HP-SEE

Инфраструктура за високопроизводителни пресмятания за изследователските общности в Югоизточна Европа

www.hp-see.eu

Еднодневно обучение
25 Февруари 2013, София
Съвместно организирано по проекти:
SuperCA++, HP-SEE

HP-SEE
High-Performance Computing Infrastructure for South East Europe's Research Communities

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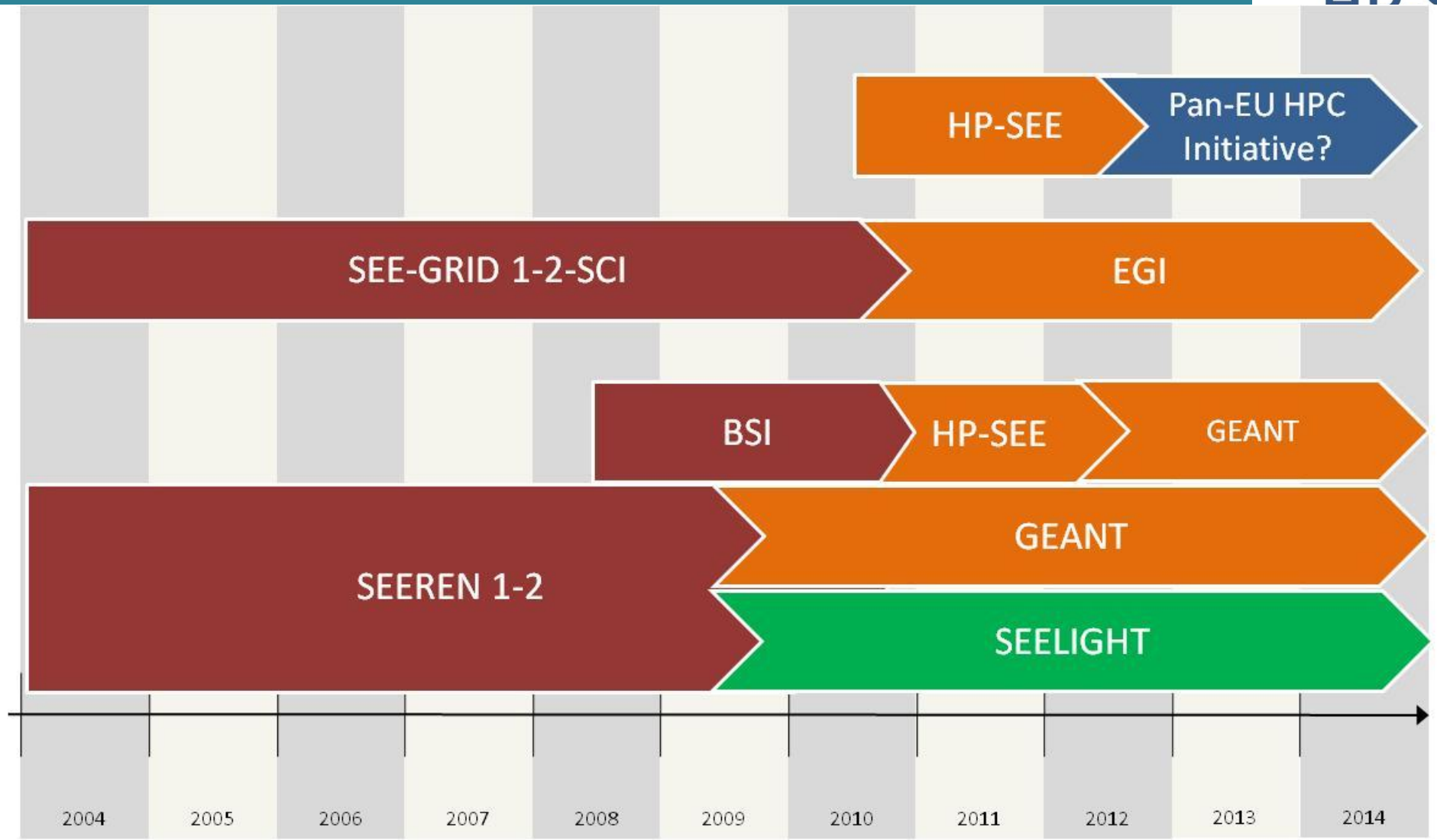
СТРУКТУРА НА 7РП (програми и инструменти)

