HP-SEE

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

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

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The structure of FP7

- **Cooperation**
- **Ideas**
- **People**
- **Capacities**
  - **Research Infrastructures**
  - **Research for the benefits of SMEs**
  - **Regions of Knowledge**
  - **Research Potential**
  - **Science and Society**
  - **International Cooperation**
  - **Support for the Coherent Development of Research Policies**

HP-SEE

- **Contract n°:** RI-261499
- **Project type:** CP & CSA
- **Start date:** 01/09/2010
- **Duration:** 24 months
- **Funding from the EC:** 2 100 000 €
- **Total funded effort, PMs:** 539.5
- **Web site:** www.hp-see.eu

HP-SEE Partnership

Contractors (14)

GRNET	Coordinating Contractor	Greece
IPP-BAS	Contractor	Bulgaria
IFIN-HH	Contractor	Romania
TUBITAK ULAKBIM	Contractor	Turkey
NIIFI	Contractor	Hungary
IPB	Contractor	Serbia
UPT	Contractor	Albania
UOBL ETF	Contractor	Bosnia-Herzegovina
UKIM	Contractor	FYROM
UOM	Contractor	Montenegro
RENAM	Contractor	Moldova (Republic of)
IIAP NAS RA	Contractor	Armenia
GRENA	Contractor	Georgia
AZRENA	Contractor	Azerbaijan

Third Party / JRU mechanism used
associate universities / research centres

HP-SEE Vision: sustainability

Seismology, Meteorology, Environment

Comp physics, Comp chem, Life sciences

User / Knowledge layer

SEE-GRID → EGI

HP-SEE→PRACE

GEANT & SEE-LIGHT

HP-SEE

- ❑ The aim of the project is to link existing and upcoming HPC facilities in the region in a common infrastructure.
- ❑ As a complementary action, the project will establish and maintain GEANT link for Caucasus.
- ❑ The HPC infrastructure will be opened to a wide range of new user communities, including those of less-resourced countries, fostering collaboration and providing advanced capabilities to researchers, with an emphasis on strategic groups in computational physics, chemistry and life sciences.
- ❑ The project will support establishment of national HPC initiatives, and act as a SEE bridge for PRACE

Project objectives

- O1 – Empowering multi-disciplinary virtual research communities

  enable application porting and support for SEE major scientific fields

- O2 – Deploying integrated infrastructure for virtual research communities

  edify and operate the regional HPC infrastructure

- O3 – Policy development and stimulating regional inclusion in pan-European HPC trends

  enable integration and compatibility of and between national /regional / pan-European HPC infrastructures -> PRACE

- O4 – Strengthening the regional and national human network

  creation of sustainable VRCs; take-up/maintenance of eInfrastructure services by communities

Objective 1 – Empowering multi-disciplinary virtual research communities

- ❑ Engage regional multi-disciplinary research communities from the region
- ❑ In a number of scientific fields with needs in massively parallel execution on powerful computing resources
- ❑ Porting and support of the applications
- ❑ Pave the way for new communities' involvement in HPC usage
- ❑ Already identified communities
    - ❑ Computational physics, Computational chemistry, Life sciences
- ❑ Opening up access to the regional infrastructure to countries without HPC infrastructure
- ❑ Prepare applications for PRACE inclusion

- ❑ **Metric: 22 apps deployed by the end of the project**

- Provide and Operate the integrated South-East European eInfrastructure
- Operating
  - HPC infrastructure
  - Specific end-user services
- Establishing the continuation of the GÉANT link to Caucasus
- Provide a regional Tier-1 for PRACE and an interface to PRACE
- Effective integration of the regional end-to-end eInfrastructure
- **Metric: The increase in the computing power during the lifetime of the project**

Objective 3 – Policy development and stimulating regional inclusion in pan-European HPC trends

- Ensure SEE countries' access to regional and if needed European HPC facilities
  - Via sustainable organizational and operational models
- Organizational models at National and Regional Level
- Analyse issues regarding integration and compatibility of and between:
  - National HPC infrastructures
  - Regional infrastructures
  - Pan-European infrastructures
- Setup of national HPC task forces
- Resource sharing across administrative domains as well as scientific fields
- **No quantifiable metric for this objective**

Objective 4 – Strengthening the regional and national human network

- Reach out to as wide as possible range of local and national virtual communities
- Strong Dissemination and Training campaign
- Target primarily communities of Computational physics, Computational chemistry, Life sciences
- Maintain communication channels and PR material

- **Metrics:**
  - **2 regional training events**
  - **5 national level training events in Principal partner countries**

