HP-SEE

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

PRACE Workshop on HPC Approaches on Life Sciences and Chemistry
Sofia, Bulgaria, 16-02-2012

www.hp-see.eu

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

The HP-SEE initiative is co-funded by the European Commission under the FP7 Research Infrastructures contract no. 261499

Overview

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

- HP-SEE facts
- Who are HP-SEE partners
- History of collaboration in region
- What HP-SEE does
- How it's done
- Key results:
  - Management
  - Infrastructure
  - Software stack and technologies
  - **Research applications**
  - Training and dissemination
  - HPC initiatives
- Long term vision

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for South East Europe's Research Communities

- **Contract n° :** RI-261499
- **Project type:** CP & CSA
- **Call**: INFRA-2010-1.2.3: VRCs
- **Start date:** 01/09/2010
- **Duration:** 24 + 9 months
- **Total budget:** 3 885 196 €
- **Funding from the EC:** 2 100 000 €
- **Total funded effort, PMs:** 539.5
- **Web site:** www.hp-see.eu

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HP-SEE Partnership

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Contractors (14)

GRNET	Coordinating Contractor	Greece
IICT-BAS	Contractor	Bulgaria
IFIN-HH	Contractor	Romania
TÜBİTAK-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 Partnership

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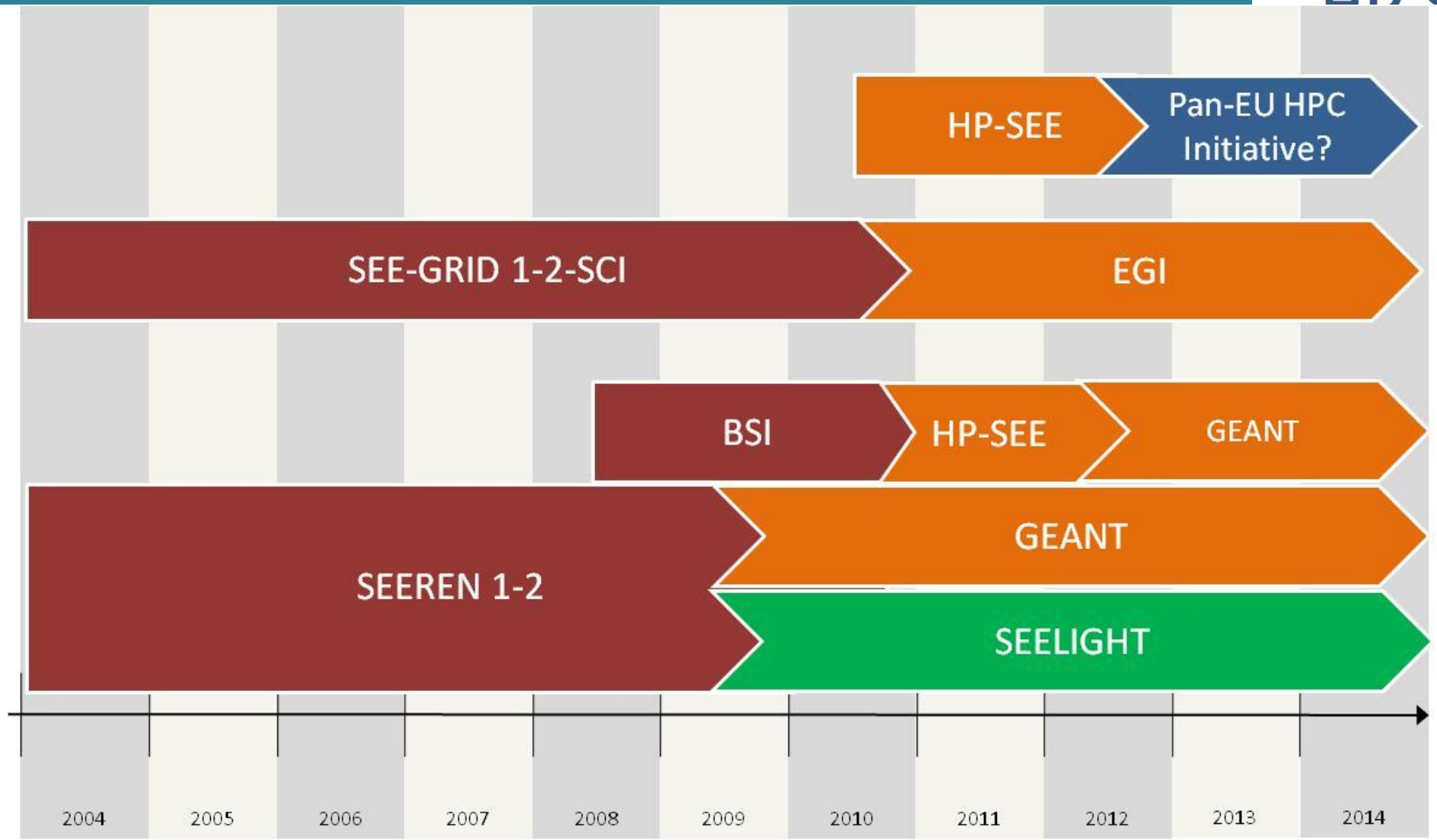
Context: the Timeline



