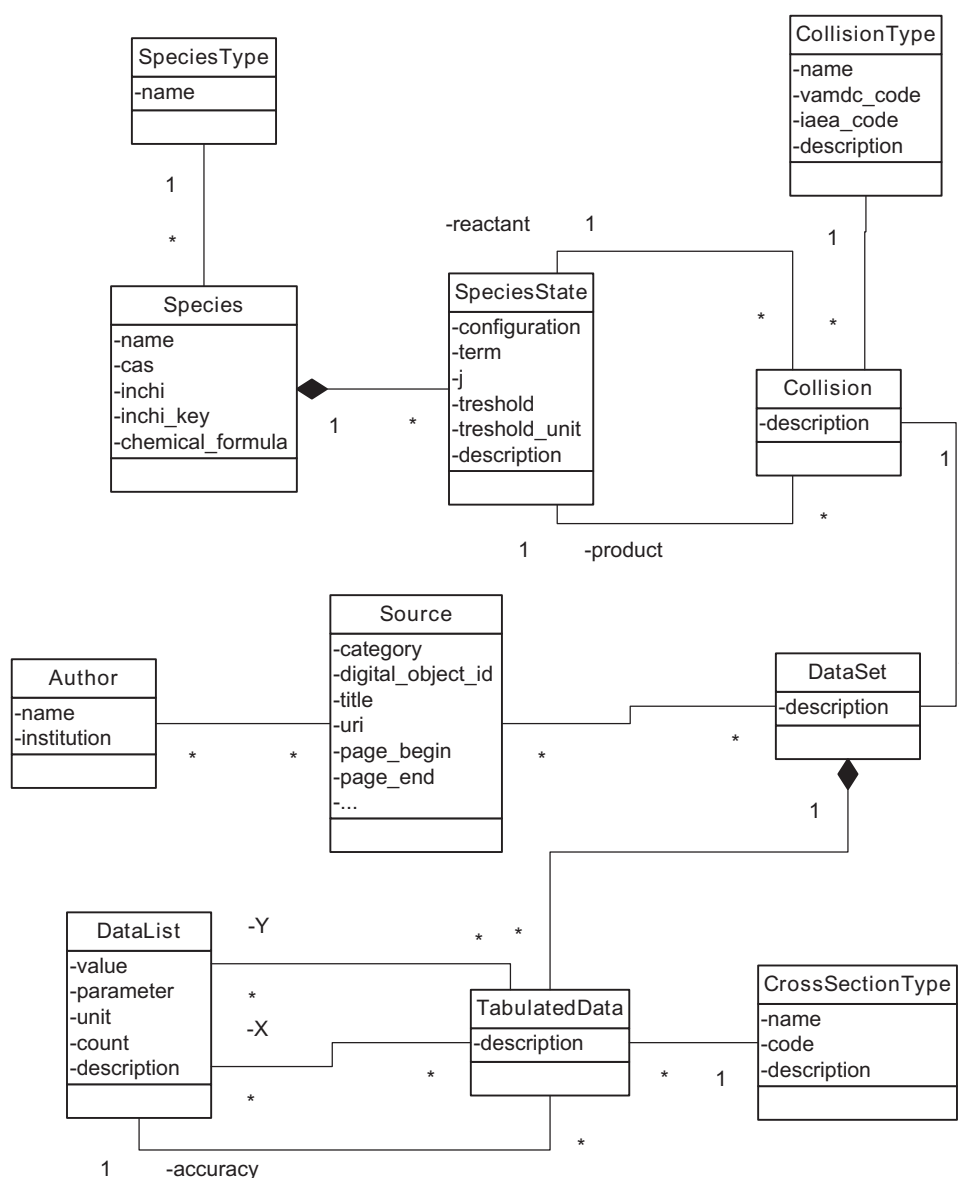


Fig. 1. The data model of BEAMDB, the Belgrade electron/molecule database, with entities and attributes. The relationships of one-to-one, one-to-many and many-to-many are shown.

(such as NIST bibliographic database on Atomic Transition Probabilities [9]) and those that maintain actual data sets of evaluated and recommended values [10]. A new era of data accessibility opened with the idea of the Virtual Atomic and Molecular Data Centre (VAMDC) [11] that creates a common portal for different data bases in the field which use the same data protocol for exchanging and representing data in the format of so the called “xsams” xml files (XML Schema for Atomic & Molecular Spectroscopy [12]). VAMDC now provides a scientific data e-infrastructure enabling easy access to atomic and molecular data [13].

While there is a vast amount of structural and transition data in the current VAMDC data bases, the number of collisional data bases is currently rather small. Our goal is to make a functional data base that will maintain data on electron/atom and molecule interactions. These data are in the form of differential and integral cross sections for elastic scattering and electronic excitation processes. In addition energy loss spectra as relative intensities of scattered electrons versus electron energy loss at the fixed impact electron energy and scattering angle are stored in the present data base since these may be important for direct comparison with theory and useful in determin-

ing ‘total’ energy transfer into a medium. The aim of BEAMDB was to create a specialised node within VAMDC consortium and RADAM database and this goal has been achieved.

2. The Belgrade database (BEAMDB)

The first ideas for developing a Belgrade data base came through a combination of the research interests of those involved in the development of expert and information systems and those producing A&M data in Belgrade. It was realised that the establishment of such an A&M database would both facilitate data analysis and ensure the long term curation of measured sets of data in electron atom/molecule interactions. The process model was defined and further developed from the context level to several hierarchical levels each of them represented by the data flow diagram [14]. This relational data model was then developed and ultimately implemented.

The present data base follows the VAMDC data model which defines A&M processes in domain of three classes: radiative,

LACP@IPB e/Mol RADAM DATABASE
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Laboratory for Atomic Collision Processes

Collision Type:

Species:

Species State (product):

Cross Section Type:

```

-<XSAMSData xmlns="http://vamdc.org/xml/xsams/1.0" xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
xmlns:cml="http://www.xml-cml.org/schema" xsi:schemaLocation="http://vamdc.org/xml/xsams/1.0 http://vamdc.org/xml/xsams/1.0">
+<Sources> </Sources>
+<Species> </Species>
+<Processes> </Processes>
</XSAMSData>

```

Fig. 2. A screen shot of the BEAMDB database at Belgrade server station.

non-radiative and collisional. BEAMDB follows the protocols defined for presentation of data for collisional processes. In collisions there are always a reactant and a product. In the case of BEAMDB one of the reactants and one of the products is an electron. The target in the reactant side could be either an atom or a molecule but it is always assumed to be in the ground level state. For molecules it is assumed that the target is in an ensemble of rotationally excited states that corresponds to the molecule being in thermal equilibrium at the temperature that is evidenced under the entity of 'environment temperature'. The product after the interaction with an electron can be either in the ground state (elastic scattering) or in an excited state, at present only electronic state excitations are included but also other types of inelastic processes (e.g., vibrational excitation or ionisation) can easily be added as database develops.

The data model of the Belgrade electron/molecule data base (BEAMDB) is shown in Fig. 1 in which the relationships between entities of one-to-one and one-to-many are shown. The principle adopted for data storage is that only those data that have been previously published and so have been subject to a formal refereeing procedure, should be included. This principle follows from discussion amongst A&M community and is a consensus of the views of the data providers, who measure and calculate these A&M data. For such reasons the sources of the data are therefore included in the data base with all their crucial entities (authors, journal, volume, pages, doi, Bibtext). Atoms and molecules are covered by the entity 'Species' and are characterised by their state i.e., 'SpeciesState' entity. The data itself are organised within 'DataSets' which include 'TabulatedData' of cross sections or spectroscopic data.

This database is a natural extension of VAMDC software which provides infrastructure for implementing atomic and molecular data as a web service. VAMDC software is implemented in Django, a Python-based web framework which offers forward and reverse database generation, automatised object-relational mapping, loose coupling of software modules, automatic administrative interface, extensible templating system and other advanced features. The relational database of choice is MySQL, the web server is Nginx and Python application server is Gunicorn, hosted on a Linux machine.

VAMDC software requires customisation in terms of writing data models, mapping fields in the database to keywords in VAMDC dictionaries and adapting query functions to connect the xml generator with the database. Dictionaries are lists of names which identify certain type of data, key-value pairs that indicate which attributes could be used in filtering the data on user's end ("restrictables") and what kind of data can be returned from the database end ("returnables").

In cases where the generator does not support desired xml output out-of-the-box, it can be overridden. For the BEAMDB node, we had to provide 3-dimensional data structure represented with two X axes and one Y axis. Such data structure is supported in xsams schema but not implemented in VAMDC generator, which expects single X and Y axes. For such specific needs, VAMDC software allows writing a function named *XML()* on the specific entity in the model that needs alteration. In this way, a generator is bypassed and desired custom output can be controlled by the node owner which adds flexibility and removes potential bottleneck in software development.

Access to the data is possible via Table Access Protocol (TAP), a Virtual Observatory standard of a web service or via AJAX-enabled web interface (<http://servo.aob.rs/emol/>). Relying on JQuery (a javascript framework) libraries, the web interface allows asynchronous access to database which enhances the dynamic nature of the application. Both queries return data in xsams format.

3. Data sets

A screen shot of BEAMDB Database at Belgrade server station is shown in Fig. 2. Since the intention of the authors was to easily identify what kind of electron collisional data could be retrieved, the front page of BEAMDB is created in such manner that it consists of simple and small number (four) combo-boxes. Within the field entity entitled 'Collision Type' one can choose between 'Elastic' and 'Electronic Excitation' or 'Energy-loss Spectrum' and 'Total Scattering'. One also can select under the entity 'Species' all available atomic and molecular targets that are currently maintained in the data base. After selecting one of the targets, automatically the

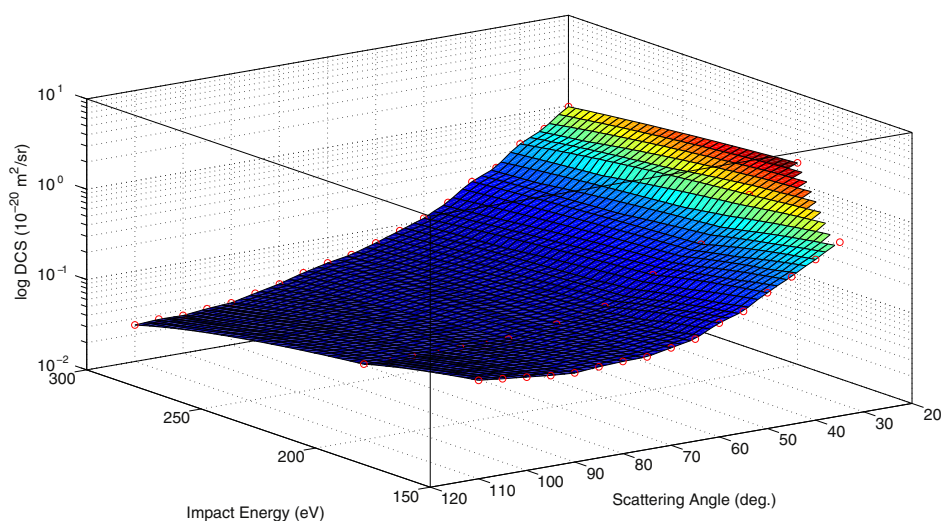


Fig. 3. Differential cross section (DCS) surface versus impact electron energy and scattering angle for elastic scattering from formamide. The DCS is in units of 10^{-20} m²/srad, the impact energy is expressed in eV and the scattering angle in degrees. The data points are represented by open circles while the connecting lines are interpolated values.

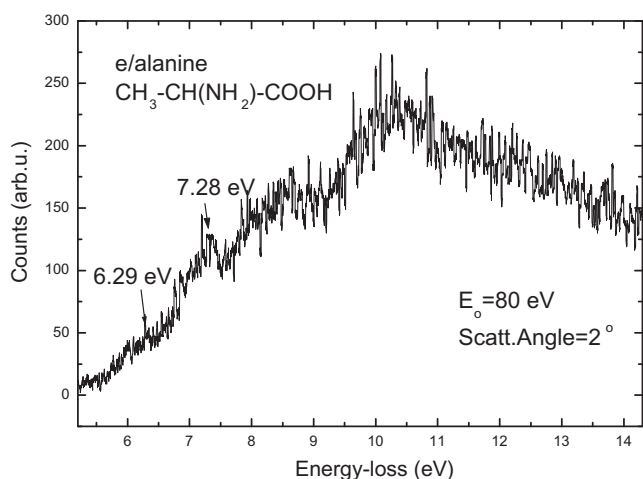


Fig. 4. An energy loss spectrum of 80 eV electrons scattered at the angle of 2° from alanine, CH₃-CH(NH₂)-COOH, molecule.

tific literature and contains a unique set of data within the VAMDC consortium. It is therefore contributing to the e-infrastructure that has been created the VAMDC project. The aim of this database is to be accessible to, and be used by, the wider scientific community and its accessibility through VAMDC will allow this.

Another aim of the BEAMDB database is to facilitate the evaluation of data undertaken by the Electron-Molecule Data Board (eMol-board), a team of experts that meets regularly and perform critical analysis of published electron/molecule data on specific molecular targets. The combination of data sets within this database and other databases that contain collisional data (e.g., [19]) with data reviews (e.g., [2,20]) will facilitate the task of eMol-board to provide recommended cross-section values and consider future data needs [13].

The BEAMDB is also included in the wider scope of RADAM data base which covers the specific needs of radiation community. The RADAM data base [21] has five distinctive areas that cover complex processes met in radiation damage i.e., photon, ion, electron/positron interactions, multi-scale processes and biological effects [5]. In future, the present electron interaction database may be used

to make a clone database that would maintain the same structure but would curate positron interaction data sets.

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SPEEDUP Code for Calculation of Transition Amplitudes via the Effective Action Approach

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Abstract. We present Path Integral Monte Carlo C code for calculation of quantum mechanical transition amplitudes for 1D models. The SPEEDUP C code is based on the use of higher-order short-time effective actions and implemented to the maximal order $p=18$ in the time of propagation (Monte Carlo time step), which substantially improves the convergence of discretized amplitudes to their exact continuum values. Symbolic derivation of higher-order effective actions is implemented in SPEEDUP Mathematica codes, using the recursive Schrödinger equation approach. In addition to the general 1D quantum theory, developed Mathematica codes are capable of calculating effective actions for specific models, for general 2D and 3D potentials, as well as for a general many-body theory in arbitrary number of spatial dimensions.

AMS subject classifications: 81Q05, 81Q15, 65Y04, 65B99

Key words: Transition amplitude, effective action, path integrals, Monte Carlo.

1 Introduction

Exact solution of a given many-body model in quantum mechanics is usually expressed in terms of eigenvalues and eigenfunction of its Hamiltonian

$$\hat{H} = \sum_{i=1}^M \frac{\hat{\mathbf{p}}_i^2}{2m_i} + \hat{V}(\hat{\mathbf{q}}_1, \dots, \hat{\mathbf{q}}_M), \quad (1.1)$$

but it can be also expressed through analytic solution for general transition amplitude $A(\mathbf{a}, \mathbf{b}; T) = \langle \mathbf{b} | e^{-iT\hat{H}/\hbar} | \mathbf{a} \rangle$ from the initial state $|\mathbf{a}\rangle$ to the final state $|\mathbf{b}\rangle$ during the time of

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propagation T . Calculation of transition amplitudes is more suitable if one uses path integral formalism [1–3], but in principle, if eigenproblem of the Hamiltonian can be solved, one should be able to calculate general transition amplitudes, and vice versa. However, mathematical difficulties may prevent this, and even more importantly, exact solutions can be found only in a very limited number of cases. Therefore, use of various analytic approximation techniques or numerical treatment is necessary for detailed understanding of the behavior of almost all models of interest.

In numerical approaches it could be demanding and involved to translate numerical knowledge of transition amplitudes to (or from) eigenstates, but practically can be always achieved. It has been implemented in various setups, e.g. through extraction of the energy spectra from the partition function [2–5], and using the diagonalization of space-discretized matrix of the evolution operator, i.e. matrix of transition amplitudes [6–10]. All these applications use the imaginary-time formalism [11, 12], typical for numerical simulations of such systems.

Recently introduced effective action approach [13–17] provides an ideal framework for exact numerical calculation of quantum mechanical amplitudes. It gives systematic short-time expansion of amplitudes for a general potential, thus allowing accurate calculation of short-time properties of quantum systems directly, as has been demonstrated in [8–10]. For numerical calculations that require long times of propagation to be considered using e.g. Monte Carlo method, effective action approach provides improved discretized actions leading to the speedup in the convergence of numerically calculated discretized quantities to their exact continuum values. This has been also demonstrated in Monte Carlo calculations of energy expectation values using the improved energy estimators [5, 18].

In this paper we present SPEEDUP codes [19] which implement the effective action approach, and which were used for numerical simulations in [4, 5, 8–10, 13–17]. The paper is organized as follows. In Section 2 we briefly review the recursive approach for analytic derivation of higher-order effective actions. SPEEDUP Mathematica codes capable of symbolic derivation of effective actions for a general one- and many-body theory as well as for specific models is described in detail in Section 3, while in Section 4 we describe SPEEDUP Path Integral Monte Carlo C code, developed for numerical calculation of transition amplitudes for 1D models. Section 5 summarizes presented results and gives outlook for further development of the code.

2 Theoretical background

From inception of the path integral formalism, expansion of short-time amplitudes in the time of propagation was used for the definition of path integrals through the time-discretization procedure [2, 3]. This is also straightforwardly implemented in the Path Integral Monte Carlo approaches [20], where one usually relies on the naive discretization of the action. Several improved discretized actions, mainly based on the Trotter formula

and its generalizations, were developed and used in the past [21–23]. A recent analysis of this method can be found in Jang et al [24]. Several related investigations dealing with the speed of convergence have focused on improvements in short-time propagation [25, 26] or the action [27]. More recently, split-operator method has also been developed [28–32], later extended to include higher-order terms [33–36], and systematically improved using the multi-product expansion [37–39].

The effective action approach is based on the ideal discretization concept [16]. It was introduced first for single-particle 1D models [13–15] and later extended to general many-body systems in arbitrary number of spatial dimensions [5, 17]. This approach allows systematic derivation of higher-order terms to a chosen order p in the short time of propagation.

Recursive method for deriving discretized effective actions, established in [17], is based on solving the underlying Schrödinger equation for the amplitude. It has proven to be the most efficient tool for treatment of higher-order expansion. In this section we give brief overview of the recursive method, which will be implemented in Mathematica in the next section. We start with the case of single particle in 1D, used in the SPEEDUP C code. Throughout the paper we will use natural system of units, in which \hbar and all masses are set to unity.

2.1 One particle in one dimension

In the effective action approach, transition amplitudes are expressed in terms of the ideal discretized action S^* in the form

$$A(a, b; T) = \frac{1}{\sqrt{2\pi T}} e^{-S^*(a, b; T)}, \quad (2.1)$$

which can be also seen as a definition of the ideal action [16]. Therefore, by definition, the above expression is correct not only for short times of propagation, but for arbitrary large times T . We also introduce the ideal effective potential W ,

$$S^*(a, b; T) = T \left[\frac{1}{2} \left(\frac{b-a}{T} \right)^2 + W \right], \quad (2.2)$$

reminiscent of the naive discretized action, with the arguments of the effective potential (a, b, T) usually written as $W\left(\frac{a+b}{2}, \frac{b-a}{2}; T\right)$, to emphasize that we will be using mid-point prescription.

However, ideal effective action and effective potential can be calculated analytically only for exactly solvable models, while in all other cases we have to use some approximative method. We use expansion in the time of propagation, assuming that the time T is small. If this is not the case, we can always divide the propagation into N time steps, so that $\varepsilon = T/N$ is small. Long-time amplitude is then obtained by integrating over all short-time ones,

$$A(a, b; T) = \int dq_1 \cdots dq_{N-1} A(a, q_1; \varepsilon) A(q_1, q_2; \varepsilon) \cdots A(q_{N-1}, b; \varepsilon), \quad (2.3)$$

paving the way towards Path Integral Monte Carlo calculation, which is actually implemented in the SPEEDUP C code.

If we consider general amplitude $A(q, q'; \varepsilon)$, introduce the mid-point coordinate $x = (q + q')/2$ and deviation $\bar{x} = (q' - q)/2$, and express A using the effective potential,

$$A(q, q'; \varepsilon) = \frac{1}{\sqrt{2\pi\varepsilon}} e^{-\frac{2}{\varepsilon}\bar{x}^2 - \varepsilon W(x, \bar{x}; \varepsilon)}, \quad (2.4)$$

the time-dependent Schrödinger equation for the amplitude leads to the following equation for W

$$W + \bar{x}\bar{\partial}W + \varepsilon\partial_\varepsilon W - \frac{1}{8}\varepsilon\partial^2W - \frac{1}{8}\varepsilon\bar{\partial}^2W + \frac{1}{8}\varepsilon^2(\partial W)^2 + \frac{1}{8}\varepsilon^2(\bar{\partial}W)^2 = \frac{1}{2}(V_+ + V_-), \quad (2.5)$$

where $V_\pm = V(x \pm \bar{x})$, i.e. $V_- = V(q)$, $V_+ = V(q')$. The short-time expansion assumes that we expand W to power series in ε to a given order, and calculate the appropriate coefficients using Eq. (2.5). We could further expect that this results in coefficients depending on the potential $V(x)$ and its higher derivatives. However, this scheme is not complete, since the effective potential depends not only on the mid-point x , but also on the deviation \bar{x} , and the obtained equations for the coefficients cannot be solved in a closed form. In order to resolve this in a systematic way, we make use of the fact that, for short time of propagation, deviation \bar{x} is on the average given by the diffusion relation $\bar{x}^2 \propto \varepsilon$, allowing double expansion of W in the form

$$W(x, \bar{x}; \varepsilon) = \sum_{m=0}^{\infty} \sum_{k=0}^m c_{m,k}(x) \varepsilon^{m-k} \bar{x}^{2k}. \quad (2.6)$$

Restricting the above sum over m to $p-1$ leads to level p effective potential $W_p(x, \bar{x}; \varepsilon)$ which gives expansion of the effective action S_p^* to order ε^p , and hence the level designation p for both the effective action and the corresponding potential W_p . Thus, if the diffusion relation is applicable (which is always the case in Monte Carlo calculations), instead of the general double expansion in \bar{x} and ε , we are able to obtain simpler, systematic expansion in ε only.

As shown previously [13–15], when used in Path Integral Monte Carlo simulations for calculation of long time amplitudes according to Eq. (2.3), use of level p effective action leads to the convergence of discretized amplitudes proportional to ε^p , i.e. as $1/N^p$, where N is the number of time steps used in the discretization.

If we insert the above level p expansion of the effective potential to Eq. (2.5), we obtain the recursion relation derived in [17],

$$\begin{aligned} 8(m+k+1)c_{m,k} &= (2k+2)(2k+1)c_{m,k+1} + c''_{m-1,k} - \sum_{l=0}^{m-2} \sum_r c'_{l,r} c'_{m-l-2,k-r} \\ &\quad - \sum_{l=1}^{m-2} \sum_r 2r(2k-2r+2)c_{l,r} c_{m-l-1,k-r+1}, \end{aligned} \quad (2.7)$$

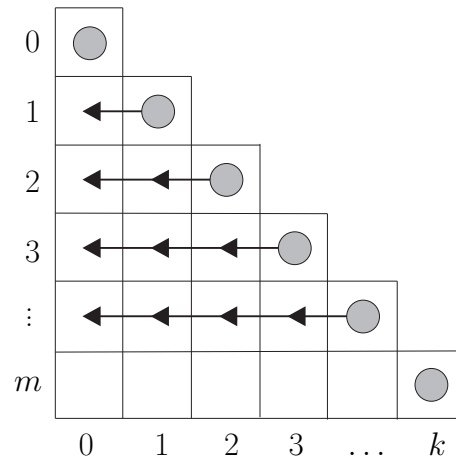


Figure 1: Order in which the coefficients $c_{m,k}$ are calculated: diagonal ones from Eq. (2.8), off-diagonal from recursion (2.7).

where the sum over r goes from $\max\{0, k-m+l+2\}$ to $\min\{k, l\}$. This recursion can be used to calculate all coefficients $c_{m,k}$ to a given level p , starting from the known initial condition, $c_{0,0} = V$. The diagonal coefficients can be calculated immediately,

$$c_{m,m} = \frac{V^{(2m)}}{(2m+1)!} \tag{2.8}$$

and for a given value of $m=0, \dots, p-1$, the coefficients $c_{m,k}$ follow recursively from evaluating (2.7) for $k=m-1, \dots, 1, 0$, as illustrated in Fig. 1.

2.2 Extension to many-body systems

The above outlined approach can be straightforwardly applied to many-body systems. Again the amplitude is expressed through the effective action and the corresponding effective potential, which now depends on mid-point positions and deviations of all particles. For simplicity, these vectors are usually combined into $D \times M$ dimensional vectors \mathbf{x} and $\bar{\mathbf{x}}$, where D is spatial dimensionality, and M is the number of particles. In this notation,

$$A(\mathbf{q}, \mathbf{q}'; \epsilon) = \frac{1}{(2\pi\epsilon)^{DM/2}} e^{-\frac{2}{\epsilon}\bar{\mathbf{x}}^2 - \epsilon W(\mathbf{x}, \bar{\mathbf{x}}; \epsilon)}, \tag{2.9}$$

where initial and final position $\mathbf{q} = (\mathbf{q}_1, \dots, \mathbf{q}_M)$ and $\mathbf{q}' = (\mathbf{q}'_1, \dots, \mathbf{q}'_M)$ are analogously defined $D \times M$ dimensional vectors. Here we will not consider quantum statistics of particles. The required symmetrization or antisymmetrization must be applied after transition amplitudes are calculated using the effective potential.

Many-body transition amplitudes satisfy $D \times M$ -dimensional generalization of the time-dependent Schrödinger equation, which leads to the equation for the effective po-

tential similar to Eq. (2.5), with vectors replacing previously scalar quantities,

$$W + \bar{\mathbf{x}} \cdot \bar{\partial} W + \varepsilon \partial_\varepsilon W - \frac{1}{8} \varepsilon \partial^2 W - \frac{1}{8} \varepsilon \bar{\partial}^2 W + \frac{1}{8} \varepsilon^2 (\partial W)^2 + \frac{1}{8} \varepsilon^2 (\bar{\partial} W)^2 = \frac{1}{2} (V_+ + V_-). \quad (2.10)$$

The effective potential for short-time amplitudes again can be written in the form of the double expansion in ε and $\bar{\mathbf{x}}$. However, it turns out to be advantageous to use the expansion

$$W(\mathbf{x}, \bar{\mathbf{x}}; \varepsilon) = \sum_{m=0}^{\infty} \sum_{k=0}^m \varepsilon^{m-k} W_{m,k}(\mathbf{x}, \bar{\mathbf{x}}), \quad (2.11)$$

and work with fully contracted quantities $W_{m,k}$

$$W_{m,k}(\mathbf{x}, \bar{\mathbf{x}}) = \bar{x}_{i_1} \bar{x}_{i_2} \cdots \bar{x}_{i_{2k}} c_{m,k}^{i_1, \dots, i_{2k}}(\mathbf{x}), \quad (2.12)$$

rather than with the respective coefficients $c_{m,k}^{i_1, \dots, i_{2k}}$. In this way we avoid the computationally expensive symmetrization over all indices i_1, \dots, i_{2k} . After inserting the above expansion into the equation for the effective potential, we obtain the recursion relation which represents a generalization of previously derived Eq. (2.7) for 1D case, and has the form

$$\begin{aligned} 8(m+k+1)W_{m,k} &= \partial^2 W_{m-1,k} + \bar{\partial}^2 W_{m,k+1} - \sum_{l=0}^{m-2} \sum_r (\partial W_{l,r}) \cdot (\partial W_{m-l-2,k-r}) \\ &\quad - \sum_{l=1}^{m-2} \sum_r (\bar{\partial} W_{l,r}) \cdot (\bar{\partial} W_{m-l-1,k-r+1}). \end{aligned} \quad (2.13)$$

The sum over r runs from $\max\{0, k-m+l+2\}$ to $\min\{k, l\}$, while diagonal quantities $W_{m,m}$ can be calculated directly,

$$W_{m,m} = \frac{1}{(2m+1)!} (\bar{\mathbf{x}} \cdot \partial)^{2m} V. \quad (2.14)$$

The above recursion disentangles, in complete analogy with the previously outlined case of one particle in 1D, and is solved in the order shown in Fig. 1.

3 SPEEDUP Mathematica codes for deriving the higher-order effective actions

The effective action approach can be used for numerically exact calculation of short-time amplitudes if the effective potential W_p can be analytically derived to sufficiently high values of p such that the associated error is smaller than the required numerical precision. The error ε^p for the effective action, obtained when level p effective potential is used, translates into $\varepsilon^{p-DM/2}$ for a general many-body short-time amplitude. However, when amplitudes are calculated using the Path Integral Monte Carlo SPEEDUP C

code [19], which will be presented in the next section, the errors of numerically calculated amplitudes are always proportional to $\varepsilon^p \sim 1/N^p$, where N is number of time-steps in the discretization of the propagation time T .

Therefore, accessibility of higher-order effective actions is central to the application of this approach if it is used for direct calculation of short-time amplitudes [8–10], as well as in the case when PIMC code is used [4, 5, 18]. However, increase in the level p leads to the increase in complexity of analytic expressions for the effective potential. On one hand, this limits the maximal accessible level p by the amount of memory required for symbolic derivation of the effective potential. On the other hand, practical use of large expressions for W_p may slow down numerical calculations, and one can opt to use lower than the maximal available level p when optimizing total CPU time required for numerical simulation. The suggested approach is to study time-complexity of the algorithm in practical applications, and to choose optimal level p by minimizing the execution time required to achieve fixed numerical precision.

We have implemented efficient symbolic derivation of higher-order effective actions in Mathematica using the recursive approach. All source files described in this section are located in the `Mathematica` directory of the SPEEDUP code distribution.

3.1 General 1D Mathematica code

SPEEDUP code [19] for symbolic derivation of the effective potential to specified level p is implemented in Mathematica [40], and is available in the `EffectiveAction-1D.nb` notebook. It implements the algorithm depicted in Fig. 1 and calculates the coefficients $c_{m,k}$ for $m = 0, \dots, p-1$ and $k = m, \dots, 0$, starting from the initial condition $c_{0,0} = V$. For a given value of m , the diagonal coefficient $c_{m,m}$ is first calculated from Eq. (2.8), and then all off-diagonal coefficients are calculated from the recursion (2.7).

In this code the potential $V(x)$ is not specified, and the effective potential is derived for a general one-particle 1D theory. The resulting coefficients $c_{m,k}$ and the effective potential are expressed in terms of the potential V and its higher derivatives. Level p effective potential, constructed as

$$W_p(x, \bar{x}; \varepsilon) = \sum_{m=0}^{p-1} \sum_{k=0}^m c_{m,k}(x) \varepsilon^{m-k} \bar{x}^{2k}, \quad (3.1)$$

contains derivatives of V to order $2p-2$.

The only input parameter of this Mathematica code is the level p to which the effective potential should be calculated. As the code runs, it prints used amount of memory (in MB) and CPU time. This information can be used to estimate the required computing resources for higher values of p . The calculated coefficients can be exported to a file, and later imported for further numerical calculations. As an illustration, the file `EffectiveAction-1D-export-p5.m` contains exported definition of all the coefficients $c_{m,k}$ calculated at level $p=5$, while the notebook `EffectiveAction-1D-matching-p5.nb`

contains matching output from the interactive session used to produce the above $p = 5$ result.

The execution of this code on a typical 2 GHz CPU for level $p = 10$ requires 10-15 MB of RAM and several seconds of CPU time. We have successfully run this code for levels as high as $p = 35$ [19]. SPEEDUP C code implements effective actions to the maximal level $p = 18$, with the size of the corresponding C function around 2 MB. If needed, higher levels p can be easily implemented in C and added to the existing SPEEDUP code.

3.2 General 2D and 3D Mathematica code

Although we have developed Mathematica code capable of deriving effective actions for a general many-body theory in arbitrary number of spatial dimensions, in practical applications in 2D and 3D it can be very advantageous to use simpler codes, able to produce results to higher levels p than the general code [9, 10].

This is done in files `EffectiveAction-2D.nb` and `EffectiveAction-3D.nb`, where the recursive approach is implemented directly in 2D and 3D. Execution of these codes requires more memory: for $p = 10$ effective action one needs 60 MB in 2D case, while in 3D case the needed amount of memory increases to 860 MB. On the other hand, the execution time is several minutes for 2D code and around 30 minutes for 3D code.

The distribution of the SPEEDUP code contains exported $p = 5$ definitions of contractions $W_{m,k}$ for both 2D and 3D general potential, as well as matching outputs from interactive sessions used to generate these results.

3.3 Model-specific Mathematica codes

When general expressions for the effective actions, obtained using the above described SPEEDUP Mathematica codes, are used in numerical simulations, one has to specify the potential V and its higher derivatives to order $2p - 2$ in order to be able to calculate transition amplitudes. Such approach is justified for systems where the complexity of higher derivatives increases. However, for systems where this is not the case, or where only a limited number of derivatives is non-trivial (e.g. polynomial interactions), it might be substantially beneficial to specify the potential at the beginning of the Mathematica code and calculate the derivatives explicitly when iterating the recursion.

Using this approach, one is able to obtain coefficients $c_{m,k}$ and the effective potential W directly as functions of the mid-point x . This is implemented in the notebooks `EffectiveAction-1D-AHO.nb` and `EffectiveAction-2D-AHO.nb` for the case of anharmonic oscillators in 1D and 2D,

$$V_{1D-AHO}(x) = \frac{A}{2}x^2 + \frac{g}{24}x^4, \quad (3.2)$$

$$V_{2D-AHO}(x) = \frac{A}{2}(x^2 + y^2) + \frac{g}{24}(x^2 + y^2)^2. \quad (3.3)$$

These codes can be easily executed within few seconds and with the minimal amounts of memory even for $p = 20$. For 1D anharmonic oscillator we have successfully calculated effective actions to excessively large value $p = 144$, and in 2D to $p = 67$ [19], to illustrate the advantage of this model-specific method.

Similar approach can be also used in another extreme case, when the complexity of higher derivatives of the potential V increases very fast, so that entering the corresponding expressions to the code becomes impractical. Even in this situation expressions for effective actions can be usually simplified using some appropriate model-specific ansatz. The form of such ansatz can be deduced from the form of model-specific effective potentials, and then used to simplify their derivation. Such use-case is illustrated in the SPEEDUP Mathematica code for the modified Pöschl-Teller potential,

$$V_{1D-MPT}(x) = -\frac{\lambda}{(\cosh \alpha x)^2}. \quad (3.4)$$

For this potential, the coefficients $c_{m,k}$ of the effective potential can be expressed in the form

$$c_{m,k}(x) = \sum_{l=0}^m d_{m,k,l} \frac{(\tanh \alpha x)^{2l}}{(\cosh \alpha x)^{2m-2l+2}}, \quad (3.5)$$

and newly introduced constant coefficients $d_{m,k,l}$ can be calculated using the model-specific recursion in `EffectiveAction-1D-MPT.nb`. The form of the ansatz (3.5) is deduced from the results of executing general 1D Mathematica code, with the model-specific potential (3.4) defined before the recursion calculation of the coefficients is performed. Using this approach, we were able to obtain maximal level $p = 41$ effective action [19].

3.4 General many-body Mathematica code

SPEEDUP Mathematica code for calculation of effective action for a general many-body theory is implemented using the `MathTensor` [41] package for tensorial calculations in Mathematica. This general implementation required some new functions related to the tensor calculus to be defined in the source notebook `EffectiveAction-ManyBody.nb` provided with the SPEEDUP code.

The function `GenNewInd[n]` generates the required number n of upper and lower indices using the `MathTensor` function `UpLo`, with the assigned names `up1, lo1, ...`, as well as lists `upi` and `loi`, each containing n strings corresponding to the names of generated indices. These new indices are used in the implementation of the recursion for calculation of derivatives of $W_{m,k}$, contractions of the effective potential, and for this reason had to be explicitly named and properly introduced.

The expressions obtained by iterating the recursion contain large numbers of contractions, and function `NewDefUnique[contr]` replaces all contracted indices with the newly-introduced dummy ones in the contraction `contr`, so that they do not interfere with the calculation of derivatives in the recursion. This is necessary since the derivatives in recursion do not distinguish contracted indices from non-contracted ones if their names

happen to be generated by the function `GenNewInd`. Note that the expression `contr` does not have to be full contraction, i.e. function `NewDefUnique` will successfully act on tensors of any kind if they have contracted indices, while it will leave them unchanged if no contractions are present.

The function `NewDerivativeVec[contr, vec, ind]` implements calculation of the first derivative of the tensor `contr` (which may or may not contain contracted indices, but if it does, they are supposed to be uniquely defined dummy ones, which is achieved using the function `NewDefUnique`). The derivative is calculated with respect to vector `vec` with the vectorial index `ind`. The index `ind` can be either lower or upper one, and has to be generated previously by the function `GenNewInd`.

