Научном већу Института за физику

Београд, 15. мај 2019. године

Предмет: Молба за покретање поступка за реизбор у звање истраживач сарадник

мольа

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

У прилогу достављам:

- 1. мишљење руководиоца пројекта са предлогом комисије за реизбор у звање;
- 2. кратку стручну биографију;
- 3. кратак преглед научне активности;
- 4. списак објављених радова и других публикација;
- 5. копије објављених радова и других публикација;
- 6. уверење о последњем овереном и уписаном семестру на докторским студијама;
- 7. одлуку Већа научних области природно-математичких наука Универзитета у Београду о прихватању предлога теме докторске дисертације.

С поштовањем,

Диан Вздраговић

Душан Вудраговић

Научном већу Института за физику у Београду

Београд, 15. мај 2019. године

Предмет: Мишљење руководиоца пројекта о реизбору Душана Вудраговића у звање истраживач сарадник

Душан Вудраговић је запослен у Лабораторији за примену рачунара у науци, у оквиру Центра изузетних вредности за изучавање комплексних система Института за физику у Београду и ангажован је на пројекту основних истраживања Министарства просвете, науке и технолошког развоја Републике Србије OH171017, под називом "Моделирање и нумеричке симулације сложених вишечестичних физичких система". На поменутом пројекту ради на темама из проучавања особина диполних Бозе-Ајнштајн кондензата и развоју нумеричких метода за њихов опис под руководством др Антуна Балажа. 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 реизбор Душана Вудраговића у звање истраживач сарадник.

За састав комисије за реизбор Душана Вудраговића у звање истраживач 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) академик Милан Дамњановић, редовни професор Физичког факултета Универзитета у Београду

Руководилац пројекта

At-no др Антун Балаж

др Антун Балаж научни саветник

Кратка биографија Душана Вудраговића

Душан Вудраговић је рођен 3. маја године у Сремској Митровици. 1980. 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 смеру Физика језгра и честица на Физичком факултета Универзитета у Београду је уписао 2012. године, а под руководством др Антуна Балажа ради на темама везаним за ултрахладне квантне гасове и на развоју нумеричких метода за паралелне рачунарске системе.

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. Поред пројекта основних истраживања ОН171017 којим руководи др Антун Балаж, делимично је ангажован и на интегрисаном пројекту ИИИ43007, у оквиру потпројекта којим руководи др Александар Богојевић. У оквиру међународне сарадње ангажован је на Хоризонт 2020 пројекту SMARTCHAIN (*Towards Innovation - driven and smart solutions in short food supply chains*).

Од претходног избора у звање Душан Вудраговић је објавио 2 рада категорије M21a, 1 саопштење M33 и 2 саопштења категорије M34.

Кратак преглед научне активности Душана Вудраговића

Душан Вудраговић је започео свој истраживачки рад под менторством др Антуна Балажа 2012. године на Институту за физику у Београду у Лабораторији за примену рачунара у науци. Студент је докторских студија на Физичком факултету Универзитета у Београду на смеру Физика језгра и честица, а ради на темама везаним за ултрахладне квантне гасове.

Истраживачки рад је започео развојем нумеричке симулације за израчунавање стационарних и нестационарних, временски зависних решења Грос-Питаевски једначине – једначине која описује својства Бозе-Ајнштајн кондензата на ниским температурама. Симулација омогућава пропагацију Грос-Питаевски једначине у имагинарном и реалном времену, а базирана је на Кренк-Николсоновој методи. Кондензат је могуће разматрати једнодимензионално, дводимензионално, цилиндричносиметрично, сферно-симетрично и потпуно анизотропно у три димензије. Свака опција је паралелизована и оптимизована за рад са неколико популарних компајлера.

Стандардна Грос-Питаевски једначина је нелинеарна парцијална диференцијална једначина која описује Бозе-Ајнштајн кондензоване системе са краткодометном интеракцијом у теорији средњег поља. Уколико атоми интерагују и дугодометном диполном интеракцијом, Грос-Питаевски једначина постаје парцијална интегралнодиференцијална једначина. Душан Вудраговић је учествовао у развоју комплексног алгоритма за решавање овакве једначине.

Развијене алгоритме Душан Вудраговић је применио за разматрање појаве Фарадејевих таласа у квази једнодимензионалним ⁵²Cr и ¹⁶⁴Dy Бозе-Ајнштајн кондензатима. Таласне густине индуковане периодичном модулацијом потенцијалне јаме разматрао је нумеричким и Гаусовим варијационим методама.