SEE eInfrastructure Activities – past 8 years

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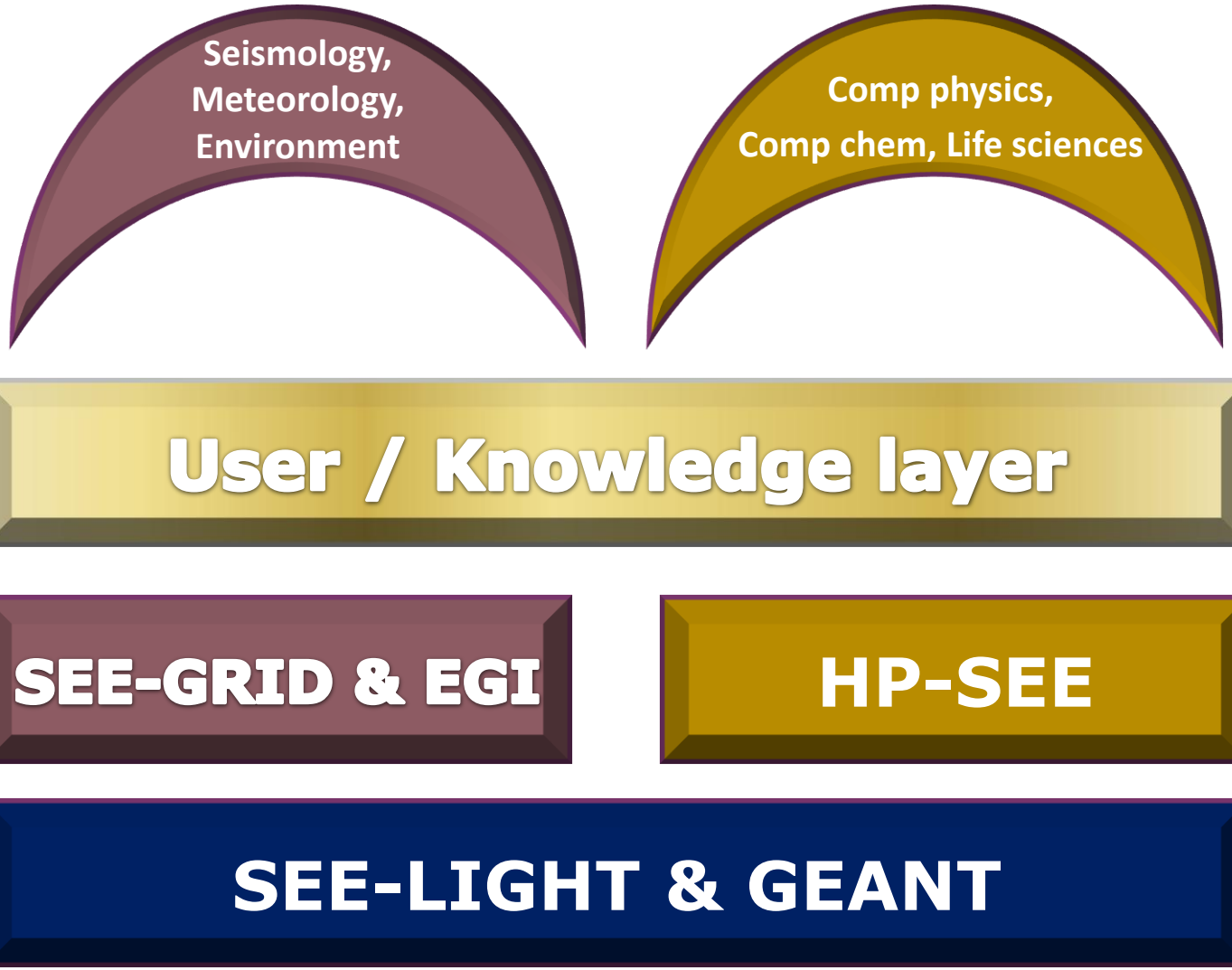
- **SEEREN1/2:** regional inter-NREN connectivity and GEANT links [DGINFSO]
- **BSI:** Southern Caucasus links [DGINFSO]
- **SEELIGHT:** lambda facility in SEE [Greek HiperB]
- *Result: sustainable national & regional networks, most countries in GEANT*