Finally, the function `NewLaplacianVec[contr, vec]` implements the Laplacian of the tensor `contr` with respect to the vector `vec`, i.e. it performs the calculation of contractions of the type

$$\frac{\partial}{\partial \text{vec}_i} \frac{\partial}{\partial \text{vec}^i} \text{contr}. \quad (3.6)$$

After all described functions are defined, the execution of the code proceeds by setting the desired level of the effective action p , generating the needed number of named indices using the function call `GenNewInd[2 p + 2]`, and then by performing the recursion according to the scheme illustrated in Fig. 1. The use of `MathTensor` function `CanAll` in the recursion ensures that the obtained expressions for $W[m, k]$ will be simplified if possible. This is achieved in `MathTensor` by sorting and renaming all dummy indices using the same algorithm and trying to simplify the expression obtained in such way. By default, `Mathematica` will distinguish contracted indices in two expressions if they are named differently, and `MathTensor` works around it using the renaming scheme implemented in `CanAll`.

The computing resources required for the execution of the many-body SPEEDUP `Mathematica` code depend strongly on the level of the effective action. For example, for level $p = 5$ the code can be run within few seconds with the minimal memory requirements. The notebook with the matching output of this calculation is available as `EffectiveAction-ManyBody-matching-p5.nb`, and the exported results for $W[m, k]$ are available in `EffectiveAction-ManyBody-export-p5.m`. We were able to achieve maximal level $p = 10$ [19], with the CPU time of around 2 days on a recent 2 GHz processor. The memory used by `Mathematica` was approximately 1.6 GB.

Note that exporting the definition of the effective potential from `Mathematica` to a file will yield lower and upper indices named `ll1`, `uu1`, etc. In order to import previous results and use them for further calculations with the provided `Mathematica` code, it is necessary to replace indices in the exported file to the proper index names used by the function `GenNewInd`. This is easily done using `find/replace` feature of any text editor. Prior to importing definition of the effective potential, it is necessary to initialize `MathTensor` and all additional functions defined in the notebook `EffectiveAction-ManyBody.nb`, and to generate the needed number of named indices using the function call `GenNewInd[2p+2]`.

4 SPEEDUP C codes for Monte Carlo calculation of 1D transition amplitudes

For short times of propagation, the effective actions derived using the above described Mathematica codes can be directly used. This has been extensively used in [8, 9], where SPEEDUP codes were applied for numerical studies of several lower-dimensional models and calculation of large number of energy eigenvalues and eigenfunctions. The similar approach is used in [10], where SPEEDUP code was used to study properties of fast-rotating Bose-Einstein condensates in anharmonic trapping potentials. The availability of a large number of eigenstates allowed not only precise calculation of global properties of the condensate (such as condensation temperature and ground state occupancy), but also study of density profiles and construction of time-of-flight absorption graphs, with the exact quantum treatment of all available eigenfunctions.

However, in majority of applications the time of propagation cannot be assumed to be small. The effective actions are found to have finite radius of convergence [8], and if the typical propagation times in the considered case exceed this critical value, Path Integral Monte Carlo approach must be used in order to accurately calculate the transition amplitudes and the corresponding expectation values [4, 18]. As outlined earlier, in this case the time of propagation T is divided into N time steps, such that $\varepsilon = T/N$ is sufficiently small and that the effective action approach can be used. The discretization of the propagation time leads to the following expression for the discretized amplitude

$$A_N^{(p)}(a, b; T) = \int \frac{dq_1 \cdots dq_{N-1}}{(2\pi\varepsilon)^{N/2}} e^{-S_N^{(p)}}, \quad (4.1)$$

where $S_N^{(p)}$ stands for the discretized level p effective action,

$$S_N^{(p)} = \sum_{k=0}^{N-1} \left[\frac{(q_{k+1} - q_k)^2}{2\varepsilon} + \varepsilon W_p(x_k, \bar{x}_k; \varepsilon) \right], \quad (4.2)$$

and $q_0 = a$, $q_N = b$, $x_k = (q_{k+1} + q_k)/2$, $\bar{x}_k = (q_{k+1} - q_k)/2$.

Level p discretized effective action is constructed from the corresponding effective potential W_p , calculated as power series expansion to order ε^{p-1} . Since it enters the action multiplied by ε , this leads to discretized actions correct to order ε^p , i.e. with the errors of the order ε^{p+1} . The long-time transition amplitude $A_N^{(p)}(a, b; T)$ is a product of N short-time amplitudes, and its errors are expected to scale as $N \cdot \varepsilon^{p+1} \sim 1/N^p$, as has been shown in [5, 13–15] for transition amplitudes, and in [5, 18] for expectation values, calculated using the corresponding consistently improved estimators.

4.1 Algorithm and structure of the code

SPEEDUP C source is located in the `src` directory of the code distribution [19]. It uses the standard Path Integral Monte Carlo algorithm for calculation of transition amplitudes.

The trajectories are generated by the bisection algorithm [20], hence the number of time-steps N is always given as a power of two, $N = 2^s$. When the amplitude is calculated with 2^s time steps, we can also easily calculate all discretized amplitudes in the hierarchy $2^{s-1}, \dots, 2^0$ at no extra cost. This requires only minor additional CPU time and memory, since the needed trajectories are already generated as subsets of maximal trajectories with 2^s time-steps.

The trajectory is constructed starting from bisection level $n = 0$, where we only have initial and final position of the particle. At bisection level $n = 1$ the propagation is divided into two time-steps, and we have to generate coordinate q of the particle at the moment $T/2$, thus constructing the piecewise trajectory connecting points a at the time $t = 0$, q at $t = T/2$, and b at $t = T$. The coordinate q is generated from the Gaussian probability density function centered at $(a+b)/2$ and with the width $\sigma_1 = \sqrt{T/2}$. The procedure continues iteratively, and each time a set of points is added to the piecewise trajectory. At each bisection level n the coordinates are generated from the Gaussian centered at midpoint of coordinates generated at level $n - 1$, with the width $\sigma_n = \sqrt{T/2^n}$. To generate numbers η from the Gaussian centered at zero we use Box-Müller method,

$$\eta = \sqrt{-2\sigma_n^2 \ln \zeta_1} \cos 2\pi \zeta_2, \quad (4.3)$$

where numbers ζ_1 and ζ_2 are generated from the uniform distribution on the interval $[0,1]$, using the SPRNG library [42]. If the target bisection level is s , then at bisection level $n \leq s$ we generate 2^{n-1} numbers using the above formula, and construct the new trajectory by adding to already existing points the new ones, according to

$$q[(1+2i) \cdot 2^{s-n}] = \eta_i + \frac{q[i \cdot 2^{s-n+1}] + q[(i+1) \cdot 2^{s-n+1}]}{2}, \quad (4.4)$$

where i runs from 0 to $2^{n-1} - 1$. This ensures that at bisection level s we get trajectory with $N = 2^s$ time-steps, consisting of $N + 1$ points, with boundary conditions $q[0] = a$ and $q[N] = b$. At each lower bisection level n , the trajectory consists of $2^n + 1$ points obtained from the maximal one (level s trajectory) as a subset of points $q[i \cdot 2^{s-n}]$ for $i = 0, 1, \dots, 2^n$.

The use of trajectories generated by the bisection algorithm requires normalization factors from all Gaussian probability density functions with different widths to be taken into account. This normalization is different for each bisection level, but can be calculated easily during the initialization phase.

The basic C code is organized in three source files, `main.c`, `p.c` and `potential.c`, with the accompanying header files. The file `potential.c` (its name can be changed, and specified at compile time) must contain a user-supplied function `V0()`, defining the potential V . For a given input value of the coordinate, `V0()` should initialize appropriate variables to the value of the potential V and its higher derivatives to the required order $2p - 2$. When this file is prepared, SPEEDUP code can be compiled and used. The distributed source contains definition of 1D-AHO potential in the file `potential.c`, the same as in the file `1D-AHO.c`.

The execution of the SPEEDUP code starts with the initialization and allocation of memory in the `main()` function, and then the array of amplitudes and associated MC error estimates for each bisection level $n = 0, \dots, s$ is calculated by calling the function `mc()`. After printing the output, `main()` deallocates used memory and exits. Function `mc()` which implements the described MC algorithm is also located in the file `main.c`, as well as the function `distr()`, which generates maximal (level s) trajectories.

The function `mc()` contains main MC sampling loop. In each step new level s trajectory is generated by calling the function `distr()`. Afterwards, for each bisection level n , function `func()` is invoked. This function is located in the file `p.c`, and returns the value of the function e^{-S} , properly normalized, as described earlier. This value (and its square) is accumulated in the MC loop for each bisection level n and later averaged to obtain the estimate of the corresponding discretized amplitude and the associated MC error.

The function `func()` makes use of C implementation of earlier derived effective actions for a general 1D potential. For a given trajectory at the bisection level n , `func()` will first initialize appropriate variables with the values of the potential and its higher derivatives (to the required level $2p-2$) by calling the user-supplied function `V0()`, located in the file `potential.c`. Afterwards the effective action is calculated according to Eq. (4.2), where the effective potential is calculated by the function `Wp()`, located in the file `p.c`. The desired level p of the effective action is selected by defining the appropriate pre-processor variable when the code is compiled.

In addition to this basic mode, when SPEEDUP code uses general expression for level p effective action, we have also implemented model-specific mode, described earlier. If effective actions are derived for a specific model, then user can specify an alternative `p.c` file to be used within the directory `src/models/<model>`, where `<model>` corresponds to the name of the model. If this mode is selected at compile time, the compiler will ignore `p.c` from the top `src` directory, and use the model-specific one, defined by the user. The distributed source contains model definitions for 1D-AHO and 1D-MPT potentials in directories `src/models/1D-AHO` and `src/models/1D-MPT`. Note that in this mode the potential is specified directly in the definition of the effective potential, and therefore the function `V0()` is not used (nor the `potential.c` file).

4.2 Compiling and using SPEEDUP C code

SPEEDUP C source can be easily compiled using the `Makefile` provided in the top directory of the distribution. The compilation has been thoroughly tested with GNU, Intel and IBM XLC compilers. In order to compile the code one has to specify the compiler which will be used in the `Makefile` by setting appropriately the variable `COMPILER`, and then to proceed with the standard command of the type `make <target>`, where `<target>` could be one of `all`, `speedup`, `sprng`, `clean-all`, `clean-speedup`, `clean-sprng`.

The SPRNG library [42] is an external dependency, and for this reason it is located in the directory `src/deps/sprng4.0`. In principle, it has to be compiled only once, after the compiler has been set. This is achieved by executing the command `make sprng`. After-

wards the SPEEDUP code can be compiled and easily linked with the already compiled SPRNG library. Note that if the compiler is changed, SPRNG library has to be recompiled with the same compiler in order to be successfully linked with the SPEEDUP code.

To compile the code with level $p=10$ effective action and user-supplied function $V0()$ located in the file `src/1D-AH0.c`, the following command can be used:

```
make speedup P=10 POTENTIAL=1D-AH0.c
```

If not specified, `POTENTIAL=potential.c` is used, while the default level of the effective action is $P=1$. To compile the code using a model-specific definition of the effective potential, instead of the `POTENTIAL` variable, we have to appropriately set the `MODEL` variable on the command line. For example, to compile the supplied `p.c` file for 1D-MPT model located in the directory `src/models/1D-MPT` using the level $p=5$ effective action, the following command can be used:

```
make speedup P=5 MODEL=1D-MPT
```

All binaries compiled using the `POTENTIAL` mode are stored in the `bin` directory, while the binaries for the `MODEL` mode are stored in the appropriate `bin/models/<model>` directory. This information is provided by the `make` command after each successful compilation is done.

The compilation is documented in more details in the supplied `README.txt` files. The distribution of the SPEEDUP code also contains examples of compilation with the GNU, Intel and IBM XLC compilers, as well as matching outputs and results of the execution for each tested compiler, each model, and for a range of levels of the effective action p .

Once compiled, the SPEEDUP code can be used to calculate long-time amplitudes of a system in the specified potential V . If executed without any command-line arguments, the binary will print help message, with details of the usage. The obligatory arguments are time of propagation T , initial and final position a and b , maximal bisection level s , number of MC samples N_{mc} and `seed` for initialization of the SPRNG random number generator. All further arguments are converted to numbers of the `double` type and made available in the array `par` to the function $V0()$, or to the model-specific functions in the file `src/models/<model>/p.c`. The output of the execution contains calculated value of the amplitude for each bisection level $n=0, \dots, s$ and the corresponding MC estimate of its error (standard deviation). At bisection level $n=0$, where no integrals are actually calculated and the discretized $N=1$ amplitude is simply given by an analytic expression, zero is printed as the error estimate.

Fig. 2 illustrates the typical results obtained from the SPEEDUP code on the example of 1D-MPT theory. In this figure we can see the convergence of numerically calculated amplitudes with the number of time-steps N to the exact continuum value, obtained in the limit $N \rightarrow \infty$. Such convergence is obtained for each level p of the effective action used. However, the convergence is much faster when higher-order effective action is used. Note that all results corresponding to the one value of level p on the graph are obtained from a single run of the SPEEDUP code with the maximal bisection level $s=10$. The simplest way to estimate the continuum value of the amplitude is to fit numerical

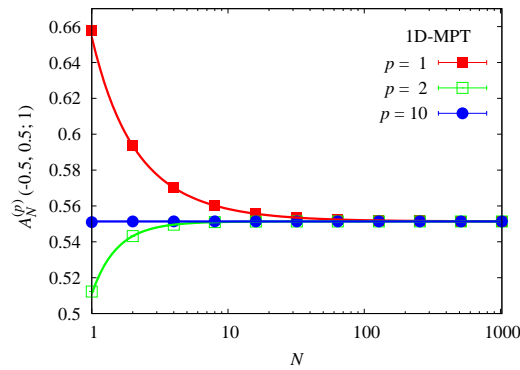


Figure 2: Convergence of SPEEDUP Monte-Carlo results for the transition amplitude $A_N^{(p)}(-0.5, 0.5; 1)$ of 1D-MPT potential as a function of the number of time steps N , calculated with level $p=1, 2, 10$ effective actions, with the parameters of the potential $\lambda=\alpha=1$. The full lines give the fitted functions (4.5), where the constant term A_p corresponds to the continuum-theory amplitude $A(-0.5, 0.5; 1)$. The number of Monte-Carlo samples was $N_{MC}=10^6$.

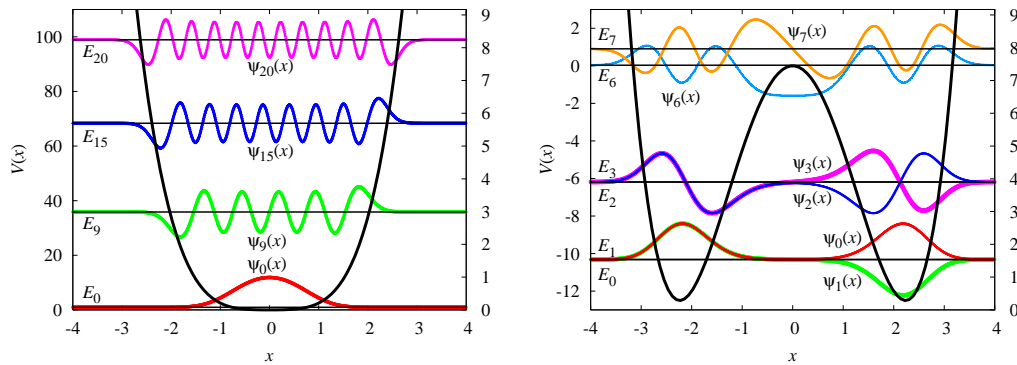


Figure 3: (left) The anharmonic potential 1D-AHO, its energy eigenvalues (horizontal lines) and eigenfunctions, obtained by direct diagonalization of the space-discretized matrix of the evolution operator with level $p=21$ effective action and parameters $A=1, g=48$. The discretization cutoff was $L=8$, spacing $\Delta=9.76 \cdot 10^{-4}$, and time of propagation $t=0.02$. (right) Results for the double-well potential, $A=-10, g=12, L=10, \Delta=1.22 \cdot 10^{-3}$, $t=0.1$. On both graphs, left y -axis corresponds to $V(x)$ and energy eigenvalues, while scale on the right y -axis corresponds to values of eigenfunctions, each vertically shifted to level with the appropriate eigenvalue.

results from single run of the code to the appropriate level p fitting function [13–15],

$$A_N^{(p)} = A^{(p)} + \frac{B^{(p)}}{N^p} + \frac{C^{(p+1)}}{N^{p+1}} + \dots \quad (4.5)$$

The constant term obtained by fitting corresponds to the best estimate of the exact amplitude which can be found from the available numerical results.

As mentioned earlier, the effective action approach can be used for accurate calculation of a large number of energy eigenstates and eigenvalues by diagonalization of the space-discretized matrix of transition amplitudes [6–10]. Fig. 3 illustrates this for the case

of an anharmonic and double-well potential. The graph on the left gives several eigenvalues and eigenstates for 1D-AHO potential with $A = 1$ and quartic anharmonicity $g = 48$, while the graph on the right gives low-lying spectrum and eigenfunctions of the double-well potential, obtained for $A = -10$, with the moderate anharmonicity $g = 12$. More details on this approach, including study of all errors associated with the discretization process, can be found in [8,9].

5 Conclusions

In this paper we have presented SPEEDUP Mathematica and C codes, which implement the effective action approach for calculation of quantum mechanical transition amplitudes. The developed Mathematica codes provide an efficient tool for symbolic derivation of effective actions to high orders for specific models, for a general 1D, 2D and 3D single-particle theory, as well as for a general many-body systems in arbitrary number of spatial dimensions. The recursive implementation of the code allows symbolic calculation of extremely high levels of effective actions, required for high-precision calculation of transition amplitudes.

For calculation of long-time amplitudes we have developed SPEEDUP C Path Integral Monte Carlo code. The C implementation of a general 1D effective action to maximal level $p = 18$ and model-specific effective actions provide fast $1/N^p$ convergence to the exact continuum amplitudes.

Further development of the SPEEDUP C codes will include parallelization using MPI, OPENMP and hybrid programming model, C implementation of the effective potential to higher levels p , as well as providing model-specific effective actions for relevant potentials, including many-body systems.

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Development of Grid e-Infrastructure in South-Eastern Europe

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Abstract Over the period of six years and three phases, the SEE-GRID programme has established a strong regional human network in the area of distributed scientific computing and has set up a powerful regional Grid infrastructure. It attracted a number of user communities and applications from diverse fields from countries throughout the South-Eastern Europe. From the infrastructure point view, the first project phase has established a pilot Grid infrastructure with more than 20 resource centers in 11 countries. During the subsequent two phases of the project,

the infrastructure has grown to currently 55 resource centers with more than 6,600 CPUs and 750 TBs of disk storage, distributed in 16 participating countries. Inclusion of new resource centers to the existing infrastructure, as well as a support to new user communities, has demanded setup of regionally distributed core services, development of new monitoring and operational tools, and close collaboration of all partner institution in managing such a complex infrastructure. In this paper we give an overview of the development and current status of SEE-GRID regional infrastructure and describe its transition to the NGI-based Grid model in EGI, with the strong SEE regional collaboration.

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Keywords Grid · e-Infrastructure ·
Distributed computing

1 Introduction

The transition of the traditional science to e-Science is fueled by the ever increasing need for processing of exceedingly large amounts of data and exponentially increasing computational requirements: in order to realistically describe and solve real-world problems, numerical simulations are becoming more detailed, experimental sciences use more sophisticated sensors to make precise measurements; and shift from the

individuals-based science work towards collaborative research model now starts to dominate.

Computing resources and services able to support needs of such a new model of scientific work are available at different layers: local computing centers, national and regional computing centers, and supercomputing centers. The gap between the needs of various user communities and dispersed computing resources able to satisfy their requirements is effectively bridged by introduction of Grid technology on the top of the networking layer and local resource management layers.

Computing Grids are conceptually not unlike electrical Grids. In an electrical Grid, the wall outlets allow us to link to and use an infrastructure of resources, which generate, distribute, and bill for electrical power. When we connect to the electrical Grid, we do not need to know details on the power plant currently generating the electricity we use. In the same way Grid technology uses middleware layer to coordinate and organize into one logical resource a set of available distributed computing and storage resources across a network, allowing users to access them in a unified fashion. The computing Grids, like electrical Grids, aim to provide users with easy access to all the resources they need, whenever they need them, regardless of the underlying physical topology and management model of individual clusters.

Grids address two distinct but related goals: providing remote access to information technology (IT) assets, and aggregating processing and storage power. The most obvious resources included in Grids are processors (CPUs) and data storage systems, but Grids also can encompass various sensors, applications, and other advanced types of resources. One of the first commonly known Grid initiatives was the SETI@HOME project, which solicited several millions of volunteers to download a screensaver, which was able to use idle processor time to analyze the astronomical data in the search for extraterrestrial life.

In the past six years the European Commission has funded, through a number of targeted initiatives, activation of new user communities and enabling collaborative research across a number of fields in order to close existing technological and scientific gaps. In addition, this helps in bridging the digital divide, stimulating research

and consequently alleviating the brain drain in the less-developed regions of Europe. This was especially successful in the South-Eastern Europe (SEE), where a number of such initiatives show excellent results. In the Grid arena, the South-East European GRid e-Infrastructure Development (SEE-GRID) series of projects [1, 2], through its first two 2-year phases, has established a strong human network in the area of scientific computing and has set up a powerful regional Grid infrastructure, attracting large number of applications from diverse fields from countries throughout the South-Eastern Europe. The third 2-year phase of the SEE-GRID programme, SEE-GRID-SCI [3] project, has aimed and succeeded in having a catalytic effect on a number of SEE user groups, with a strong focus on the key seismological, meteorological, and environmental communities.

One of the main successes of the SEE-GRID programme is cumulative structuring effort on the establishment of National Grid Initiatives (NGIs) in SEE countries and collaborative work on achieving sustainable model of operation, supported strongly from national funding sources. The regional SEE-GRID initiative has also supported and coordinated a successful transition of all SEE countries from the centralized operations model to the NGI-based EGI infrastructure, which is clearly visible from the participation of all partner countries in the 4-year EGI-InSPIRE project [4].

2 Resource Centers

The regional Grid infrastructure operated by SEE-GRID-SCI project was built on top of the pilot infrastructure established by the first SEE-GRID project (2004–2006), which was since then substantially extended and enlarged in terms of resources and number of Grid sites, and upgraded in terms of the deployed middleware and core services provided to existing and new user communities during the SEE-GRID-2 project (2006–2008).

The operations activity adopted the pragmatic model of the 2-layered infrastructures in which mature sites were migrated to the EGEE [5]

production infrastructure, while the start-up sites from new institutes and user communities were incubated within the SEE-GRID infrastructure until they were ready to follow the requirements of the full-scale production infrastructure. In this way, both SEE-wide and national-level applications were able to benefit from the computing resources of both infrastructures, by mainly using the pilot infrastructure in the incubation phase and production infrastructure later, when they reach the production phase. Moreover, this approach ensured that smaller sites, typical for the region, have a chance to be a part of the regional SEE-GRID infrastructure acting as an incubator for their maturing into EGEE production.

As applications developed in the region have matured, new Virtual Organizations (VOs) have spun off with the relevant core services supported by the SEE-GRID-SCI operations activity SA1. Discipline-specific services were deployed in multiple instances (for failover and for achieving load-balancing through a wide geographic distribution) over the e-Infrastructure and operationally maintained and supported by SA1. Sophisticated operational tools, some of them being developed within the joint research activity JRA1 of the

SEE-GRID-SCI project, were used to enhance infrastructure performance.

SEE-GRID-SCI project has continued to operate and further extend, develop and improve this infrastructure, with the aim to cater for the needs of all activated user communities in the region, with special emphasis on the three identified target areas: meteorology, seismology, and environmental sciences. Apart from computing and storage resources made available to these user communities, SA1 activity provided and maintained a set of existing and new operational and monitoring tools so as to ensure proper operation of the infrastructure, and a set of primary and secondary core services for all deployed VOs in order to ensure optimal geographical distribution according to the underlying network structure, load sharing, and quality of the service to end users.

Currently SEE-GRID-SCI infrastructure encompasses approximately 55 Grid sites, more than 6600 CPUs, and around 750 TBs of available data storage capacity, which is illustrated in Fig. 1, with further details given in Table 1. Overall number of CPUs has grown from 2400 at the beginning of the SEE-GRID-SCI project in May 2008 to cur-



Fig. 1 Overview of the SEE-GRID-SCI infrastructure

Table 1 SEE-GRID-SCI computing and storage resources

Country	Total number of CPUs	Total storage [TB]
Greece	1,200	66.8
Bulgaria	1,210	42.3
Romania	120	4.0
Turkey	2,380	528.0
Hungary	8	2.0
Albania	34	1.3
Bosnia-Herzegovina	80	1.1
FYR of Macedonia	80	4.1
Serbia	974	97.0
Montenegro	40	0.6
Moldova	24	6.5
Croatia	44	0.2
Armenia	424	0.2
Georgia	16	0.1
Total	6,634	754.2

rently more than 6600, while the number of dedicated CPUs for SEE-GRID-SCI VOs is currently around 1500. Grid operations activity successfully maintains such a large, geographically disperse and ever-growing infrastructure, harmonizing its operation with the pan-European EGEE/EGI infrastructure. In addition to this, one of the most important achievements of SA1 activity is transfer of knowledge and Grid know-how to all participating countries, and support to their NGI operation teams to reach the level of expertise needed for sustainable NGI-based operational model in EGI.

After the completion of the SEE-GRID-SCI project in April 2010, the regional Grid infrastructure was seamlessly integrated to the EGI infrastructure, and continues to support all deployed Virtual Organizations (VOs) and applications developed during the 6-year SEE-GRID programme. The strong human network remains in place and still supports on-going transition of all countries to independent NGI operations through the SEE Regional Operations Centre. The catch-all SEE-GRID Certification Authority will continue its operation until all the countries from the region deploy their own national certification authorities. In terms of Grid operations, currently almost all (with only a few exceptions) NGI operations teams and infrastructures are fully validated by EGI teams, while validation for the remaining

SEE countries is expected to finish within a few months, i.e. by mid-2011.

3 User Communities

The core objective of the SEE-GRID-SCI project was to engage user communities from different regional countries in close collaboration. This strategy had a structuring effect for crucial regional communities. The target applications were selected from core earth science disciplines in the region, namely, seismology, meteorology and environmental protection. Thus, the focus of the project was to engage these three core cross-border communities in the research fields crucial for the region, structured in the form of Virtual Organizations (VO):

- Seismology VO had six applications ranging from Seismic Data Service to Earthquake Location Finding, from Numerical Modelling of Mantle Convection to Seismic Risk Assessment [6–12].
- Meteorology VO, with two large-scale applications, follows an innovative approach to weather forecasting that uses a multitude of weather models and bases the final forecast on an ensemble of weather model outputs. The other problem tackled within this VO is the reproduction/forecasting of the airflow over complex terrain [13–21].
- Environmental Protection VO supports eight applications focusing on environmental protection/response and environment-oriented satellite image processing [22–32].

In the Seismology VO, the work was organized around the development of Seismic Data Server (SDS) application services, providing distributed storage and serving of seismic data from different partner countries, logical organization and indexing of distributed seismic data, and programming tools (called iterators) that provide easy access to seismic data. In terms of applications, the focus was on gridification of five seismology applications from different South-eastern European countries: Seismic Risk Assessment (SRA), Numerical Modeling of Mantle Convection (NMMC3D), Fault Plane Solution (FPS),

Earthquake Location Finding (ELF) and Massive Digital Seismological Signal Processing with the Wavelet Analysis (MDSSP-WA).

In the Meteorology VO, with the aim to contribute to the improvement of the forecasts in the Mediterranean, among other techniques, the regional ensemble forecasting technique has been explored in the frame of the SEE-GRID-SCI. Indeed the regional ensemble forecasting system built over the Mediterranean, involves the need of large infrastructure that was not easily available at medium-scale research centres and institutions. For that reason, the Grid infrastructure was explored for its ability to support the high CPU and storage needs of such a regional ensemble forecasting system. This application allowed the meteorological entities participating in the project to assess the probability of a particular weather event to occur. This information is being made freely available (to the participants and to the general public, etc) through the project web page, helping thus when needed, to make the necessary decisions based on this probabilistic information. In addition, another set of applications permitted the entities participating in the project to improve the quality of the understanding and forecasting of the airflow over regions characterized by the complex terrain. Further an important benefit of this application is the possibility offered to use this model for operational weather forecasting. Operational weather forecasting model chains based on this model have been developed in the frame of this project over Bosnia and Herzegovina, Armenia and Georgia. This is considered as an important benefit for the meteorological services of the aforementioned countries that did not have up to now the infrastructure support to run op-

erationally weather forecasting models for their region.

The Environmental VO has dealt with several important problem areas in the domain of environmental modeling and environmental protection and the applications developed within the VO advanced the scientific knowledge and affected the policy and decision-making process, responding to the EU directives and national priorities. New modeling techniques and algorithms were employed in several of the applications, using the power of the Grid in order to increase the spatial and temporal resolution and obtain more adequate representation of the natural processes under investigation. In other applications, established techniques were used, combined with filters and scripts developed by the project partners in order to accommodate these systems to the specifics of the Balkan region. The beneficiaries of the systems developed during the projects lifetime include not only environmental scientists, but also the relevant governmental and international organizations, for example the international air quality monitoring bodies. By employing the Grid to increase the resolution these applications are now starting to target new beneficiaries like municipal authorities, small and medium enterprises and media. For many of the applications the validation of the models and standardizing the computational processes has been an important achievement, since the methodological aspect of these studies was a challenging one, especially in the Balkan region.

Figure 2 gives some details on the size of activated user communities, and the distribution of computing resources they have utilized during the project lifetime. Overall, during the period 2008–

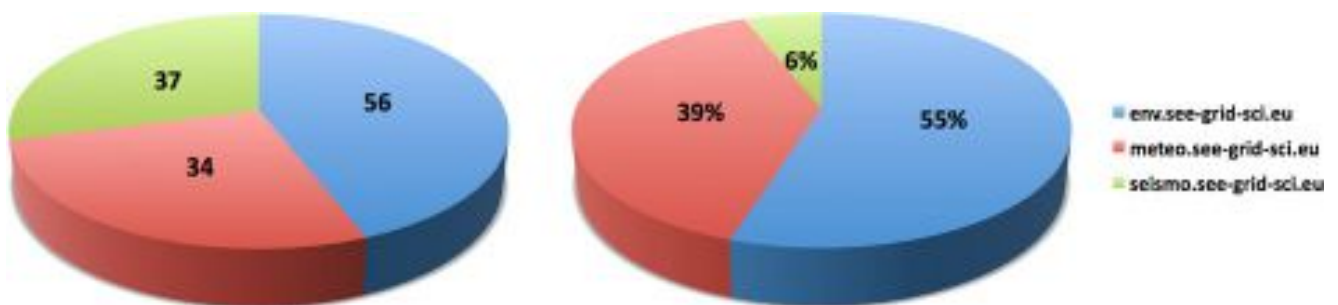


Fig. 2 The distribution of the size of three target user communities (*left*, number of end users per VO), and the distribution of the computing resources used by VOs (*right*)

2010, SEE-GRID-SCI project has provided more than 22.5 million elapsed CPU hours or 2,566 CPU years, and more than 4.5 million jobs were executed on the regional infrastructure. Out of this, SEE-GRID-SCI and national VOs amounted to 16.4 million CPU hours or 1,872 CPU years (73%). The total utilization of dedicated resources (based on the average number of 1050 available CPUs) was quite high, around 89%, and this has attracted the growth of supported user communities, and enabled them to achieve the enormous amount of new scientific results, as can be seen by the large number of scientific papers published in per-reviewed research journals [33–38] and presented at numerous scientific conferences [6–32]. The project itself has organized SEE-GRID-SCI User Forum in December 2009, where the most significant results were presented.

4 Core Services

To operationally provide computational and storage resource to the three target scientific commu-

nities supported by the SEE-GRID-SCI project, three different VOs have been created: METEO, SEISMO, and ENV VO. The support for these VOs, as well as to the catch-all SEEGRID VO, has been configured on all Resource Centres participating in the regional infrastructure, and a set of core services was installed and deployed by SA1 activity, as illustrated in Fig. 3.

For each VO a primary and secondary VO Management Service (VOMS) has been deployed and maintained by institutes involved in the corresponding VO application development. Additionally, a set of core Grid services was deployed in order to support job management operations (Workload Management System—WMS, Logging and Bookkeeping—LB), Grid information system (Berkeley Database Information Index—BDII), data storage and transfer operations (Logical File Catalog—LFC, File Transfer Service—FTS, ARDA Metadata Grid Application—AMGA), and management of digital credentials (MyProxy—PX). Deployment details of primary core Grid services are given in Table 2.

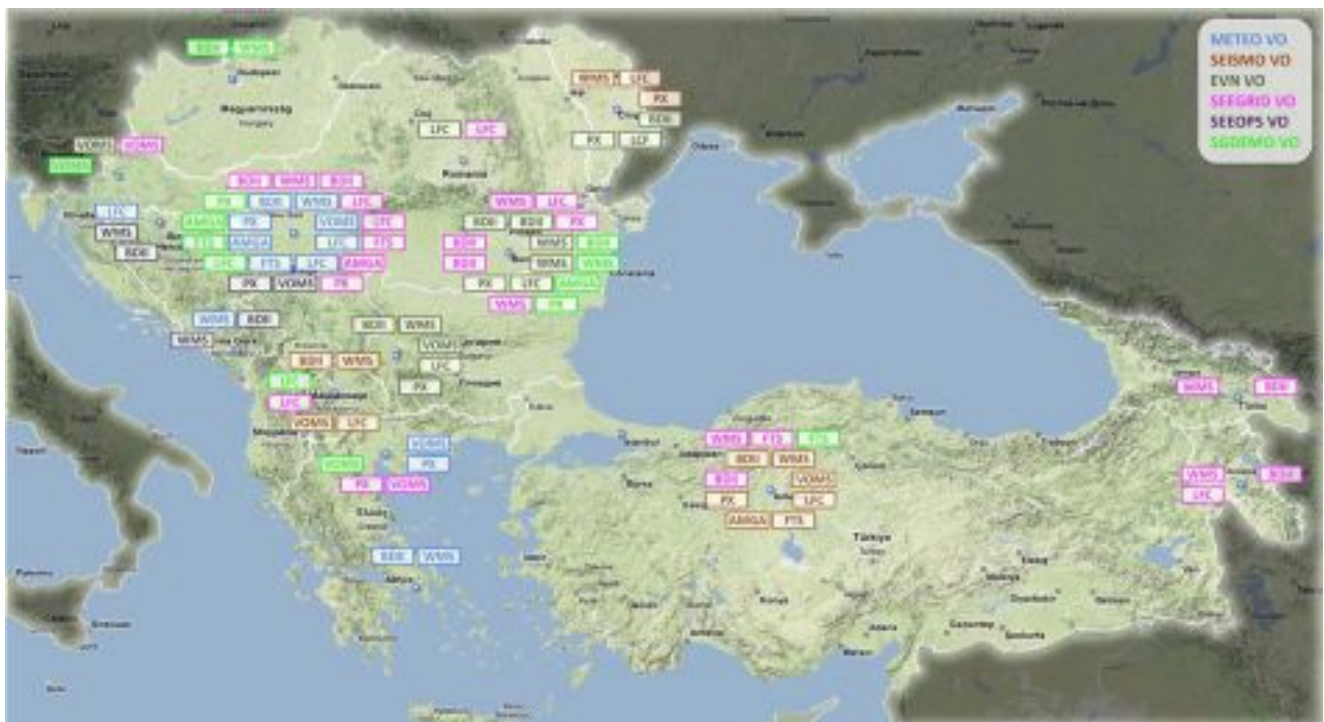


Fig. 3 Geographical distribution of core services

Table 2 List of primary core services deployed per VO

Service	METEO VO	ENV VO	SEISMO VO
VOMS	voms.grid.auth.gr	voms.ipp.acad.bg	voms.ulakbim.gov.tr
WMS & LB	wms.ipb.ac.rs	wms.ipp.acad.bg	wms.ulakbim.gov.tr
BDII	bdii.ipb.ac.rs	bdii.ipp.acad.bg	bdii.ulakbim.gov.tr
LFC	grid02.rcub.bg.ac.rs	lfc01.mosigrid.utcluj.ro	lfc.ulakbim.gov.tr
FTS	grid16.rcub.bg.ac.rs		fts.ulakbim.gov.tr
AMGA	grid16.rcub.bg.ac.rs		amga.ulakbim.gov.tr
PX	myproxy.ipb.ac.rs	myproxy.ipp.acad.bg	myproxy.ulakbim.gov.tr

5 Grid Operations

This section gives brief description of operational procedures and key tools developed during the course of the SEE-GRID programme. In addition, a number of operational tools have been developed, improved and deployed by the SEE-GRID-SCI SA1 activity and used in day-to-day infrastructure management, as illustrated in Fig. 4. Table 3 lists all currently deployed tools including those used for monitoring of the infrastructure, some of which are described in more detail in the next section, while Fig. 4 gives their geographical distribution, as well as distribution of respon-

sibilities for their deployment and maintaining. The interactions and collaboration on the development and usage of described tools with other Grid initiatives/projects are emphasized wherever applicable.

