

**Инфраструктура за високопроизводителни
пресмятания за изследователските общности в
Югоизточна Европа**

HP-SEE
www.hp-see.eu



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

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HP-SEE

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

СТРУКТУРА НА 7РП (програми и инструменти)



HP-SEE

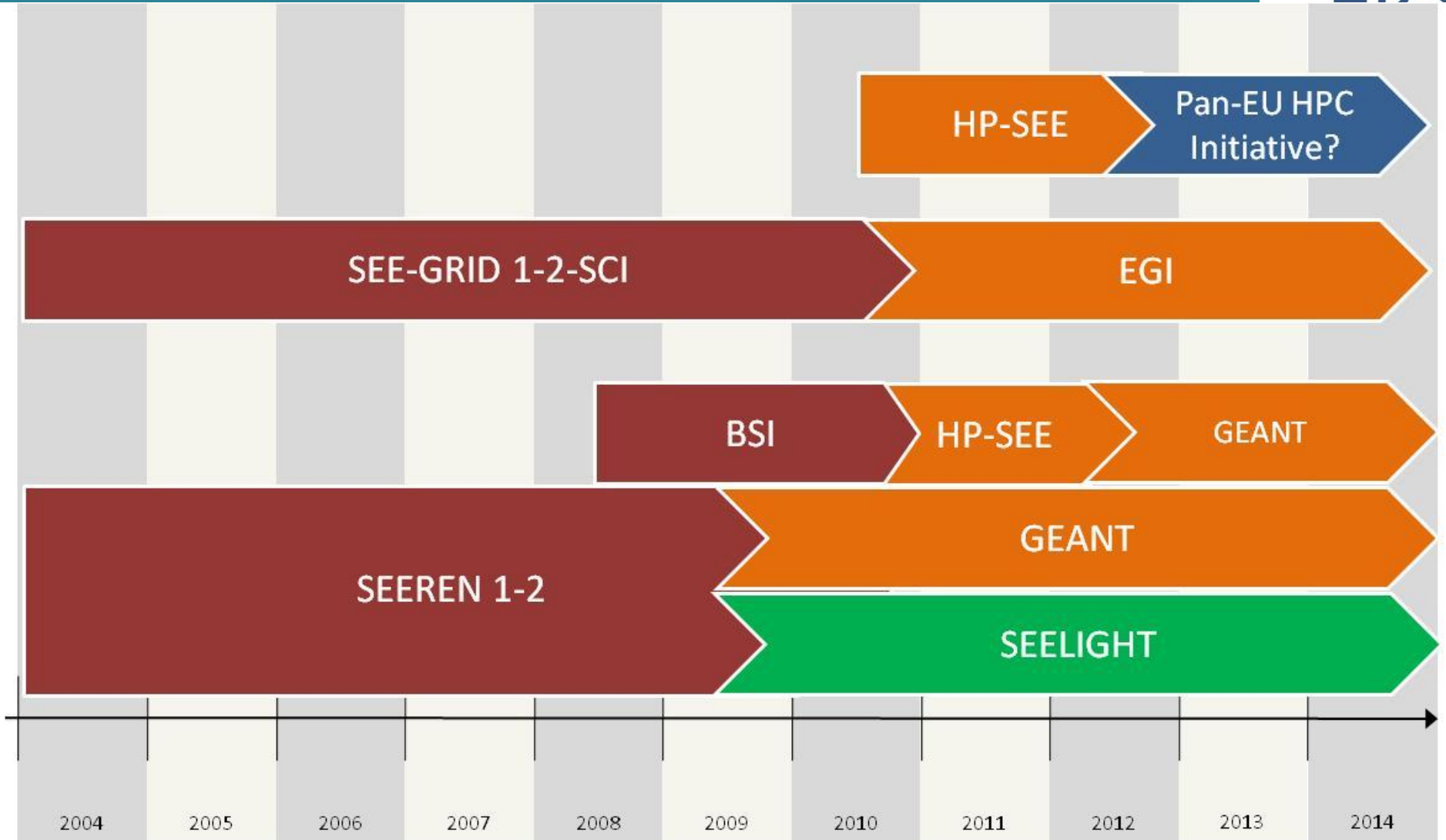
High-Performance Computing Infrastructure
for South East Europe's Research Communities

- ❑ **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
Building Infrastructure
for Research Communities



HP-SEE Консорциум



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

Членове на консорциума

Greek Research & Technology Network

**Институт по информационни и комуникационни технологии,
Българска академия на науките**

"Horia Hulubei" National Institute of Research and Development for
Physics and Nuclear Engineering