- **SEEGRID1/2:** regional Grid infrastructure, building NGIs and user communities
- **SEE-GRID-SCI:** eInfrastructure for large-scale environmental science user communities: meteorology, seismology, environmental protection. Inclusion of Caucasus. [DGINFSO]
- *Result: sustainable national Grids, all countries within European Grid Initiative*

- **HP-SEE**: regional HPC interconnection and 2nd generation Caucasus link
- *Expected result: stable national HPC centers, (hierarchical) model in collaboration with PRACE and DEISA*

- **SEERA-EI:** regional programme managers collaboration towards common eInfrastructure vision, strategy and regional funds [DGRTD]
- *Result: common regional policy, identifying long-term national-level funds and regional funds to complement EC funds*

Context: the Model - Converged Communication & Service Infrastructure for South-East Europe



HP-SEE Project Objectives

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- Objective 1 – Empowering multi-disciplinary virtual research communities
- Objective 2 – Deploying integrated infrastructure for virtual research communities
  - Including a GEANT link to Southern Caucasus
- Objective 3 – Policy development and stimulating regional inclusion in pan-European HPC trends
- Objective 4 – Strengthening the regional and national human network

Work Organization - PERT

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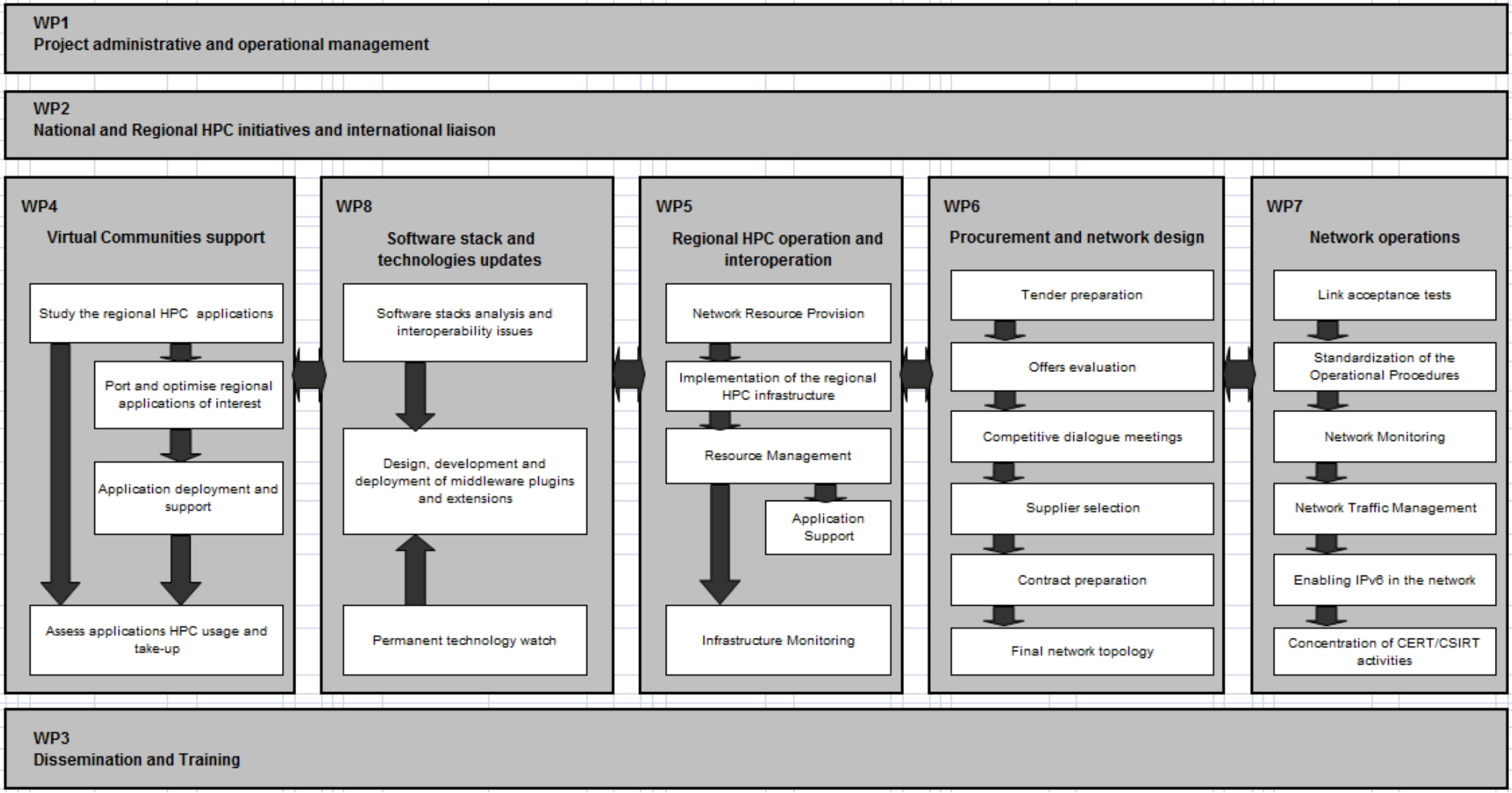