Recognizing that improvements in the quality and shaping-up of the SEE-GRID infrastructure are an important and continuous effort, necessary for the successful work of SEE-GRID application developers, as well as for the usage of our infrastructure by the existing user communities, the pro-active monitoring of Grid sites in the region was organized through rotating shifts by SA1 country representatives (Grid Infrastructure

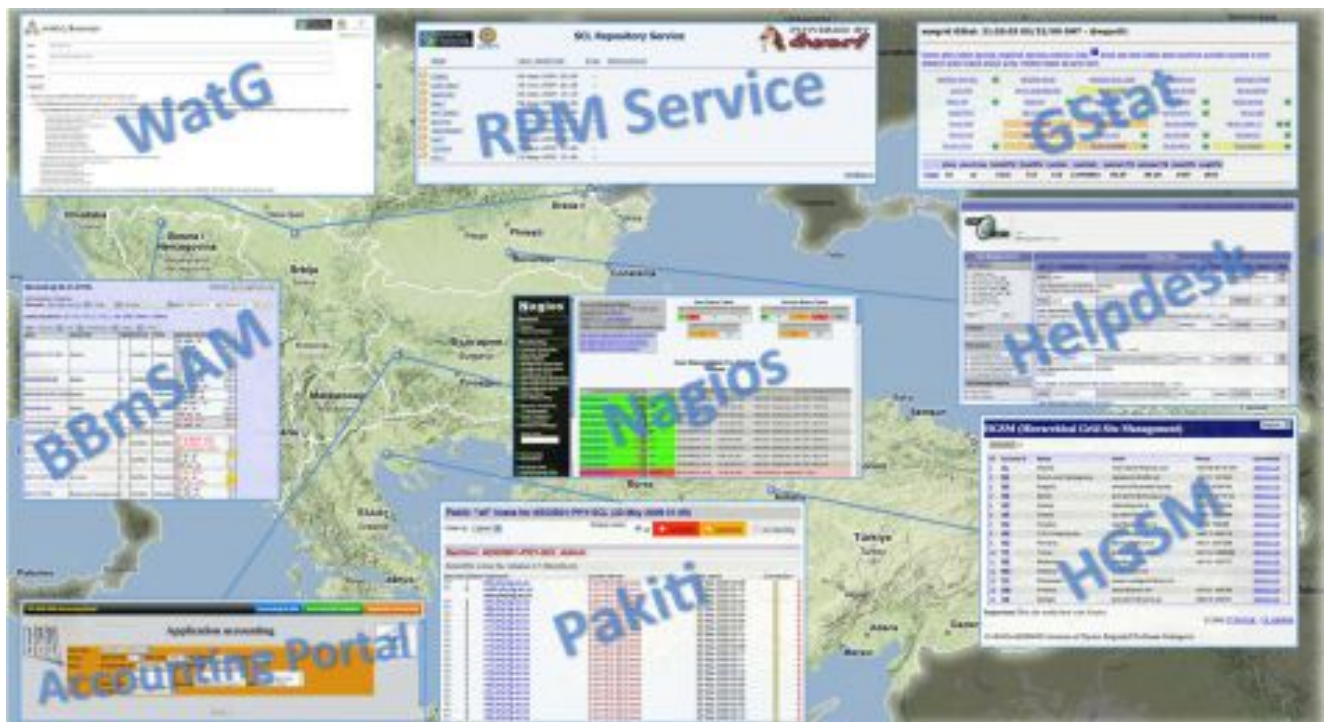


Fig. 4 Geographical distribution of SEE-GRID operational and monitoring tools

Table 3 Deployment of operational and monitoring tools in the SEE-GRID infrastructure

Service	Service URL
HGSM	https://hgsm.grid.org.tr/
BBmSAM	https://c01.grid.etfbl.net/bbmsam/
BBmobileSAM	https://c01.grid.etfbl.net/bbmsam/mobile.php
Gstat	http://gstat.gridops.org/gstat/seegrid/
Accounting Portal	http://gserv4.ipp.acad.bg:8080/AccountingPortal/
Nagios	https://portal.ipp.acad.bg:7443/seegridnagios/
Googlemap	http://www.grid.org.tr/eng/
MonALISA	http://monitor.seegrid.grid.pub.ro:8080/
Real Time Monitor	http://gridportal.hep.ph.ic.ac.uk/rtm/applet.html
WatG Browser	http://watgbrowser.scl.rs:8080/
WMS Monitoring Tool	http://wmsmon.scl.rs/
Repository Service	http://rpm.egee-see.org/yum/SEE-GRID/
Dwarf	https://dwarf.scl.rs/
Grid-Operator-On-Duty	http://wiki.egee-see.org/index.php/SG_GOOD
Helpdesk	http://helpdesk.see-grid.eu/
SEE-GRID Wiki	http://wiki.egee-see.org/index.php/SEE-GRID_Wiki
P-Grade Portal	http://portal.p-grade.hu/multi-grid

Managers—GIMs). During each shift, the corresponding GIM is designated as Grid-Operator-On-Duty, or GOOD [39].

Basically, the idea is that each GIM (i.e. GIM team from one country) is on duty during one week overseeing the infrastructure and opening trouble tickets in the SEE-GRID Helpdesk to sites from all countries where operational problems are identified using the available monitoring tools. Of course, all GIMs are expected to continually monitor and provide support to sites from their countries—this is their day-to-day duty, in addition to regular regional GOOD shifts. Details of the organization of GOOD shifts are given at the SEE-GRID Wiki [39, 40]. For problems identified by GOODs, trouble tickets were created in the SEE-GRID Helpdesk [42], and site managers were expected to deal with such operational problems and provide feedback on the steps taken. Typically, simple problems were resolved within one working day, while for more complex issues typical resolution time was up to three working days.

On the request of applications which need MPI support on sites, GOODs are expected to test MPI setup on all SEE-GRID sites which support MPI. The MPI setup tests are performed at least once a week, and GOODs ensure that the test parallel jobs run at the same time on at least two WNs (to test ssh setup as well). More details

can be found on the Wiki page on Testing MPI support [40].

In this section we describe two selected tools used for Grid operations: HGSM database (used for maintaining the database of Grid resources and personnel), Dwarf portal related to software development and repositories (especially important in maintaining updated of Grid middleware and application software).

5.1 HGSM

Hierarchical Grid Site Management—HGSM [43] is a web based management application primarily geared towards Grid site administrators. At the beginning it was designed to store static information about Grid sites and personnel responsible for the sites, but later it evolved to the central information hub, also used for other Grid monitoring and checking services.

The idea behind the HGSM is to reflect the natural hierarchy present in the infrastructure. For each supported infrastructure, HGSM has a ROC (Regional Operational Centers) associated with it at the top. These ROCs contain the countries that participate in a particular infrastructure. Grid sites of each country are listed under the respective country tree, and all details related to a specific Grid site can be viewed under the respective site entry in the web front end of HGSM (Fig. 5). The

HGSM (Hierarchical Grid Site Management) English

SEEGRID »

ID	Country Id	Name	email	Phone	Comments
1	AL	Albania	neki.frasheri@gmail.com	+355 66 22 59 467	Admins List
2	BA	Bosnia and Herzegovina	badaboom@etbi.net	+387 51 221860	Admins List
3	BG	Bulgaria	emanouil@parallel.bas.bg	+359 2 9796783	Admins List
4	RS	Serbia	grid-admin@ipb.ac.rs	+381 11 3713152	Admins List
5	GR	Greece	ilabos@gnet.gr	+302107474248	Admins List
6	HR	Croatia	lcp-admin@ib.hr	+385 1 4561168	Admins List
7	HU	Hungary	log2@ipds.sztaki.hu	+361 2 796066	Admins List
8	MK	FYR of Macedonia	boroj@i.edu.mk	+389 70 326718	Admins List
9	RO	Romania	stanciu@grid.icl.ro	+40 21 2241266	Admins List
10	TR	Turkey	grid@ulakbim.gov.tr	+90 312 2960363	Admins List
11	ME	Montenegro	lukaf@cg.ac.yu	+381 81 242777	Admins List
12	MD	Moldavia	svv@renam.md		Admins List
13	CH	Switzerland	dusan.vudragovic@cern.ch		Admins List
14	AM	Armenia	grid-admin@sci.am	+374 94 361138	Admins List
15	GE	Georgia	grid-admin@grens.ge	+995 32 250591	Admins List
16	AZ	Azerbaijan	ai.ismayilov@ieeo.org		Admins List

Important: This site works best with Firefox

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/C=RS/O=AEGIS/OU=Institute of Physics Belgrade/CN=Dusan Vudragovic

Fig. 5 Overview of HGSM portal

management personnel information is also stored for each organizational level (ROC, country, site), containing contacts with both administrative and management privileges.

While HGSM holds vast information about Grid sites and core services, it also contains personal information for named contacts (names, e-mail addresses and phone numbers). To properly protect this information, HGSM uses a digital certificate-based authentication system. HGSM server only authorizes people with a valid Grid certificate to view the information in HGSM web front-end. Editing information is only allowed to authorized personnel with administrative privileges. The authorization is organized in a hierarchical manner, so that an administrator at the higher level can manage every aspect (including the administrators) at lower organizational levels.

HGSM has already been used by communities and projects other than SEE-GRID, e.g., by the Deployment of Remote Instrumentation Infrastructure—DORII project [44], as well as by the Spanish and Portuguese NGIs [45].

5.2 Dwarf

Web-based Dwarf tool is composed of the Dwarf web portal [46], Dwarf modules and Dwarf data-

base. Using the Public Key Infrastructure (PKI), Dwarf framework provides digital certificate-based management of RPM uploading and creation of APT and YUM repositories. The Dwarf web portal home page, shown in Fig. 6, gives an overview of repository structure together with information on the context of each repository, and latest build's timestamp.

From the Dwarf web portal, properly authenticated and authorized user can perform the following operations on the repository:

- Create and change repository structure: Users can create paths to new distributions and components, by specifying their names. In the current implementation of the Dwarf framework, the users are able to create APT and YUM repositories, as well as to create a MIRROR to an existing remote repository.
- Package uploading: Users can upload different software packages, but only to sections of the repository for which they are authorized as contributors.
- Build repository: After each RPM upload, a user should re-build the repository structure. If not, Dwarf system will do it automatically, through a cron job.



Fig. 6 Overview of the SEE-GRID Dwarf web portal

Dwarf modules are implemented as bash scripts which handle appropriate build actions on various repositories.

After a new APT repository structure is created from the Dwarf web portal, the RPMs must be indexed to create the APT database. This is done by the APT Dwarf module, which uses the `genbasedir` tool for this purpose. It analyzes RPM packages in a directory tree and builds information files so that that directory tree can be used as a proper APT repository.

The Dwarf database contains information on security (authentication and authorization), repositories types and metadata, mirror repositories, and logging information. Dwarf database contains metadata repository information on build's timestamps, contexts, and descriptions of the repositories, as well as repository types. The rules for creation of mirror repositories are also kept in the Dwarf database. In addition, for security and auditing reasons, the database contains a log of all user-initiated actions. The Dwarf database is realized using the MySQL database technology.

Once the repository is constructed, it is made available by HTTP and FTP servers configured and working on the Dwarf web portal. The DWARF framework provides configurations that should be included in the local HTTP and FTP servers configuration files in order to provide the context of repositories.

6 Monitoring of SEE-GRID Infrastructure

The monitoring of the heterogeneous and widely geographically dispersed Grid infrastructure is an essential task for achieving the required quality of service to supported user communities. This has been defined through the SEE-GRID Service Level Agreement (SLA), which has served as a prototype for the later adopted EGEE SLA. The monitoring of the performance of sites is not only used for formal assessment of the conformance to SLA, but also for day-to-day Grid operations, since various monitoring tools provide the main channel for identification and diagnostics of operational problems by Grid Operators on Duty and

GIMs. The most important such tools are listed in Table 3, and we briefly describe them in this section. To illustrate how the conformance of availabilities of Grid services to the adopted SLA was monitored and assessed, Fig. 7 gives overview of the availability monitoring results for the second year of the SEE-GRID-SCI project (May 2009 to April 2010). Using the BBmSAM tool (described below), precise measurement of the availability of all services was systematically done, and detailed results were provided at different levels or granularity: per service, per site, per country, and per SEE-GRID infrastructure. For example, the overall availability of resources (weighted by the CPU number of individual clusters) for the last four quarters increased from around 78% in Q5 (May–July 2009) to around 89% in Q8 (February–April 2010). Strict enforcement of SLA lead to a steady increase in the availability and reliability of Grid services offered to our target user communities.

6.1 BBmSAM

Availability monitoring of the infrastructure is carried out using the Service Availability Monitoring—SAM [47] framework developed in EGEE project [5], which is further developed and extended by SEE-GRID series of projects and deployed by its SA1 activity. The original SAM system consists of server and client components which communicate using web services. The client

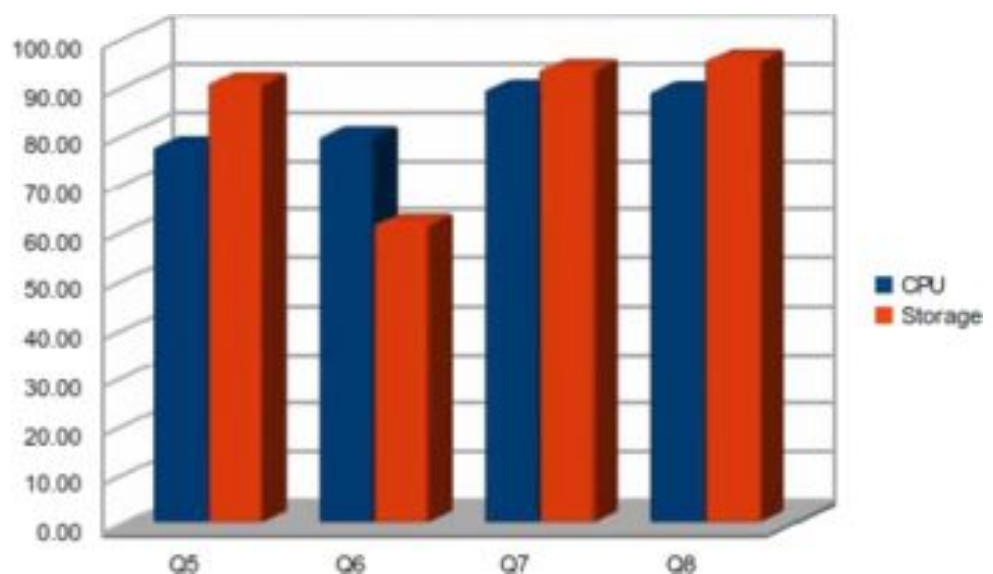
initiates periodical tests of the infrastructure and publishes data to the server which stores them in the Oracle database. Main change in the SAM framework in its adaptation for the SEE-GRID community was its porting to MySQL, suitable for the deployment in the region and in line with the SEE-GRID open source philosophy.

BBmSAM [48–50] Platform is a web application coded in PHP and using the MySQL Database as data storage back-end (although any standard-compliant SQL database server could be used, since it does not rely on any of MySQL-specific features). It has been tested under Apache HTTPD and Microsoft IIS web servers, and should work with any web server supporting PHP (at least through CGI). Main features of BBmSAM system are:

- Use of unaltered client and sensor components of EGEE SAM system.
- Synchronization with central HGSM service.
- Use of free and open source technologies.

BBmSAM client and sensors are the same as ones used in the standard EGEE SAM distribution, and they operate in identical way. In designing BBmSAM portal and dependent web services, special care was taken so that the solution would be compatible with EGEE/EGI tools and practices. This was achieved by implementing the same web services in PHP/MySQL implementation as

Fig. 7 Overview of availability of Grid services within the SEE-GRID-SCI infrastructure per quarter in the second (final) year of the project (May 2009 to April 2010)



the ones used in the original Java/Oracle-based SAM.

Main part of the BBmSAM web front-end, shown in Fig. 8, is a summary of current results for all tested Grid sites, containing site names, countries and other relevant details for each service.

6.2 SEE-GRID Accounting Portal

Accounting Portal [51] is a web-service based utility to collect and statistically present information

on the CPU accounting data for the SEE-GRID computing resources. Its main purpose is to collect and manage accounting data for the sites in SEE-GRID infrastructure. Recently a new publisher was released, capable of collecting and processing data for parallel MPI jobs, which are not properly accounted for when using the standard publisher provided by gLite. The accounting processing structure is based on two services: MPI log parser and accounting publisher. The MPI log parser tool processes PBS Server logs and inserts the data on MPI jobs in the MPI accounting database on the

SITE	COUNTRY	TIER	STATUS	TYPE	SERVICE STATUS
AEGIS01-IPB-SCL	Serbia	1	Certified	Production	CE: ce64 - ok 2.0 d SE: se - ok 15.2 d SRM: se - ok 1.0 d LFC: lfc - ok 3.1 d SRMv2: se - ok 3.0 d LFC_C: lfc - ok 3.0 d LFC_L: lfc - ok 3.0 d MPI: ce64 - ok 31+
AEGIS02-RCUB	Serbia	2	Certified	Production	CE: grid01 - ok 1.3 d SE: grid15 - ok 6.6 d SRM: grid15 - ok 12.3 h LFC: grid02 - ok 3.1 d LFC_C: grid02 - ok 3.0 d MPI: grid01 - ok 30.5 d
AEGIS03-ELEF-LEDA	Serbia	1	Certified	Production	CE: grid01 - ok 2.0 d SE: grid02 - ok 15.2 d SRM: grid02 - ok 1.0 d SRMv2: grid02 - ok 3.0 d MPI: grid01 - ok 31+
AEGIS04-KG	Serbia	1	Certified	Production	CE: cluster1 - ok 2.0 d SE: se - ok 2.3 d SRM: se - ok 2.3 d MPI: cluster1 - ok 31+
AEGIS05-ETFBG	Serbia	2	Certified	Production	CE: grid-ce - ok 2.0 d SE: grid-ce - ok 3.0 d
AEGIS06-AOB	Serbia	2	Uncertified	Production	
AEGIS08-IPB-DEMO	Serbia	2	Uncertified	Candidate	CE: ce-demo - ok 2.0 d SE: se-demo - ok 5.2 d SRM: se-demo - ok 5.2 d SRMv2: se-demo - ok 3.0 d MPI: ce-demo - ok 31+
AEGIS09-FTN-KM	Serbia	2	Uncertified	Production	
AEGIS11-MISANU	Serbia	2	Uncertified	Candidate	CE: ce - ok 2.0 d MPI: ce - ok 31+

Fig. 8 Overview of the SEE-GRID BBmSAM web portal

MON node. Afterwards, the accounting publisher aggregates the data from the standard accounting database and MPI database and sends it to the central accounting portal database. The publisher is based on an independent module architecture which allow the two modules (MPI and standard serial) to work independently, so that sites that do not support MPI can use the same publisher.

New web front-end interface of the accounting portal (Fig. 9) is created to dynamically generates account statistics and charts. It is written in Adobe Flex and Java and implements the MVC design pattern. The View module of the portal is written in Flex, offering an interactive environment with dynamic visualization of the accounting data managed in tables, bar and pie charts. The Interface module is a Java web service which accepts input parameters such as data type, job type, period, rows and columns for the tables. In addition, it is capable of filtering the data by VO, country and site, offering more flexible data organization. It can also generate SQL queries based on the pro-

vided parameters and extract required data from the accounting database. The data are returned in XML form, suitable for import to a variety of other applications. The web portal is hosted on a web server running under Apache Tomcat with installed Apache Axis web-service framework.

6.3 WatG Browser

The What is at the Grid—WatG Browser [52] is a web-based Grid Information System (GIS) visualization application providing detailed overview of the status and availability of various Grid resources in a given gLite-based e-Infrastructure. It is able to query and present data obtained from Grid information systems at different layers: from local resource information system for a particular Grid service (GRIS), to the Grid site information system (site BDII), and to the top-level information system for the whole Grid infrastructure (top-level BDII).

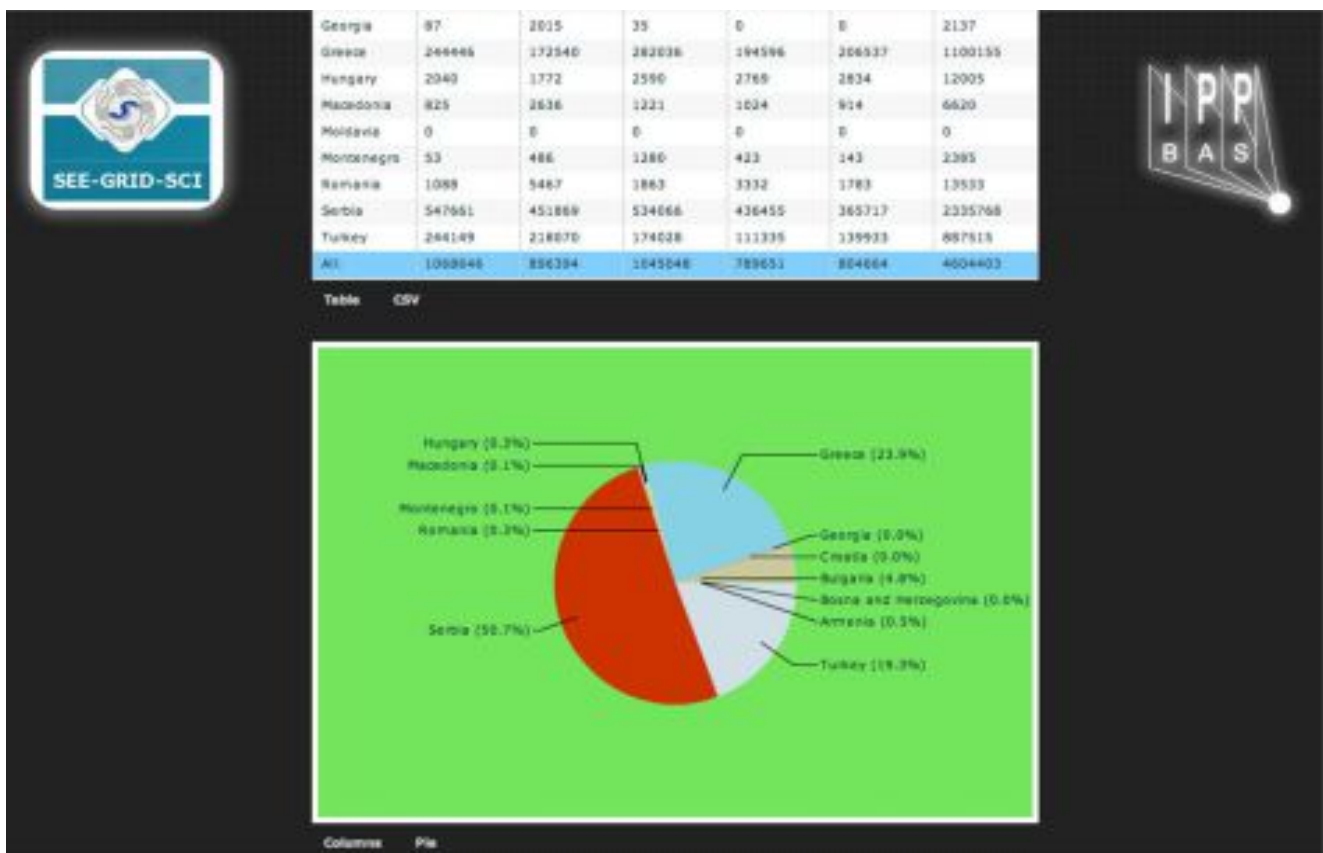


Fig. 9 Overview of the SEE-GRID accounting portal

The efficient implementation of WatG Browser allows quick and easy navigation through entries and objects of the LDAP tree retrieved by the specified query, even if the size of the output is huge and hierarchically very complex. Highly responsibility is achieved with implementation of partial refreshes and asynchronization of a web page. A partial refresh of WatG application can be observed when an interaction event is triggered, for example click on the plus icon of the LDAP tree. The server processes the information and returns a limited response specific to the data it receives, for example LDAP's subtree that requires given condition. One may notice that WatG server does not send back an entire page, like the conventional “click, wait and refresh” web applications. Instead, WatG client updates the page based on the response. This means that only part of the page is updated. In other words, WatG's initial page (Fig. 10) is treated like a template: WatG server and client exchange the data and the client updates parts of the template based on the data it receives from the server. Another way to

think about it is to consider WatG application as driven by events and data, whereas conventional web applications are driven by pages. Asynchronization of the WatG application is reflected in the fact that after sending data to the server, the client can continue processing while the server does its processing in the background. During all this, a user can continue interacting with the client without noticing interruption or a lag in the response. For example, a user can click on any plus or minus icon even during the loading, and in that way a new request will be created and executed afterwards. The client does not have to wait for a response from the server before continuing, as is the case in the traditional, synchronous approach. The WatG Browser is deployed by SCL [53] and publicly available at the address given in [52].

6.4 WMS Monitoring Tool

The complex task of computing resources discovery and management on behalf of user applications in the gLite Grid environment is done by the



Fig. 10 Overview of WatG Browser

Workload Management System (WMS) service. WMS monitoring tool WMSMon [54] provides reliable, site-independent, centralized, and uniform monitoring of gLite WMS services.

WMSMon tool, developed and deployed by SCL [53], is based on the collector-agent architecture that ensures monitoring of all properties relevant for successful operation of gLite WMS service and triggering of the alarms if certain monitored parameter values exceed predefined limits. In addition, the tool provides links to the appropriate troubleshooting guides when problems are identified.

WMSMon tool consists of two parts of software. The first one, WMSMon Agent, should be installed on all monitored WMS services, and locally aggregates the values of all relevant parameters described in the previous section. The second component of WMSMon software is WMSMon Collector, installed on a specific ma-

chine equipped with the web server and gridFTP client, with the aim to collect the data from all WMSMon Agents and to provide web interface to the graphical presentation of the collected data.

WMSMon web portal presents information from diverse WMS sources in a unified way, as can be seen in Fig. 11. The main page provides the aggregated status view of all monitored WMS services from the target Grid infrastructure. This part of the portal presents the data in a simplified way, with the emphasis on WMS services identified not to work properly. The portal also provides links to pages with detailed information and graphs for each monitored WMS service. These pages contain the latest data, as well as historical data presented in the graphical form.

In addition to the main WMSMon instance deployed by SCL [53], other instances of WMSMon are installed and used at Grid Operations Centre at CERN [55] and at NIKHEF [56].

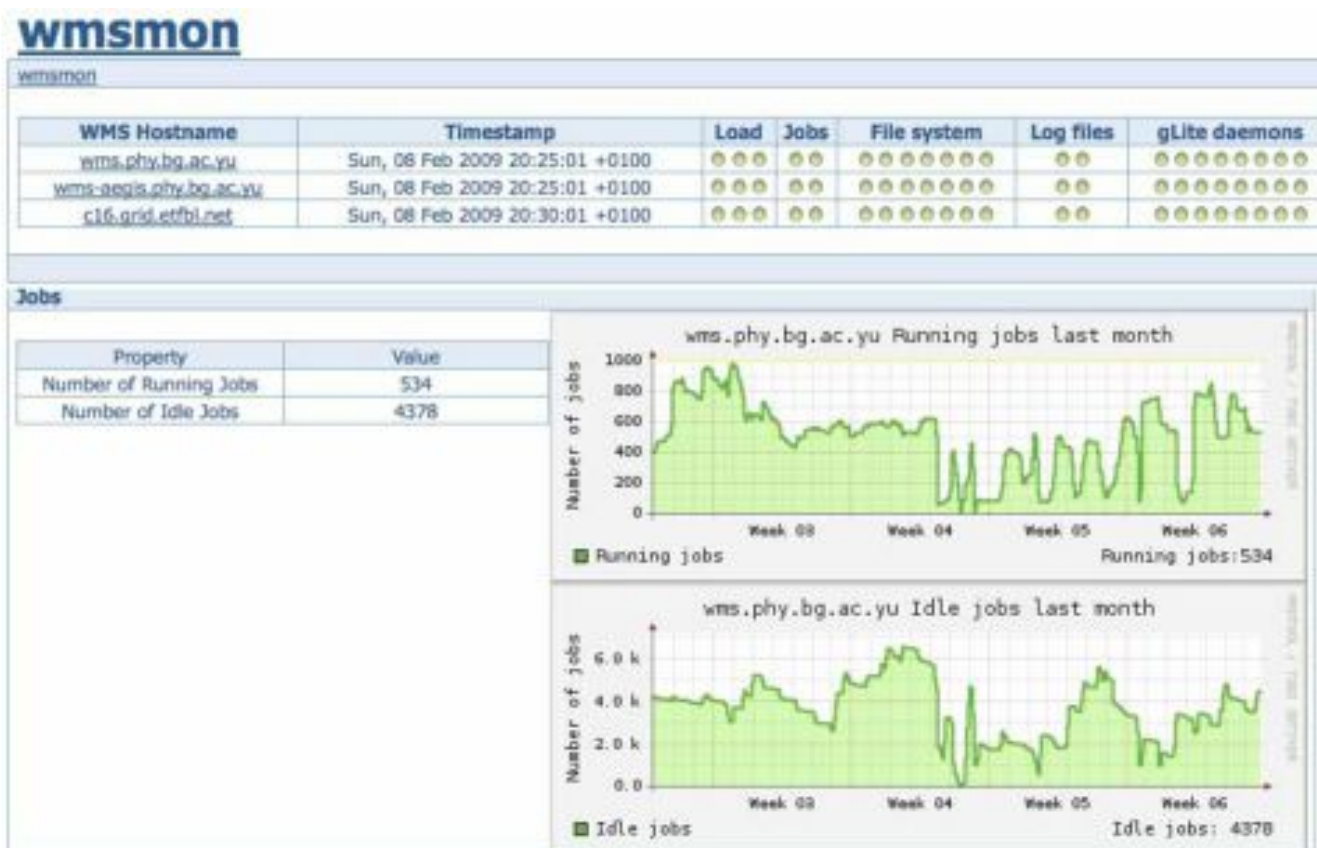


Fig. 11 Overview of WMSMon Portal

7 SEE Involvement in High Performance Computing

The Grid developments in the region, described in this paper, are currently being complemented with supercomputing/High-Performance Computing (HPC) actions. The HP-SEE project [57] (High-Performance Computing Infrastructure for South East Europe's Research Communities) is currently work across several strategic lines of action. First, it is linking the existing HPC facilities in the region into a common infrastructure, and providing operational and management solutions for it. Second, it is striving to open this infrastructure to a wide range of new user communities, including those of non-resourced countries, fostering collaboration and providing advanced capabilities to more researchers, with an emphasis on strategic groups in computational physics, computational chemistry and life sciences. Finally, it acts as a catalyst for establishment of national HPC initiatives, and will act as a SEE bridge for DEISA [58], also presented in this edition, as well as PRACE [59] infrastructure.

Figure 12 depicts the multi-dimensional regional e-Infrastructure in South-East Europe, where HP-SEE effectively adds the new Research Infrastructure: HPC infrastructure and knowledge/user layer, on top of the existing network plane, and parallel to the existing Grid plane, thus

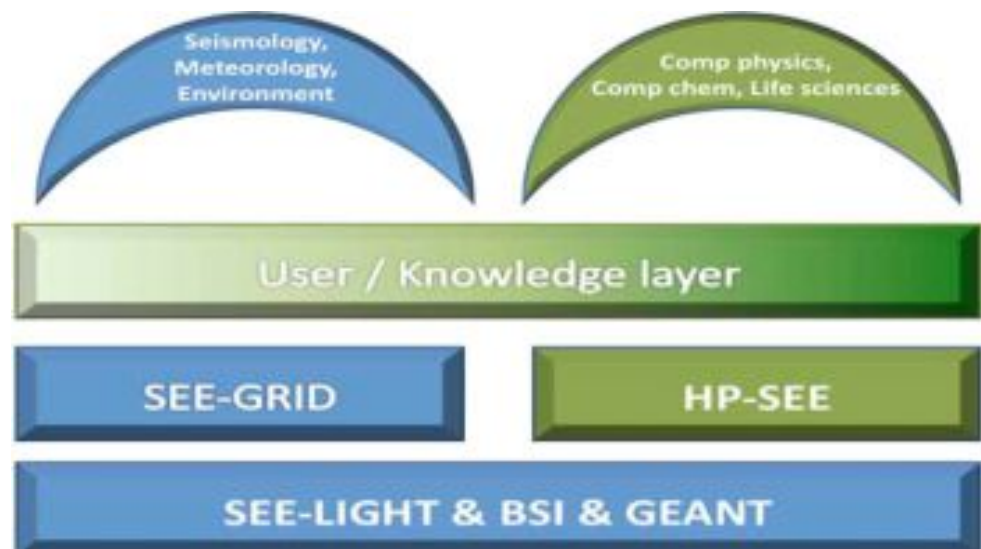
Table 4 Current and planned computing power (TFlops) by HP-SEE countries (double precision for CPU and single precision for GPU)

Country	2010	2011	2012
Greece	0	40	80
Serbia	0	20	40
Bulgaria	25	30+8 GPU	40+20 GPU
Romania	10	20+100 GPU	30+100 GPU
Hungary	1	30	60
Overall	36	140+108 GPU	250+120 GPU

optimising all layers and further enabling a wide range of new cross-border e-Science applications to be deployed over the regional e-Infrastructure. This approach effectively creates an integrated e-Infrastructure for new virtual research communities, and provides a platform for collaboration between ICT engineers and computational scientists dealing with the infrastructure on one hand, and on the other the scientists from diverse scientific communities in the region.

It should be noted that this vision will provide an integrated infrastructure, where Grid and HPC layers and not mutually exclusive but rather complementary, and tailored for the type of applications supported. Table 4 gives the overview of the current and planned HPC resources that will be available to the HP-SEE Virtual Research Communities within the project.

Fig. 12 SEE e-Infrastructure with HPC, and new user communities



The available resources will be integrated into a common infrastructure available for the regional Virtual Research Communities. The current and planned HPC infrastructure is heterogeneous, comprising of BlueGene supercomputers, Intel/AMD clusters and enhanced with GPU computing accelerators. Concerning the middleware deployments, we believe the upcoming Unified Middleware Distribution, which will combine Unicore, gLite and ARC will be well suited for the regional HPC infrastructure, taking into account the current situation, where various combinations of these middleware stacks with batch systems and workflow management systems exist. The regional HP-SEE infrastructure will be operated through the operations centre that will be established within the project, which will carry out analysis, requirements capture and evaluation, and deployment of the existing solutions for system management of the regional infrastructure; will identify missing components, and provide optimal solutions. Solutions by system vendors and successful developments from European projects, especially DEISA, and PRACE, will be taken into account. Wherever possible the existing solutions will be adapted and enhanced for deployment in the regional infrastructure. A set of operational tools will be deployed, including user administration, accounting, distributed data management, security, authentication and authorization, monitoring of distributed resources, resource management and allocation, and helpdesk for user support.

The identified target user communities include computational physics, computational chemistry and life sciences. Computational physics is represented by 8 applications from 6 countries and covers the fields of many-body condensed matter physics, including modeling of electron transport, modeling of complex gas dynamics and convection, plasma physics and image processing. Computational chemistry community includes 7 applications from 6 countries, covering the fields of molecular dynamics and simulations, and materials science. Life sciences community has 7 applications from 5 countries, covering the fields of computational biology, computational genomics, computational biophysics and DNA sequencing.

8 Transition to EGI and Conclusions

Over the period of six years and three phases, the SEE-GRID programme aimed at creating independent and sustainable NGIs in each country of the South-Eastern Europe. That has allowed all the countries to participate as full-fledged members of the wider European Grid infrastructure realized through the series of EGEE projects and currently by the European Grid Initiative, EGI [4]. EGI is established as a coordinating organization for the European Grid Infrastructure, based on the federation of individual NGIs, aiming to support a wide variety of multi-disciplinary user communities. To facilitate the above aim, the SEE-GRID programme has focused both at stimulating the support to policy makers as well as for creating sustainable operational structures in each of the countries in the region.

In particular, on the policy level, the last two years of the SEE-GRID programme have focused on monitoring and improving the status of NGIs in partner countries, and providing support for their evolution and integration into the environment standardized by EGI, aiming to achieve sustainability as active partners in this new pan-European collaboration model. This effort resulted in one of main successes of the project, with all countries of the region currently members or associate members of EGI and participating as partners in the EGI-InSPIRE project.