The Scientific & Technological Research Council of Turkey

National Information Infrastructure Development Office

Institute of Physics Belgrade

Polytechnic University of Tirana

University of Banja Luka

SS. Cyril & Methodius University of Skopje

University of Montenegro

Research & Educational Networking Association of Moldova

Institute for Informatics & Automation Problems,
National Academy of Sciences of Armenia

Georgian Research & Educational Networking Association

Azerbaijan Research and Education Association

Абривиатура

GRNET

IICT-BAS

IFIN-HH

TUBITAK ULAKBIM

NIIF

IPB

PuoT

UoBL ETF

UKIM

UOM

RENAM

IIAP-NAS-RA

GRENA

AZRENA

GR

BG

RO

TR

HU

RS

AL

BA

MK

ME

MD

AM

GE

AZ

Трети страни / JRU механизъм

11 университета / изследователски центрове

HP-SEE проект (Основни Резултати)



HP-SEE

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Contract n°: **RI-261499**

Start date: **01/09/2010**

Duration: **36 months**

Funding from the EC: **2.1 M €**

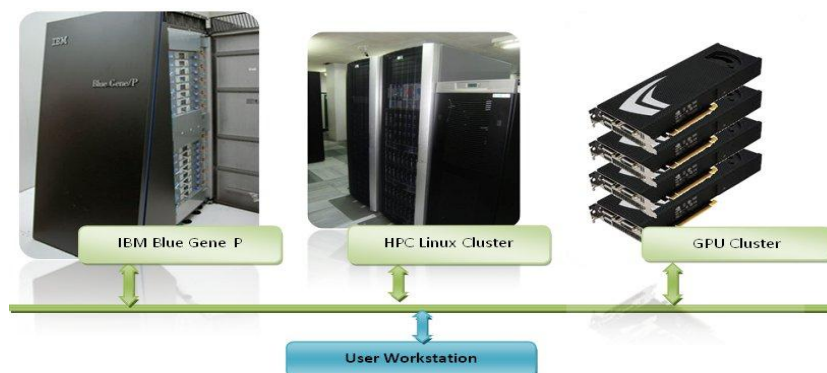
Total budget: **3.9 M €**

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

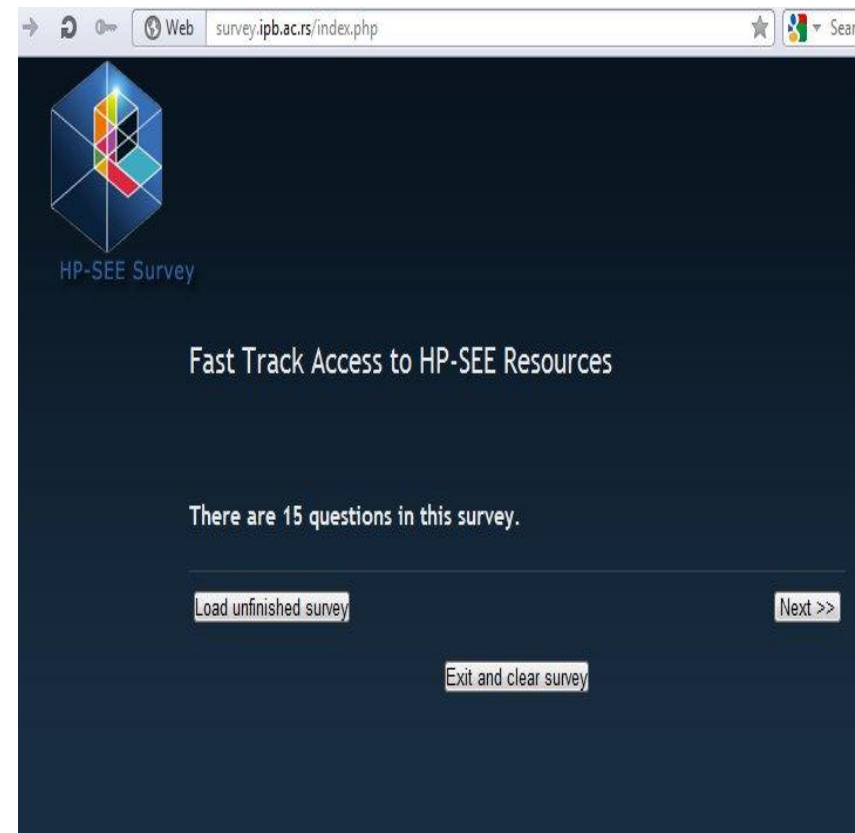
Резултати на проекта



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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