Work Organization

| Work Package	WP Title	Lead
WP1	Management	GRNET
WP2	National and Regional HPC initiatives and international liaison	GRNET
WP3	Dissemination and training	IPB
WP4	Virtual Research Communities support	IFIN-HH
WP5	Regional HPC infrastructure operations	IICT-BAS
WP6	Procurement and network design	GRNET
WP7	Network Operations	TUBITAK-ULAKBIM
WP8	Software stack and technologies updates	NIIFI

Work Organization – PETR
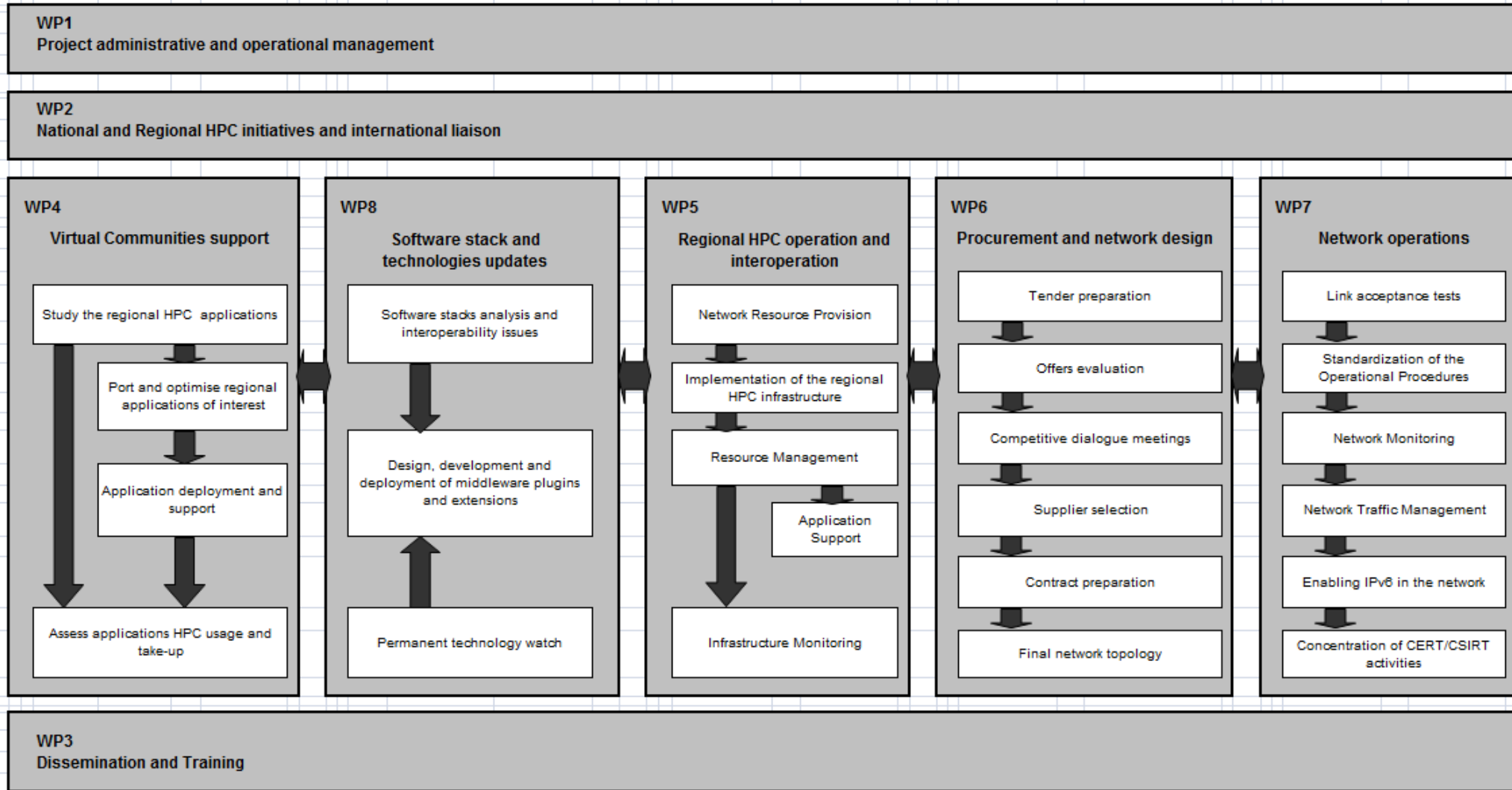
Existing and Planned infrastructure

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

❑ Resource commitments per country

Country	Tflops		
	2010	**2011**	**2012**
Greece	0	40	80
Bulgaria	Planned 25/**available 30** Planned 0**/ (available 8 GPU)**	30+8 GPU	40+20 GPU
Romania	10	20+100 GPU	30+100 GPU
Hungary	1	30	60
Serbia	0	20	40
OVERALL	**36**	**140 +108 GPU**	**250+120 GPU**

Current and planned computing power (double precision for CPU and single for GPU)
The metric in this context is the increase in the computing power during the lifetime of the project, with specific dates, as given in B1.3.3.