On the operational level, the focus of SEE-GRID was to create and increase the capacity of Grid resources in the region, create independent and stable operational structures, increase the availability of Grid resources, deploy core services in all countries of the region, as well as to develop geographically distributed network of Grid experts able to provide operational and application level support to end users. At the end of the 6th year of the SEE-GRID programme, all SEE countries are providing such an operational infrastructure for the local and international user communities from the pan-European EGI infrastructure, either as independent NGIs or as a part of the South-Eastern Europe Regional Operations Centre.

We describe below the procedure taken by most of the countries in the region in order to

become fully independent operational NGIs from the technical point of view. The new NGIs use EGIs Grid Operations Database, GOCDB [60] to register their NGI management structure, sites and operational personnel. Most of the SEE NGIs base their operational portal on the central portal that is provided by EGI, performing operations via the NGI view that it offers. In cases like the Greek NGI, a standalone operational portal has been setup. During the course of the SEE-GRID projects the regional Helpdesk was based on OneOrZero as it has also been discussed in Section 4. The SEE-GRID Helpdesk by the end of the SEE-GRID projects was fully integrated with GGUS and therefore it is a candidate system for NGIs, to use as their national Helpdesk solution integrated with the Global Grid User Support, GGUS [61]. Further to that Request Tracker, RT [62] has been integrated with GGUS and can offer the same functionality. Based on the above the NGIs of the regional can select which helpdesk solution to use (either directly GGUS, OneOrZero, or RT). Since infrastructure monitoring in EGI has moved from SAM to Nagios, all new NGIs install and operate their own instance of Nagios that integrates with the rest of EGIs monitoring systems. Finally, SEE NGIs use the Unified Middleware Distribution (UMD) as a central repository for installing basic middleware components while still use the regional repository or even some national repositories, for software packages that are tailored to specific needs of their countries and are not available in UMD.

Towards the end of the SEE-GRID-SCI project (May 2010) all NGIs of the project where migrated to EGEE/EGI via the SEE-ROC, utilizing the existing ROC infrastructure and services. Since May 2010 and up to now (January 2011) almost all the NGIs have migrated to the EGI operational model. The average time for an NGI to migrate its operational structure from SEE-ROC to EGI is between 1 and 3 months.

The SEE-GRID programme had pivotal role in bridging the digital divide in the SEE region, in spearheading regional research collaborations, and in creating a strong human network in ICT field paving the way towards full integration of the region into the European Research Area (ERA). This work continues with the HP-SEE project

[57], that aims at bringing together the national HPC infrastructures in the region of South Eastern Europe and the regional Virtual Research Communities of Computational Physics, Computational Chemistry and Life Sciences. Enabling of those user communities to get access to HPC resources for their scientific work is the prime goal of this new project, and demonstrates the success of SEE-GRID series of projects in involving scientists from the region in the development and production use of distributed research infrastructures.

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Article

Faraday and Resonant Waves in Dipolar Cigar-Shaped Bose-Einstein Condensates

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Abstract: Faraday and resonant density waves emerge in Bose-Einstein condensates as a result of harmonic driving of the system. They represent nonlinear excitations and are generated due to the interaction-induced coupling of collective oscillation modes and the existence of parametric resonances. Using a mean-field variational and a full numerical approach, we studied density waves in dipolar condensates at zero temperature, where breaking of the symmetry due to anisotropy of the dipole-dipole interaction (DDI) plays an important role. We derived variational equations of motion for the dynamics of a driven dipolar system and identify the most unstable modes that correspond to the Faraday and resonant waves. Based on this, we derived the analytical expressions for spatial periods of both types of density waves as functions of the contact and the DDI strength. We compared the obtained variational results with the results of extensive numerical simulations that solve the dipolar Gross-Pitaevskii equation in 3D, and found a very good agreement.

Keywords: Bose-Einstein condensate; pattern formation; dipole-dipole interaction; parametric resonance; interaction effects

1. Introduction

After pioneering experiments that realized Bose-Einstein condensates (BEC) in systems with weak contact interactions, it took a decade of work on improvements of experimental techniques to enable measurement of effects of the dipole-dipole interaction (DDI) that exist between atoms or molecules with a permanent or induced electrical or magnetic dipole moment. The very first such experiment was realized in 2005 with chromium atoms ^{52}Cr [1], followed by the experiments with atoms with much larger magnetic moments, such as dysprosium ^{164}Dy [2] and erbium ^{168}Er [3]. Furthermore, the dipolar BECs comprised of polar molecules with much stronger electrical [4] and magnetic [5] dipole moments were also realized. While the contact interaction is symmetric and has a short-range, the DDI between atoms or molecules is anisotropic and long-range. These features are responsible for a whole series of new phenomena that appear in ultracold dipolar gases [6]. If we take into account that the strength of the contact interactions can be varied over many orders of magnitude using the Feshbach resonance [7] technique, and that the DDI strength can be also tuned using a fast rotating magnetic or electric field [8,9], it is easy to see that such a versatility of dipolar quantum gases is unparalleled and makes them an obligatory element in a toolbox for engineering quantum devices and sensors.

Bose-Einstein condensates are usually termed quantum fluids, which encompasses a broader range of physical systems where quantum effects are either dominant or very much pronounced. Despite their name, some of quantum fluids do not share the trademark property of classical fluids, incompressibility. In fact, the BECs are made of rarefied gases, but their fluid-like behavior stems from the quantum coherence of such systems. Therefore, while in classical fluids density modulations can

be excited only under extreme conditions, in quantum fluids the density waves represent one of the natural collective excitations. They appear due to nonlinearity in ultracold quantum gases, and can be induced by a harmonic modulation of the trap frequencies or interaction strengths. However, the motivation for study of such excitations comes from the classical phenomenon of Faraday waves, which may appear on the surface of the shallow layer of liquid under certain conditions. Namely, if the container with the liquid is harmonically oscillated in a vertical direction, the wave patterns may emerge, depending on the ratio of the liquid depth and the container size, as well as depending on the modulation frequency. This phenomenon was first studied and described by Michael Faraday at the beginning of 19th century [10]. The interest for this type of excitations arose again during the 1980s, as a consequence of the study of nonlinear liquids. In the context of ultracold gases, Faraday waves were first investigated theoretically in 2002 by Staliunas [11]. After these theoretical and numerical results for the systems with contact interaction, where it was assumed that the interaction strength is harmonically modulated, the Faraday waves were first measured in BEC experiments with ^{87}Rb in 2007 by Engels [12], and more recently with ^7Li by Hulet and Bagnato [13,14]. In the first experiment, the radial part of the harmonic trap was modulated, while the other two experiments have modulated the contact interaction strength. However, qualitatively, this leads to the same type of density waves.

Parametric driving of system parameters can lead to pattern formation not only in BECs, where Faraday waves are experimentally observed in cigar-shaped condensates [12–14], but also in helium cells [15]. The actual experimental observation of this phenomenon in 2007 was preceded by numerical studies starting in 2002 [11,16–20], all focusing on systems with short-range, contact interactions. More recently, Faraday waves have been studied in dipolar [21–23] and two-component condensates, including the systems with spatially-dependent contact interaction [24,25]. Numerical studies of Faraday waves have also been extended to mixtures of Bose and Fermi gases [26], as well as Fermi gases exhibiting superfluid behavior [27,28].

Faraday waves in ultracold gases are a consequence of the existence of parametric resonances in the system. While the spatial period of these waves depends on the geometry of the system and other parameters, the frequency of their oscillations is constant and is two times smaller than the modulation frequency. This is a characteristic of all parametric resonant phenomena, and in the variational approach leads to the Mathieu's differential equation [29], which gives the observed ratio of the frequency of Faraday waves and the modulation. The Faraday density waves with half of the modulation frequency are not the only nonlinear excitation of the system. In a driven system, there are always excitations with the same frequency as the modulation. However, they become resonant when the modulation frequency corresponds to one of the collective modes or the trap frequencies, or their linear combination. The resonant waves develop in the system and grow exponentially [30], faster than the Faraday waves. Therefore, these two phenomena can be easily distinguished, not only by comparing their frequencies, but also the corresponding onset times. We note that resonant behavior can appear not only due to the modulation of the interaction strength or the trapping potential, but also due to its spatial modulation [31–40].

In the context of dipolar BECs, the study of Faraday waves was limited mostly to their excitation spectrum in one-dimensional and two-dimensional systems [21], while the properties of resonant waves, to the best of our knowledge, have not been studied yet. In Section 2, we develop a mean-field variational approach for the dynamics of a driven dipolar BEC at zero temperature and identify the instability of the system leading to the emergence of Faraday and resonant waves. Using this approach, we derive analytic expressions for the dependence of density wave properties on the strength of the contact and the dipole-dipole interaction. In Section 3, we numerically study how such waves develop and can be characterized in ultracold systems of three experimentally relevant magnetic dipolar species: chromium ^{52}Cr , erbium ^{168}Er , and dysprosium ^{164}Dy . In Section 4, the analytically obtained expressions for the spatial period of Faraday are compared to results of the extensive numerical simulations, which solve the full three-dimensional mean-field equations for a dipolar BEC. The emergence of resonant

waves and comparison of the corresponding analytical and numerical results is given in Section 5. Finally, Section 6 summarizes our conclusions and presents outlook for future research.

2. Variational Approach

We consider the system in an experimentally-inspired setup, where the condensate is confined into a cigar-shaped harmonic trap, with the equilibrium frequencies $\omega_x = 2\pi \times 7$ Hz, $\omega_y = \omega_z = \Omega_0 = 2\pi \times 160.5$ Hz. These are typical values taken from Reference [12]. The dipole moments of the atoms are assumed to be oriented along z direction, i.e., orthogonal to the weak-confinement axis x (which we refer to as the longitudinal axis), since this maximizes the stability of the system. To ensure stability of the system, we consider the condensate to have $N = 10^4$ atoms for all three species. The driving of the system is achieved by harmonic modulation of the radial ($y - z$) part of the trap,

$$\omega_y(t) = \omega_z(t) = \Omega_0 (1 + \epsilon \sin \omega_m t), \quad (1)$$

where $\epsilon = 0.1 - 0.2$ is the modulation amplitude and ω_m is the modulation frequency.

For a variational study of Faraday and resonant waves in dipolar condensates, we use a modification of the Gaussian ansatz [16–20,23–25,30,41,42] to capture the induced density waves in the longitudinal, weak-confinement direction x ,

$$\psi(x, y, z, t) = A e^{-\frac{x^2}{2u_x^2} - \frac{y^2}{2u_y^2} - \frac{z^2}{2u_z^2} + ix^2\phi_x + iy^2\phi_y + iz^2\phi_z} [1 + (\alpha + i\beta) \cos kx], \quad (2)$$

where the normalization of the wave function to unity is ensured by the prefactor

$$A \equiv A(u_x, u_y, u_z, \alpha, \beta, k) = \frac{1}{\pi^{3/4} \sqrt{u_x u_y u_z}} \frac{\sqrt{2}}{\sqrt{2 + \alpha^2 + \beta^2 + 4\alpha e^{-k^2 u_x^2/4} + (\alpha^2 + \beta^2) e^{-k^2 u_x^2}}}. \quad (3)$$

The above variational ansatz involves eight variational parameters $\{u_i, \phi_i, \alpha, \beta\}$, which are functions of time. The parameters u_i represent the condensate widths, while ϕ_i are the conjugated phases, which are necessary to properly describe the system's dynamics. Note that these phases can be omitted when we are interested only in the ground state. The multiplicative factor $1 + (\alpha + i\beta) \cos kx$ describes the density modulation along x direction, and the variational parameters α and β represent the real and the imaginary part of the amplitude of the wave. The wave vector k , which is related to the spatial period ℓ of the density waves by $\ell = 2\pi/k$, is not treated here as a variational parameter. We determine its value from the condition for the instability emergence, which leads to Faraday or resonant waves.

The use of the Gaussian variational ansatz corresponds to the weak interaction regime with low density of atoms, while the Thomas-Fermi profile is more appropriate for systems with high particle density. Although the emergence of Faraday and resonant waves leads to higher particle densities, we still use the Gaussian ansatz in all regimes. This is done since we are mostly interested just in the onset of longitudinal density modulations, but also for mathematical convenience. Let us note that tunability of all variational parameters may improve the accuracy of the applied approximation. Nevertheless, the use of this ansatz can be fully justified only a posteriori, by comparison with numerical results [16].

Note that we use the dimensionless units, where a chosen referent frequency ω_r defines the length scale through the harmonic oscillator length $\sqrt{\hbar/(m\omega_r)}$, where m is the mass of the corresponding atomic species, the time scale as $1/\omega_r$, and the energy scale as $\hbar\omega_r$. The trapping frequencies are also expressed in units of ω_r through the trap aspect ratios $\gamma = \omega_x/\omega_r$, $\nu = \omega_y/\omega_r$, and $\lambda = \omega_z/\omega_r$, as well as the modulation frequency $\eta_m = \omega_m/\omega_r$. We choose below the value $\omega_r = \Omega_0$, corresponding to $\nu = \lambda = 1$, but for now we keep all three aspect ratios as free parameters, for generality.

If we insert the modified Gaussian ansatz (Equation (2)) into the Lagrangian density that yields the dipolar Gross-Pitaevskii equation, we can express the Lagrangian of the system as a sum of five terms. The first term reads

$$L_1(t) = \frac{i}{2} \int d\mathbf{r} (\psi^* \dot{\psi} - \psi \dot{\psi}^*) = -\frac{1}{2} \left(u_x^2 \dot{\phi}_x + u_y^2 \dot{\phi}_y + u_z^2 \dot{\phi}_z \right) - \frac{\alpha \dot{\beta} - \beta \dot{\alpha}}{2 + \alpha^2 + \beta^2}, \quad (4)$$

while the kinetic and the potential energy terms yield, respectively,

$$L_2(t) = \frac{1}{2} \int d\mathbf{r} \psi^* \Delta \psi = -\frac{1}{4} \left(\frac{1}{u_x^2} + \frac{1}{u_y^2} + \frac{1}{u_z^2} + 4u_x^2 \phi_x^2 + 4u_y^2 \phi_y^2 + 4u_z^2 \phi_z^2 \right) - \frac{(\alpha^2 + \beta^2) k^2}{2(2 + \alpha^2 + \beta^2)}, \quad (5)$$

$$L_3(t) = - \int d\mathbf{r} \left(\frac{1}{2} \gamma^2 x^2 + \frac{1}{2} v^2 y^2 + \frac{1}{2} \lambda^2 z^2 \right) |\psi|^2 = -\frac{1}{4} \left(\gamma^2 u_x^2 + v^2 u_y^2 + \lambda^2 u_z^2 \right). \quad (6)$$

The contact interaction term corresponds to

$$L_4(t) = -2\pi N a_s \int d\mathbf{r} |\psi|^4 = -\frac{N a_s}{\sqrt{2\pi} u_x u_y u_z} \left(1 + \frac{\alpha^4 + 16\alpha^2 + 2\alpha^2 \beta^2 + \beta^4}{2(2 + \alpha^2 + \beta^2)^2} \right), \quad (7)$$

where a_s is the s -wave scattering length of atoms, expressed in units of the harmonic oscillator length. The Lagrangian term that corresponds to the DDI energy is given by

$$L_5(t) = -\frac{3N a_{\text{dd}}}{2} \int d\mathbf{r} d\mathbf{r}' \psi^*(\mathbf{r}) \psi^*(\mathbf{r}') U_{\text{dd}}(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}), \quad (8)$$

where the dipolar potential reads $U_{\text{dd}}(\mathbf{r}) = (1 - 3 \cos^2 \theta)/r^3$, θ is the angle between the dipoles' orientation (z axis) and vector \mathbf{r} , and a_{dd} is the DDI interaction strength, that depends on the dipole moment of atoms d and their mass m as $a_{\text{dd}} = \mu_0 m d^2 / (12\pi \hbar^2)$. Note that it is conveniently expressed in units of length and cast into a dimensionless quantity as outlined above. However, due to the spatial modulation term in the modified Gaussian ansatz, it is not possible to perform exact integration and obtain $L_5(t)$. Using the convolution theorem, the DDI term can be written as

$$L_5(t) = -\frac{3N a_{\text{dd}}}{2(2\pi)^3} \int d\mathbf{k} \mathcal{F}[U_{\text{dd}}](\mathbf{k}) \mathcal{F}[|\psi|^2]^2(\mathbf{k}), \quad (9)$$

where \mathcal{F} stands for the Fourier transform, and

$$\mathcal{F}[|\psi|^2](\mathbf{k}) = B(k_x, u_x, \alpha, \beta, k) e^{-\frac{1}{4}(k_x^2 u_x^2 + k_y^2 u_y^2 + k_z^2 u_z^2)}. \quad (10)$$

The coefficient B can be explicitly calculated and reads

$$B(k_x, u_x, \alpha, \beta, k) = \frac{4 + 4(e^{-\frac{k}{4}(k-2k_x)u_x^2} + e^{-\frac{k}{4}(k+2k_x)u_x^2})\alpha + (2 + e^{-k(k-k_x)u_x^2} + e^{-k(k+k_x)u_x^2})(\alpha^2 + \beta^2)}{2 \left[2 + 4e^{-\frac{1}{4}k^2 u_x^2} \alpha + (1 + e^{-k^2 u_x^2})(\alpha^2 + \beta^2) \right]}. \quad (11)$$

To proceed further, we take into account that the condensate width in the weak confinement direction is large compared to the other widths, as well as compared to the spatial period of the density waves, such that $ku_x \gg 1$. We also take into account that the wave amplitude is small immediately after the waves emerge, such that $\alpha, \beta \ll 1$. Since the integral over \mathbf{k} in Equation (9) cannot be analytically performed even using these approximations, we replace B^2 , stemming from the square of the Fourier transform $\mathcal{F}[|\psi|^2]$, by its average over k_x , and neglect all terms proportional to $e^{-k^2 u_x^2/8}$ and its powers, as already argued that ku_x is a large quantity. The integration over \mathbf{k} can now proceed smoothly, yielding

$$L_5(t) = \frac{Na_{\text{dd}}}{\sqrt{2\pi} u_x u_y u_z} f\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) \left(1 - \frac{8\alpha^2}{(2 + \alpha^2 + \beta^2)^2}\right), \quad (12)$$

where f is the standard dipolar anisotropy function [43].

Now that we have the explicit expression for the Lagrangian of the system $L(t) = \sum_{i=1}^5 L_i(t)$, we can derive the corresponding Euler-Lagrange equations. We assume that the wave amplitudes α and β are small, such that their quadratic and higher order terms can be neglected in the equations of motion. The three equations for the phases yield $\phi_i = \dot{u}_i / (2u_i)$ and can be used to eliminate the phases ϕ_i from the corresponding set of equations for the condensate widths u_i , which have the form of the second order differential equations,

$$\ddot{u}_x + \gamma^2 u_x - \frac{1}{u_x^3} - \sqrt{\frac{2}{\pi}} \frac{N}{u_x^2 u_y u_z} \left[a_s - a_{\text{dd}} f\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) + a_{\text{dd}} \frac{u_x}{u_z} f_1\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) \right] = 0, \quad (13)$$

$$\ddot{u}_y + \nu^2 u_y - \frac{1}{u_y^3} - \sqrt{\frac{2}{\pi}} \frac{N}{u_x u_y^2 u_z} \left[a_s - a_{\text{dd}} f\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) + a_{\text{dd}} \frac{u_y}{u_z} f_2\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) \right] = 0, \quad (14)$$

$$\ddot{u}_z + \lambda^2 u_z - \frac{1}{u_z^3} - \sqrt{\frac{2}{\pi}} \frac{N}{u_x u_y u_z^2} \left[a_s - a_{\text{dd}} f\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) - a_{\text{dd}} \frac{u_x}{u_z} f_1\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) - a_{\text{dd}} \frac{u_y}{u_z} f_2\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) \right] = 0, \quad (15)$$

where f_1 and f_2 are partial derivatives of the anisotropy function with respect to the first and the second argument. The Euler-Lagrange equation for the variational parameter β yields $\beta = 2\alpha/k^2$, which we use to eliminate β from the corresponding equation for the parameter α , as was done with the phases. With this, the equation for α turns out to be the second order differential equation,

$$\ddot{\alpha} + \left[\frac{k^4}{4} + \sqrt{\frac{2}{\pi}} \frac{N}{u_x u_y u_z} \left(a_s + a_{\text{dd}} f\left(\frac{u_x}{u_z}, \frac{u_y}{u_z}\right) \right) k^2 \right] \alpha = 0. \quad (16)$$

In the context of variational analysis of Faraday and resonant waves, the above equation of motion for the wave amplitude α is usually cast into the form of the Mathieu-like equation [29]

$$\ddot{\alpha} + [a(k) + \epsilon b(k) \sin 2\tau] \alpha = 0. \quad (17)$$

This equation can be solved perturbatively in the small modulation amplitude ϵ . Assuming a solution in the form of a harmonic oscillator

$$\alpha(\tau, \epsilon) = P(\epsilon\tau) \cos\left(\tau\sqrt{a(k)}\right) + Q(\epsilon\tau) \sin\left(\tau\sqrt{a(k)}\right), \quad (18)$$

we obtain that functions P and Q are exponentials of the form $e^{\pm i\zeta\epsilon\tau}$, where ζ is a complex number. The existence of the imaginary part of ζ leads to the instability, i.e., to the exponential growth of the wave amplitude, which yields Faraday or resonant waves. It was shown in Reference [29] that the nonvanishing imaginary part of ζ appears for $a(k) = n^2$, where $n \in \mathbb{N}$, and this represents the mathematical form of the instability condition.

To cast Equation (16) into the Mathieu-like form (Equation (17)), we need to take into account that the radial trap frequencies are modulated, such that the corresponding trap aspect ratio is given by $\nu(t) = \lambda(t) = \lambda_0(1 + \epsilon \sin \eta_m t)$, where $\lambda_0 = \Omega_0/\omega_r$. This generates the dynamics of the system and we need to obtain approximate expressions for the condensate widths in order to get explicit form of the quantities $a(k)$ and $b(k)$. We assume that the condensate width u_x slowly varies, and can be taken to be constant at the onset of instability. We also assume that second derivatives of the radial widths

u_y and u_z , with respect to time, can be neglected, since they are proportional to the small modulation amplitude ϵ . Furthermore, for simplicity, we assume $u_y \approx u_z \equiv u_\rho$, which now satisfies the modified Equation (14) or (15) in the form

$$\lambda^2(t)u_\rho^4 = 1 + \sqrt{\frac{2}{\pi}} \frac{N}{u_x} \left[a_s + \frac{a_{dd}}{2} f_s \left(\frac{u_\rho}{u_x} \right) - a_{dd} f'_s \left(\frac{u_\rho}{u_x} \right) \right], \tag{19}$$

where $f_s(x) = f(x, x)$. On the right-hand side of the above equation, we assume that the ratio u_ρ/u_x is constant and equal to the corresponding ratio for the ground state, which can be calculated from Equations (13)–(15). If we express u_ρ^2 from Equation (19), and use it to estimate the quantity $u_y u_z \approx u_\rho^2$ in Equation (16), we obtain the equation for the variational parameter α in the form

$$\ddot{\alpha} + \left[\frac{k^4}{4} + \frac{\Lambda k^2}{4} \lambda(t) \right] \alpha = 0, \tag{20}$$

where Λ is given by

$$\Lambda = \frac{4\sqrt{\frac{2}{\pi}} N \left[a_s - \frac{a_{dd}}{2} f_s \left(\frac{u_\rho}{u_x} \right) \right]}{u_x \left\{ 1 + \sqrt{\frac{2}{\pi}} \frac{N}{u_x} \left[a_s + \frac{a_{dd}}{2} f_s \left(\frac{u_\rho}{u_x} \right) - a_{dd} f'_s \left(\frac{u_\rho}{u_x} \right) \right] \right\}^{1/2}}. \tag{21}$$

After inserting the explicit form for $\lambda(t)$ into Equation (20), we still need to make a variable change $\eta_m t \rightarrow 2\tau$ in order to transform it into the Mathieu-like Equation (17). This finally yields the expressions for the coefficients $a(k)$ and $b(k)$,

$$a(k) = \frac{k^4}{\eta_m^2} + \frac{\lambda_0 \Lambda k^2}{\eta_m^2}, \quad b(k) = \frac{\lambda_0 \Lambda k^2}{\eta_m^2}. \tag{22}$$

As previously discussed, the instability condition for the Faraday waves reads $a(k) = 1$, which can be used to calculate the wave vector of density waves shortly after their emergence,

$$k_F = \sqrt{-\frac{\lambda_0 \Lambda}{2} + \sqrt{\frac{\lambda_0^2 \Lambda^2}{4} + \eta_m^2}}. \tag{23}$$

This represents our analytical result for the wave vector k_F and the spatial period $\ell_F = 2\pi/k_F$ of the Faraday waves, which can be directly compared with numerical or experimental results. Let us also stress that the above analysis is consistent with the main characteristic of the Faraday waves, namely, that their oscillation frequency is half that of the driving frequency. This can be concluded according to $\tau = \eta_m t/2$ and Equation (18), where we see that indeed the solution of the derived Mathieu-like equation oscillates with the frequency whose aspect ratio is $\eta_m/2$, i.e., with the frequency $\omega_m/2$.

If the modulation frequency is close to one of the characteristic oscillation modes of the system, it will exhibit resonant behavior, which is suppressed for an arbitrary value of the modulation frequency. While the system’s dynamics will certainly include the Faraday mode at the frequency $\omega_m/2$ even close to a resonance, the resonant mode with the frequency ω_m will have a larger amplitude and will develop much faster. Although it is clear that the above analysis would break down, the condition for the emergence of resonant waves still corresponds to $a(k) = 2^2$, i.e., the wave vector of the resonant wave is given by

$$k_R = \sqrt{-\frac{\lambda_0 \Lambda}{2} + \sqrt{\frac{\lambda_0^2 \Lambda^2}{4} + 4\eta_m^2}}. \tag{24}$$

In that case, according to $\tau = \eta_m t/2$ and Equation (18), the resonant density wave will oscillate with the frequency whose aspect ratio is $(\eta_m/2)\sqrt{2} = \eta_m$, i.e., with the frequency ω_m . Depending on the system's parameters, higher resonant modes can also appear corresponding to the conditions $a(k) = n^2$, where n is an integer, corresponding to the oscillation frequencies $n\omega_m/2$.

3. Faraday Waves in Chromium, Erbium, and Dysprosium Condensates

To study Faraday waves in dipolar condensates, we performed extensive numerical simulations of the real-time dynamics and solved the dipolar Gross-Pitaevskii equation using the programs described in References [44–52]. The parameters of these simulations match the physical parameters of BECs of chromium ^{52}Cr , erbium ^{168}Er , and dysprosium ^{164}Dy , which, respectively, have the dipole moments $d = 6\mu_B$, $d = 7\mu_B$, and $d = 10\mu_B$, where B is the Bohr magneton. The corresponding background s -wave scattering lengths are $a_s = 105a_0$, $a_s = 100a_0$, and $a_s = 100a_0$, where a_0 is the Bohr radius. We used these interaction strengths, unless otherwise specified.

As discussed previously, Faraday waves are expected as a main excitation mode of the system when the modulation frequency ω_m does not match any of the characteristic frequencies of the system. For this reason, we used the value $\omega_m = 200 \times 2\pi$ Hz, for which we verified that these conditions are satisfied. To characterize the density waves, we typically analyze their FFT spectra in the time-frequency and spatial-frequency domains. However, instead of directly analyzing their density profiles, for FFT, it is advantageous to have a clearer signal, which can be obtained by considering only the density variations compared to the initial state, i.e., the ground state of the system, before the modulation is switched on. Therefore, Figure 1 shows time dependence of the integrated density profile variations in the weak confinement direction $\delta n(x, t) = n(x, t) - n(x, t = 0)$. Here, $n(x, t)$ is the column density profile calculated by integrating the 3D condensate density $|\psi|^2$ over the radial coordinates y and z .

The emergence of spatial patterns is clearly visible for all three atomic species after around 150 ms. This is consistent with earlier experimental observations [12–14] and theoretical results [16,24,25]. The density waves in x direction from Figure 1 take time to develop and are a result of the transfer of energy from the modes that are directly excited in the radial directions, where the trap is modulated. On the other hand, the density waves in the radial directions (which are not shown here) emerge immediately after the modulation is switched on at $t = 0$, and their frequency is equal to the modulation frequency. By looking at Figure 1, we can even estimate the main oscillation frequency, e.g., counting the number of maxima or minima in a given time interval. For instance, in the last 50 ms in each of the panels in Figure 1, we count five periods, which corresponds to the frequency $100 \times 2\pi$ Hz = $\omega_m/2$. This is a distinguishing characteristic of Faraday waves, and therefore we can directly determine that in this case the system develops this type of collective oscillations.

However, this way we can determine only the main excitation modes. The dynamics of the system contains other modes as well, and over the time they can develop and even start to dominate the behavior of the system. Therefore, it is important to analyze the spectra in more detail. This is done in Figure 2 for all integrated density profile variations, separately for each spatial direction. For simplicity, the FFT analysis is performed for the profiles at the trap center. As expected, in the weak confinement direction (left column of Figure 2), the main excitation mode has a frequency $\omega_m/2$. In addition to this, we observe two other modes, at ω_m and $3\omega_m/2$. This is expected from the theoretical analysis in Section 2, but could not be discerned directly from the density profiles or their variations.

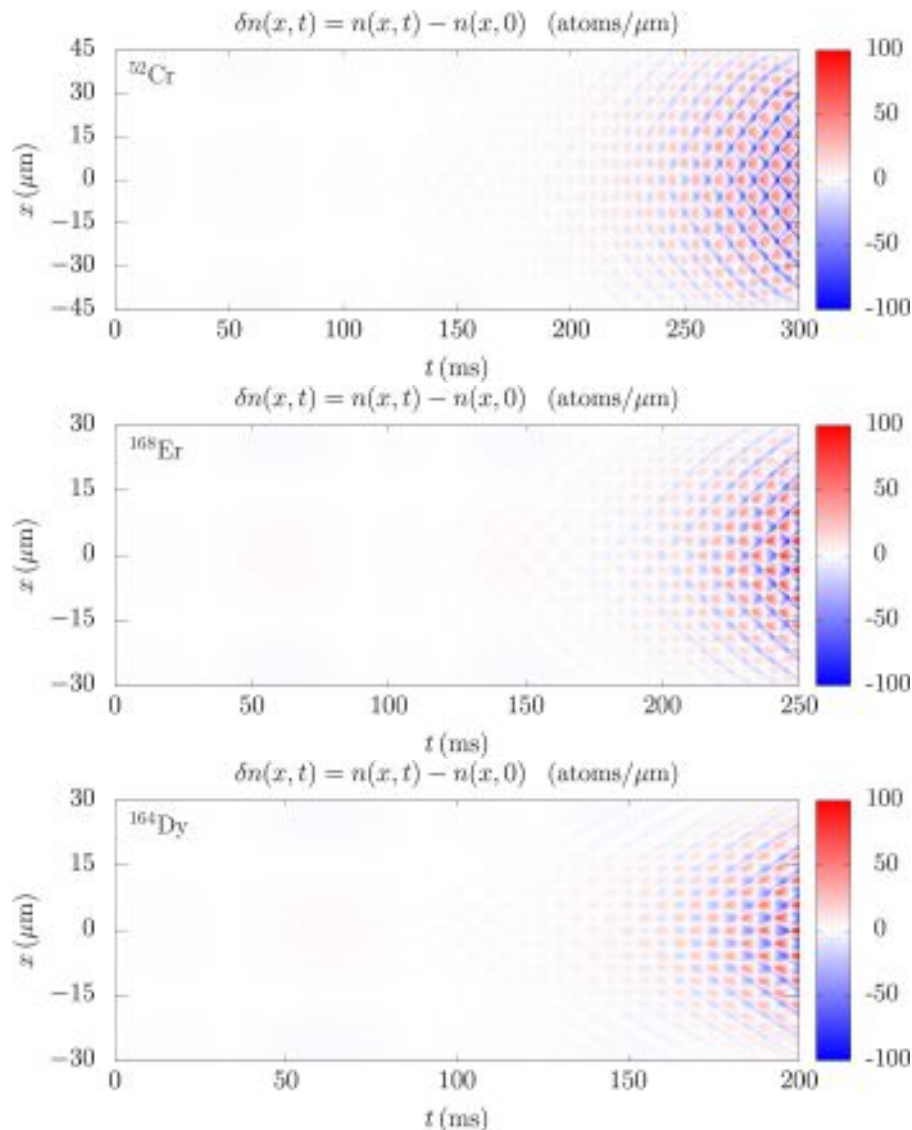


Figure 1. Time evolution of the integrated density profile variation $\delta n(x, t)$ in the weak-confinement direction for a BEC of chromium ^{52}Cr (**top**), erbium ^{168}Er (**middle**), and dysprosium ^{164}Dy (**bottom**), for the modulation frequency $\omega_m = 200 \times 2\pi$ Hz and amplitude $\epsilon = 0.2$, and the system parameters given in Section 2.

In the Fourier spectra of the integrated density profile variations in the radial directions (middle and right columns of Figure 2), we see a somewhat richer set of excitation modes. In addition to the main mode corresponding to the trap modulation at ω_m , we see that also the breathing mode is excited at the frequency $\omega_B \approx 321 \times 2\pi$ Hz. This value can be calculated by linearizing the equations of motion from Section 2. The spectra prominently contain the second modulation harmonic at $2\omega_m$ as well. We also see some other peaks, for instance the small peak at around $120 \times 2\pi$ Hz, which can be due to the linear combination of the modes $\omega_B - \omega_m$. However, such an identification would require further theoretical and numerical analysis, which is out of the scope of the present paper.

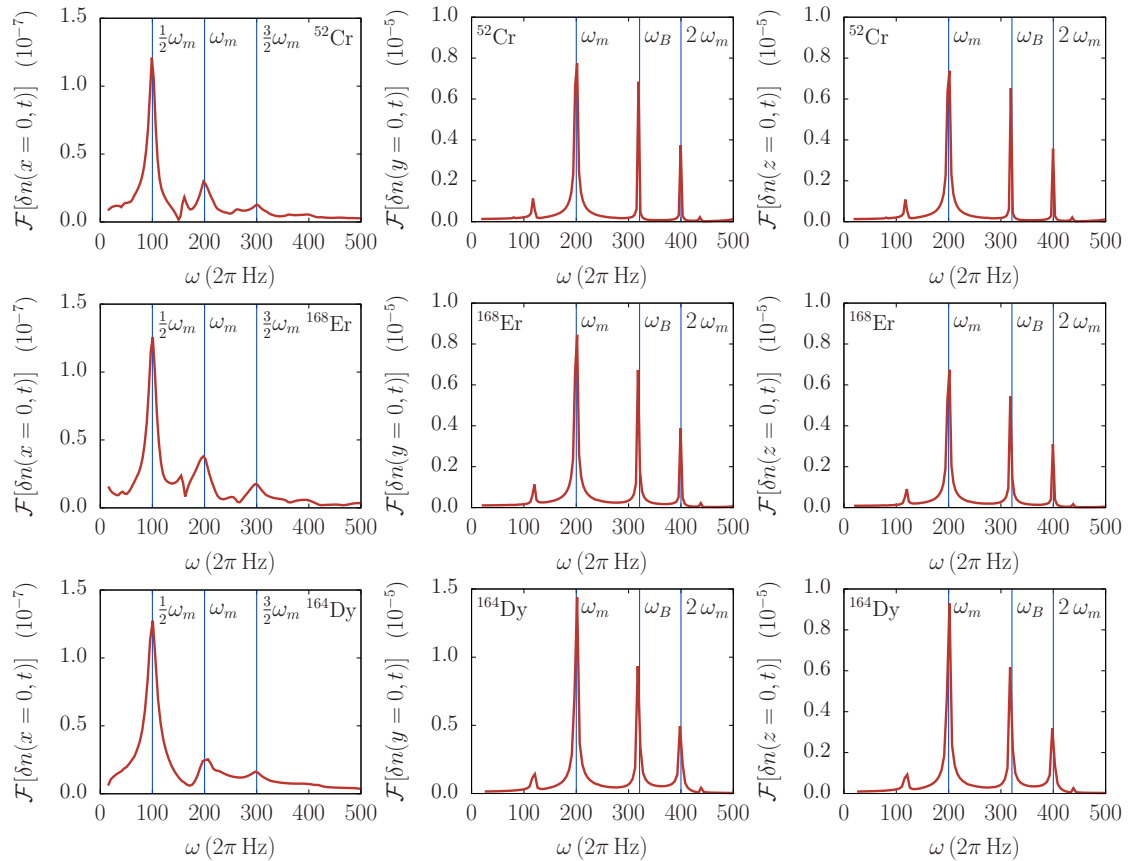


Figure 2. The Fourier spectrum in the time-frequency domain of the integrated 1D density profile variations of Faraday waves at the trap center $\delta n(x = 0, t)$ in x direction (**left column**), $\delta n(y = 0, t)$ in y direction (**middle column**), and $\delta n(z = 0, t)$ in z direction (**right column**) for a BEC of chromium ^{52}Cr (**top row**), erbium ^{168}Er (**middle row**), and dysprosium ^{164}Dy (**bottom row**). Vertical blue lines represent theoretical predictions, where $\omega_m/2$ corresponds to Faraday waves, ω_m , $3\omega_m/2$, and $2\omega_m$ to resonant waves, and ω_B is the variational result for the breathing mode frequency, which is obtained by linearization of the equations of motion from Section 2.