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- 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

The collage displays several key components of the HP-SEE infrastructure:

- SCL Grid Monitoring:** Reports on SCL Grid Load and Memory usage for Wed, 10 Aug 2011.
- Geographic Map:** Shows the HP-SEE network footprint across Central Europe, including countries like Slovakia, Hungary, Romania, and Bulgaria.
- Helpdesk Interface:** A ticket management system with columns for Host, Service, Status, Last Check, Duration, Attempts, and Status Information.
- Lemon Web Monitoring:** Dashboards for CPU and network utilization across different clusters.
- RT at a glance:** A dashboard for Real Time (RT) ticket management, showing priority tickets, newest unowned tickets, and bookmarked tickets.
- HP-SEE Accounting Portal:** A system for resource accounting, featuring tables of usage data and a pie chart for new data.

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Виртуални изследователски общности



UD CEE

- 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



HD-SEE

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



HD-SEE

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



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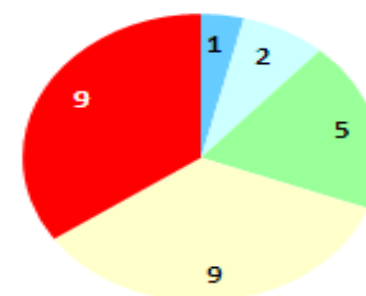
European Computing Infrastructure
for the Research Communities

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

APPLICATIONS PROGRESS DURING Y1

STAGES	
CONCEPT	CONCEPT
ALPHA	ALPHA
BETA	BETA
TESTING	TESTING
DEPLOYMENT	DEPLOYMENT
PRODUCTION	PRODUCTION

STATISTICS - M12



Accounting data



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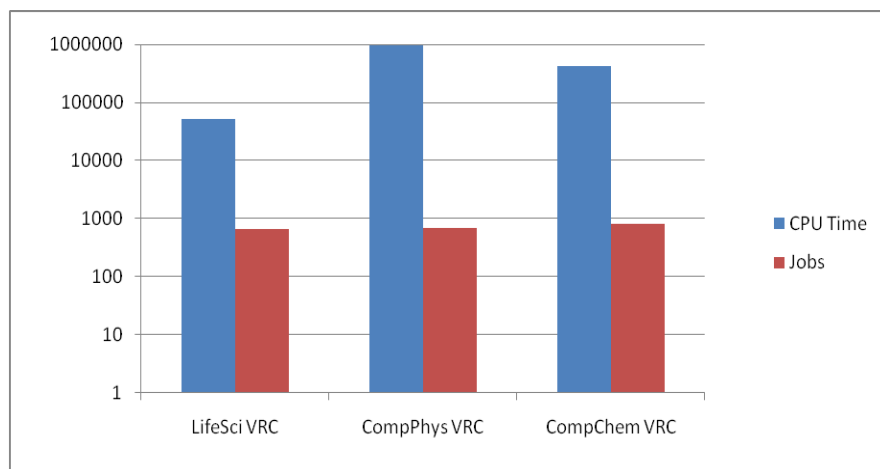