Regional HPC infrastructure operations

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Integrated provision of state-of-the-art eInfrastructure services to the end users

- ❑ Ensure computing, storage and application-specific resources for the user community
- ❑ Authentication and authorization mechanisms and joint regional operations
- ❑ Smooth interaction with the regional networking layer
- ❑ Deploy a set of operational tools covering:
  - User administration
  - Accounting
  - Distributed data management
  - Security
  - Monitoring
  - Resource management and allocation
  - Helpdesk

Introduction to VRCs

- **Comput. Physics**
  IFIN-HH,
  6 countries,
  8 appls.

- **Comput. Chemistry**
  IPP-BAS,
  6 countries,
  7 appls.

- **Life Sciences**
  GRNET,
  5 countries,
  7 appls.

Country	Physics	Chemistry	Life Sciences	TOTAL
Albania	1			1
Armenia			1	1
Bosnia-Herzegovina		1		1
Bulgaria	2	2		4
Georgia			1	1
Greece		1	2	3
Hungary			2	2
Moldova	1			1
Montenegro			1	1
FYR of Macedonia	1	1		2
Romania	2	1		3
Serbia	1	1		2
TOTAL	8	7	7	22

Description of Computational Physics applications

Country	Proposed name (DoW)	Domains	# of candidate appls.
Albania	Computational Resources for Lattice QCD	HE&P Phys.	1
Bulgaria	Computer Simulation of Complex Gas Flows in Micro-sized Channels and Domains	Fluid dynamics, micro-devices mod.	2
	Simulation of Electron Transport	Cond. Matter, nanoelectronics	
Moldova	Adaptive Mesh Refinement	General purpose	1
FYR Macedonia	Study of atomic collisions of highly charged ions in plasma	Plasma Phys.	1
Romania	Dissemination, Developing and Deploying of Graphics Processing Unit	HE&P Phys., Electro-magn., Astrophys.	2
	Feature Extraction from Satellite Images Using a Hybrid Computing Architecture	Geophysics, Meteorology	2
Serbia	Numerical study of ultra-cold quantum gases	Cond. Matter, Atomic Phys.	1
TOTAL	8		10

Description of Computational Chemistry applications

Country	Proposed name (DoW)	Domains	# of candidate appls.
Bosnia-Herzegovina	Design of a chemical reactors, burners, boilers or furnaces	CFD	1
Bulgaria	Principal Component Analysis of the Conformational Interconversions in large-ring Cyclodextrins	Quantum Chem	2
	Molecular design of platinum group metal complexes as potential non-classical cisplatin analogues	Quantum Chem.	
Greece	Design of fullerene and metal-diothiolene-based materials for photonic applications	Quantum Chem., Cond. Matter Phys	1
FYR Macedonia	Quantum Mechanical Computer Simulation of Condensed Phases	Quantum Chem., Cond. Matter Phys	1
Romania	Simulation and modelling of biomolecules.	Biophys., Biochem.	1
Serbia	Molecular-orbital simulations of chemical reactions	Quantum Chem.	1
TOTAL	7		7

Description of Life Sciences applications

Country	Proposed name (DoW)	Domains	# of candidate appls.
Armenia	Simulations for Biological Model Membranes and Surfactant Systems	Biophys., Biochem.	1
Greece	Network models of short and long term memory	.	2
	Searching for novel miRNA genes and their targets	Genomics	
Georgia	Modeling of biochemical processes for realization of thin and purposeful synthesis	Biochemistry	1
Hungary	Sequence analysis genomics application	Genomics	2
	Comparative genomics application		
Montenegro	DNA sequence analysis	Bioinformatics	1
TOTAL	7		7

OBS: all applications are multidisciplinary ! (O1)

Computer Simulation of Complex Gas Flows in Micro-sized Channels and Domains (CSCG):

❑ The computer simulation uses parallel numerical algorithms based on MPI strategy:

  ❑ Finite Volume Method SIMPLE-TS, algorithm developed by K. Shterev and S. Stefanov

  ❑ Direct Simulation Monte Carlo (DSMC) algorithm developed by S. Stefanov

  The overall objective of the work is to develop a robust and accurate modeling tool that can be used to design and optimize micro-devices that operate in the non-equilibrium transition gas flow regime. These tools have application in biomedicine (modeling certain kinds of robotic devices). Achieving good parallel efficiency with this type of applications is hard if at all possible without the use of high-performance low-latency MPI interconnect. The application requires high amount of overall CPU time, not available to the application developers at present.