Розенсвајг нестабилност у ¹⁶⁴Dy Бозе-Ајнштајн кондензатима услед јаких магнетних диполних момената атома омогућава разматрање квантних ферофлуида. Уколико се контактна интеракција нагло смањи (нпр. изненадном променом јачине магнетног поља у ком се кондензат налази) тако да дипол-дипол интеракција постане доминантна, може доћи до формирања уређених структура у форми капљица (налик на кристале). Како Грос-Питаевски једначина не може да објасни настанак Розенсвајг нестабилност, потребно ју је проширити трочестичним интеракцијама или квантним флуктуацијама. Душан Вудраговић је учествовао у развоју овог приступа.

Од претходног избора у звање Душан Вудраговић је објавио 2 рада категорије M21a, 1 саопштење M33 и 2 саопштења категорије M34.

Списак радова Душана Вудраговића

Радови након претходног избора у звање

Радови у међународним часописима изузетних вредности (М21а)

- 1. Luis E. Young-S., P. Muruganandam, S. K. Adhikari, V. Loncar, **D. Vudragovic**, and A. Balaz, *OpenMP GNU and Intel Fortran programs for solving the timedependent Gross-Pitaevskii equation*, Comput. Phys. Commun. **220**, 503 (2017).
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- B. P. Marinkovic, V. Vujcic, G. Sushko, D. Vudragovic, S. Djordjevic, S. Ivanovic, M. Nesic, D. Jevremovic, 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).
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Саопштења са међународних скупова штампана у целини (М33)

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- D. Vudragovic, A. Balaz, A. Belic, C. Kourkoumelis, D. Fassouliotis, and S. Vourakis, *Hybrid Pupil's Analysis Tool for Interactions in ATLAS*, MIPRO 2010, Opatia, Croatia, 24-28 May 2010.
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- 3. D. Vudragovic, V. Slavnic, A. Balaz, and A. Belic, *WMSMON GLite WMS Monitoring Tool*, MIPRO 2009, Opatia, Croatia, 25-29 May 2009.
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Монографска студија/поглавље у књизи М11 или рад у тематском зборнику водећег међународног значаја (М13)

- 1. **D. Vudragovic**, and A. Balaz, *Science gateway for the Serbian condensed matter physics community*, Science gateways for distributed computing infrastructures, Ed. Peter Kacsuk, p. 209-220, Springer (2014).
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Монографска студија/поглавље у књизи М12 или рад у тематском зборнику водећег међународног значаја (М14)

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Computer Physics Communications 220 (2017) 503–506



Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

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



COMPUTER PHYSICS

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ARTICLE INFO

Article history: Received 11 July 2017 Accepted 14 July 2017 Available online 10 August 2017

Keywords:

Bose–Einstein condensate Gross–Pitaevskii equation Split-step Crank–Nicolson scheme Intel and GNU Fortran programs Open Multi-Processing OpenMP 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 nonstationary solutions, respectively. The present OpenMP programs are designed for computers with multicore 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) 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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http://dx.doi.org/10.1016/j.cpc.2017.07.013

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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 generalpurpose 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 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 | GNU | Intel | GNU | Intel | GNU | Intel | GNU |
| | time | time | time | time | time | time | speedup | 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 |

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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). © 2017 Elsevier B.V. All rights reserved.

Acknowledgments

V.L., D.V., and A.B. acknowledge support by the Ministry of Education, Science, and Technological Development of the Republic of Serbia under projects ON171017 and III43007. P.M. acknowledges support by the Science and Engineering Research Board, Department of Science and Technology, Government of India under project no. EMR/2014/000644. S.K.A. acknowledges support by the CNPq of Brazil under project 303280/2014-0, and by the FAPESP of Brazil under project 2012/00451-0. Numerical tests were partially carried out on the PARADOX supercomputing facility at the Scientific Computing Laboratory of the Institute of Physics Belgrade.

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Computer Physics Communications 204 (2016) 209-213



Contents lists available at ScienceDirect

Computer Physics Communications

journal homepage: www.elsevier.com/locate/cpc

OpenMP Fortran and C programs for solving the time-dependent Gross-Pitaevskii equation in an anisotropic trap



COMPUTER PHYSICS

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ARTICLE INFO

Article history: Received 22 February 2016 Received in revised form 9 March 2016 Accepted 22 March 2016 Available online 6 April 2016

Keywords:

Bose-Einstein condensate Gross-Pitaevskii equation Split-step Crank-Nicolson scheme Real- and imaginary-time propagation C program Fortran program OpenMP Partial differential equation

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 supersedes versions AEDU_v1_0 and

AEDU_v2_0, but not AEDU_v3_0, which is MPI-parallelized version.

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http://dx.doi.org/10.1016/j.cpc.2016.03.015 0010-4655/© 2016 Elsevier B.V. All rights reserved.