HP-SEE
High-Performance Computing Infrastructure for South East Europe's Research Communities

- Сътрудничество / Cooperation
- Идеи / Ideas
- Хора / People
- Капацитети / Capacities
  - Изследователски инфраструктури / Research Infrastructures
  - Изследвания в подкрепа на МСП / Research for the benefits of SMEs
  - Региони на знанието / Regions of Knowledge
  - Научен потенциал / Research Potential
  - Науката в обществото / Science and Society
  - Международно сътрудничество / International Cooperation
  - Кохерентно развитие на политиките / Support for the Coherent Development of Research Policies

Регионално сътрудничество – история



HP-SEE Консорциум

HP-SEE

Членове на консорциума	Абривиатура	Страна
Greek Research & Technology Network	GRNET	GR
Институт по информационни и комуникационни технологии, Българска академия на науките	**IICT-BAS**	**BG**
"Horia Hulubei" National Institute of Research and Development for Physics and Nuclear Engineering	IFIN-HH	RO
The Scientific & Technological Research Council of Turkey	TUBITAK ULAKBIM	TR
National Information Infrastructure Development Office	NIIF	HU
Institute of Physics Belgrade	IPB	RS
Polytechnic University of Tirana	PuoT	AL
University of Banja Luka	UoBL ETF	BA
SS. Cyril & Methodius University of Skopje	UKIM	MK
University of Montenegro	UOM	ME
Research & Educational Networking Association of Moldova	RENAM	MD
Institute for Informatics & Automation Problems, National Academy of Sciences of Armenia	IIAP-NAS-RA	AM
Georgian Research & Educational Networking Association	GRENA	GE
Azerbaijan Research and Education Association	AZRENA	AZ

Трети страни / JRU механизъм

11 университета / изследователски центрове

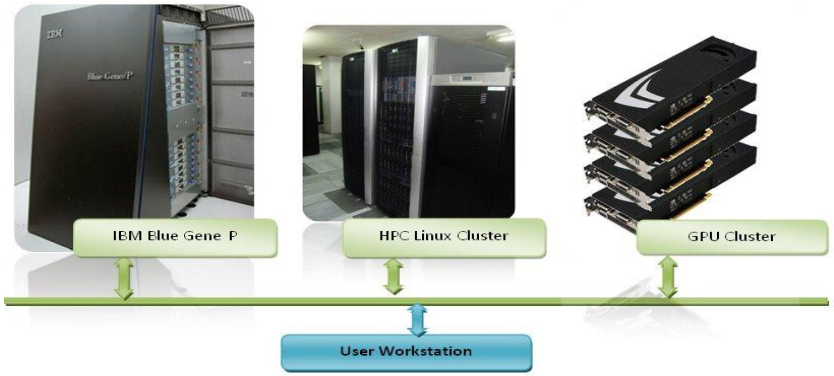
HP-SEE проект (Основни Резултати)

HP-SEE
High-Performance Computing Infrastructure for South East Europe's Research Communities

Contract n°: RI-261499
Start date: 01/09/2010
Duration: 36 months
Funding from the EC: 2.1 M €
Total budget: 3.9 M €

Funding from EC to Bulgaria: 196 K €
Requested Support from BgNSF: 75 K €
Received from BgNSF so far: 15 K €

- Съществуващите високопроизводителни изчислителни средства в региона са свързани в обща инфраструктура.
- Проектът установи и поддържа GEANT връзката за Кавказкия регион.
- Високопроизводителната изчислителна инфраструктура на ЮИЕ е достъпна за широк обхват от нови потребителски общества, включително и тези идващи от страните с по-малко изчислителни ресурси.