Key results: Management

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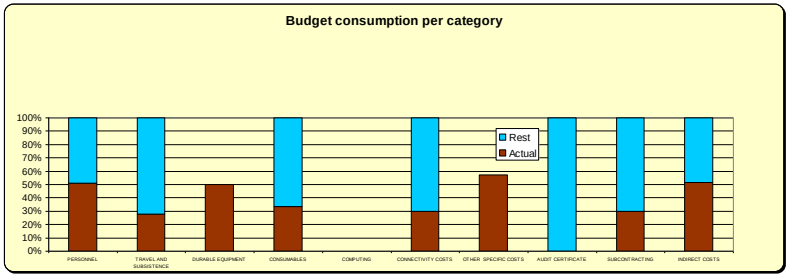
- Complex but efficient management structure with 14 partners and a number of third parties.
- 5 project Steering Committee meetings held collocated with large project events such as trainings
- 9-month project prolongation implemented, to cover the South Caucasus link duration.
- Collaborations with PRACE and LinkSceem

WP1 activities description

WP Name	**Project administrative and operational management**														**WP1**
Start date	1/9/2010			**End Date**	31/8/2012					**Duration**				24 months	
Responsible	Ognjen Prnjat									GRNET-GR					
Participants	GRNET-GR	IPP-BAS	IFIN-HH	BITAK-ULAK	NIIFI	IPB	UPT	UoBL ETF	UKIM	UOM	RENAM	SAP_NAS_RA	GRENA	AZRENA	**TOTAL**
Planned person-months	12,00	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	0,50	**18,50**
Task Name	**Organize meetings**														**1.1**
Planned start date	1/9/2010			**Planned end date**	31/8/2010					**Planned duration**				24 months	
Actual start date	1/9/2010			**Actual end date**						**Actual duration**					
Responsible	Ognjen Prnjat									GRNET-GR					
Participants	GRNET-GR	IPP-BAS	IFIN-HH	BITAK-ULAK	NIIFI	IPB	UPT	UoBL ETF	UKIM	UOM	RENAM	SAP_NAS_RA	GRENA	AZRENA	**TOTAL**
Planned person-months	0,50	0,25	0,25	0,25	0,25	0,25	0,25	0,25	0,25	0,10	0,25	0,25	0,25	0,25	**3,60**

Input	Objectives	Output
Venue information	Organisation of kick-off meeting	Meeting minutes. M1
From: Host		To: HP-SEE consortium
Participants	Regular management and technical meetings (quarterly)	Meeting minutes
From: HP-SEE consortium		To: HP-SEE consortium
Presentations	Review meetings	Review results, M2, M3
From: HP-SEE consortium		To: HP-SEE consortium
Agenda topics	Project technical reviews	Meeting logistics
From: Coordinator, HP-SEE consortium		To: HP-SEE consortium