While the Fourier analysis in the time-frequency domain can be used to determine the character of the induced density waves (Faraday, collective, and resonant), the analysis in the spatial-frequency domain enables us to characterize the density patterns and calculate their spatial period. This is illustrated in Figure 3 for Faraday waves for all three considered atomic species. The integrated density profile variations are analyzed at appropriate times, which are determined to correspond to the evolution stage when Faraday waves have fully emerged, but the system is still far from the violent dynamics that inevitably follows after the long driving period.

In all three panels of Figure 3, the main peak corresponds to the wave vector k_F of the Faraday waves, and we see significant differences: for ^{52}Cr , we obtained $k_F = 0.57 \mu\text{m}^{-1}$, yielding the spatial period $\ell_F = 2\pi/k_F = 11.02 \mu\text{m}$; for ^{168}Er , we obtained $k_F = 0.98 \mu\text{m}^{-1}$ and $\ell_F = 6.41 \mu\text{m}$; and, for ^{164}Dy , we obtained $k_F = 1.10 \mu\text{m}^{-1}$ and $\ell_F = 5.71 \mu\text{m}$. The variational analysis presented in Section 2 yields results which are in good agreement with the numerical ones, namely $k_F = 0.51 \mu\text{m}^{-1}$ for ^{52}Cr , $k_F = 0.91 \mu\text{m}^{-1}$ for ^{168}Er , and $k_F = 1.06 \mu\text{m}^{-1}$ for ^{164}Dy . These variational results are shown in Figure 3 by vertical blue lines, which illustrate their agreement with the Fourier analysis. The presented spectra also contain some additional peaks that correspond to other geometrical features of the analyzed density profile variations, such as the condensate widths and their higher harmonics, as well as the higher harmonics of the Faraday waves periods, and linear combinations of all of these. However, they are not of interest for our analysis and we did not study them further.

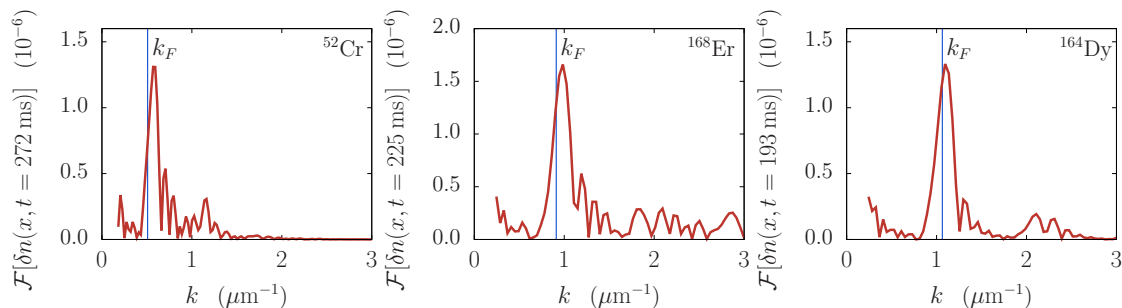


Figure 3. The Fourier spectrum in the spatial-frequency domain of the integrated 1D density profile variations of Faraday waves in x direction $\delta n(x, t = 272 \text{ ms})$ for ^{52}Cr (left), $\delta n(x, t = 225 \text{ ms})$ for ^{168}Er (middle), and $\delta n(x, t = 193 \text{ ms})$ for ^{164}Dy (right) BECs with $N = 10^4$ atoms. The corresponding density profile variations are shown in Figure 1. Vertical blue lines represent theoretical predictions for the wave vector k_F of the Faraday waves, Equation (23).

Note that the spatial period of Faraday waves can also be determined by directly looking at the density profile variations in Figure 1, and estimating the spacing between the consecutive minima or maxima at the appropriate evolution time. For instance, for chromium, we count three minima over the spatial extent of $30 \mu\text{m}$, yielding an estimate $\ell_F \approx 10 \mu\text{m}$, and similarly for other species. Obviously, such estimates are not as precise as the Fourier analysis results, and therefore we rely on FFT spectra to systematically determine the spatial periods of Faraday waves and their functional dependencies on the contact and the DDI strength.

4. Interaction Effects and Properties of Faraday Waves

In the previous section, we show how the Fourier analysis can be used to calculate the spatial period of Faraday waves. Next, we systematically studied the interaction effects, namely how the contact and the DDI strength affect the properties of generated density waves. First, we explored the influence of the contact interaction on the emergence time and the spatial period of Faraday waves for a fixed value of the DDI strength. In experiments, this can be achieved by employing the Feshbach resonance technique, which allows tuning a_s by changing the external magnetic field, thus changing the electronic structure of atoms and their scattering properties.

The existence of Faraday waves is a consequence of nonlinearity of the system, i.e., the presence of the contact and the DDI terms in the Hamiltonian. In a linear system, described by the pure Schrödinger equation, the harmonic modulation of the trap in the radial direction would not be transferred into the longitudinal direction. Therefore, the emergence time of Faraday waves (and other types of density waves in the longitudinal direction) critically depends on the strength of interatomic interactions. However, if interaction strengths become sufficiently large, the emergence time is less sensitive to their changes. Since the DDI is strong in erbium and dysprosium, we can expect that the emergence time of Faraday waves significantly depends on the contact interaction strength only in chromium, where a_{dd} is small.

This is illustrated in Figure 4, where we see the density profile variations for chromium for three different values of a_s . Let us first note that the amplitude of density variations is much smaller in the top panel for $a_s = 60 a_0$ than in the middle panel for $a_s = 80 a_0$, and significantly smaller than in the bottom panel for $a_s = 150 a_0$. This is also evident from the fact that in the top and middle panel we can clearly see the quadrupole collective oscillation mode, which has a frequency of around $\omega_Q = 12 \times 2\pi \text{ Hz}$. This can be estimated from the figure and compared to the variational value of ω_Q , which can be obtained by linearizing the equations of motion in Section 2. When the interaction is sufficiently large, the amplitude of Faraday waves is much larger than those of the collective modes, and they cannot be even discerned in the bottom panel in Figure 4. Only for a weak interaction the amplitude of the Faraday waves is comparable to the amplitude of the collective modes, and this is why we can see them all for small values of a_s .

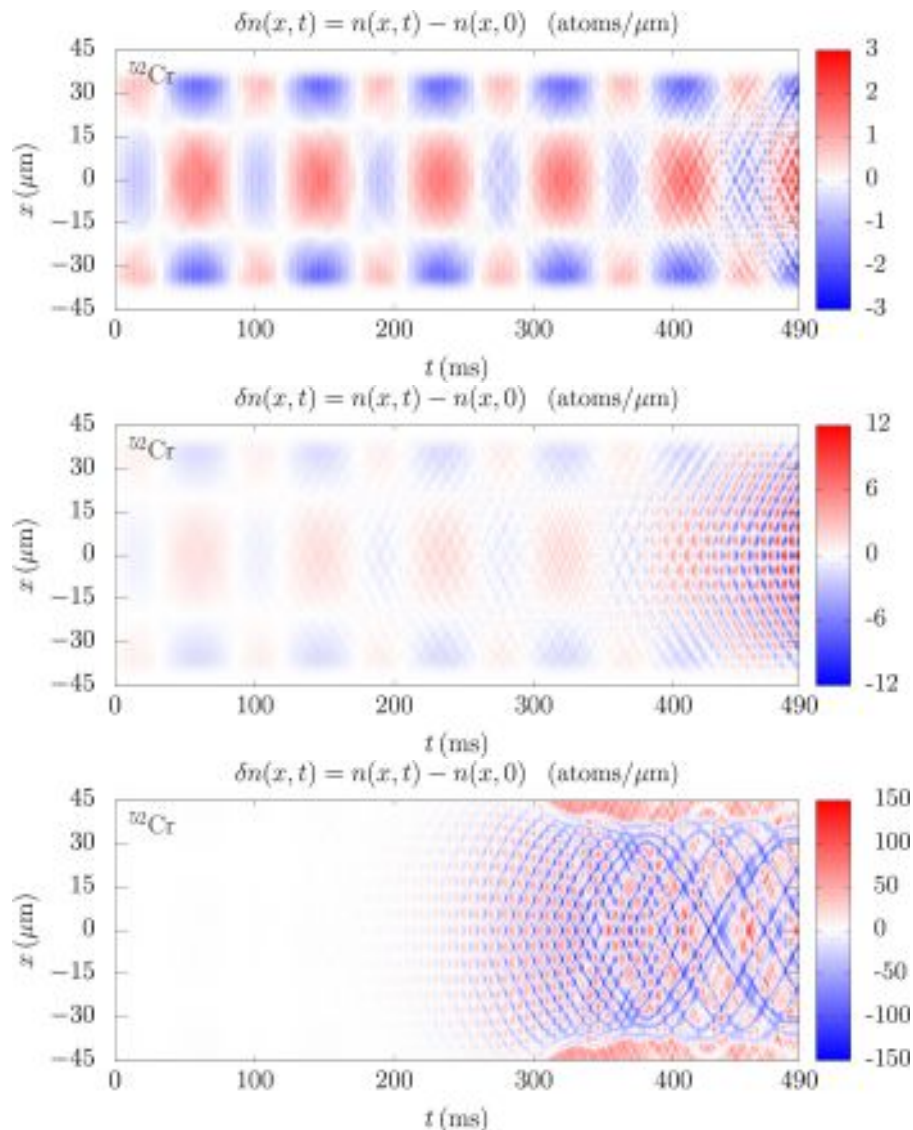


Figure 4. Emergence of Faraday waves for different strengths of the contact interaction: $a_s = 60 a_0$ (top), $a_s = 80 a_0$ (middle), and $a_s = 150 a_0$ (bottom) for a BEC of ^{52}Cr . We observe that Faraday waves emerge faster as the contact interaction strength increases.

As with all other excitations, Faraday waves start to develop immediately after the modulation is switched on. The question on their emergence time is related to their amplitude, which is time-dependent and grows exponentially, as can be seen from the solution (Equation (18)) of the Mathieu-like equation that describes the dynamics of the Faraday density oscillations. The imaginary part of the parameter ζ in Equation (18) is responsible for the exponential growth of the Faraday waves' amplitude, which is not the case for collective modes. Therefore, in practical terms, the definition of the emergence time of Faraday waves is always arbitrary and can be expressed as a time needed for the density variations to reach a certain absolute or relative (compared to the total density) value. One can even relate this to the experimental point of view, where there is a threshold for the density variations that can be observed, due to measurement errors. However, in numerical simulations, there are no such limitations and one can easily use an arbitrary definition to estimate the emergence time of density waves. The more relevant quantity to study would be the exponent that governs the growth of the wave amplitude, which depends on the interaction strength.

Now, we turn our attention to spatial features of the Faraday waves. Figure 5 presents the dependence of the wave vector k_F on the s -wave scattering length a_s for all three considered species.

We also show the variational results for the dependence $k_F(a_s)$ derived in Section 2. The agreement is very good, with errors of the order of 10–15%. We stress that the derived variational expression closely follows the numerical results not only by their values, but, more importantly, also their functional dependence properly.

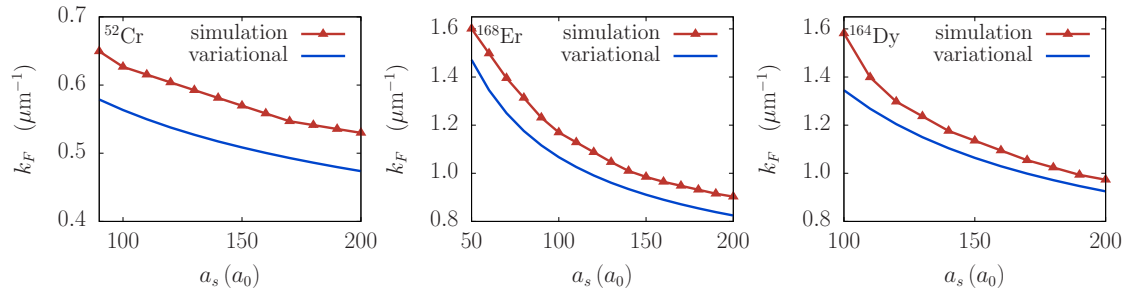


Figure 5. Wave vector of the Faraday waves k_F as a function of the contact interaction strength for a BEC of ^{52}Cr (left), ^{168}Er (middle), and ^{164}Dy (right), for a fixed DDI strength. Red upper triangles were numerically obtained values using the FFT analysis as in Figure 3, and blue lines are the variational results according to Equation (23).

Next, we studied the effects of the DDI strength for a fixed value of the contact interaction. Figure 6 shows the corresponding dependence of k_F on a_{dd} . In contrast to the contact interaction dependence, where k_F is a decreasing function of a_s , here we see that k_F increases as the DDI strength is increased. Figure 6 also shows the variational results, where the level of agreement with the numerically obtained results is different, with errors as small as 7% for chromium and up to around 25% for erbium and dysprosium for largest values of a_{dd} . Due to complex approximations made in the derivation of variational results, in particular those related to the DDI term, the obtained functional dependence is not as good as in the case of contact interaction, but still provides reasonable estimates of the wave vector values for the Faraday waves.

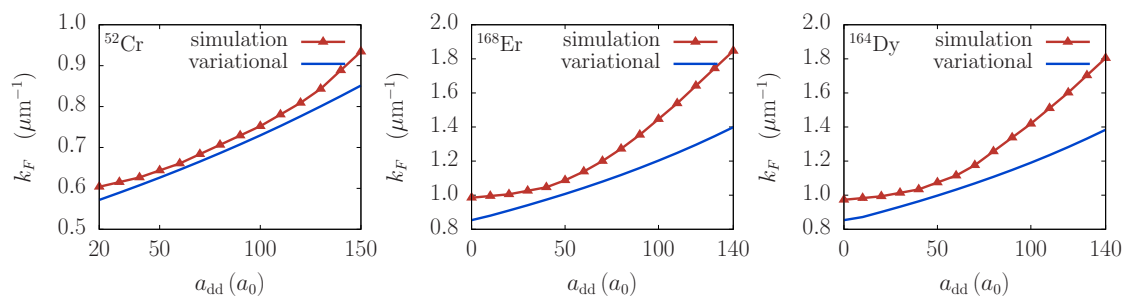


Figure 6. Wave vector of the Faraday waves k_F as a function of the DDI strength for a BEC of ^{52}Cr (left), ^{168}Er (middle), and ^{164}Dy (right), for a fixed contact interaction strength. Red upper triangles represent numerically obtained values using the FFT analysis as in Figure 3, and blue lines are the variational results according to Equation (23).

5. Resonant Waves

In the presence of interactions, various excitation modes in dipolar BECs are coupled and the energy pumped into the system by periodic driving can be transferred from the driving direction to other, orthogonal directions. In the previous section, we show this for non-resonant driving, when the harmonic modulation in the radial direction was transferred to the longitudinal direction in the form of Faraday waves, which were the main excitation mode generated. The main distinguishing property of these excitations is halving of the oscillation frequency, i.e., the induced density waves have the frequency $\omega_m/2$. Next, we studied the other important case, when the modulation frequency is resonant, such that the induced density waves have the same frequency. This happens when ω_m is close to one of the characteristic frequencies of the system, e.g., one of the frequencies of the collective

oscillation modes or one of the trap frequencies. Although Faraday waves and all other collective oscillation modes are also excited in this case, the largest amplitude corresponds to resonant waves with the frequency ω_m . When generated, these resonant waves dominate the behavior of the system and make all other excitations negligible for the dynamics.

Figure 7 shows the integrated density profile variation of ^{168}Er for a resonant wave induced by a harmonic modulation of the radial part of the trapping potential at $\omega_m = \Omega_0$, i.e., when the modulation frequency coincides with the radial trapping frequency. The density waves in this case develop much more quickly than for the non-resonant modulation and are clearly visible already after 55 ms. Due to a violent dynamics that emerges in the system very quickly, it is not easy to estimate the frequency of the waves directly from Figure 7, as was possible before. Therefore, we relied on the Fourier analysis in the time-frequency domain, as presented in the left panel of Figure 8. The obtained FFT spectrum clearly shows that the main excitation mode has the frequency equal to ω_m . We also see that the spectrum is continuous, practically without distinct individual peaks, and only the second harmonic at $2\omega_m = 321 \times 2\pi$ Hz yields a small local maximum. This demonstrates that the system is far from the regime of small perturbations, where individual excitation modes can be observed.

In the right panel of Figure 8, we see the Fourier spectrum in the spatial-frequency domain, which yields the wave factor k_R of resonant waves. The FFT results give the value $k_R = 1.59 \mu\text{m}^{-1}$ and the corresponding spatial period $\ell_R = 2\pi/k_R = 3.95 \mu\text{m}$ for ^{168}Er . In the figure we also present the variational result $k_R = 1.40 \mu\text{m}^{-1}$, calculated using Equation (24). The agreement is again quite good, which indicates that the variational approach developed in this paper can be reliably used not only for the Faraday waves, but also for the resonant waves.

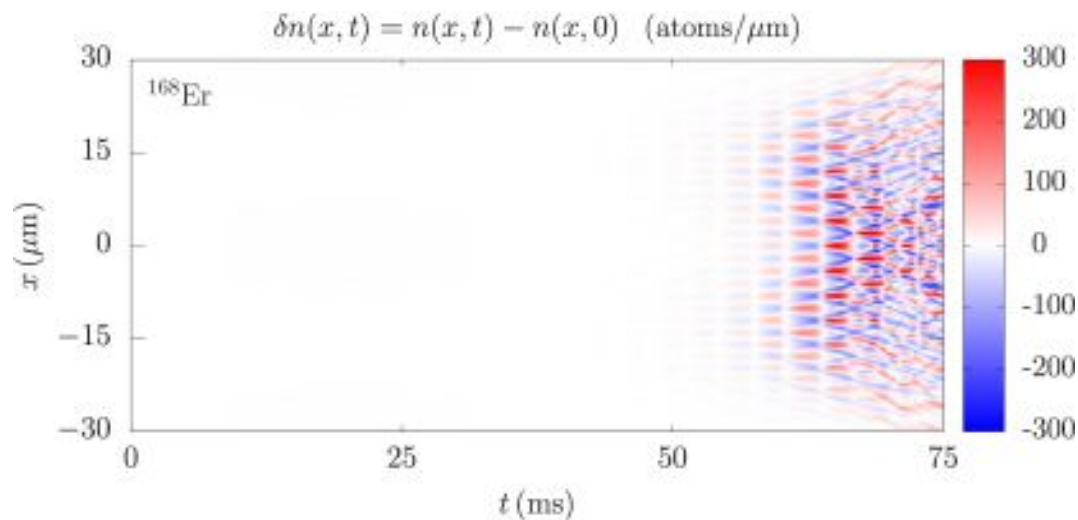


Figure 7. Time evolution of the integrated density profile variation in the weak confinement direction for a BEC of ^{168}Er , with the modulation frequency equal to the weak confinement frequency, $\omega_m = \Omega_0$. We observe resonant behavior corresponding to the first harmonic of the resonant frequency Ω_0 , which sets in after around 55 ms.

This can also be concluded from Figure 9, which presents the results for the dependence of the resonant wave vector k_R on the contact and the DDI strength. The agreement between the numerical and variational results is of the order of 10% over the whole experimentally relevant domain. We see similar behavior for the resonant waves as for the Faraday ones, namely the wave vector decreases as the contact interaction strength increases, while the opposite is true for the DDI. Again, the functional dependence obtained from the variational approach properly describes the numerical results, thus confirming that Equation (24) can be used to calculate spatial period of resonant waves.

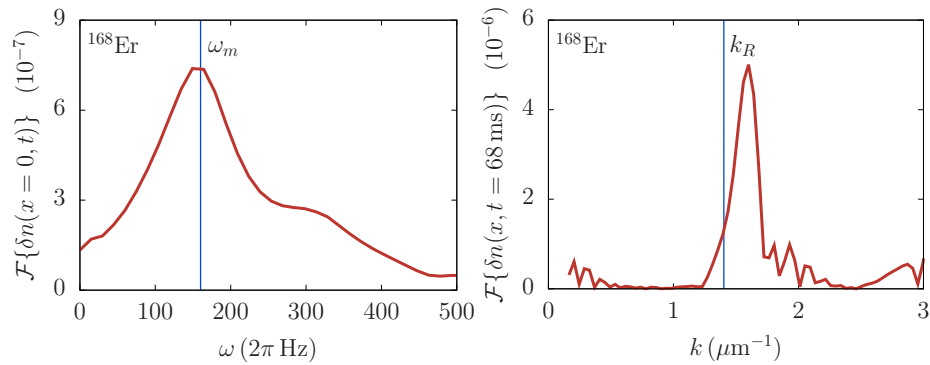


Figure 8. The Fourier spectrum of the integrated 1D density profile variations $\delta n(x, t)$ at the trap center in the time-frequency domain (**left**), and of the density profile variations in x direction $\delta n(x, t = 68 \text{ ms})$ in the spatial-frequency domain (**right**) of resonant waves for a BEC of ^{168}Er . Vertical blue line in the left panel represents the modulation frequency ω_m , while in the right panel it corresponds to the theoretical prediction for the wave vector k_R of the resonant waves, Equation (24).

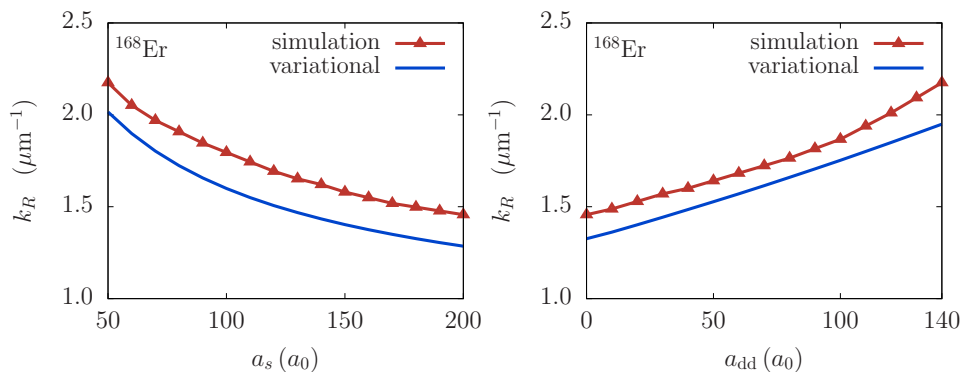


Figure 9. Wave vector of the resonant waves k_R as a function of the contact (**left**) and the DDI (**right**) strength for a BEC of ^{168}Er . The results in the left panel are obtained for a fixed DDI strength, and similarly in the right panel a fixed contact interaction strength is used. In both panels, red upper triangles represent numerically obtained values using the FFT analysis as in the right panel of Figure 8, and blue lines are the variational results according to Equation (24).

It is interesting to note that resonant behavior appears not only under conditions mentioned above, when ω_m is equal to one of the characteristic frequencies, but also when it matches their higher harmonics. Figure 10 illustrates this for ^{168}Er , which is harmonically modulated at twice the radial trapping frequency, $\omega_m = 2\Omega_0 = 321 \times 2\pi \text{ Hz}$. In this case, the amplitude of the resonant mode grows even more quickly and significant density variations can be observed already after 30 ms. Therefore, we see that the modulation at the second harmonic yields even more violent dynamics than the first harmonic. The Fourier analysis in the time-frequency domain reveals that the main excitation mode again has a frequency of Ω_0 , but the mode at $\omega_m = 2\Omega_0$ is also present. From the experimental point of view, resonant driving is very dangerous and leads to the destruction of the system in a matter of tens of milliseconds. While numerical simulations can be performed for longer time periods, the atoms leave the condensate due to a large, resonant transfer of energy to the system. As the condensate is depleted, the mean-field description of the system breaks down and it can no longer be simulated by the dipolar Gross-Pitaevskii equation.

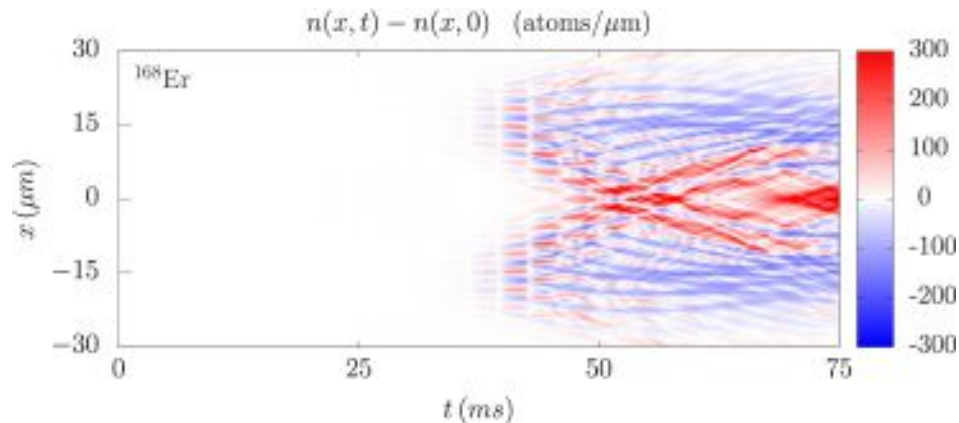


Figure 10. Time evolution of the integrated density profile variation in the weak confinement direction for a BEC of ^{168}Er . The modulation frequency is equal to twice the weak confinement frequency, $\omega_m = 2\Omega_0$. We observe resonant behavior corresponding to the second harmonic of the resonant frequency Ω_0 , which sets in more quickly than the first harmonic, already after around 30 ms.

6. Conclusions

We investigated here the Faraday and resonant density waves in ultracold dipolar Bose-Einstein condensates for experimentally relevant atomic species with the permanent magnetic dipole moment: chromium ^{52}Cr , erbium ^{168}Er , and dysprosium ^{164}Dy . The interplay of the contact and the dipole-dipole interaction in such systems is a hot research topic today, but detailed understanding of their dynamics and even their stability is still lacking. Our results contribute to variational and numerical description of driven dipolar systems and their properties, which are important for ongoing experiments, and will be of particular interest as the strongly dipolar regime becomes experimentally available.

To describe the dynamics of the Faraday and resonant waves in dipolar BECs, we relied here on the variational approach introduced in Ref. [16] (and references therein), which was already used in various setups [17–20,23–25,30,41,42]. This approach is based on the Gaussian variational ansatz and includes the condensate widths and the conjugated dynamical phases as parameters. The ansatz also includes the density modulations in order to capture the dynamics of density waves. Using our variational approach, the obtained equations for the dynamical evolution of the system are cast into the form of the Mathieu-like differential equation. This allowed us to identify the most unstable solutions of the Mathieu's equation with the Faraday and the resonant waves, which we observed numerically. Based on this idea, we derived analytical expressions for the periods of these two types of density waves. Performing the FFT analysis of the results of extensive numerical simulations, we were able to calculate the corresponding periods numerically, as functions of the contact and the dipole-dipole interaction strength. The comparison of variational and numerical results shows very good agreement and demonstrates that the derived analytical expressions provide full understanding of the properties of density waves in dipolar condensates.

In the future, we plan to study onset times for the emergence of Faraday and resonant waves, and in particular the corresponding exponents and their dependence on the contact and the DDI. It is well known that the periodic driving of a dipolar system may lead to its collapse, and we plan to investigate if recently observed quantum droplets, that appear as a result of stabilization due to quantum fluctuations, may also appear in a scenario which leads to Faraday waves.

Author Contributions: Conceptualization, methodology, software, validation, formal analysis, writing—original draft preparation, and writing—review and editing, both authors; investigation, data curation, and visualization, D.V.; and resources, supervision, project administration, and funding acquisition, A.B.

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VI-SEEM DREAMCLIMATE SERVICE

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Abstract. Premature human mortality due to cardiopulmonary disease and lung cancer is found in epidemiological studies to be correlated to increased levels of atmospheric particulate matter. Such negative dust effects on the human mortality in the North Africa – Europe – Middle East region can be successfully studied by the DREAM dust model. However, to assess health effects of dust and its other impacts on the environment, a detailed modelling of the climate for a period of one year in a high-resolution mode is required. We describe here a parallel implementation of the DREAM dust model, the DREAMCLIMATE service, which is optimised for use on the high-performance regional infrastructure provided by the VI-SEEM project. In addition to development and integration of this service, we also present a use-case study of premature mortality due to desert dust in the North Africa – Europe – Middle East region for the year 2005, to demonstrate how the newly deployed service can be used.

Key words: DREAM model, dust effects, human mortality, VI-SEEM project, application service

AMS subject classifications. 68W10, 68M14, 68N30

1. Introduction. Exposure to airborne mineral dust particles can significantly influence human health. Atmospheric dust particles are primarily driven by mesoscale and synoptic processes, and may be present in high concentrations near the sources and carried over long distances while having adverse health effects. Drought and desertification, as climate-related changes and human activities such as changes in land use, affect potential dust sources of fine particulate matter in arid areas. Therefore, numerical modelling with sufficiently high resolution of the processes of the atmospheric dust cycle that drive dust emissions and transport is a useful approach to assessment of the potential health effects of exposure to dust.

The previously developed Dust REgional Atmospheric Modeling (DREAM) system [1] is a component of a comprehensive atmospheric model designed to simulate and predict the atmospheric cycle of mineral dust aerosols. The DREAM provides a climatology of dust based on long-term re-analysis of the model. It is widely used by the research and operational dust forecasting communities in more than 20 countries, including its recent use in a series of NASA-funded projects [2, 3, 4, 5] dealing with health aspects of dust suspended in the air. The Institute of Physics Belgrade group, which is a partner in the Sand and Dust Storm Warning Advisory and Assessment System (SDS-WAS) project of the World Meteorological Organization, uses DREAM to provide daily dust forecasts to the SDS-WAS model inter-comparisons and validation activities. Also, it is used for investigation on how fine particulate matter contributes to air pollution in North Africa – Europe – Middle East region.

To assess health effects of dust in the region and other dust impacts on the environment, it is usual to consider at least a one-year modelling climatology for the given region. In this case this was achieved by solving the DREAM model in a high-resolution mode with the horizontal grid resolution of 15 km. Such a high resolution model is capable to accurately describe the behaviour of small-scale dust sources in the desert areas (Sahara, Middle East), as well as the mesoscale atmospheric conditions. However, due to numerical complexity it requires a parallelised version of the DREAM code, which we created and optimised for usage on high-performance computing infrastructures available today.

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In parallel to development of the DREAM model, a number of initiatives were crucial for enabling high-quality climate research in the region. This was achieved by providing e-Infrastructure resources, application support and training through the VI-SEEM project [6], funded by the EU H2020 programme. The project brings together regional e-Infrastructures in order to build capacity and better utilise synergies, as well as to provide improved service within a unified virtual research environment for several inter-disciplinary scientific user communities. The overall aim is to offer a user-friendly integrated e-Infrastructure platform for regional cross-border scientific communities in climatology, life sciences, and cultural heritage. This includes integration of computing, data, and visualisation resources, as well as services, models, software solutions and tools. The VI-SEEM virtual research environment provides the support to scientists in a full lifecycle of collaborative research.

By efforts of the DREAM code developers and the VI-SEEM support team, the DREAM model was successfully refactored and tuned for usage on high-performance computing infrastructures in a form of the DREAMCLIMATE service, presented here. Section 2 briefly describes the DREAM model, which is capable of producing results in the required high-resolution mode for a one year period. The DREAMCLIMATE service is presented in detail in Section 3, while Section 4 describes produced datasets and main results. By using an order of magnitude finer DREAM model grid than available before, we perform a detailed analysis of dust impacts to public health.

2. DREAM model. Premature human mortality due to cardiopulmonary disease and lung cancer is found in epidemiological studies to be correlated to increased levels of atmospheric particulate matter, in particular to long-term exposure to particulate matter with an aerodynamic diameter smaller than $2.5 \mu\text{m}$. In order to estimate the premature mortality caused by the long-term exposure to airborne desert dust, we use results of the DREAM gridded model dust climatology of fine particulate matter and dust concentrations. This analysis follows the previous study [7] that indicates that there is a large number of premature deaths by cardiopulmonary disease and a significant number of deaths by lung cancer, mostly in the dust belt region neighbouring Sahara and Middle East deserts.

The DREAM model is developed as an add-on component of a comprehensive atmospheric model and is designed to simulate and/or predict the atmospheric cycle of mineral dust aerosols. It solves a coupled system of the Euler-type partial differential nonlinear equations for dust mass continuity, one equation for each particle size class, which is one of the governing prognostic equations in an atmospheric numerical prediction model [8, 9, 10]. The DREAM model takes into account all major processes of the atmospheric dust cycle. During the model simulation, calculation of the surface dust emission fluxes is made over the model cells declared as deserts. A viscous sub-layer parameterisation regulates the amount of dust mass emission for a range of near-surface turbulent regimes. Once injected into the air, dust aerosols are driven by the atmospheric dynamics and corresponding physical quantities: by turbulence in the early stage of the process, when dust is lifted from the ground to the upper levels; by winds in later phases of the process, when dust travels away from the sources; and finally, by thermodynamic processes, rainfall and land cover features that provide wet and dry deposition of dust over the Earth surface.

The model is implemented as a bundle of Fortran programs and libraries. These components are divided into three groups: the preprocessing system, the model operational system, and post-processing and visualisation tools. The preprocessing consists of two phases. The first is the setup in which the simulation domain, model configuration and interpolation of terrestrial data are defined. These parameters are mostly hard-coded and any change to parameters in this phase requires recompilation. The second stage of preprocessing is interpolation of the meteorological input data from the global meteorological model to the current simulation domain, as well as a setup of initial boundary conditions for the dust model. The model operational system is the main component, and it runs the numerical integration program. Post-processing and visualisation tools include GrADS [11] with conversion from Arakawa E-grid to geo-referenced grid and plots.

The code is predominantly written in the style of the Fortran 77 standard. Some of the more pressing constraints of the standard were the lack of support for dynamic memory allocation and command line arguments. These two constraints required for a number of parameters to be hard-coded. As a consequence, this limited the number of users who could use the application independently, and the number of parallel tests that could be ran at once. Recompilation also requires a deep technical knowledge of the implementation itself, which reduces

usability and dissemination of the model.

3. DREAMCLIMATE service. Within the framework of the VI-SEEM project, the DREAM model was successfully re-factored and tuned for usage on high-performance computing infrastructures. The DREAMCLIMATE service was developed and deployed using the VI-SEEM infrastructure modules. Configuration of the considered physical system is separated from the source code of the application, and all relevant parameters are grouped into a single configuration file. Such an improved configuration approach enabled more user-friendly way to configure various model setups, without the need for each user to dive into the code and technical details of the implementation. This also enables multiple users to run their model instances independently. Important additional improvements include significant reduction of the disk-space consumption, as well as standardisation of its usage through an environment-module approach.

Configuration files follow the format of the Python configuration parser, which is a convenient, flexible, and powerful way for parsing configuration files. It uses simple INI style configuration syntax, i.e., a text file with a basic structure composed of sections, properties, and values. Parameters are divided into sections which are designated by square brackets. Within one section, each parameter is specified in a separate line and its name and value are delimited by the equals sign. In-line comments are also permissible and corresponding lines begin with a semicolon. In addition to this, a support for variable interpolation is included as well.

The DREAM processing stages remain similar to the original version of the code, and consist of the pre-processing, the model operational processing, and the post-processing phase. Majority of changes are related to reducing the complexity of configuration in the setup stage of preprocessing. In a typical use-case, a user begins the simulation project by loading the environment module for the DREAMCLIMATE service, which sets the environment paths for the commands used to initialise and prepare the DREAM model simulation. Afterwards, by invoking the `dreamclimate_init` script the default configuration file is created in the working directory and files needed for a configuration of the local simulation instance are created in the `.dreamclimate` subdirectory. After the parameters are set in the configuration file, the `dreamclimate_reconfig` script is called to execute the setup stage, which encapsulates recompilation of the components, depending on the parameters changed. The resulting binaries, which are used to run simulation, are placed in the `.dreamclimate/bin` directory. This step isolates each user's simulation instance from others and enables multiple instances to work without interference. The next step in this stage generates and interpolates vegetation and soil texture for the forecast domain, by calling the `gt30mounth`, `gt30source`, `gt30vegetadirect`, `text4eta`, and `texteta` components.