Country	Center	Cores	Teraflops
Bulgaria			
	BG Blue Gene/P	8192	27.85
	HPCG	**576**	**3.23**
Macedonia			
	FINKI SC	2016	9
Hungary			
	Pecs SC	1152	10
	Debrecen SC	3078	18
	Szeged	2112	14
Romania			
	InfraGRID	400	2.5
	IFIN_BIO	256	2.72
	IFIN_BC	368	3.9
	NCIT	562	3.4
	UVT Blue Gene/P	4096	13.9
Serbia			
	PARADOX	672	6.26
TOTAL		**23624**	**115.26**

Резултати на проекта

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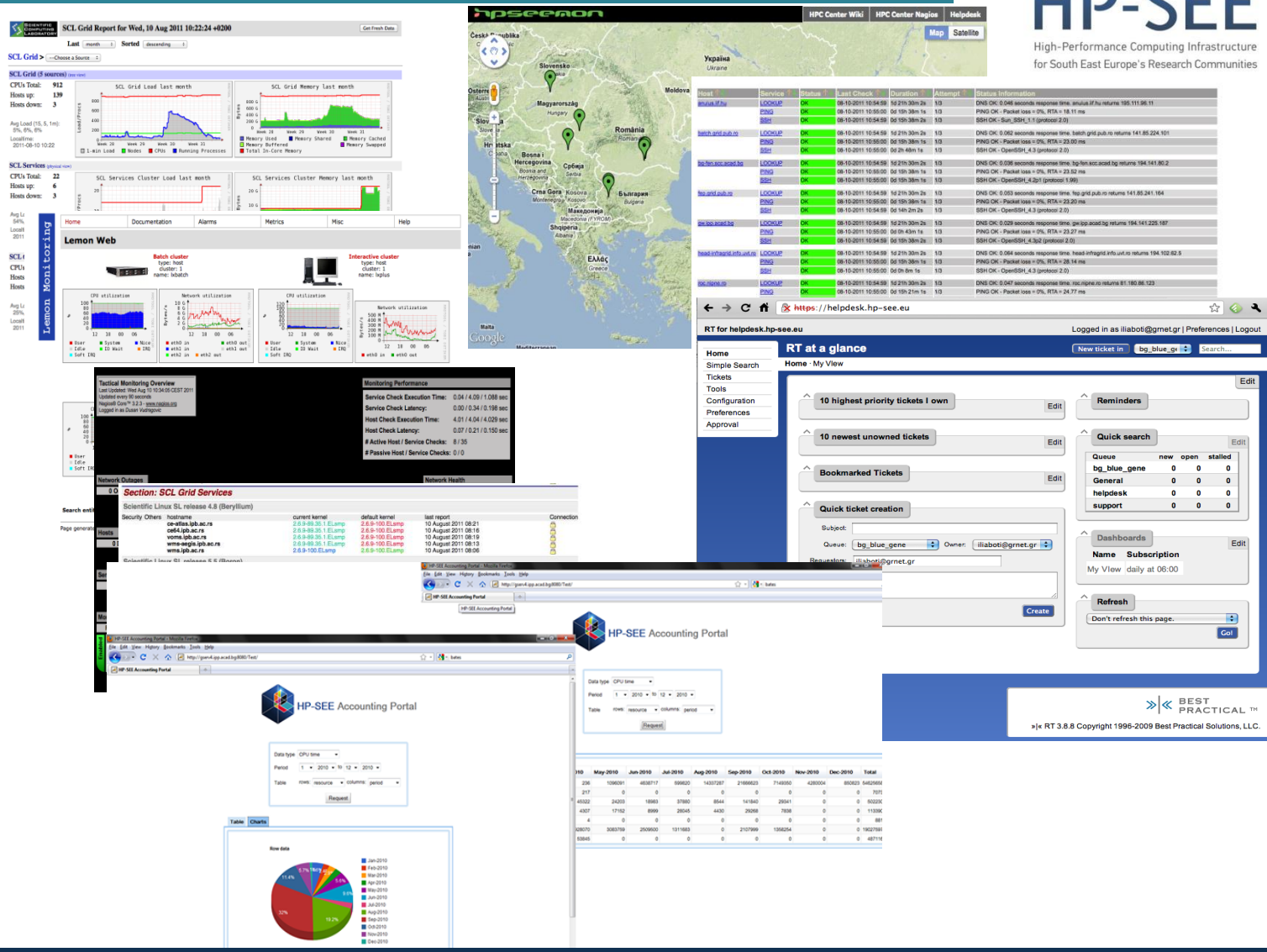
- Фокусът от сътрудничество при изграждането на HPC инфраструктурата в ЮИЕ е върху 3 стратегически групи от изследователи в региона (26 приложения):
  - **изчислителната физика, изчислителната химия и науките за живота.**
- Пилотен конкурс за включване на нови приложения проведен от 5 септември до 7 октомври 2012: – постъпили 20 приложения от 9 страни, удобрени 13 приложения.
- Ускорен процес (fast-track process) за включване на нови потребители
- http://hp.see.eu
- http://survey.ipb.ac.rs/index.php?sid=19757