Results are obtained on the High Performance cluster at IICT-BAS using parallel version of the TS algorithm on 250 cores.

Research related to MEMS.
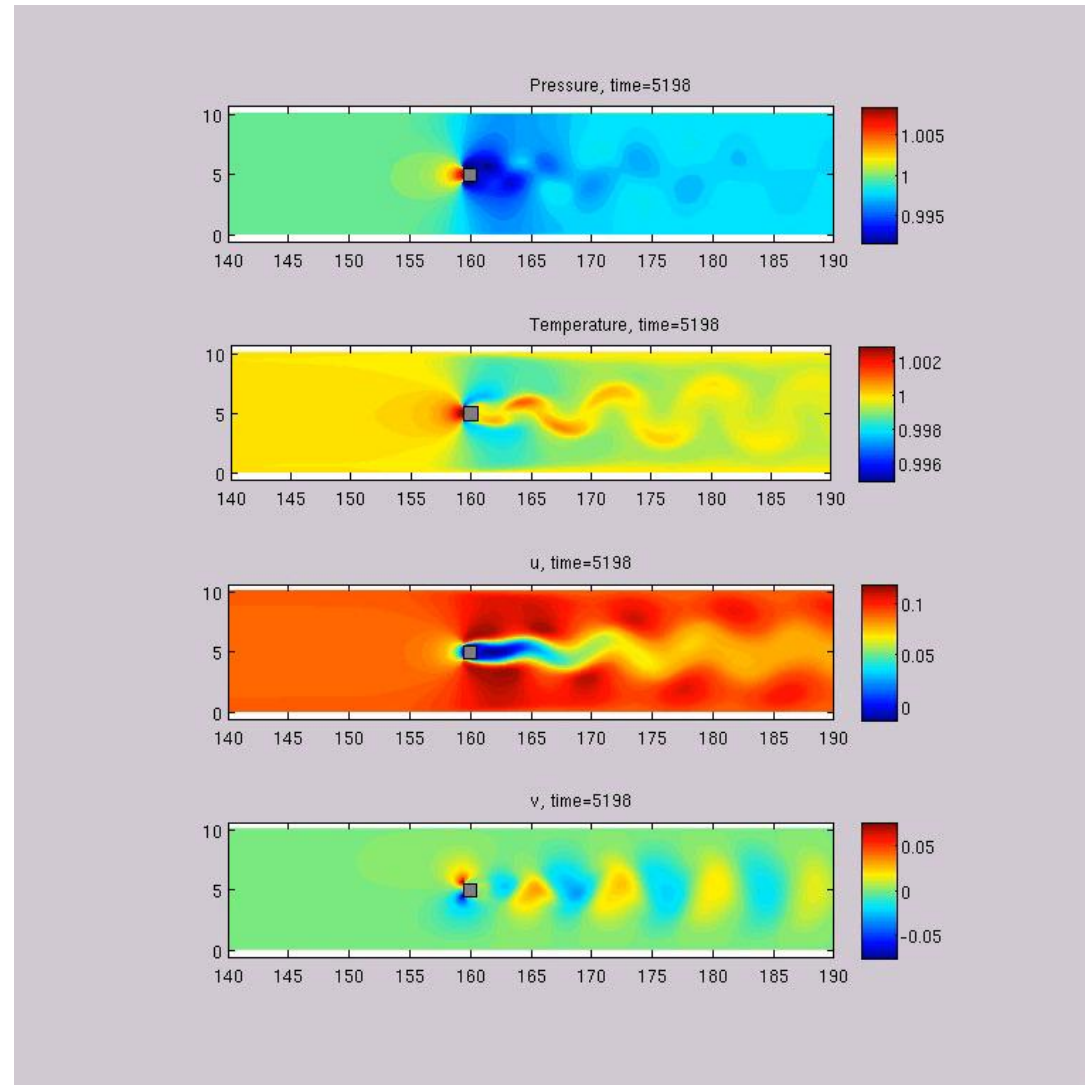
Perspectives for collaboration

- The HP-SEE project ensures access for scientists from the domains of computational chemistry, life sciences and computational physics to state of the art high performance computing facilities in the region.
- Scientists and organizations from the region can leverage this possibility when applying for EU projects.
- Other applications with high computational requirements can be supported in the future.
- The project and its stuff can provide advanced training and education in the domains of high performance computing, parallel algorithms and usage of application software.