After the setup, preprocessing continues by invoking the `dreamclimate_preproc` script whose role is to prepare input data for the Eta model grid. This script invokes the following components:

- `climsst` – horizontal grid (IMT, JMT) Eta model indexing from the SST as a function of the month,
- `anecw` – horizontal grid (IMT, JMT) Eta model indexing from global initial data,
- `pusiWRF` – set of the vertical variables and vertical interpolation of the pressure to sigma surfaces,
- `const` – conversion of the initial fields in Eta model coordinates from 2D horizontal (IMT, JMT) indexing to 1D (IMJM), definition of dummy initial boundary soil moisture and temperature values, and calculation of the constants needed for the 1D version of the soil model,
- `dboco` – creation of the boundary condition files,
- `gfdlco2` – interpolation of the transmission functions grid, for which the transmission functions have been pre-calculated, to the grid structure.

This preprocessing step produces binary files interpolated to the model grid (i.e., Arakawa E-grid) in the output directory specified in the configuration file. All the routines of the model itself, which describe atmospheric processes including the dust cycle, are built into the main executable file. This is a parallel MPI program that runs the simulation and is submitted to the job scheduling system using the job description script, which is automatically generated earlier in the setup stage. The post-processing includes the conversion of the main GrADS output file from the Arakawa E-grid to the GrADS grid. These steps are handled by the `dreamclimate_post-process` script.

Many of the configuration parameters in the generated configuration file have sensible default values, to minimise the need for users to search through lengthy lists of output file locations. The domain parameters of interest for configuring the model itself, inside the ALLINC section, are:

- `TLM0D` – longitude of the centre point of the domain,

- TPH0D – latitude of the centre point of the domain,
- WBD – western boundary of the domain with respect to the centre point (always less than 0),
- SBD – southern boundary of the domain with respect to the centre point (always less than 0),
- DLMD – longitudinal model grid resolution,
- DPHD – latitudinal model grid resolution,
- DTB – time step of the model, which depends on DLMD and DPHD values by means of the Courant-Friedrichs-Lewy (CFL) criteria,
- LM – the number of vertical levels.

Another set of commonly changed model parameters are dimensions of the model grid. These are grouped in the PARMETA section of the configuration file:

- IM – the number of mass grid points along the first row, essentially half of the total number of grid points in the west-east direction, due to the horizontal staggering of mass and wind points,
- JM – the number of rows in the north-south direction.

These parameters also influence the number of processes and the topology of the MPI parallel execution.

The rest of the parameters in the configuration file specify paths for input, output and intermediate files. With these paths defined during configuration, a significant reduction in disk space usage was achieved, as the data files no longer need to be copied together with the code, and no longer have to be in fixed relative locations.

The DREAMCLIMATE service is deployed during the first VI-SEEM development access call at the PARADOX high-performance computing cluster [12], hosted by the Scientific Computing Laboratory, Center for the Study of Complex Systems of the Institute of Physics Belgrade. This cluster is part of the VI-SEEM infrastructure, and consists of 106 working nodes. Working nodes (HP ProLiant SL250s Gen8) are configured with two Intel Xeon E5-2670 8-core Sandy Bridge processors, at a frequency of 2.6 GHz and 32 GB of RAM. The total number of CPU-cores available in the cluster is 1696, and each working node contains an additional GP-GPU card (NVIDIA Tesla M2090) with 6 GB of RAM. The peak computing power is 105 TFlops. The PARADOX provides a data storage system, which consists of two service nodes (HP DL380p Gen8) and 5 additional disk enclosures. One disk enclosure is configured with 12 SAS drives of 300 GB each (3.6 TB in total), while the other four disk enclosures are configured each with 12 SATA drives of 2 TB (96 TB in total), so that the cluster provides around 100 TB of storage space. Storage space is distributed via a Lustre high-performance parallel file system that uses Infiniband QDR interconnect technology, and is available on both working and service nodes.

Although the DREAMCLIMATE code is a copyright-protected software, it can be obtained for research purposes with the permission of the principal investigator (S. Ničković). Therefore, the DREAMCLIMATE service source code is only internally available at the VI-SEEM code repository [13], as well as a module at the PARADOX cluster software repository. Transfer of the software to third parties or its use for commercial purposes is not permitted, unless a written permission from the author is received.

4. Produced datasets and results. Using the DREAMCLIMATE service at PARADOX during the first VI-SEEM call for production use of resources and services, we produced a dataset with the aerosol optical thickness and surface dust concentration for the one-year period. We selected the year 2005 for this analysis, which serves as an example and demonstrates usability of DREAMCLIMATE service. The dataset covers wide region of North Africa, Southern Europe and Middle East in 30 km horizontal resolution with 28 vertical levels, and is made publicly available via the VI-SEEM data repository [14].

In addition to this initial dataset, we also produced a dataset with a higher resolution of 15 km for the same region and period of time. The global mean DREAMCLIMATE-modelled dust concentration for year 2005 is presented in Fig. 4.1.

Using the human health impact function introduced in Refs. [15, 16], we can relate the changes in pollutant concentrations to the changes in human mortality, and estimate the global annual premature mortality due to airborne desert dust. For this, we use as a baseline the mortality rate estimated by the World Health Organization (WHO) Statistical Information System on the country-level based on the International Classification of Diseases 10th Revision (ICD-10) classification, and regional data from the WHO Global burden of disease for countries with no data. Population statistics we used for the year 2005 is based on the United Nations Department of Economic and Social Affairs (UNDES 2011) database, while gridded global population numbers

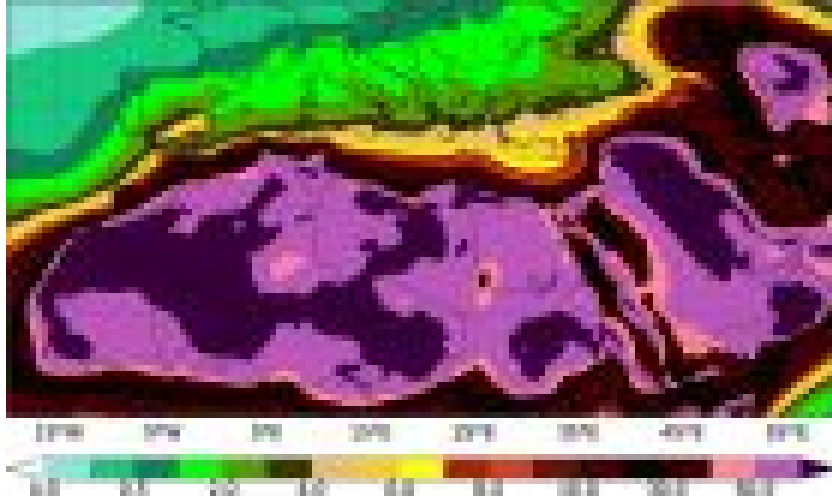


FIG. 4.1. Calculated mean dust concentrations in $\mu\text{g}/\text{m}^3$, obtained from the DREAMCLIMATE model. The model integration area covers region of North Africa, Southern Europe and Middle East, with 15 km horizontal resolution in 28 vertical levels for the year 2005.

TABLE 4.1
Total CPD and LC premature mortalities for the threshold concentrations between 0 and $10 \mu\text{g}/\text{m}^3$.

Baseline concentration (in $\mu\text{g}/\text{m}^3$)	0	5.0	7.5	10
CPD premature mortality (in thousands)	765	615	567	524
LC premature mortality (in thousands)	14.8	10.2	9.1	8.4

are taken from the Columbia University Center for International Earth Science Information Network (CIESIN) database. We used the population cohort of 30 years and older in the health impact function.

Applying the health impact function to the considered population, the DREAM model output suggests a significant contribution of desert dust to premature human mortality. For the global background of dust concentration of $7.5 \mu\text{g}/\text{m}^3$ i.e., threshold below which no premature mortality occurs, the estimated premature mortality (per grid cell) by cardiopulmonary disease (CPD) and lung cancer (LC) is illustrated in Fig. 4.2. In total, around 570,000 premature deaths in the model domain are predicted to occur during a one-year period, as a negative consequence of dust. According to our results, top five countries with the highest induced CPD-mortality in the year 2005 are: Egypt with 74,000; Iraq with 67,000; Iran with 50,000; Nigeria with 46,000; Sudan with 45,000. On the other hand, top five countries with the highest induced LC-mortality in the same year are: Iraq with 1,200; Iran with 900; Sudan with 800; Egypt with 800; Uzbekistan and Turkey with 500 premature deaths each.

We also investigated the sensitivity of our results on the value of the threshold concentrations, which is above assumed to be $7.5 \mu\text{g}/\text{m}^3$. Table 4.1 gives the obtained total CPD and LC premature mortalities for the threshold concentrations between 0 and $10 \mu\text{g}/\text{m}^3$. This analysis is presented to showcase capabilities of the model and the developed DREAMCLIMATE service, and can be efficiently used to study desired regions and time periods if the required input data are provided.

5. Conclusions. Using the VI-SEEM project infrastructure and services, we have successfully re-factored the DREAM atmospheric model. We have developed and implemented the DREAMCLIMATE service, which is tuned for usage on high-performance computing infrastructures available today. In order to demonstrate a typical use-case, we have produced a dataset with the aerosol optical thickness and surface dust concentration for the one-year period for the wide region of North Africa, Southern Europe and Middle East. We have used

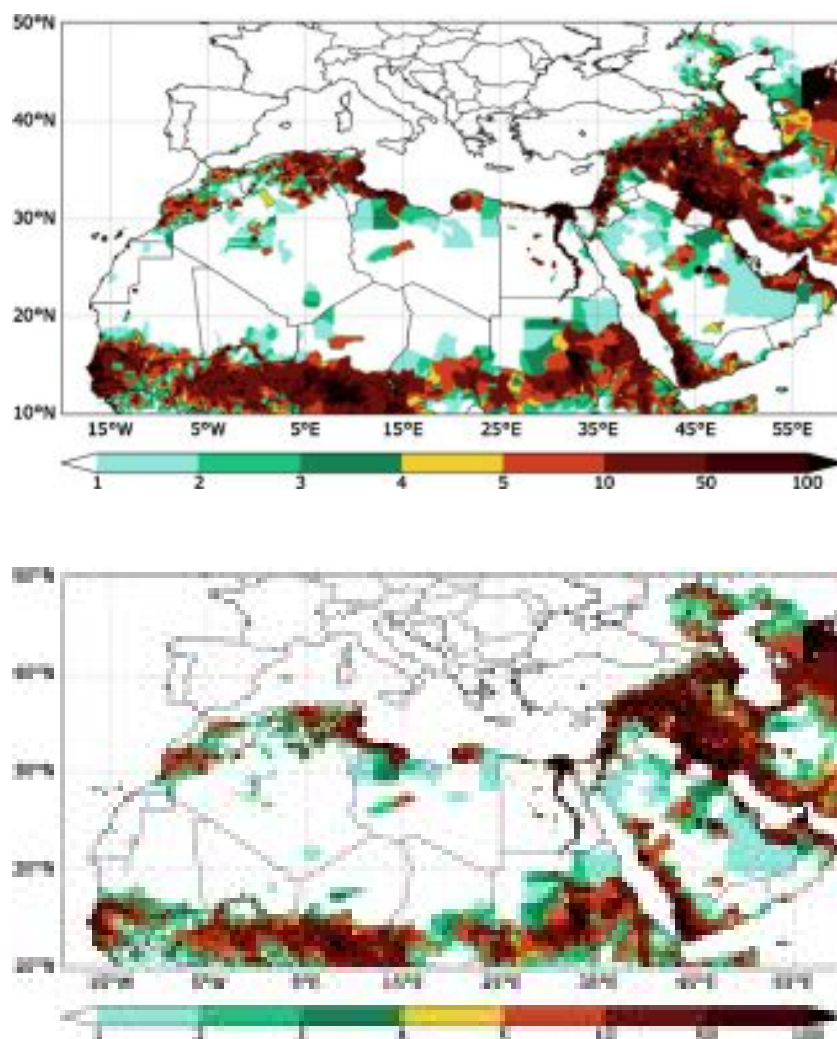


FIG. 4.2. Estimated global premature mortality per grid cell by cardiopulmonary disease (top) and lung cancer (down) due to the long-term exposure to desert dust with an aerodynamic diameter smaller than $2.5 \mu\text{m}$, calculated by the VI-SEEM DREAMCLIMATE service.

both the 30 km and the 15 km horizontal resolution, with 28 vertical levels. To showcase how results of the DREAMCLIMATE service can be applied, using the human health impact function and calculated global fine particulate matter concentrations, we have estimated the premature mortality caused by the long-term exposure to airborne desert dust with an aerodynamic diameter smaller than $2.5 \mu\text{m}$ for the year 2005 in the considered region. The results show that the large total number of premature deaths (around 570,000) in the model domain is mainly due to cardiopulmonary disease, but a significant number of deaths is also caused by lung cancer. The model also shows high sensitivity of the results on the threshold concentration, which is a significant parameter of relevance to public health.

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E-INFRASTRUCTURES FOR LARGE-SCALE COLLABORATIONS

VI-SEEM Virtual Research Environment

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In the last decade, a number of initiatives were crucial for enabling high-quality research in both South-East Europe and Eastern Mediterranean region. This was achieved by providing e-Infrastructure resources, application support and training in these two areas. VI-SEEM project brings together these e-Infrastructures to build capacity and better utilize synergies, for an improved service provision within a unified virtual research environment for the inter-disciplinary scientific user communities in those regions. The overall aim is to provide user-friendly integrated e-Infrastructure platform for regional cross-border scientific communities in climatology, life sciences, and cultural heritage. This includes linking computing, data, and visualization resources, as well as services, models, software and tools. The VI-SEEM virtual research environment provides the scientists and researchers with the support in a full lifecycle of collaborative research: accessing and sharing relevant research data, using it with provided codes and tools to carry out new experiments and simulations on large-scale e-Infrastructures, and producing new knowledge and data. The VI-SEEM consortium brings together e-Infrastructure operators and scientific communities in a common endeavor that will be presented in this talk. We will also point out how the audience may benefit from this newly created virtual research environment.

Underlying e-Infrastructure of the VI-SEEM project consists of heterogeneous resources - HPC resources - clusters and supercomputers with different hardware architectures, Grid sites, Clouds with possibility to launch virtual machines (VMs) for services and distributed computing, and storage resources with possibility for short and long-term storage. The heterogeneous nature of the infrastructure presents management challenges to the project's operational team, but is also an advantage for the users because of its ability to support different types of applications, or different segments of the same application. These are modern, state-of-the-art technologies for computing, virtualization, data storage and transfer.

Efficient management of the available computing and storage resources, as well as interoperability of the infrastructure is achieved by a set of operational tools. Static technical information, such as name, geographical location, contact and downtime information, list of service-endpoints provided by a particular resource center within the infrastructure etc., is manually entered and made available through the VI-SEEM GOCDDB database. Based on this information, project monitoring system is able to automatically trigger execution of monitoring service probes, and to enable efficient access to results of the probes via a customized monitoring web portal. Using standardized metrics, the VI-SEEM accounting system accumulates and reports utilization of the different types of



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resources. User support and service-related problems are resolved mainly through the helpdesk system, but via a technical mailing list as well. The VI-SEEM source code repository contains all codes developed within the project, while the technical wiki collects technical documentation, know-hows, best practices, guidelines, etc.

A solid but flexible IT service management is one of the keystones of the foundation for the service-oriented design. The specifics of the federated environment, such as the one found in the VI-SEEM consortium, impose requirements for service management tools that cannot be met using common off-the-shelf solutions. Hence, special care is taken in the design and the implementation of easy to use, custom solutions that are tailor-made for the scientific communities. Our application-level and data services are managed through the VI-SEEM service portfolio management system. It has been developed to support the service portfolio management process within the project as well as to being usable for other infrastructures, if required. The main requirements for the creation of this tool have been collected from the service management process design, and it is designed to be compatible with the FitSM service portfolio management.

The VI-SEEM authentication and authorization infrastructure relies on the Login service. It enables research communities to access VI-SEEM e-Infrastructure resources in a user-friendly and secure way. More specifically, the VI-SEEM Login allows researchers whose home organizations participate in one of the eduGAIN federations to access the VI-SEEM infrastructure and services using the same credentials they are using at their home institutions. Furthermore, the VI-SEEM Login supports user authentication through social identities, enabling even those users who do not have a federated account at home institutions to be able to seamlessly access the VI-SEEM services without compromising the security of the VI-SEEM infrastructure.

The provided infrastructure resources and services are mainly used through the development access, as well as through the calls for production use of resources and services. The VI-SEEM development access facilitates the development and integration of services by the selected collaborating user communities: climatology, life sciences, and cultural heritage. In this process, applications are given access to the infrastructure and necessary computational resources for a six-month period, during which application developers are expected to develop and integrate relevant services. The calls for production use of resources and services target specific communities and research groups that have already began development of their projects. These calls are intended for mature projects, which require significant resources and services to realize their workplans. Therefore, a significant utilization of the VI-SEEM resources comes from the calls for production use of resources and services, and an order-of-magnitude smaller utilization comes from the development access.

Federating Computation and Storage Resources to support Agricultural Science Communities

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ABSTRACT

Agricultural sciences are one of the largest and most significant examples of Big Data research communities. The development of this research field brings about demands for larger, more powerful and trustable computing infrastructures to support the work of agricultural scientists. On the other hand, Cloud and Grid technologies have emerged in the last decade as a way to integrate large-scale data infrastructures. In the present work, we describe a federation of large computation and storage infrastructures developed within the agINFRA project, and the interfaces to use them. The new data infrastructure and its interfaces allow different user profiles to access and take advantage of applications and services to manage, process, navigate, and visualize trustable information on agricultural science topics.

Keywords: Grid computing, cloud computing, federation, interfaces, big data.

1. INTRODUCTION

Agricultural sciences are one of the largest and most significant examples of Big Data research communities in growth the past decade. As the size of our knowledge grows and the science becomes more and more interconnected, the complexity of the scientific

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inquiry increases. Also, science is becoming largely digital - it needs to deal with ever increasing amounts of data and computational power. To engage the technological challenges of the scientific practice, it is necessary to efficiently build computing compounds that bring data analysis and processing to a new level.

The agINFRA data infrastructure aims to enhance the co-operation, data sharing, federation and data exchange between research communities in the agricultural sciences by providing a robust new data infrastructure to compliment the building of trust and federation between agricultural researchers, enhancing the field and creating new opportunities for joint work and research sharing.

2. THE AGINFRA INFRASTRUCTURE

AgINFRA has been conceived as a sustainable data infrastructure for agricultural research. The project addresses implementation of services relevant for a wide range of users: from infrastructure providers, developers of data processing and data management software, data providers, information managers, librarians, developers of high-level portals, to end-users (researchers, educators, citizens). Design of the infrastructure relies on adaptation of the existing resources, their customization, and the development of new components that will ensure balance in the system and its seamless use.

2.1 Science Gateways

On top of the Grid and Cloud infrastructure, the layer of Science gateways (SG) provides seamless access to the distributed infrastructure for software developers. Two different Science gateway architectures are deployed within the agINFRA project. Together, they address different usage patterns and requests, and complement each other in providing advanced grid access mechanisms.

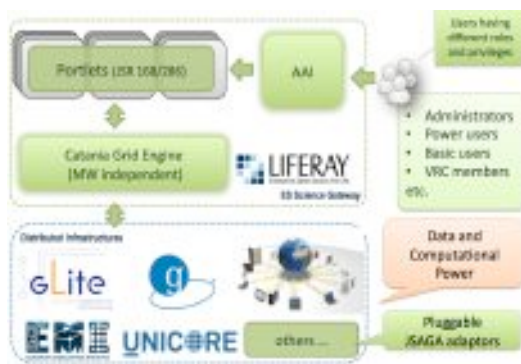


Figure 1. Catania SG Architecture



Figure 2. gUSE architecture

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The Catania Science Gateway, shown in Figure 1, provides a full-featured environment accessing with single software architecture to many distributed infrastructure resources. It also allows creating high-level user interfaces able to submit and control Grid jobs, manage data and metadata content, manage Cloud nodes, provide both secure and anonymous access to the Cloud hosted services and more in general avoid its user community to deal directly with the technicalities and the complexities of each specific distributed infrastructures.

SZTAKI has developed the gUSE (grid User Support Environment), shown in Figure 2, which is a grid virtualization environment providing a scalable set of high-level Grid services by which interoperability between Grids and user communities can be achieved. Incorporating a more flexible workflow concept and enabling its distribution on clusters and different Grid sites, gUSE is aimed to extend the objectives and features of P-GRADE Portal based on Liferay. SZTAKI is currently developing a generic-purpose gateway technology as a toolset to provide seamless access to major computing, data and networking infrastructures and services in Europe including clusters, supercomputers, and grids, academic and commercial clouds.

The SZTAKI SG implementation focuses on the management of complex job workflows, while the Catania SG implementation focuses on user membership management through the adoption of the Identity Federations and Identity Providers approach, allowing the single sign-on across many supported institutions, but also offering a vertical interface to all user levels.

2.2 AGINFRA STORAGE BACKEND

In parallel to the two general-purpose SG implementations, agINFRA RESTful gateway⁹ is provided as well, as a third agINFRA layer. This gateway is developed within the project, and its main responsibilities are cataloging, off-line processing, and management of data. As a catalog facility, agINFRA RESTful gateway keeps user's configurations of Grid-ported applications, datasets' metadata information and locations, arbitrary user-defined metadata information, and allows querying of these information.

The gateway carries out automatic replication of datasets, ensures the existence of the same dataset on different storage systems, and its exposure through the HTTP protocol. Instead of perpetual reorganization of schemas, the database back-end has been migrated to the document-oriented data model. Due to several additional features, such as offline replication, Multi-Version Concurrency Control, incremental replication, fault-tolerance, we have decided to replace MySQL with CouchDB¹⁰ technology. Existing tables and rows are reorganized into CouchDB JSON documents that could be now directly transferred via REST API incorporated in CouchDB.

⁹ agINFRA RESTful gateway documentation, <http://agro.ipb.ac.rs/>

¹⁰ CouchDB official web site, <http://couchdb.apache.org/>



2.3 Public Clouds

Some of the proposed agINFRA services require an on-demand delivery of service with a sort of interactive response such as agriDrupal and Omeka data components. The grid was initially designed to support long-term job runs, rather than online response capabilities. The integrated approach of agINFRA, requires also that the services (on Virtual Machines) should be available with an user friendly access to the infrastructure. For these reasons, agINFRA is able to connect with Cloud infrastructures, such as CLEVER (TUSA et al., 2010) and OKEANOS (KOUKIS et al. 2013).

3. LAYERED ARCHITECTURE

The conceptual architecture of agINFRA is depicted in Figure 3. On the top of the infrastructure lay the integrated services, existing portals that provide to end-users with high quality information on a specific topic or sub-domain of an agricultural science. Considered integrated service examples in agINFRA are Organic.Edunet (MANOUSELIS et al., 2009) portal, AGRIS (SUBIRATS et al., 2008) and CIARD RING (PESCE et al., 2011).

In a layer conceptually below integrated services are the data components, software packages that provided advanced data processing, management, visualization and navigation capabilities to users and integrated service managers.

If we look at the grid infrastructure conceptually in terms of APIs, the Figure 3, depicts its main elements. Web-based components and integrated services use APIs to access the infrastructure service layer.

In turn, these services use existing generic Grid resources. It should be noted that here the term “API” is used in a broad sense, as it includes any kind of interface exposed by the infrastructure, including REST APIs, exposure in the form of RDF LD, as well as any other mechanism for exposing data management and processing services.

In Figure 5 there is a detail of the agINFRA infrastructure showing how IS and data components can access two kinds of services Conceptually, there are four subsystems inside the infrastructure that fulfill different missions. The functional data flow and interactions with data components is shown in Figure 5.

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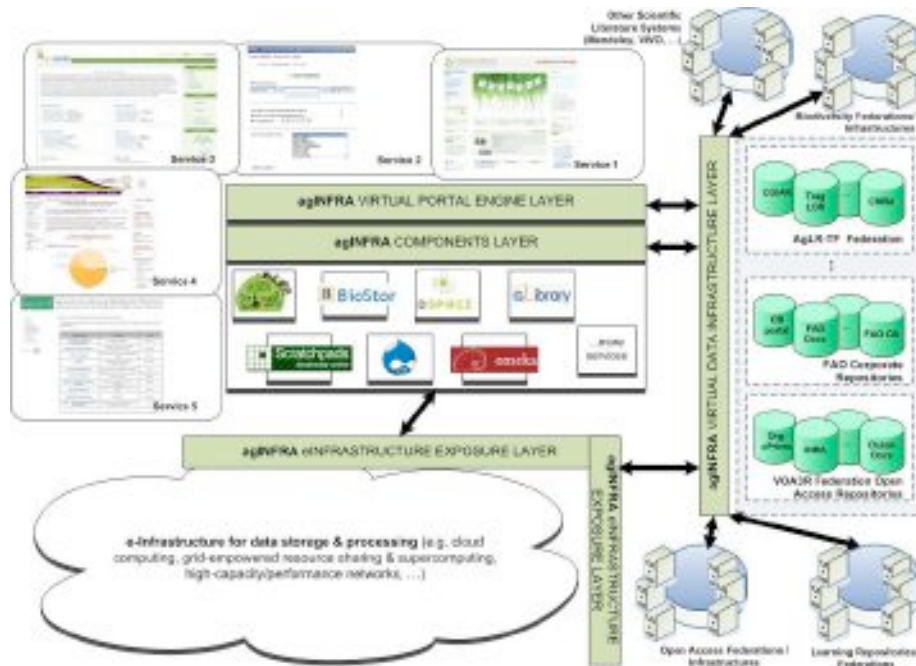


Figure 3. Conceptual infrastructure

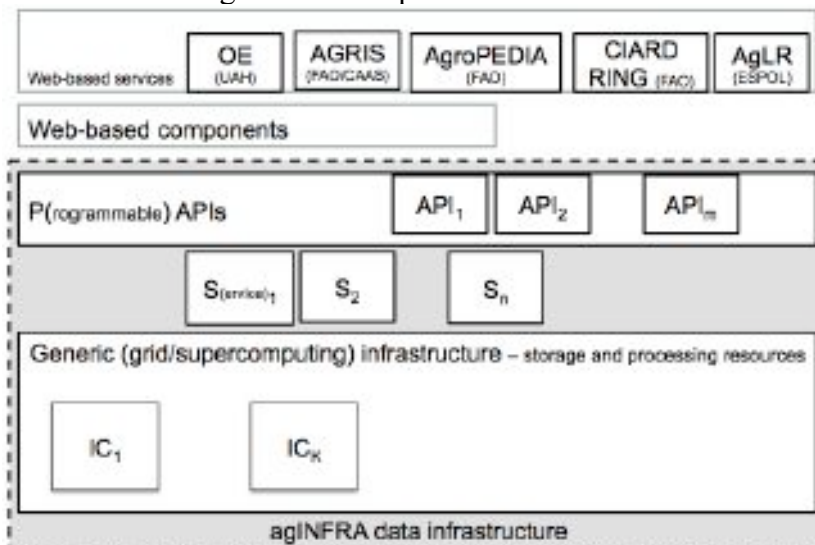


Figure 4. Layered view

The Data Management layer (DML) is responsible for the creation, update and management of datasets, including their metadata and actual contents when required. The DML offers a Dataset API externally and also to the rest of the internal elements, and acts as a central repository of datasets, its versions and derivatives. The Data Processing Layer (DPL) carries out the execution of offline jobs over the data. These jobs are scheduled using grid middlewares and provide users with non-interactive powerful computation services. The Data Transformation Layer (DTL) deals with metadata schema transformation services. These functions are key to interlink datasets

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and ensure interoperability of data. This adds an important value to the available content. Finally, the Data Exposure Layer (DEL) is in charge of exposing content and metadata in LD, allowing machines to consume high-quality integrated data and services.

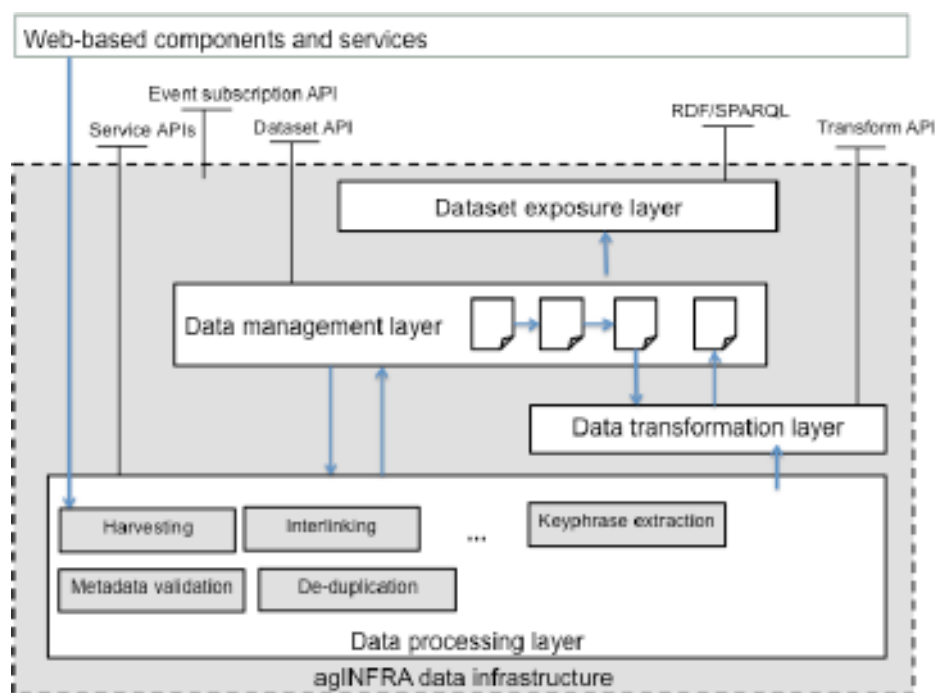


Figure 5. Functional data flow

4. RELATED WORK

Among the wide range of agINFRA related projects, the iPlant Collaborative (GOOF et al., 2011) is one of excellent examples of e-Infrastructures designed to solve challenges, here in particular for plant science. It successfully merges the plant biology tools and services for data analysis, mining and visualization, workflow and education resources. The project develops applications to support remote collaborations and virtual organizations.

The agINFRA science gateways provided by INFN and SZTAKI are an analogy to the iPlant DE. The science gateway technologies provide various modules for web-based graphical user interface creation, user-friendly data management, visual workflow construction, and application deployment in the Grid and HPC environments. In addition, science gateway frameworks, through Grid technology, supply authentication and authorization mechanism that naturally enables easy integration of geographically distributed new computing and storage resources. Furthermore, existing Grid components afford high-level meta-scheduling, workflow execution, task tracking, data and metadata catalogues, replication of data, delegation and renewal of credentials, accounting functionality, etc.



Environment provided by iPlant Atmosphere could be compared with gLite user interface machine (UI). Currently, in agINFRA UI machines can be used remotely at the infrastructure partners' resource centers through command line interfaces, and in some cases by VNC. The other possibility for a user is to install gLite-UI VM image locally at a personal computer. Such gLite-UI image is provided by INFN, and is available for download. Beside the standard gLite interface, this VM image can include particular agINFRA applications and tools. In both cases, user is provided with application programming interfaces (APIs), for software development or for specific data analysis. Furthermore, user is able to access to all agINFRA computing and storage resources, to use all previously installed applications, and to create various tasks workflows.

Under the scope of agINFRA, the SemaGrow¹¹ project aims to develop data intensive techniques to boost the real-time performance of global agricultural data infrastructures, achieving scalability when querying distributed and big data agricultural data repositories.

5. CONCLUSIONS

This paper describes the technical achievements of the project agINFRA. We have shown how existing technologies can be customized and integrated to set up the foundations to build an advanced data infrastructure to support agricultural science communities. This data infrastructure has been conceived as a set of layers that group different functionalities to manage datasets. These layers provide services that process, retrieve, store, transform and publish heterogeneous data easily.

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Ground state and collective modes of dipolar BECs

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We study the effects of the dipole-dipole interaction on the ground state and collective modes of quasi-one-dimensional dipolar Bose-Einstein condensates of atomic gases of chromium ^{52}Cr , erbium ^{168}Er , and dysprosium ^{164}Dy . Through extensive numerical simulations and detailed variational treatment, we analyze the dependence of condensate widths on the dipole-dipole interaction strength, as well as the interaction-induced frequency shifts of collective oscillation modes. Furthermore, we show that the Gaussian variational approach gives a good qualitative description of the system's ground state, and an excellent quantitative description of the condensates' low-lying excitation modes.

Parallel solvers for dipolar Gross-Pitaevskii equation

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We present serial and parallel semi-implicit split-step Crank-Nicolson algorithms for solving the dipolar Gross-Pitaevskii equation [1, 2], used for study of ultracold Bose systems with the dipole-dipole interaction. Six parallel algorithms will be presented: C implementation parallelized with OpenMP targeting single shared memory system [3], CUDA implementation targeting single Nvidia GPU [4], hybrid C/CUDA implementation combining the two previous approaches, and their parallelizations to distributed memory systems using MPI [5]. We first give an overview of the split-step Crank-Nicolson method and describe how the dipolar term is computed using FFT, which forms the basis of all presented algorithms. We then move on to describing the concepts used in each of the parallel implementations, and finally present a performance evaluation of each algorithm. In our tests OpenMP implementation demonstrates a speedup of 12 on a 16-core workstation, CUDA version has a speedup of up to 13, hybrid version has a speedup of up to 16, while the MPI parallelization yields a further speedup of 16 for the OpenMP/MPI version, speedup of 10 for the CUDA/MPI version, and speedup of 6 for the hybrid version.

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Q 17: Quantum Gases: Bosons I

Time: Tuesday 11:00–13:00

Location: e001

Group Report

Q 17.1 Tue 11:00 e001

Rosensweig instability and solitary waves in a dipolar Bose-Einstein condensate — ●MATTHIAS WENZEL, HOLGER KADAU, MATTHIAS SCHMITT, IGOR FERRIER-BARBUT, and TILMAN PFAU — 5. Physikalisches Institut and Center for Integrated Quantum Science and Technology, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany

Ferrofluids show unusual hydrodynamic effects due to the magnetic nature of their constituents. For increasing magnetization a classical ferrofluid undergoes a Rosensweig instability and creates self-organized ordered surface structures or droplet crystals.

In the experiment we observe a similar behavior in a sample of ultracold dysprosium atoms, a quantum ferrofluid. By controlling the short-range interaction with a Feshbach resonance we can induce a finite-wavelength instability due to the dipolar interaction.

Subsequently, we observe the spontaneous transition from an unstructured superfluid to an ordered arrangement of droplets by in situ imaging. These patterns are surprisingly long-lived and show hysteretic behavior. When transferring the sample to a waveguide we observe mutually interacting solitary waves. Time-of-flight measurements allow us to show the existence of an equilibrium between dipolar attraction and short-range repulsion. In addition we observe interference between droplets.

In conclusion, our system shows both superfluidity and translational symmetry breaking. This novel state of matter is thus a possible candidate for a supersolid ground state.

Q 17.2 Tue 11:30 e001

Rosensweig instability due to three-body interaction or quantum fluctuations? — VLADIMIR LONČAR¹, DUŠAN VUDRAGOVIĆ¹, ●ANTUN BALAŽ¹, and AXEL PELSTER² — ¹Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Serbia — ²Physics Department and Research Center OPTIMAS, Technical University of Kaiserslautern, Germany

In the recent experiment [1], the Rosensweig instability was observed in a ¹⁶⁴Dy Bose-Einstein condensate, which represents a quantum ferrofluid due to the large atomic magnetic dipole moments. After a sudden reduction of the scattering length, which is realized by tuning the external magnetic field far away from a Feshbach resonance, the dipolar quantum gas creates self-ordered surface structures in form of droplet crystals. As the underlying Gross-Pitaevskii equation is not able to explain the emergence of that Rosensweig instability, we extend it by both three-body interactions [2-4] and quantum fluctuations [5]. We then use extensive numerical simulations in order to study the interplay of three-body interactions as well as quantum fluctuations on the emergence of the Rosensweig instability.

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Q 17.3 Tue 11:45 e001

Phonon to roton crossover and droplet formation in trapped dipolar Bose-Einstein condensates — ●FALK WÄCHTLER and LUIS SANTOS — Institut für Theoretische Physik, Leibniz Universität Hannover, Hannover, Germany

The stability, elementary excitations, and instability dynamics of dipolar Bose-Einstein condensates depend crucially on the trap geometry. In particular, dipolar condensates in a pancake trap with its main plane orthogonal to the dipole orientation are expected to present under proper conditions a roton-like dispersion minimum, which if softening induces the so-called roton instability. On the contrary, cigar-shape traps are expected to present no dispersion minimum, and to undergo phonon (global) instability if destabilized. In this talk we investigate by means of numerical simulations of the non-local non-linear Schrödinger equation and the corresponding Bogoliubov-de Gennes equations the stability threshold as a function of the trap aspect ratio, mapping the crossover between phonon and roton instability. We will discuss in particular how this crossover may be observed in destabilization ex-

periments to reveal rotonization.