Key results: HPC infrastructure

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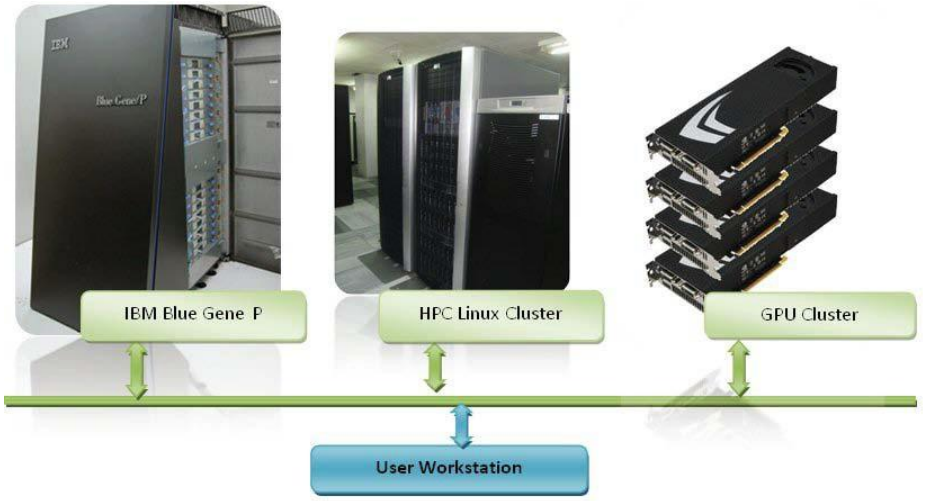
Country	Center	Computing Cores	Teraflops
Bulgaria			
	BG Blue Gene/P	8192	27.85
	HPCG	576	3.23
FYR of Macedonia			
	FINKI SC	2016	9
Hungary			
	NIIFI SC	144	0.5
	Pecs SC	1152	10
	Debrecen SC	3078	18
	Szeged	2112	14
Romania			
	InfraGRID	400	2.5
	IFIN_BIO	256	2.72
	IFIN_BC	368	3.9
	NCIT	562	3.4
	UVT Blue Gene/P	4096	13.9
Serbia			
	PARADOX	672	6.26
TOTAL		**23624**	**115.26**