Operational and user support tools

- Operational monitoring:
  - site-level monitoring tools (Ganglia, Lemon, Nagios, Pakiti)
- Top level monitoring implemented by newly HP-SEE plug-ins (Nagios monitoring systems)
- Helpdesk
- Accounting information system



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Виртуални изследователски общности

- Изчислителна физика
  IFIN-HH,
  7 страни,
  12 приложения
- Изчислителна химия
  ИИКТ-БАН,
  6 страни,
  7 приложения
- Науки за Земята
  GRNET,
  5 страни,
  7 приложения

СТРАНА	Изч. Физика	Изч. Химия	Науки за Земята	Общо
Албания	2			2
Армения			1	1
Босна&Хер	1	1		2
България	2	2		4
Грузия			1	1
Гърция		1	2	3
Унгария			2	2
Молдова	1			1
Черна Г.			1	1
Македония	1	1		2
Румъния	4	1		5
Сърбия	1	1		2
12	12	7	7	26

Приложения в изчислителната физика

Country	Application name	Acronym	Partner
Albania	**Geophysical Inversion Modeling**	GIM	PUoT
	Hadron Masses from Lattice QCD	HMLQCD	UT
Bosnia-Herz	Self Avoiding Hamiltonian Walk on Gaskets	SFHG	UoBL
Bulgaria	**Computer Simulation of Complex Gas Flows in Micro-sized Channels and Domains**	**SIMPLE-TS 2D**	**IM-BAS**
	Simulation of Electron Transport	**SET**	**IICT-BAS**
Moldova	Parallel algorithm and program for the solving of continuum mechanics equations using Adaptive Mesh Refinement	AMR-PAR	IMI-ASM
FYR of Macedonia	Genetic algorithms in atomic collisions	GENETATOMIC	UKIM
Romania	Fractal Algorithms for MAss Distribution / High energy physics Algorithms on GPU	FAMAD /HAG	ISS
	Feature Extraction from Satellite Images Using a Hybrid Computing Architecture	EagleEye	UPB
	Parallel Fuzzy C Means for classification/Feature detection category	FuzzyCmeans	UVT
Serbia	**Numerical study of ultra-cold quantum gases**	**NUQG**	**IPB**
7	**12**		**11**

Приложения в изчислителната химия

Country	Application name	Acronym	Partner
Bosnia-Herzegovina	CFD Analysis of Combustion	CFDOF	UoBL
Bulgaria	Principal Component Analysis of the Conformational Interconversions in large-ring Cyclodextrins	PCACIC	IOCCP-BAS
	Molecular design of platinum group metal complexes as potential non-classical cisplatin analogues	MDCisplatin	IMB-BAS
Greece	Design of fullerene and metal-diothiolene-based materials for photonic applications	FMD-PA	NHRF
FYR Macedonia	**Hybrid Classical/Quantum Molecular Dynamics – Quantum Mechanical Computer Simulation of Condensed Phases**	HC-MD-QM-CS	UKIM
Romania	Integrated System for Modeling and data analysis of complex Biomolecules	ISyMAB	IFIN-HH
Serbia	Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation in chemistry	CompChem	UoB
6	7		7

Приложения - науки за Земята

HP-SEE

Country	Application name	Acronym	Partner
Armenia	Molecular Dynamics Study of Complex systems	MDSCS	IIAP-NASRA
Greece	Computational Models of Short and Long Term Memory	CMSLTM	IMBB-FORTH
	Searching for novel miRNA genes and their targets	miRs	
Georgia	Modeling of biochemical processes for realization of thin and purposeful synthesis	MSBP	TSU / GRENA
Hungary	Deep sequencing for short fragment alignment	DeepAligner	MTA –SZTAKI/ OU-Biotech Group
	In-silico Disease Gene Mapper	DiseaseGene	
Montenegro	DNA Multicore Analysis	DNAMA	SC&CS/LCBB
5	7		7