In a second part, motivated by recent experiments on droplet formation in Stuttgart, we introduce large conservative three-body interactions, and study how these forces affect the destabilization dynamics. We will discuss the ground-state physics of the individual droplets, and the crucial role that is played by the interplay between internal droplet energy, external center-of mass energy of the droplets, and energy dissipation in the nucleation of droplets observed in experiments.

Q 17.4 Tue 12:00 e001

Lattice Physics with Ultracold Magnetic Erbium — ●SIMON BAIER¹, MANFRED J. MARK^{1,2}, DANIEL PETER¹, KIYOTAKA AIKAWA¹, LAURIANE CHOMAZ^{1,2}, ZI CAI², MIKHAIL BARANOV², PETER ZOLLER^{2,3}, and FRANCESCA FERLAINO^{1,2} — ¹Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria — ²Institut für Quantenoptik und Quanteninformatik, Österreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria — ³Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, 6020 Innsbruck, Austria

Strongly magnetic atoms are an ideal systems to study many-body quantum phenomena with anisotropic and long-range interactions. Here, we report on the first observation of the manifestation of magnetic dipolar interaction in extended Bose-Hubbard (eBH) dynamics by studying an ultracold gas of Er atoms in a three-dimensional optical lattice. We drive the superfluid-to-Mott-insulator (SF-to-MI) quantum phase transition and demonstrate that the dipolar interaction can favor the SF or the MI phase depending on the orientation of the atomic dipoles. The system is well described by the individual terms of the eBH Hamiltonian. This includes the onsite interaction, which, additional to the isotropic contact interaction, can be tuned with the dipole-dipole interaction by changing the dipole orientation and the shape of the onsite Wannier functions. We find for the first time the presence of the nearest-neighbor interaction between two adjacent particles. Future work will investigate dipolar effects with erbium molecules and fermions as well as spin physics in our lattice system.

Q 17.5 Tue 12:15 e001

Strong-wave-turbulence character of non-thermal fixed points in Bose gases — ●ISARA CHANTESANA^{1,2,3} and THOMAS GASENZER^{2,3} — ¹Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany — ²Kirchhoff Institut für Physik, INF 227, 69120 Heidelberg, Germany — ³ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany

Far-from equilibrium dynamics of a dilute Bose gas is studied by means of the two-particle irreducible effective action formalism. We investigate the properties of non-thermal fixed points predicted previously, which are related to non-perturbative strong wave turbulence solutions of the many-body dynamic equations. Instead of using a scaling analysis, we study the Boltzmann equation of the scattering integral by means of direct integration equation for sound waves. In this way we obtain a direct prediction of the scaling behaviour of the possible fixed-point solutions in the context of sound-wave turbulence. Implication for the real-time dynamics of the non-equilibrium system are discussed.

Q 17.6 Tue 12:30 e001

Evidence of Non-Thermal Fixed Points in one-dimensional Bose gases — ●SEBASTIAN ERNE^{1,2,4}, ROBERT BÜCKER⁴, WOLFGANG ROHRINGER⁴, THOMAS GASENZER^{1,2,3}, and JÖRG SCHMIEDMAYER⁴ — ¹Institut für Theoretische Physik, Ruprecht-Karls-Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany — ²ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt, Germany — ³Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg, Germany — ⁴Vienna Center for Quantum Science and Technology (VCQ), Atominstytut, TU Wien, Vienna, Austria

This work investigates the rapid cooling quench over the dimensional- and quasicondensate-crossover. Analyzing experiments performed at the Atominstytut, we study the relaxation of such a far-from equilibrium system. The early stage of condensate formation is dominated

Faraday Waves in Dipolar Bose-Einstein Condensates

Dušan Vudragović^a and Antun Balaž^a

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Abstract. We study the emergence of Faraday waves in quasi-one-dimensional dipolar Bose-Einstein condensates of ^{52}Cr and ^{164}Dy subject to periodic modulation of the radial confinement. We investigate through extensive numerical simulations and detailed variational treatment the effects of the strong dipolar interaction on the spatial and time-period of the Faraday waves. Unlike in the case of homogeneous [1] or inhomogeneous contact interactions [2], the emergence of Faraday waves is found to further destabilize the condensate in the presence of strong dipolar interaction. The interesting effect of spatial period variation of generated density patterns is observed numerically and studied within the Gaussian variational approach.

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1. Balaž, A., and Nicolin, A. I., *Phys. Rev. A* **85**, 023613 (2012).
2. Balaž, A., Paun, R., Nicolin, A. I., Balasubramanian, S., and Ramaswamy, R., *Phys. Rev. A* **89**, 023609 (2014).

semiclassical approximation and derive with this self-consistency equations between the disorder ensemble-averages of particle density and condensate density. Invoking, furthermore, the Thomas-Fermi approximation we obtain results that reproduce for weak disorder the seminal results of a Bogoliubov theory of dirty bosons [1-3], but do not yield for strong disorder a Bose-glass phase. Afterwards, we go beyond the Thomas-Fermi approximation and perform a full numerical treatment of the self-consistency equations based on the Crank-Nicolson split-step semi-implicit imaginary-time propagation [4], which yields a quantum phase transition to a Bose-glass phase for strong disorder [5].

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- [1] K. Huang, H.-F. Meng, Phys. Rev. Lett. 69, 644 (1992).
- [2] G. M. Falco, A. Pelster, R. Graham, Phys. Rev. A 75, 063619 (2007).
- [3] G. M. Falco, A. Pelster, R. Graham, Phys. Rev. A 76, 013624 (2007).
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- [5] P. Navez, A. Pelster, R. Graham, Appl. Phys. B 86, 395 (2007).

Faraday Waves in Dipolar Bose-Einstein Condensates

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We present the emergence of Faraday waves in cigar-shaped ^{52}Cr and ^{164}Dy Bose-Einstein condensates. These density waves are induced by periodic modulation of the frequency of the trapping potential. We study through extensive numerical simulations and detailed variational treatment the effects of the strong dipolar interaction on the spatial and time-period of the Faraday waves. Unlike in the case of homogeneous [1] or inhomogeneous contact interactions [2], the emergence of Faraday waves is found to further destabilize the condensate in the presence of strong dipolar interaction. The interesting effect of spatial period variation of generated density patterns is observed numerically and studied within the Gaussian variational approach.

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- [2] A. Balaž et al., Phys. Rev. A 89, 023609 (2014).

Q 12: Quantum Gases: Bosons II

Time: Monday 14:30–16:30

Location: P/H2

Q 12.1 Mon 14:30 P/H2

Dynamics of Bose-Einstein condensates in a one-dimensional correlated disorder potential — ●JUAN PABLO RAMÍREZ VALDES¹, ANDREAS BUCHLEITNER^{1,2}, and THOMAS WELLENS¹ — ¹Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Herman-Herder-Str. 3, 79104 Freiburg, Germany — ²Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität, Albertstr. 19, 79104 Freiburg

We study the expansion of an initially confined one-dimensional Bose-Einstein condensate in a weak random potential with finite correlation length. At long times, the expansion comes to a halt due to destructive interferences leading to Anderson Localization [1]. We develop an improved analytical description of the asymptotic disorder-averaged condensate density, which we compare to the results of numerical simulations based on a finite-element discrete variable representation. In particular, we thereby analyze the influence of inter-atomic interactions on the localization properties.

[1] L. Sanchez-Palencia, D. Clément, P. Lugan, P. Bouyer, G. V. Shlyapnikov, and A. Aspect, *Phys. Rev. Lett.* **98**, 210401 (2007).

Q 12.2 Mon 14:45 P/H2

Growing bosonic Laughlin states in a lattice — FABIAN GRUSD^{1,2}, ●FABIAN LETSCHER¹, MOHAMMAD HAFEZI^{3,4}, and MICHAEL FLEISCHHAUER¹ — ¹Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — ²Graduate School Materials Science in Mainz, Gottlieb-Daimler-Strasse 47, 67663 Kaiserslautern, Germany — ³Joint Quantum Institute, NIST/University of Maryland, College Park, Maryland 20742, USA — ⁴ECE Department and Institute for Research in Electronics and Applied Physics, University of Maryland, College Park, Maryland 20742, USA

We present a scheme for the preparation of highly correlated Laughlin states in bosonic lattice systems. The scheme is based on the idea of growing such states by adding weakly interacting composite fermions along with magnetic flux quanta one by one. The topologically protected Thouless pump is used to create two localized flux quanta resulting in a hole excitation, which is subsequently filled by a single boson using a coherent pump. A single boson together with one flux quantum forms a composite fermion. Using our protocol, filling $\nu = 1/2$ Laughlin states can be grown in a time increasing linearly with the particle number N and strongly suppressed number fluctuations. Furthermore, we analyse the scaling of the fidelity with particle number N , including particle loss and nonadiabatic transitions. We present exact numerical simulations in small lattice systems to show the feasibility of our scheme.

Q 12.3 Mon 15:00 P/H2

Twisted superfluidity in optical lattices — ●OLE JÜRGENSEN, KLAUS SENSTOCK, and DIRK-SÖREN LÜHMANN — Institut für Laserphysik, Universität Hamburg

An unconventional quantum phase with a complex order parameter has been observed recently in a hexagonal optical lattice [1] but still lacks a conclusive theoretical understanding. We show how correlated pair tunneling in the extended Bose-Hubbard model can drive the transition to this *twisted* superfluid phase. We present the full phase diagram showing a multitude of quantum phases including checkerboard insulators, supersolids and pair superfluids. Furthermore, off-site interactions support dimerized insulator phases where particles are delocalized on several lattice sites. For two components we find twisted superfluid phases already for surprisingly small pair-tunneling amplitudes. Interestingly, this ground state shows an infinite degeneracy ranging continuously from a supersolid to a twisted superfluid.

[1] P. Soltan-Panahi *et al.*, *Nature Physics* **8**, 71 (2012).

Q 12.4 Mon 15:15 P/H2

Bose-Hubbard ladder subject to effective magnetic field: geometry and dynamics — ●WLADIMIR TSCHISCHIK, RODERICH MOESSNER, and MASUD HAQUE — Max Planck Institute for the Physics of Complex Systems, Dresden

Motivated by a recent experimental realization of an optical lattice system with an effective magnetic field (Atala *et al.*, *Nature Physics* **10**, 588 (2014)), we study a Bose-Hubbard system on a two-leg lad-

der with complex hopping amplitudes. This system shows a quantum phase transition already without interactions. We examine and present differences between the periodic, open-boundary, and harmonically trapped cases. We present a striking "slowing down" effect in the collective mode dynamics near the phase transition.

Q 12.5 Mon 15:30 P/H2

Faraday Waves in Dipolar Bose-Einstein Condensates — DUŠAN VUDRAGOVIĆ and ●ANTUN BALAŽ — Scientific Computing Laboratory, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We study the emergence of Faraday waves in quasi-one-dimensional dipolar Bose-Einstein condensates of ⁵²Cr and ¹⁶⁴Dy subject to periodic modulation of the radial confinement. We investigate through extensive numerical simulations and detailed variational treatment the effects of the strong dipolar interaction on the spatial period of the Faraday waves. Unlike in the case of homogeneous [1] or inhomogeneous contact interactions [2], the emergence of Faraday waves is found to further destabilize the condensate in the presence of strong dipolar interaction. The interesting effect of spatial period doubling of generated density patterns is observed numerically and studied within the Gaussian variational approach.

[1] A. Balaž and A. I. Nicolin, *Phys. Rev. A* **85**, 023613 (2012).

[2] A. Balaž, R. Paun, A. I. Nicolin, S. Balasubramanian, and R. Ramaswamy, *Phys. Rev. A* **89**, 023609 (2014).

Q 12.6 Mon 15:45 P/H2

Ground states for the Bose-Hubbard model with flat bands — ●PETRA PUDLEINER¹ and ANDREAS MIELKE² — ¹Institute of Physics, Johannes Gutenberg University, Mainz, Germany — ²Institute for Theoretical Physics, Ruprecht-Karls University, Heidelberg, Germany

Flat band systems have been studied intensively in experiment and theory. They are a prototype for strongly correlated systems. Especially for bosons in a flat band, several interesting questions arise: What is the nature of the ground state? Are there regions in phase space where one can see a Bose transition?

The Bose-Hubbard model is used to visualize low energies on two-dimensional lattices which exhibit a lowest flat energy band. Up to the critical lattice filling constant, an eigenstate of the aforementioned band can be constructed by means of the charge density wave (CDW) as many-body ground state. Huber and Altman [1] explored ground states in the vicinity of the critical filling on the kagome lattice via a mean-field calculation; however, by restricting the calculation to a weakly interacting Hamiltonian.

The purpose of this talk is, firstly, to present similar results which are obtained by transferring their methods to the checkerboard lattice and, secondly, to demonstrate initial steps to extend to strong interactions. In this regard, one boson is added to the well-known ground state. The distribution of this additional particle seems to be localized, in contrast to the weakly interacting limit; here we observe a Bose condensation.

[1] S. Huber and E. Altman, *PRB* **82**, 184502 (2010)

Q 12.7 Mon 16:00 P/H2

Realistic matter-wave interferometry with non-unitary operators — ●LUIS FERNANDO BARRAGÁN-GIL and REINHOLD WALSER — Institut für angewandte Physik, Technische Universität Darmstadt, Hochschulestr. 4a, 64289 Darmstadt

The realization of Bose-Einstein condensates in μ -gravity conditions, at the ZARM drop tower in Bremen by the QUANTUS collaboration [1,2], has opened the possibility to measure corrections to local gravitational field of the Earth beyond the linear Earth's acceleration (g) [3,4]. This is known as the gravity gradient correction and it is the next dominant contribution found in classical Newtonian Physics as well as in general relativistic view of gravity.

We use thermal ensembles and non-unitary operator formalism [5] (particle loss, temperature, realistic detector) to implement an atom interferometer in the presence of the harmonic corrections to the gravitational potential, and look for the effects of misalignment and temperature on the fringe pattern.

[1] Quantus Collaboration <http://www.iqo.uni-hannover.de/quantus.html>

Chapter 15

Science Gateway for the Serbian Condensed Matter Physics Community

Dušan Vudragović and Antun Balaž

Abstract The Academic and Educational Grid Initiative of Serbia hosts and maintains the scientific gateway of the Serbian condensed matter physics community. The gateway is built around a code set addressing problems from the physics of ultracold quantum gases, solving the nonlinear Schroedinger equation, the Gross–Pitaevskii equation in real and imaginary time, and a path integral algorithm for estimation of quantum-mechanical transition amplitudes, which are relevant for various applications. Here we present the realization of the gateway and technologies used for its implementation.

15.1 Introduction

Condensed matter physics and materials science address problems that highly relevant for fundamental research, as well as for practical applications and society. The development of high-impact materials with enhanced and engineered properties, or research in quantum information, for example, depend on the results from these areas of physical sciences, and contribute to the IT and smartphone industry, semiconductor technology, the energy sector, and others.

Numerical simulations are now indispensable tools in science and technology, and are used to speed up the research and development while decreasing the costs. In condensed matter physics, scientists deploy a broad range of algorithms, such as solving nonlinear partial differential equations, classical and quantum Monte Carlo techniques, including solving of the Bose–Hubbard and Fermi–Hubbard models, exact diagonalization techniques for strongly correlated systems, etc. Whichever

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algorithm is used, typically it requires large-scale computing resources for simulations of relevant physical systems.

In the Serbian condensed matter physics community (CMPC), the most prominent use of computing resources is related to the three applications developed at the national level: SPEEDUP, QSPEEDUP, and GP-SCL.

SPEEDUP code (Balaz 2012-1) uses Monte Carlo-based path integral algorithms for the calculation of quantum mechanical transition amplitudes for 1D models. It is based on the use of higher-order short-time effective actions in the time of propagation (Monte Carlo time step), which substantially improves the convergence of discretized amplitudes to their exact continuum values.

QSPEEDUP code (Vudrag 2010) presents a quasi-Monte Carlo extension of the SPEEDUP code. The extended algorithm uses Sobol's set of quasi-random numbers for generation of trajectories relevant for calculation of transition amplitudes in the path integral formalism. Both applications use identical algorithm, supplied with different random number generators, which allows their unification into a single application designated as (Q)SPEEDUP.

GP-SCL (Vudrag 2012) is a set of codes parallelized using the OpenMP approach for calculating the dynamics and ground states of quantum fluids (such as Bose–Einstein condensates and superfluids). Quantum fluids represent macroscopic quantum phenomena where large numbers of atoms or molecules behave coherently, allowing special properties to emerge. In the mean-field regime, such systems can be described by a nonlinear Schroedinger equation, usually called the Gross–Pitaevskii equation (Pethick 2008). GP-SCL codes solve the time-(in) dependent Gross–Pitaevskii nonlinear partial differential equation in one, two, and three space dimensions in an arbitrary trapping potential using imaginary-time and real-time propagation. The equation is solved using the semi-implicit split-step Crank–Nicolson method by discretizing space and time, as described in Murug (2009). The discretized equation is then propagated in imaginary or real time over small time steps.

Applications have been developed by scientists from the Scientific Computing Laboratory (SCL 2014) of the Institute of Physics Belgrade (IPB 2014) and are used by an increasing number of collaborators within Serbia and also from other countries in Europe, as well as from Brazil, India, and China. The applications are deployed on the computing infrastructure provided by the Academic and Educational Grid Initiative of Serbia (AEGIS 2014), which is part of the European Grid Infrastructure (EGI 2014).

To increase the potential user base of the applications, we have decided to create the AEGIS CMPC science gateway (SG) in the framework of the SCI-BUS project (SCI-BUS 2014), to provide seamless access to the software and the data generated by the applications. This science gateway also hides the complexity of use of the Grid and applications, which was a barrier for many scientists.

15.2 Building the Science Gateway

Before the AEGIS CMPC science gateway was built and put into production, the default interface to DCI within the AEGIS CMPC was based on gLite technology provided by the European Middleware Initiative (EMI 2014). This is a command line interface, and it requires a personal certificate issued by one of recognized certificate authorities, membership in a virtual organization (VO) that supports the applications, and access to a user interface (UI) machine. A personal certificate is obtainable from the national AEGIS CA, while the Serbian AEGIS National Grid Initiative provides the VO membership service. A central UI machine is available at the IPB, but within the community personal UI virtual machines are used as well.

In this approach, the use of AEGIS CMPC applications requires preparation of a parameter input file that describes the physical system of interest. In addition, the DCI description of computational task has to be prepared as well. In a gLite-based UI machine this is typically done using the Job Description Language (JDL). Depending on machine architecture and the software stack provided by DCI in terms of available compilers, a CMPC application could be compiled locally at a UI machine or remotely at a DCI, on a target worker node. In the first case, a statically linked executable is submitted to the predefined architectures, while in the latter case the source code is transferred to the computation node, where one of the various predeployed compilers performs the compilation. A CMPC application with a physical system description from the parameter input file and with a DCI description of the computational task from the JDL file is submitted from the UI machine to the DCI by the gLite command line interface. Further job management (job cancelation, monitoring, and output retrieval) is done by the gLite command line interface as well.

This approach demands several skills: knowledge of CMPC application source codes and their parallelization techniques, knowledge of different compiler technologies, knowledge of Linux operating system and its common tools, and knowledge of gLite command line interface and DCI technology. This variety of skills, which is required for solving even trivial problems, creates a strong barrier that prevents ready use of CMPC applications within the community, and adversely affects attracting new people who are interested in numerical simulations based on the available set of codes. Since the knowledge of the underlying physics (quantum theory and Bose–Einstein condensation) and understanding of CMPC applications should be the only real requirements, the development of a scientific gateway effectively solves the identified problems and enables new users to perform numerical simulations in this field without much technical knowledge of the operating system, compiler technology, low-level DCI interface, and DCI itself. Furthermore, AEGIS CMPC SG promotes sharing of the results of simulations within the community, and in this way increases understanding of the behavior of particular physical systems of interest.

The desired level of automation of CMPC applications is achieved through the use of WS-PGRADE/gUSE (gUSE 2014) workflows. For example, typical usage of

the GP-SCL application first requires calculation of the ground state of the system, achieved by the imaginary-time propagation until convergence is reached, and then, starting from this result, one can study the dynamics of the system through the real time-propagation. A workflow concept unifies these two kinds of time-propagation algorithms into a single task, hiding the complexity from the end user. Furthermore, besides the results in the form of raw data that describe the propagation of the system in time, AEGIS CMPC scientific gateway provides visualization of the propagation in the form of graphs and movies.

In the case of the (Q)SPEEDUP codes, numerical convergence of quantum-mechanical transition amplitudes to their continuum values is achieved only when the number of Monte Carlo samples goes to infinity. The central limit theorem states that the statistical distribution of numerical results obtained using a large number of independent Monte Carlo samples is always a Gaussian. This allows automation of a process workflow for a desired maximal error of calculated transition amplitude, which is introduced as a new, more generic input parameter. In other words, for a described physical system of interest and predefined acceptable error of the result, AEGIS CMPC SG workflow provides sufficient statistics in execution of the code to achieve the desired accuracy of the amplitude.

15.3 Architecture of the Science Gateway

AEGIS CMPC science gateway has been developed to support SPEEDUP, QSPEEDUP, and GP-SCL applications. These programs are fully written in the C programming language, and do not depend on any external library. Codes could be compiled with different popular compilers: GNU's gcc compiler, Intel's icc compiler, IBM's xlc compiler, PGI's pgcc compiler, and Oracle's suncc (former Sun) compiler. Besides serial versions of the codes, parallel versions are produced as well. In the case of SPEEDUP and QSPEEDUP applications, parallelization is achieved through the message passing interface (MPI), while the GP-SCL code is parallelized using OpenMP API. All codes are accompanied by appropriate makefiles, which allow specification of the compiler, type of parallelization, and customization of compiler optimization flags. These makefiles play a significant role in the porting process, and simplify utilization of various hardware resources.

Although applications use different algorithms, from a purely technical point of view they have the common use scenario: for a particular description of physical system of interest, given in the form of a single input file, after considerable number-crunching each application produces corresponding output with numerical results. The generated numerical results are analyzed, classified, and visualized by the scientific gateway. This allows for the creation of a generic architecture for all AEGIS CMPC applications.

The generic architecture behind the AEGIS CMPC scientific gateway is illustrated in Fig. 15.1. It consists of four main blocks: the AEGIS CMPC portal, the

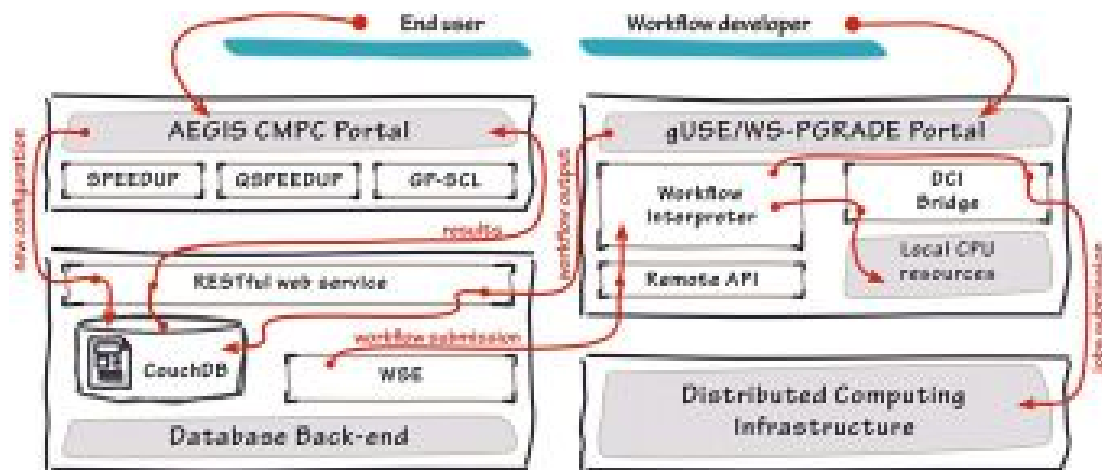


Fig. 15.1 Generic architecture behind AEGIS CMPC workflows

WS-PGRADE/gUSE portal, the database back-end, and the DCI used for calculations.

The AEGIS CMPC portal (CMPC 2014) (Fig. 15.2) is a user-oriented interface that visually unifies outputs of SPEEDUP, QSPEEDUP and GP-SCL applications. It provides a summary of collected numerical results, which is organized per application and per configuration of a physical system. In addition, the AEGIS CMPC portal allows querying of the available configurations, as well as submission of new configurations. While the submission requires authentication, browsing of the results is publicly available. Applications' configurations and results are stored in the database back-end. Communication between the portal and the database is established through a dedicated RESTful web service. On the database side, the

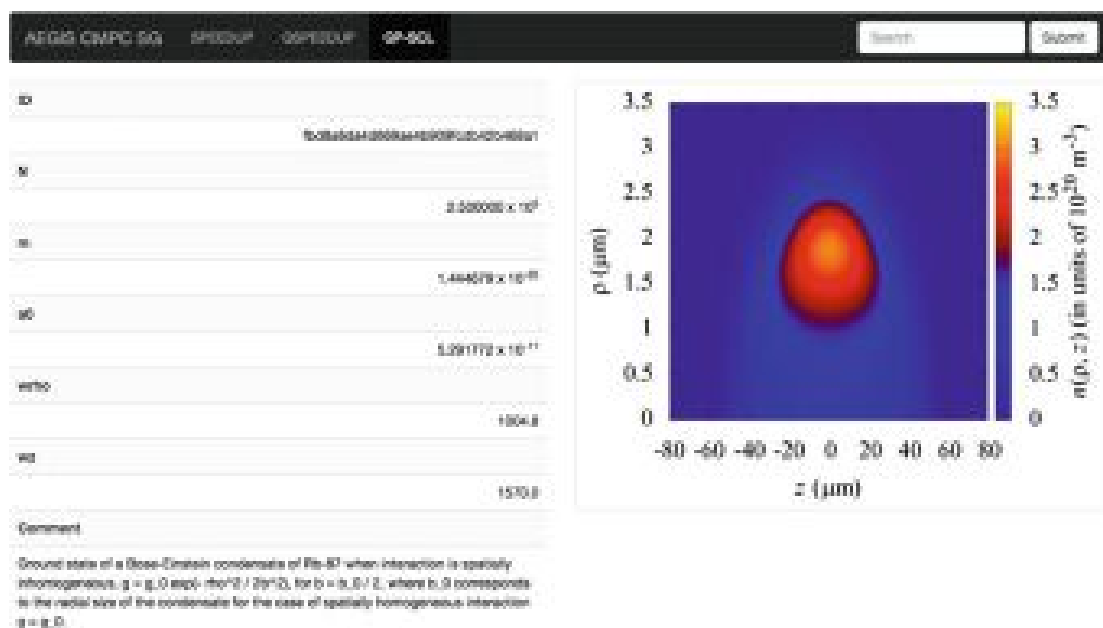


Fig. 15.2 GP-SCL view of the AEGIS CMPC Portal

workflow submission engine (WSE) daemon process looks for configurations waiting for the executions, and performs application-specific workflow submission through the WS-PGRADE/gUSE Remote API interface. The portal was developed within the Google Web Toolkit (Tacy 2013) environment using Bootstrap (Cochran 2012) front-end framework, and it was deployed through the Apache Tomcat (Brittain 2007) server (available at: <http://sci-bus.ipb.ac.rs/>).

The WS-PGRADE/gUSE Portal is a workflow developer-oriented interface based on the WS-PGRADE/gUSE technology. It allows creation of new workflows, modification of existing ones, and manual testing. Use of the portal requires a Liferay-based (Liferay 2014) account, a valid digital certificate and membership in cmpc.aegis.rs VO. Potential users are able to request Liferay-based account by filling out the generic Liferay Create Account form available at home page of AEGIS CMPC SG. The National Grid Initiative (NGI) AEGIS VOMS-admin portal provides management of cmpc.aegis.rs VO membership. The membership request form of the VOMS-admin portal requires a digital certificate, and therefore, in order to fill it out, a workflow developer has to import a personal certificate into the web browser. The AEGIS WS-PGRADE/gUSE Portal extends the default WS-PGRADE/gUSE installation with the Remote API plugin that enables usage of the core gUSE services without the WS-PGRADE user interface component. The Remote API allows one to run and manage workflows from a custom user interface, such as the AEGIS CMPC Portal.

Workflows of AEGIS CMPC applications are created within the WS-PGRADE/gUSE Portal, and are exposed for the external usage through the Remote API component. Since SPEEDUP and QSPEEDUP applications use identical algorithms, just supplied with different random number generators, both applications use a single workflow—a (Q)SPEEDUP workflow. In order to minimize the network overhead, all application binaries are preinstalled on each of DCI resource centers supporting the cmpc.aegis.rs VO. The VO software area is used for this purpose, while the installation and upgrade of particular applications is performed by VO managers.

The workflow behind the (Q)SPEEDUP application is illustrated in Fig 15.3. It has three main components:

- (Q)SPEEDUP-PREPARATION retrieves user-defined physical system configurations from the database. Retrieved JSON output is then converted to the application-specific configuration file, which is forwarded to the next process in the workflow. Together with the configuration file, technical metadata (consumed CPU time, application version, random number generator stream, etc.) produced in this part of the workflow are forwarded to the next process. This is not a CPU-intensive task, and it is executed at the server that hosts the WS-PGRADE/gUSE portal (localhost).
- (Q)SPEEDUP-EXECUTION is responsible for the application execution at the DCI, and then it retrieves the results. It equips the application with the wrapper that is able to determine the location of the preinstalled application at the DCI, supply input parameters, initiate execution, and collect results. This CPU-intensive

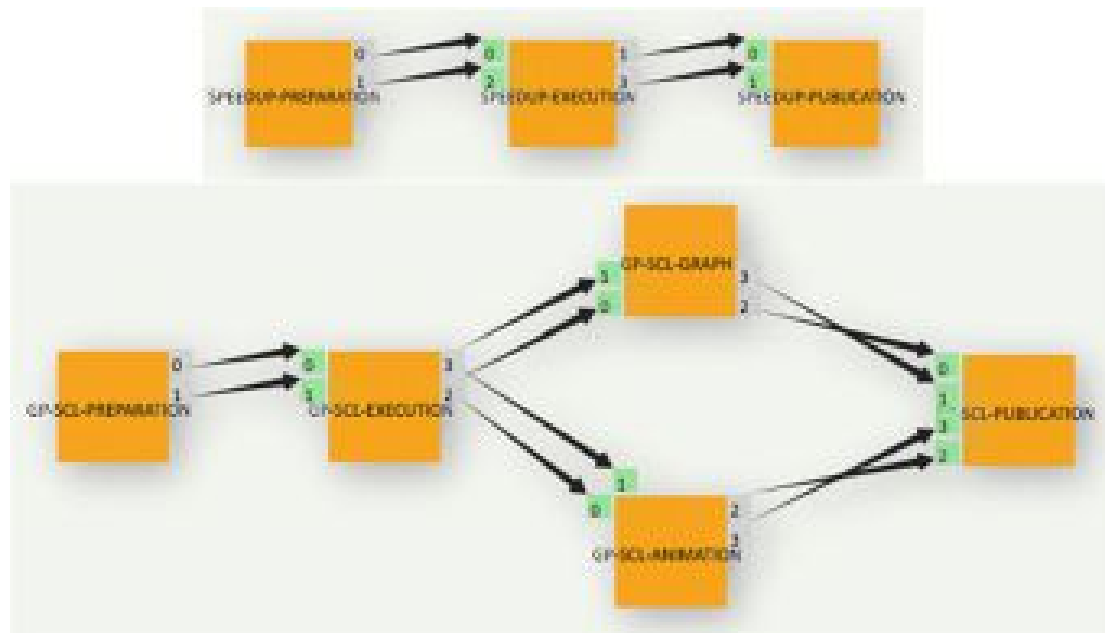


Fig. 15.3 AEGIS CMPC (Q)SPEEDUP (*top*) and GP-SCL (*bottom*) workflows

task is executed on the DCI. Outputs of the application are permanently stored on the storage elements provided by the DCI, while the workflow engine is informed of their locations.

- (Q)SPEEDUP-PUBLICATION transforms the collected results from the previous two tasks to a corresponding JSON structure, and stores the result in the database through the RESTful web service.

The AEGIS CMPC GP-SCL portlet relies on the workflow illustrated in Fig. 15.3. The workflow has the following components:

- GP-SCL-PREPARATION retrieves the physical system configuration from the database, and produces an application-specific parameter input file. The task is executed on the server hosting the WS-PGRADE/gUSE portal. Technical metadata collected in this part of the workflow are forwarded to the next process. Each node in the workflow will expand this initial metadata structure, while the last node will upload collected metadata together with the application results to the database.
- GP-SCL-EXECUTION performs submission of the simulation to the DCI and output retrieval. After the execution, the produced results are divided between two tasks running in parallel: GP-SCL-GRAPH and GP-SCL-ANIMATION. Results are permanently stored on the DCI, and only their locations are transferred back to the science gateway.
- GP-SCL-GRAPH produces graphs requested in the configuration. Graphs are produced using gnuplot-based APIs. This task is not CPU-intensive, and therefore it is performed on the local machine. Only part of the total output

produced within the GP-SCL-EXECUTION task is transferred from the DCI to the machine running the science gateway for this purpose.

- GP-SCL-ANIMATION produces animation (movie) of a dilute, trapped Bose–Einstein condensate evolution in time. This part of the workflow is CPU intensive and is executed on the DCI.
- GP-SCL-PUBLICATION accumulates results, technical metadata, graphs, and locations of the movies, and stores them in the document-oriented database.

AEGIS CMPC DB is a document-oriented database that stores configurations and numerical results from all applications supported by the science gateway. Initially, it was deployed using a relational database, but with the increase of the number of physical properties to be monitored, it has become very difficult to break-out the design of the SG into relational schemas. Instead of perpetual reorganization of schemas, the database back-end has been migrated to the document-oriented data model. Due to several additional features, such as offline replication, multiversion concurrency control, incremental replication, and fault-tolerance, MySQL technology (Harrison 2008) has been replaced by CouchDB technology (Anderson 2009).

Querying of and structuring the information available in the science gateway is realized by CouchDB views. Different views are constructed by functions that act as a mapping part of the map/reduce operation. These functions take the documents and transform them into single values that they return. CouchDB indexes the view and keep the indexes updated as new documents are added, removed, or updated.

Authentication and authorization of the requests coming to the AEGIS CMPC SG, together with the tracking and merging mechanisms, are implemented as an additional layer placed in front of the CouchDB. In order to change or add new information (POST and PUT methods), a workflow developer has to be authenticated and authorized; however, reading of information is publicly available (GET method). Authentication and authorization could be done by username/password, an X.509 certificate, or an X.509 RFC 3,820-compliant proxy certificate; this is followed by an update of the document with the JSON tracking structure. This section contains workflow developer information, the IP address of the client from which the request was triggered, and the timestamp of the action. For this reason, each document stored in AEGIS CMPC CouchDB has additional JSON structure related to the tracking mechanism.

All documents stored in CouchDB are versioned, and CouchDB determines which of the changes will be stored as the latest revision. When doing this, it does not attempt to merge the conflicting revision. A developer always decides how the merging should be done, and it is up to a developer to specify the latest revision. This task is simplified with the AEGIS CMPC CouchDB merging mechanism, and a workflow developer no longer needs to deal with the CouchDB revisions. The system automatically discovers the latest version of a particular document, and performs merging of the existing information with additional information. Existing CouchDB documents could be updated with different or new information only, which is not the case in the standard CouchDB model. In addition, the AEGIS

CMPC CouchDB instance sanctions DELETE requests in order to prevent loss of any information.

DCI used by the AEGIS CMPC SG is organized around the `cmpc.aegis.rs` VO. Establishment of a separate VO has allowed lobbying at the resource providers for additional or new resources. Also, it guarantees execution of jobs submitted from the scientific gateways in reasonable time, and provides an exact mechanism for tracking the of number of users, CPU usage, and other DCI-related statistics. The `cmpc.aegis.rs` VO is currently supported by three NGI_AEGIS Grid sites, part of EGI infrastructure (AEGIS01-IPB-SCL, AEGIS04-KG, and AEGIS11-MISANU), and by the largest HPC installation in Serbia, the PARADOX cluster, totaling to more than 2,700 CPUs and 140 TBs of storage space. Recently, AEGIS CMPC scientific gateway has been also supported by the largest HPC installation in Serbia. PARADOX cluster is equipped with 1,696 Sandy Bridge CPUs at a frequency of 2.6 GHz, 106 NVIDIA Tesla M2090 GPU cards, and 100 TBs of storage space. It is interconnected via the QDR Infiniband technology, and achieves peak computing performance of 105 TFlops.