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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.xt, 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, -speedupC = 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,

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

L.E. Y.-S. acknowledges support by the FAPESP of Brazil under project 2012/21871-7 and 2014/16363-8. D.V. and A.B. acknowledge support by the Ministry of Education, Science, and Technological Development of the Republic of Serbia under projects OI1611005, ON171017 and III43007. P.M. acknowledges support by the Science and Engineering Research Board, Department of Science and Technology, Government of India under project No. EMR/2014/000644. S.K.A. acknowledges support by the CNPq of Brazil under project 303280/2014-0, and by the FAPESP of Brazil under project 2012/00451-0.

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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 highquality 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 $2.5 \,\mu$ 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

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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 DREAM-CLIMATE 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 preprocessing, 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 Couranf-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 PARA-DOX 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 DREAMECLIMATE 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

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FIG. 4.1. Calculated mean dust concentrations in μ g/m³, 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 μ g/m³.

| Baseline concentration | | | | |
|-------------------------|------|------|-----|-----|
| $(in \ \mu g/m^3)$ | 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 μ g/m³ 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 CPDmortality 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 μ g/m³. Table 4.1 gives the obtained total CPD and LC premature mortalities for the threshold concentrations between 0 and 10 μ g/m³. 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 μ m, calculated by the VI-SEEM DREAM-CLIMATE 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 μ 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.

Acknowledgments. This work was supported by the Ministry of Education, Science, and Technological Development of the Republic of Serbia under projects ON171017 and III43007, and by the European Commission under H2020 project VI-SEEM, Grant No. 675121. Numerical simulations were run on the PARADOX supercomputing facility at the Scientific Computing Laboratory of the Institute of Physics Belgrade.

VI-SEEM DREAMCLIMATE Service

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Edited by: Aneta Karaivanova

Received: Jan 5, 2018

Accepted: Apr 12, 2018



THURSDAY, OCTOBER 26, 2017

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-guality 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 GOCDB 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.

RO-LCG 2017, Sinaia, Romania, 26-28 October 2017

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 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 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 shortrange interaction with a Feshbach resonance we can induce a finitewavelength 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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 Phys. Rev. A 86, 063609 (2012).

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 experiments 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 PETTER¹, KIYOTAKA AIKAWA¹, LAURIANE CHOMAZ^{1,2}, ZI CAI², MIKHAIL BARANOV², PE-TER ZOLLER^{2,3}, and FRANCESCA FERLAINO^{1,2} — ¹Institut für Experimentalphysik, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck, Austria — ²Institut für Quantenoptik und Quanteninformation, 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), Atominstitut, TU Wien, Vienna, Austria

This work investigates the rapid cooling quench over the dimensionaland quasicondensate-crossover. Analyzing experiments performed at the Atominstitut, we study the relaxation of such a far-from equilibrium system. The early stage of condensate formation is dominated



Република Србија Универзитет у Београду Физички факултет Д.Бр.2016/8020 Датум: 15.01.2019. године

На основу члана 161 Закона о општем управном поступку и службене евиденције издаје се

УВЕРЕЊЕ

Вудраговић (Милан) Душан, бр. индекса 2016/8020, рођен 03.05.1980. године, Сремска Митровица, Сремска Митровица-град, Република Србија, уписан школске 2018/2019. године, у статусу: самофинансирање; тип студија: докторске академске студије; студијски програм: Физика.

Према Статуту факултета студије трају (број година): три. Рок за завршетак студија: у двоструком трајању студија.

Ово се уверење може употребити за регулисање војне обавезе, издавање визе, права на дечији додатак, породичне пензије, инвалидског додатка, добијања здравствене књижице, легитимације за повлашћену вожњу и стипендије.

Овлашћено лице факултета ought



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ВЕЋЕ НАУЧНИХ ОБЛАСТИ ПРИРОДНО-МАТЕМАТИЧКИХ НАУКА

Београд, 21.5.2018. 02-04 Број 61206-1745/2-18 СЋ

На основу чл. 148. Закона о високом образовању ("Службени гласник РС", број 88/17), члана 47. став 5. тачка. 3. Статута Универзитета у Београду ("Гласник Универзитета у Београду", број 186/15-пречишћени текст и 189/16) и чл. 14. – 21. Правилника о већима научних области на Универзитету у Београду ("Гласник Универзитета у Београду", број 134/07, 150/09, 158/11, 164/11 и 165/11, 180/14, 195/16, 196/16 и 197/17), а на захтев Физичког факултета, број: 739/4 од 28.3.2018. године, Веће научних области природноматематичких наука, на седници одржаној 21.5.2018. године, донело је

од луку

ДАЈЕ СЕ САГЛАСНОСТ на предлог теме докторске дисертације ДУШАНА ВУДРАГОВИЋА, под називом: "Faraday waves in ultracold dipolar Bose gases(Фарадејеви таласи у ултрахладним диполним Бозе гасовима)", и одређивање проф. др Антуна Балажа за ментора.

ПРЕДСЕДНИК ВЕЋА

Проф. др Воја Радовановић

Доставити:

- Факултету
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