всички приложения са мултидисциплинарни

Applications Software, Libraries, Computational Methods

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- CompChem and LifeSci VRCs
  - GAMESS, AMBER, GROMACS, OpenFOAM, NetGen, FreeCAD, NAMD, AutoDock, Gaussian, CPMD, NWCHEM, MDYNAMIX, ORCA, VMD, BLAST
  - **Computational methods**: Hartree Fock(HF), density functional theory (DFT), coupled cluster CCSD(T) technique, molecular dynamics simulation (MDS), Computational Fluid Dynamics (CFD) and combustion solver (CS), Monte Carlo simulation
- CompPhys VRC
  - Fermiqcd code, LAPACK, SCALAPACK, FFTW, SPRNG, scrambled Halton and Sobol's sequences, CURAND, CUDA-SDK, Intel MKL
  - **Computational methods:** Finite Volume method (FVM), Direct MC method, spatial Fuzzy C Means algorithms, Monte Carlo and Quasi-Monte Carlo simulations, Krilov solver, Crank-Nicolson method.
- Parallel programming paradigms:
  - Message-Passing (MPI), Shared memory (OpenMP), etc.

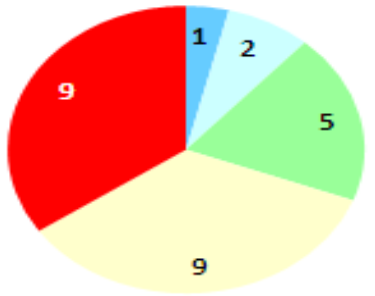
Progress of the applications

Application	VRC	M1	M2	M3	M4	M5	M6	M7	M8	M9	M10	M11	M12
AMR_PAR	CP												
CFDOF	CC												
CompChem	CC												
CMSLTM	LS												
DeepAligner	LS												
DiseaseGene	LS												
DNAMA	LS												
EagleEye	CP												
FAMAD	CP												
FMD-PA	CC												
FuzzyCmeans	CP												
GENETATOMICS	CP												
GIM	CP												
HAG	CP												
HC-MD-QM-CS	CC												
HMLQCD	CP												
ISyMAB	CC												
MDCisplatin	CC												
MDSCS	LS												
miRs	LS												
MSBP	LS												
NUQG	CP												
PCACIC	CC												
SET	CP												
SFHG	CP												
SIMPLE-TS 2D	CP												