Management of VO membership is centralized and provided by the NGI_AEGIS VOMS-admin portal. Core Grid services necessary for users to be able to access all computing and data storage resources are provided by the NGI_AEGIS as well, in particular: the BDII information system (`bdii.ipb.ac.rs`), workload management system (`wms.ipb.ac.rs`, `wms-aegis.ipb.ac.rs`), logging and bookkeeping service (`lb.ipb.ac.rs`, `lb-aegis.ipb.ac.rs`), myproxy service (`myproxy.ipb.ac.rs`), and logical file catalogue (`lfc.ipb.ac.rs`). All services are running the latest version of the middle-ware EMI 3 (Monte Bianco) release.

15.4 Usage of the Scientific Gateway

AEGIS CMPC SG achieved production mode in September 2013. Currently, there are 20 registered users, and according to the EGI accounting portal, 19,000 `cmpc.aegis.rs` VO jobs have been so far submitted from the portal. Jobs are uniformly distributed over the CMPC applications, while the average execution time per job is around 24 h.

With the introduction of the science gateway, the CPMC job success rate has dramatically increased. One of the indicators is the ratio between totally consumed CPU time and the number of jobs. Currently this ratio is approximately 23 h, which corresponds to the average execution time per job. In the case of failures, this time would be smaller. Users are allowed to tune application's configuration only, so there is not much space for changes that will lead to application crashes or an unpredictable behavior. Also, only CPU-intensive parts of the workflow are executed on the DCI, and other tasks are executed locally, on the machine running the science gateway. The success rate of the local jobs is practically 100 %, while the jobs submitted to the DCI may fail due to various infrastructure problems. For this reason, each job submitted to the DCI is configured to allow automatic resubmission.

There are two kinds of resubmissions supported by the NGL_AEGIS DCI: deep resubmission and shallow resubmission. The resubmission is deep when the job fails after it has started running on the computation node, and shallow otherwise. Both deep and shallow resubmissions are limited by default to five attempts for AEGIS CMPC SG jobs. Furthermore, even if after these five attempts (Q)SPEEDUP job fails, it will not affect the results, since they are obtained using a large number of independent jobs. For GP-SCL jobs this is not the case, and results will not be produced if the workflow node fails. This could be overseen by an additional module that monitors relations between configurations and corresponding results, and performs complete workflow resubmissions when necessary.

In this period, AEGIS CMPC SG was mainly used for:

- Study of Faraday waves in binary nonmiscible Bose–Einstein condensates (Balaz 2012-2);
- Study of Faraday waves in single-component Bose–Einstein condensates with spatially inhomogeneous atomic interactions (Balaz 2014), as well as condensates with dipolar interactions (Nikolic 2013);
- Study of fragmentation of a Bose–Einstein condensate through periodic modulation of the scattering length (Vidan 2011);
- Study of geometric resonances in Bose–Einstein condensates with two- and three-body interactions (Jibbouri 2013).

Using the numerical results obtained via the AEGIS CMPC SG and analytical variational calculations, it was shown that elongated binary nonmiscible Bose–Einstein condensates subject to periodic modulation of the radial confinement exhibit a Faraday instability, similar to that seen in one-component condensates. Modulation of the radial confinement leads to the emergence of density waves in the longitudinal direction. Considering two hyperfine states of rubidium condensates, AEGIS CMPC GP-SCL application was able to calculate two experimentally relevant stationary-state configurations: one in which the components form a dark-bright symbiotic pair (the ground state of the system), and one in which the components are segregated (first excited state). For each of these two configurations, it was shown numerically that far from resonances, the Faraday waves excited in the two components are of similar periods, emerge simultaneously, and do not impact the dynamics of the bulk of the condensate. This numerical result was confirmed analytically, and it was shown that the period of the Faraday waves can be estimated using a variational treatment of the coupled Gross–Pitaevskii equations combined with a Mathieu-type analysis for the selection mechanism of the excited waves.

Numerical study of Faraday waves in systems with spatially inhomogeneous atomic interactions has revealed that in the regime of weak inhomogeneity, the system practically behaves as in the homogeneous case. However, for the case of strong inhomogeneity, the properties of density waves substantially depend on the typical inhomogeneity scale. For systems with dipolar interaction, the stability of the ground state was found to be the major issue. Only for smaller numbers of atoms (up to several tens of thousands) is the system stable enough to support the

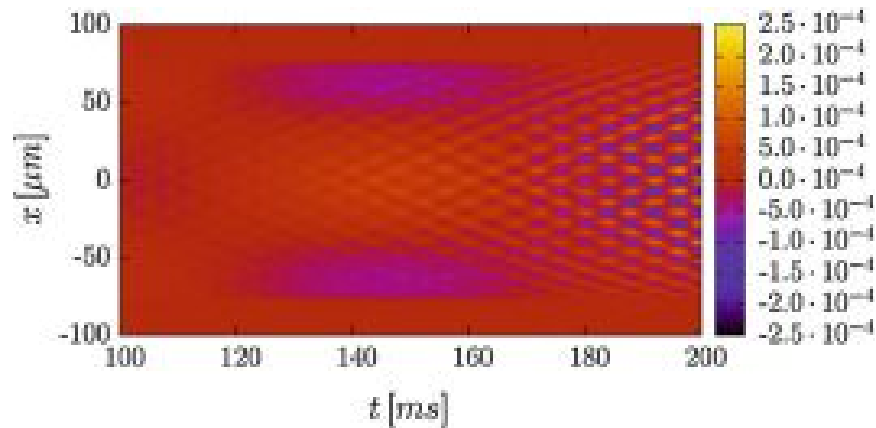


Fig. 15.4 Emergence of Faraday waves in the density profile of dipolar Bose–Einstein condensate of chromium

ground state. Harmonic modulation of the radial part of the confining potential is found again to generate Faraday density waves. For strong dipolar interaction, periods of emergent density waves (see Fig. 15.4) are found to be multiples of the corresponding periods when only contact interaction is present—a feature that has yet to be understood.

Investigation of fragmentation of Bose–Einstein condensates through periodic modulation of the scattering length is motivated by recent experimental results on the dynamics of a cigar-shaped Bose–Einstein condensate of atomic lithium. Dynamics of such system is investigated numerically, using the AEGIS CMPC SG, and analytically. It was shown that for resonant drives of large amplitude the condensate reaches a fragmented state. The fragmented state is a hybrid state of the condensate that includes a quadrupole mode on which a longitudinal resonant density wave is grafted.

Geometric resonances in Bose–Einstein condensates were investigated by solving the underlying time-dependent Gross–Pitaevskii equation for systems with two- and three-body interactions in an axially symmetric harmonic trap. For this, a recently developed analytical method (Vidan 2011) was used, as well as a detailed numerical study of a set of ordinary differential equations for variational parameters. By changing the anisotropy of the confining potential, strong nonlinear effects can be observed numerically and analytically—these are shifts in the frequencies of collective oscillation modes of the system. Additionally, coupling of collective modes can be seen, with the coupling strength strongly depending on the geometry of the system. Such results are highly relevant for experimental studies and help plan the parameters of experimental setups.

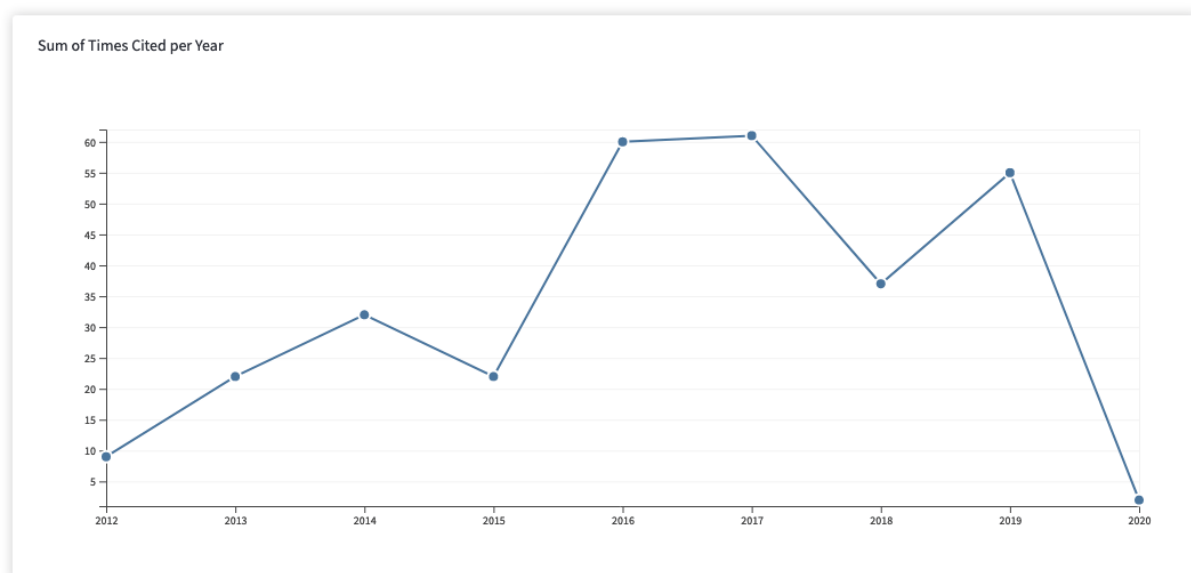
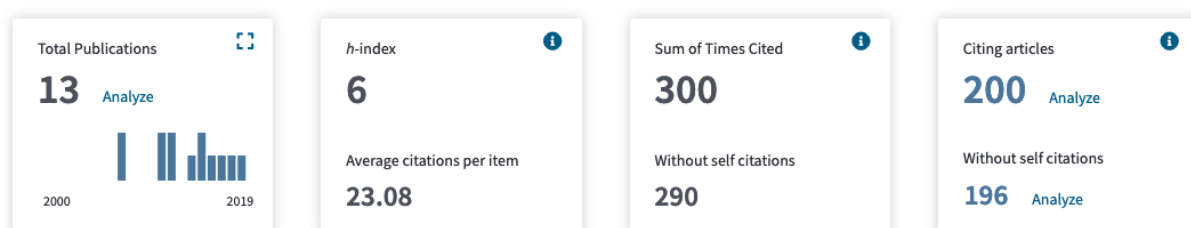
15.5 Conclusions

A new AEGIS CMPC science gateway (CMPC 2014) was developed and deployed for the Serbian condensed matter physics community in the framework of the SCI-BUS (2014) project. It was based on the WS-PGRADE/gUSE technology, and was implemented using the workflows approach. Three modules within the science gateway are responsible for managing user interaction with the supported applications (SPEEDUP, QSPEEDUP, and GP-SCL). Since September 2013, when this science gateway achieved the production status, its usage is steadily increasing, and the job success rate is high and stable.

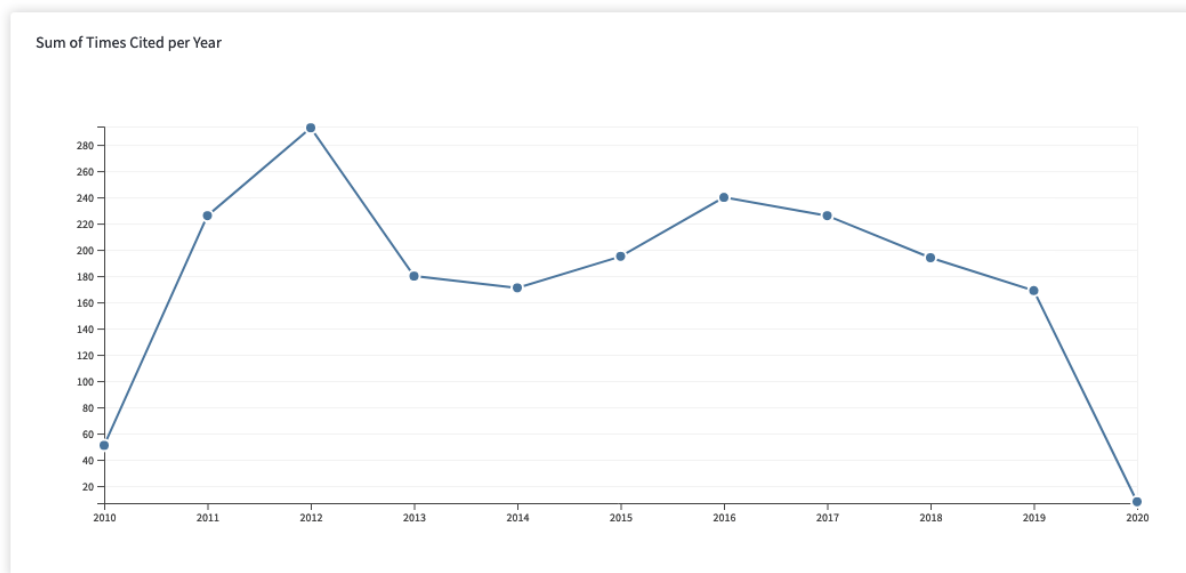
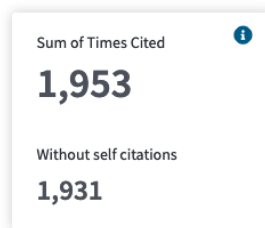
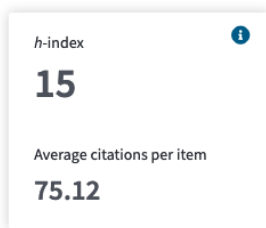
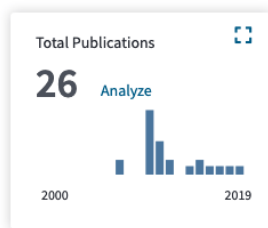
Further developments will include support for more applications used within this user community, as well as adding more workflows for specific use cases requested by the scientists. We also plan to extend support to the Serbian computational chemistry community, which is of considerable size and already uses a number of applications on computing resources of the Academic and Educational Grid Initiative of Serbia (AEGIS 2014) and European Grid Initiative (EGI 2014).

Web of Science цитираност др Душана Вудраговића

1 Цитираност без радова АТЛАС колаборације

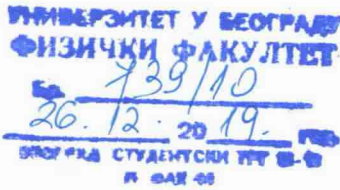
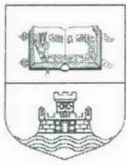


2 Цитираност са радовима АТЛАС колаборације



		2016	2017	2018	2019	2020	Total	Average Citations per Year
		240	226	194	169	8	1953	177.55
1.	Title: The ATLAS Simulation Infrastructure By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 3 Pages: 823-874 Published: DEC 2010	127	100	114	83	6	883	80.27
2.	Title: Charged-particle multiplicities in pp interactions at root s=900 GeV measured with the ATLAS detector at the LHC ATLAS Collaboration By: Aad, G.; Abat, E.; Abbott, B.; et al. Group Author(s): ATLAS Collaboration Source: PHYSICS LETTERS B Volume: 688 Issue: 1 Pages: 21-42 Published: APR 26 2010	8	6	3	4	0	148	13.45
3.	Title: C programs for solving the time-dependent Gross-Pitaevskii equation in a fully anisotropic trap By: Vudragovic, Dusan; Vidanovic, Ivana; Balaz, Antun; et al. Source: COMPUTER PHYSICS COMMUNICATIONS Volume: 183 Issue: 9 Pages: 2021-2025 Published: SEP 2012	28	23	14	18	1	141	15.67
4.	Title: Measurement of inclusive jet and dijet cross sections in proton-proton collisions at 7 TeV centre-of-mass energy with the ATLAS detector By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 71 Issue: 2 Article Number: 1512 Published: FEB 2011	5	8	7	3	0	123	12.30
5.	Title: Search for New Particles in Two-Jet Final States in 7 TeV Proton-Proton Collisions with the ATLAS Detector at the LHC By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: PHYSICAL REVIEW LETTERS Volume: 105 Issue: 16 Article Number: 161801 Published: OCT 11 2010	9	12	8	7	0	119	10.82
6.	Title: Readiness of the ATLAS Tile Calorimeter for LHC collisions By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 4 Published: DEC 8 2010	9	10	7	10	0	83	7.55
7.	Title: The ATLAS Inner Detector commissioning and calibration By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 3 Published: AUG 20 2010	6	12	8	2	0	73	6.64
8.	Title: Fortran and C programs for the time-dependent dipolar Gross-Pitaevskii equation in an anisotropic trap By: Kumar, R. Kishor; Young-S, Luis E.; Vudragovic, Dusan; et al. Source: COMPUTER PHYSICS COMMUNICATIONS Volume: 195 Pages: 117-128 Published: OCT 2015	21	18	12	12	0	67	11.17
9.	Title: Search for quark contact interactions in dijet angular distributions in pp collisions at root s=7 TeV measured with the ATLAS detector By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: PHYSICS LETTERS B Volume: 694 Issue: 4-5 Pages: 327-345 Published: JAN 3 2011	2	8	3	1	0	61	6.10
10.	Title: Measurement of the W -> lv and Z/gamma* -> ll production cross sections in proton-proton collisions at root s=7 TeV with the ATLAS detector By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: JOURNAL OF HIGH ENERGY PHYSICS Issue: 12 Article Number: 060 Published: DEC 2010	4	0	0	0	0	56	5.09

		2016	2017	2018	2019	2020	Total	Average Citations per Year
		240	226	194	169	8	1953	177.55
11.	Title: Readiness of the ATLAS liquid argon calorimeter for LHC collisions By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 3 Pages: 723-753 Published: DEC 2010	5	2	3	0	0	41	3.73
12.	Title: OpenMP Fortran and C programs for solving the time-dependent Gross-Pitaevskii equation in an anisotropic trap By: Young-S., Luis E.; Vudragovic, Dugan; Muruganandam, Paulsamy; et al. Source: COMPUTER PHYSICS COMMUNICATIONS Volume: 204 Pages: 209-213 Published: JUL 2016	7	11	9	12	0	39	7.80
13.	Title: Development of Grid e-Infrastructure in South-Eastern Europe By: Balaz, Antun; Prnjat, Ognjen; Vudragovic, Dusan; et al. Source: JOURNAL OF GRID COMPUTING Volume: 9 Issue: 2 Special Issue: SI Pages: 135-154 Published: JUN 2011	2	2	0	1	0	23	2.30
14.	Title: Performance of the ATLAS detector using first collision data By: Aad, G.; Abat, E.; Abbott, B.; et al. Group Author(s): ATLAS Collaboration Source: JOURNAL OF HIGH ENERGY PHYSICS Issue: 9 Article Number: 056 Published: SEP 2010	2	4	0	0	0	22	2.00
15.	Title: Studies of the performance of the ATLAS detector using cosmic-ray muons By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 71 Issue: 3 Article Number: 1593 Published: MAR 2011	2	2	1	2	0	19	1.90
16.	Title: OpenMP GNU and Intel Fortran programs for solving the time-dependent Gross-Pitaevskii equation By: Young-S, Luis E.; Muruganandam, Paulsamy; Adhikari, Sadhan K.; et al. Source: COMPUTER PHYSICS COMMUNICATIONS Volume: 220 Pages: 503-506 Published: NOV 2017	0	2	2	11	0	15	3.75
17.	Title: Commissioning of the ATLAS Muon Spectrometer with cosmic rays By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 3 Pages: 875-916 Published: DEC 2010	1	0	2	1	0	15	1.36
18.	Title: Drift Time Measurement in the ATLAS Liquid Argon Electromagnetic Calorimeter using Cosmic Muons By: Aad, G.; Abbott, B.; Abdallah, J.; et al. Group Author(s): ATLAS Collaboration Source: EUROPEAN PHYSICAL JOURNAL C Volume: 70 Issue: 3 Pages: 755-785 Published: DEC 2010	0	1	1	1	0	10	0.91
19.	Title: Development of collisional data base for elementary processes of electron scattering by atoms and molecules By: Marinkovic, Bratislav P.; Vujcic, Veljko; Sushko, Gennady; et al. Source: NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS Volume: 354 Pages: 90-95 Published: JUL 1 2015	1	5	0	1	1	8	1.33
20.	Title: SPEEDUP Code for Calculation of Transition Amplitudes via the Effective Action Approach By: Balaz, Antun; Vidanovic, Ivana; Stojiljkovic, Danica; et al. Source: COMMUNICATIONS IN COMPUTATIONAL PHYSICS Volume: 11 Issue: 3 Pages: 739-755 Published: MAR 2012	1	0	0	0	0	6	0.67



На основу члана 29 Закона о општем управном поступку («Службени гласник РС» број 18/2016 и 95/2018), и члана 149 Статута Универзитета у Београду - Физичког факултета, по захтеву ДУШАНА ВУДРАГОВИЋА, мастер физичара, издаје се следеће

У В Е Р Е Њ Е

ДУШАН ВУДРАГОВИЋ, мастер физичар, дана 24. децембра 2019. године, одбранио је докторску дисертацију под називом

"FARADAY WAVES IN ULTRACOLD DIPOLAR BOSE GASES"
(Фарадејеви таласи у ултрахладним диполним Бозе гасовима)

пред Комисијом Универзитета у Београду - Физичког факултета и тиме испунио све услове за промоцију у ДОКТОРА НАУКА – ФИЗИЧКЕ НАУКЕ.

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Select... ▾	12-Sep-2018	018-06-2018-0106 A Framework for Multi-Resource Fair Allocation Based on TD-DF Allocation Mechanism and Scheduling using VM in Cloud Computing File Archiving	Reject (30-Sep-2018) Archiving completed on 01-Feb- 2019 Assignments: AE: Sartori, Fabio EIC: Sicilia, Miguel-Angel GE: Not Assigned
Select... ▾	10-Jul-2018	018-06-2018-0106 Identification and Analysis of Suspicious Algorithms on Shared Memory Architecture	Major Revision (17-Sep-2018) a revision has been submitted Assignments: AE: Sicilia, Miguel-Angel EIC: Sicilia, Miguel-Angel GE: Not Assigned



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Action Links	2	19121-18	Letter	THE EFFECT OF THE ORDER OF THE BOUNDARY CONDITIONS ON THE STABILITY OF THE FINITE DIFFERENCE METHOD	Sep 28, 2018	Oct 05, 2018	Oct 19, 2018	Oct 16, 2018	18		
Action Links	2	19121-18	Letter	THE EFFECT OF THE ORDER OF THE BOUNDARY CONDITIONS ON THE STABILITY OF THE FINITE DIFFERENCE METHOD	Jul 08, 2018	Jul 09, 2018	Jul 30, 2018	Aug 07, 2018	30		

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Acknowledgement: HP-SEE User Forum 2012 is organised with the support of the European Commission through the project High-Performance Computing Infrastructure for South East Europe's Research Communities (HP-SEE), co-funded by EC (under Contract Number 261499) through the Seventh Framework Programme.

The organizers of the HP-SEE User Forum 2012 would like to thank the National Library of Serbia for the permission to use their premises and for organizational support.

High performance computing in function of business enhancement

14 Jun 2018, 09:00 → 15 Jun 2018, 18:00 Europe/Belgrade

Science Technology Park Belgrade

Description Institute of Physics Belgrade (partner in the VI-SEEM project) and the Regional Economic Development Agency for Sumadija and Pomoravlje (partner in the InnoHPC project) jointly organize dissemination event at the Science Technology Park Belgrade, Serbia on 14 and 15 June 2018. The main aims of the event is to demonstrate HPC as a general-purpose technology capable to enhance innovative capacities of enterprises, especially SMEs.

The first day is organize at the Science Technology Park Belgrade. Through the several presentations and panel discussions business development opportunities that High Performance Computing can provide to small and middle scale companies will be presented. Among the panel speakers are the representative from the Ministry of Education, Science and Technological Development of the Republic of Serbia, the directors of participating institutions, as well as coordinator of the VI-SEEM project.

On the second day of the event, participant will visit largest Serbian HPC installation (PARADOX cluster), as well as other research laboratories at the Institute of Physics Belgrade.

Dušan Vudragović [✉ dusan@ipb.ac.rs](mailto:dusan@ipb.ac.rs)

THURSDAY, 14 JUNE

09:30 → 10:00	Registration	30m
10:00 → 11:00	Panel: HPC for SMEs Speakers: Dr Aleksandar Bogojevic (Institute of Physics Belgrade, Director), Dragan Sataric (Ministry of Education, Science and Technological Development of the Republic of Serbia), Nenad Popovic (REDASP, Director), Dr Ognjen Prnjat (Greek Research and Technology Network), Radisa Vicevic (Science Technology Park Belgrade, Assistant Director)	1h
11:00 → 11:30	InnoHPC project Speaker: Jasminka Lukovic Jaglicic (Regional Economic Development Agency for Sumadija and Pomoravlje)	30m
11:30 → 12:00	InnoHPC virtual laboratories Speaker: Prof. Srdjan Skrbic (Faculty of Sciences, University of Novi Sad)	30m
12:00 → 12:30	VI-SEEM Virtual Research Environment Speaker: Dusan Vudragovic (Institute of Physics Belgrade)	30m
12:30 → 12:50	HPC resources, capabilities and applications Speaker: Dusan Vudragovic (Institute of Physics Belgrade)	20m
12:50 → 13:10	HPC resources, opportunities and applications Speaker: Dr Milos Ivanovic (Faculty of Science, University of Kragujevac)	20m
13:10 → 13:30	HPC resources, opportunities and applications Speaker: Dr Marko Dimitrijevic (Faculty of Electronic Engineering, University of Nis)	20m
13:30 → 14:30	Open questions of representatives of the SME sector and the HPC centers	1h
14:30 → 15:00	Cocktail	30m

FRIDAY, 15 JUNE

10:00 → 11:00	Presentation of the project CERN Serbia Speaker: Dr Aleksandar Bogojevic (Institute of Physics Belgrade, Director)	1h
11:00 → 14:00	Tour and presentation of scientific-research laboratories at the Institute of Physics Belgrade	3h
14:00 → 14:30	Cocktail	30m

VI-SEEM REG CL: Regional Climate training event

11-13 October 2017
 Institute of Physics, Belgrade
ipb@ipb.ac.rs

VI-SEEM Training Event

- Overview
- Timetable**
- Registration
- Photos
- Participant List

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Timetable

< Wed 11/10 Thu 12/10 Fri 13/10 All days >

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09:00	Opening and welcome Institute of Physics, Belgrade	09:00 - 09:15
	Scope and objectives of the training event Institute of Physics, Belgrade	09:15 - 09:30
	Climate Modelling & Downscaling Dr Theodoros Christoudias	
10:00	Institute of Physics, Belgrade	09:30 - 10:30
	Coffee Break Institute of Physics, Belgrade	10:30 - 11:00
11:00	The WRF-Chem Model Dr Theodore Giannaros	
	Institute of Physics, Belgrade	11:00 - 12:00
12:00	DREAMCLIMATE application usage Institute of Physics, Belgrade	12:00 - 12:30
	Lunch break Institute of Physics, Belgrade	12:30 - 13:30
13:00	Earth System Model Post-processing & Visualisation Dr Theodoros Christoudias	
14:00	Institute of Physics, Belgrade	13:30 - 14:30
	Efficient exact computations for molecular species relevant to atmospheric chemistry, climate science and drug delivery Prof. Ljupco Pejov	
15:00	Institute of Physics, Belgrade	14:30 - 15:30
	Application Level Service: The Live Access Server Institute of Physics, Belgrade	15:30 - 16:00
16:00	Coffee break Institute of Physics, Belgrade	16:00 - 16:30
	Q&A Discussion Institute of Physics, Belgrade	16:30 - 17:00
17:00	Closing remarks Institute of Physics, Belgrade	17:00 - 17:30

VI-SEEM REG LS: VI-SEEM e-Infrastructure services, Molecular Dynamics Simulations of Biomolecules and Computer-Aided Drug Design

19 Oct 2016, 09:00 → 21 Oct 2016, 15:30 Europe/Belgrade

Room 300 (Belgrade)

Description **Objective:** This interactive course will introduce participants to VI-SEEM e-Infrastructure services, and then focus on the principles and applications of biomolecular modeling, and pinpoint how biomolecular problems, such as drug design, are being currently addressed by computational techniques.

Aims:

1. Introduce VI-SEEM data and computational services, and their access methods.
2. Hands-on training in classical Molecular Dynamics (MD) simulations by examining the protein lysozyme of the NAMD program. Introduction to GROMACS.
3. Computer-aided drug design with Schrodinger Suite and ChemBioServer. An introduction to virtual screening for computer-aided drug design and application with the Schrodinger Suite software. The generated virtual screening results are then post-processed (filtered) for toxicity, chemical similarity and validity of docking pose using the ChemBioServer software (<http://bioserver-3.bioacademy.gr/Bioserver/ChemBioServer/>)

Computer-Aided Drug Design NAMD training material PARADOX-IV NAMD, VMD, and GROMACS

Participants Bojana Koteska Djordje Francuski Evdokiya Salamanova Gergana Gocheva Gjoshe Stefkov
 Jasmina Tonic Ribarska Jelena Randjelovic Kleitos Sokratous Luka Ilic Maja Simonoska Crcarevska

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WEDNESDAY, 19 OCTOBER

09:00 → 09:15	Welcome: VI-SEEM Virtual Research Environment and Services	Room 300
	start of training event Convener: Dr Antun Balaž (Institute of Physics Belgrade) slides	
09:15 → 10:00	HPC usage and software packages	Room 300
	Convener: Dusan Vudragovic (Institute of Physics Belgrade) slides	
10:00 → 10:30	VI-SEEM Source Code Repository	Room 300
	Convener: Petar Jovanović (Institute of Physics Belgrade, Serbia) slides	
10:30 → 11:00	Coffee break	30m Room 300
11:00 → 11:30	VI-SEEM Data Repository	Room 300
	Convener: Vladimir Slavnić (Institute of Physics Belgrade, Serbia) slides	
11:30 → 12:30	VI-SEEM Staging and Archiving	Room 300
	Convener: Petar Jovanović (Institute of Physics Belgrade, Serbia) slides	
12:30 → 13:30	Lunch	1h Room 300
13:30 → 14:00	Related LS e-Infrastructure initiatives: BioExcel	Room 300
	Convener: Rossen Apostolov (KTH)	
14:00 → 14:30	Introduction to VI-SEEM LS services, workflows, applications, and data sets	Room 300
	Convener: Zoe Cournia (Biomedical Research Foundation Academy Of Athens, Greece) slides	
14:30 → 15:00	Coffee break	Room 300
15:00 → 16:30	Introduction to Computer Modeling of Biomolecules	Room 300
	Convener: Zoe Cournia (Biomedical Research Foundation Academy Of Athens, Greece)	
16:30 → 18:00	Hands-on training: Visualization of Biomolecules using VMD	Room 300
	Convener: Zoe Cournia (Biomedical Research Foundation Academy Of Athens, Greece)	
20:00 → 21:00	VI-SEEM Social Dinner	1h Dva Jelena Skadarlija

THURSDAY, 20 OCTOBER

09:30 → 11:00	Hands-on training: Molecular Dynamics Simulations of the lysozyme protein using NAMD: 1. Minimization	Room 300
	Convener: Zoe Cournia (Biomedical Research Foundation Academy Of Athens, Greece)	
11:00 → 11:15	Coffee break	15m Room 300
11:15 → 13:00	Hands-on training: Molecular Dynamics Simulations using NAMD: 2. Equilibration	Room 300
	Convener: Cournia Zoe (Biomedical Research Foundation Academy Of Athens, Greece)	
13:00 → 14:00	Lunch	1h Room 300

Introduction to Parallel Programming with CUDA: "How to plow a field with 1024 chickens?", Belgrade, Serbia

Monday, 18 February 2013 from 10:00 to 14:45 (Europe/Belgrade)
at Institute of Physics Belgrade (Library)

Material Training Evaluation

Dušan Vudragović dusan@ipb.ac.rs

Monday, 18 February 2013

- 10:00 - 10:05 Opening 5'
Speaker: Dr. Antun Balaz (Institute of Physics Belgrade)
- 10:05 - 10:10 Overview of the training 5'
- 10:10 - 10:55 Introduction to heterogeneous parallel programming 45'
Speaker: Petar Jovanovic (Institute of Physics Belgrade)
Material: Slides
- 10:55 - 11:40 CUDA C overview 45'
Speaker: Dusan Stankovic (Institute of Physics, Belgrade)
Material: Slides
- 11:40 - 12:00 Coffee Break
- 12:00 - 13:00 Hands-on session: Tiled matrix multiplication (using shared memory) 1h0'
Speaker: Petar Jovanovic (Institute of Physics Belgrade)
Material: Slides
- 13:00 - 14:00 Hands-on session: Reduction on GPU 1h0'
Speaker: Dusan Stankovic (Institute of Physics, Belgrade)
Material: Slides
- 14:00 - 14:10 Coffee break
- 14:10 - 14:40 Hands-on session: Using CUDA numerical libraries 30'
Speaker: Petar Jovanovic (Institute of Physics Belgrade)
Material: Slides
- 14:40 - 14:45 End of training 5'

Tuning and Optimization of HPC Application, Belgrade, Serbia

chaired by Dusan Vudragovic (Institute of Physics Belgrade)

Friday, 1 June 2012 from 09:00 to 17:00 (Europe/Belgrade)
at Institute of Physics Belgrade (Library)

Material Paradox User Guide Training Evaluation

Dušan Vudragović dusan@ipb.ac.rs

Friday, 1 June 2012

- 09:00 - 09:05 **Opening 5'**
Speaker: Dr. Antun Balaz (Institute of Physics Belgrade)
- 09:05 - 09:10 **Overview of the Training 5'**
Speaker: Dusan Vudragovic (Institute of Physics Belgrade)
- 09:10 - 09:55 **PARADOX MPI Libraries 45'**
Speaker: Dusan Stankovic (Institute of Physics Belgrade)
Material: Codes Slides
- 09:55 - 10:40 **Intel MKL Usage 45'**
Speaker: Petar Jovanovic (Institute of Physics Belgrade)
Material: Codes Slides
- 10:40 - 10:55 **Coffee Break**
- 10:55 - 11:25 **FFTs Using FFTW and FFE Libraries 30'**
Speaker: Aleksandar Jovic (Institute of Physics Belgrade)
Material: Codes Slides
- 11:25 - 11:55 **Debugging with GDB 30'**
Speaker: Vladimir Slavnic (Institute of Physics Belgrade)
Material: Codes Slides
- 11:55 - 12:40 **TotalView Debugger 45'**
Speaker: Josip Jakic (Institute of Physics Belgrade)
Material: Slides
- 12:25 - 13:30 **Lunch Break**
- 13:30 - 14:00 **Valgrind Usage 30'**
Speaker: Josip Jakic (Institute of Physics Belgrade)
Material: Slides
- 14:00 - 14:30 **TAU Performance System 30'**
Speaker: Petar Jovanovic (Institute of Physics Belgrade)
Material: Slides
- 14:30 - 15:00 **Using the Scalasca Profiler 30'**
Speaker: Dusan Stankovic (Institute of Physics Belgrade)
Material: Slides
- 15:00 - 15:15 **Coffee Break**
- 15:15 - 15:45 **Profiling with GNU GProf 30'**
Speaker: Aleksandar Jovic (Institute of Physics Belgrade)
Material: Slides
- 15:45 - 16:15 **OpenEye Scientific Software 30'**
Speaker: Branko Drakulic (Department of Chemistry-ICTM, University of Belgrade)
Material: Slides
- 16:15 - 16:45 **Firefly Scientific Software 30'**
Speaker: Jelena Randjelovic (Faculty of Pharmacy)
Material: Slides

PARADOXical Training, 14 October 2011, Belgrade, Serbia

Friday, 14 October 2011 from 10:00 to 14:30 (Europe/Belgrade)
at Institute of Physics Belgrade (Library)

Material Evaluation Form ICTP Advanced School On Scientific Software Development
PARADOX Cluster user guide

Dušan Vudragović dusan@ipb.ac.rs

Friday, 14 October 2011

- 10:00 - 10:05 Opening 5'
- 10:05 - 10:50 Introduction to High-Performance Computing 45'
 - Clusters
 - Supercomputers
 - HPC vs Grid Computing
 - Overview of HPC projects

Speaker: Dr. Antun Balaz (Institute of Physics Belgrade)
Material: Slides
- 10:50 - 11:05 Coffee break
- 11:05 - 12:35 Hands on session: PARADOX Cluster job management 1h30'
 - Access to login node
 - Preparing job submitting scripts
 - Submitting jobs:
 - Serial jobs
 - OpenMP jobs
 - MPI jobs
 - Hybrid jobs
 - Application specific jobs (NAMD, CPMD)
 - Batch system job control and monitoring

Speaker: Nikola Grkic (Institute of Physics Belgrade)
Material: Slides
- 12:35 - 12:50 Coffee break
- 12:50 - 14:20 Hands-on session: Overview and usage of PARADOX software stack 1h30'
 - Overview of software installed
 - Compilers
 - Debuggers
 - Libraries
 - Application software
 - Using compilers (ICC, GCC, PGI)
 - Useful flags
 - Using numerical libraries
 - Intel MKL libraries (linking guide)
 - Debugging simple codes using GDB
 - Performing simple profiling using gprof
 - Finding memory leaks with Valgrind

Speaker: Vladimir Slavnic (Institute of Physics Belgrade)
Material: Slides