FIG. 2: Distribution of CPU hours and job numbers per VRC

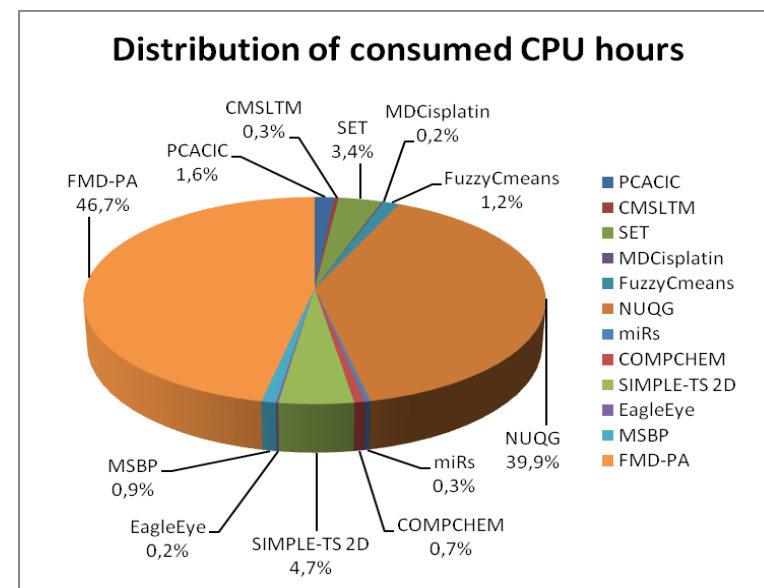


FIG. 2: Distribution of CPU hours consumed in the HP-SEE infrastructure

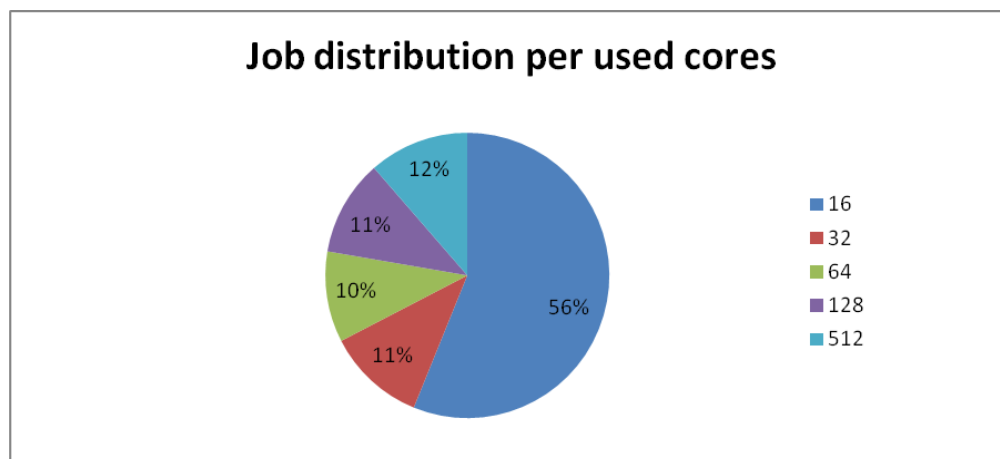


FIG. 2: Job Distribution per used cores

How to get access to HP-SEE infrastructure



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Welcome, Dobromir M. Georgiev

Profile Resources Requests

HPC Centers

HPCG	The HPCG cluster is located at IICT-BAS. It has 576 computing cores organized in 14 racks. All these servers are interconnected via a high-speed network. A smaller cluster with powerful GPU computing cards is also attached to it. The main applications are environmental modelling, computational physics, computational chemistry and materials science.
UVT	The most powerful supercomputer at HPC Center (UVT), and also in Romania. UVT's BG/P consists of a fully loaded single BlueGene/P rack that has moved to a new location. It can offer a 11.7 TFlops sustained performance.
BG	The Bulgarian Supercomputing Centre (BGSC), operates and provides access to a supercomputing infrastructure consisting of two racks, 2048 PowerPC 450 based compute nodes, 8192 processor cores and 16 TB of access memory. The Blue Gene/P supercomputer is deployed at Executive Agency for Information Systems.

Fig2: List of HPC centers

You are not registered within the HP-SEE Portal.

Please fill this form to register.

Title: Country: City: Organization: Telephone: Email: Institute:

Applications:

CompPhys VRC
 SET AMR_PAR EagleEye FAMAD
 FuzzyCmeans GENETATOMICS GIM HAG
 HMLQCD NUQG SFHG SIMPLE-TS_2D

LifeSci VRC
 CMSLTM DeepAligner DiseaseGene DNAMA
 MDSCS miRs MSBP

CompChem VRC
 CFDOF CompChem FMD-PA HC-MD-QM-CS
 ISyMAB MDCisplatin PCACIC

Fig1: Registration form



Welcome, Dobromir M. Georgiev
HP-SEE username: see-test-dg

Profile Resources Requests

Request Resources

BG - Blue Gene/P (Bulgaria)

Request form [Download](#)
Other requirements:
Upload:
CPU Time (hours):
Storage (GB):
Select group: --

HPCG - Cluster (Bulgaria)

Request form [Download](#)
Other requirements:
Upload:
CPU Time (hours):
Storage (GB):
Select group: --

UVT - Cluster (Romania)

Request form [Download](#)
Other requirements:
Upload:
CPU Time (hours):
Storage (GB):
Select group: --

Fig3: Request Forms for user account

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



- 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 кандидатстване 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 напреднали) в областите: високопроизводителни изчисления, паралелни алгоритми и употребата на приложен софтуер.