APPLICATIONS PROGRESS DURING Y1

STAGES
CONCEPT
ALPHA
BETA
TESTING
DEPLOYMENT
PRODUCTION

STATISTICS - M12



Accounting data

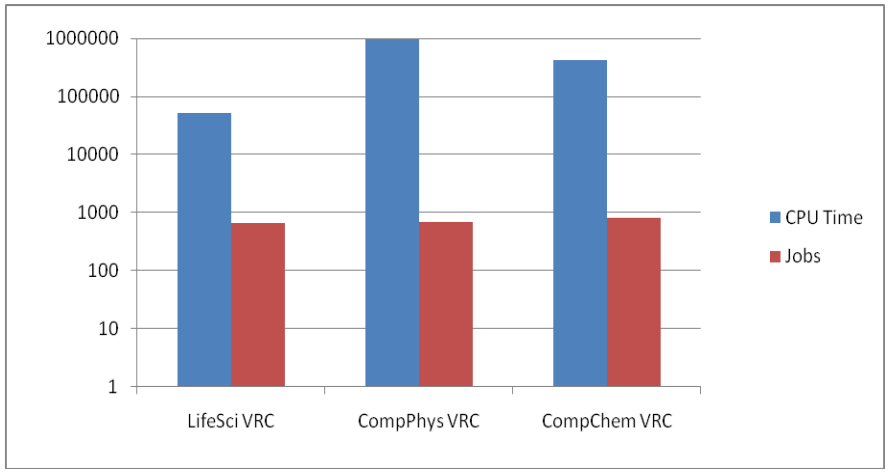


FIG. 2: Distribution of CPU hours and job numbers per VRC

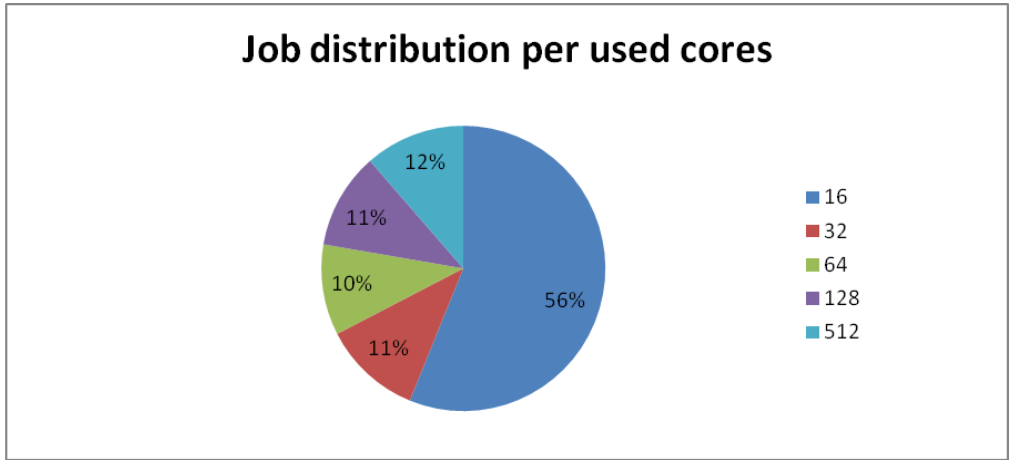


FIG. 2: Job Distribution per used cores

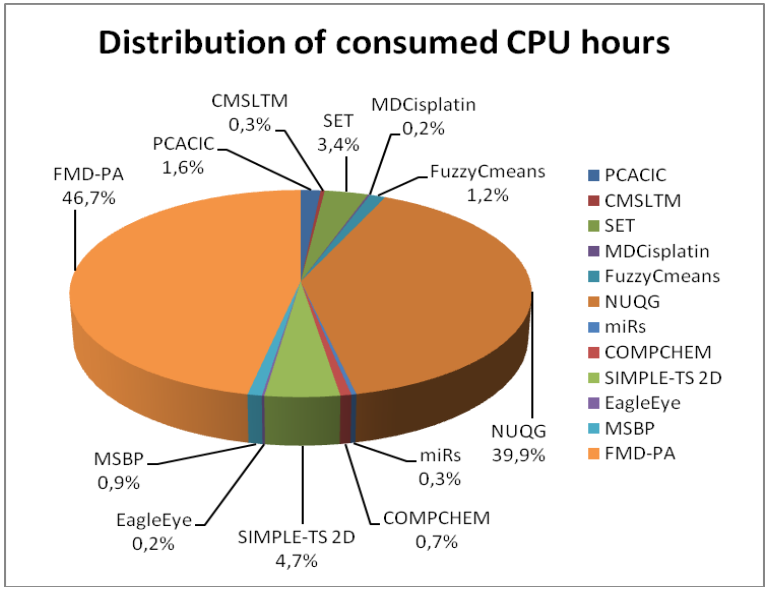


FIG. 2: Distribution of CPU hours consumed in the HP-SEE infrastructure

How to get access to HP-SEE infrastructure

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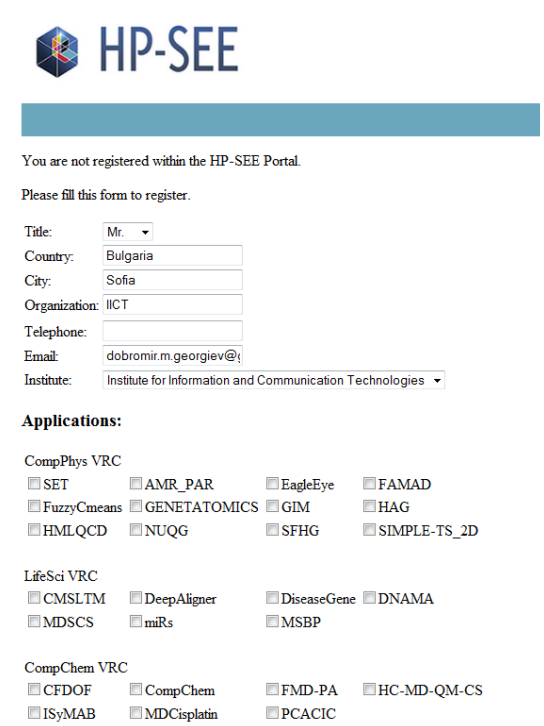

Fig1: Registration form

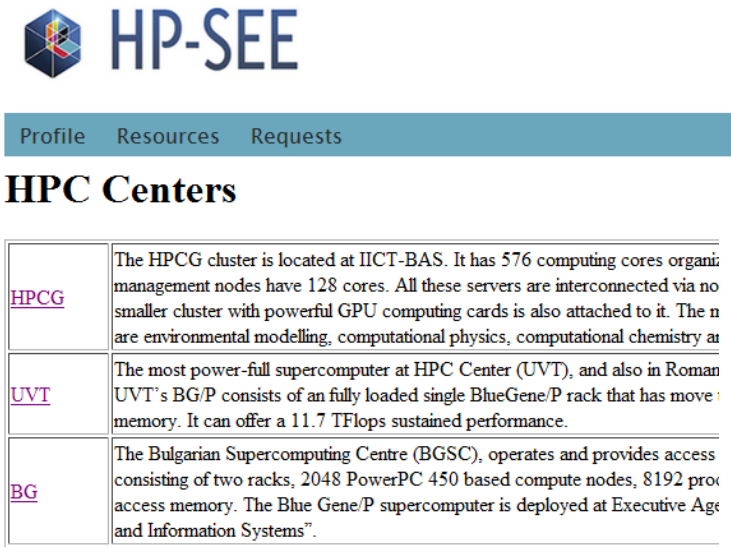

Fig2: List of HPC centers

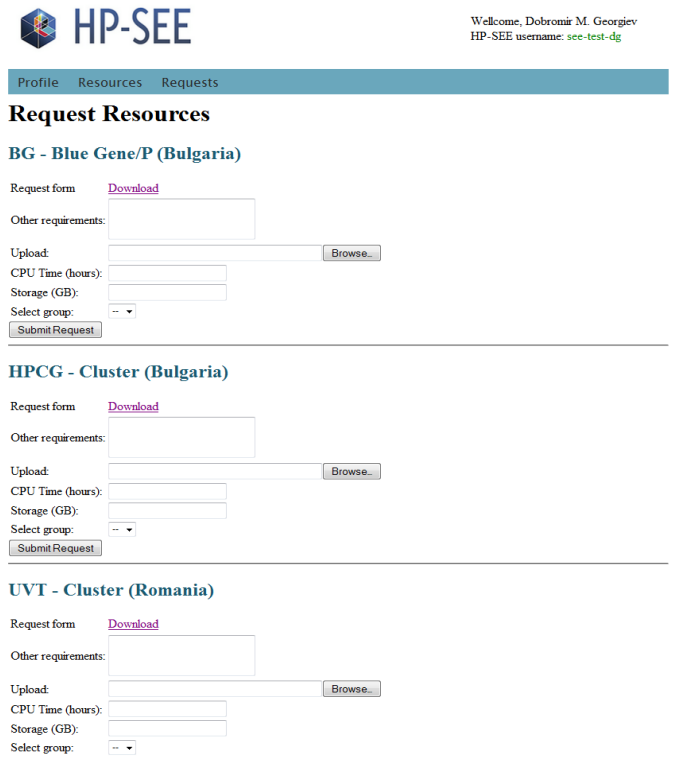

Fig3: Request Forms for user account

After users have been approved by the Application Review Committee (ARC)

Перспективи за сътрудничество

HP-SEE
High-Performance Computing Infrastructure for South East Europe's Research Communities

- HP-SEE подкрепя по-нататъшното разширяване на мрежата от специалисти на регионално и национално ниво, протягайки ръка на възможно най-широк кръг от локални и национални виртуални общности, посредством силна кампания за популяризиране и обучение.
- Учените и организациите от региона могат да получат преимущество при кандидатсване за проекти на Европейско и национално ниво.
- Други приложения изискващи високопроизводителни изчислителни ресурси също ще бъдат подкрепяни в близко бъдеще.
- Проектът дава възможност за обучение (на начинаещи и на на преднали) в областите: високопроизводителни изчисления, паралелни алгоритми и употребата на приложен софтуер.