Infrastructure operational services

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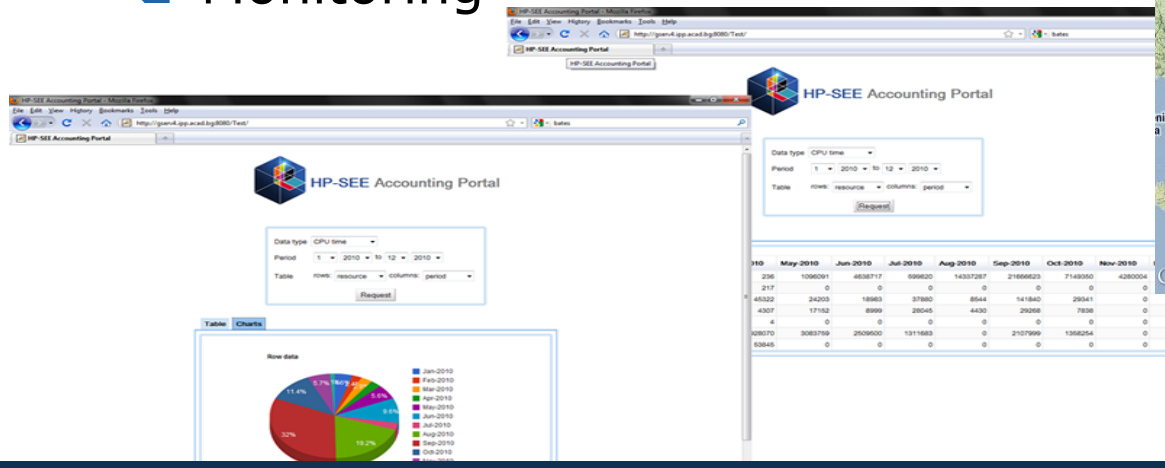
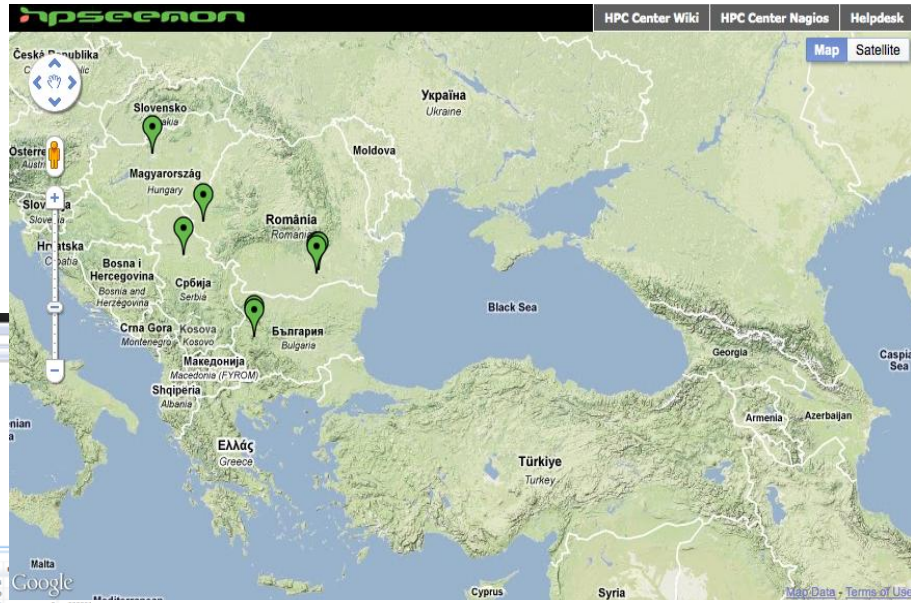
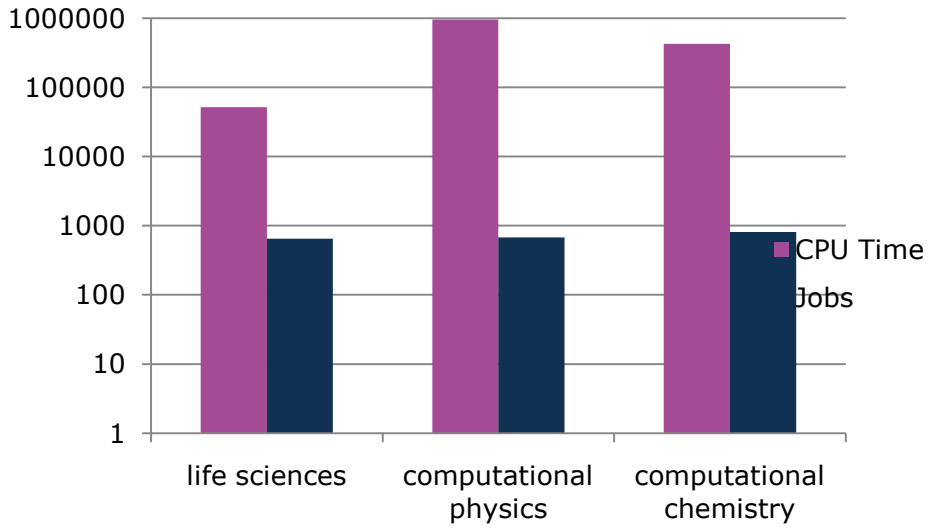
- Distributed set of services supports infrastructure operations:
  - AAA framework:
    - Resource Management System
    - ARC-LDAP service
    - Accounting System
  - Helpdesk
  - Monitoring

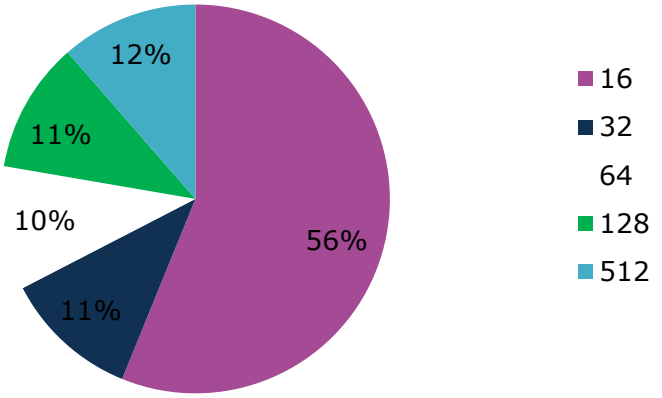


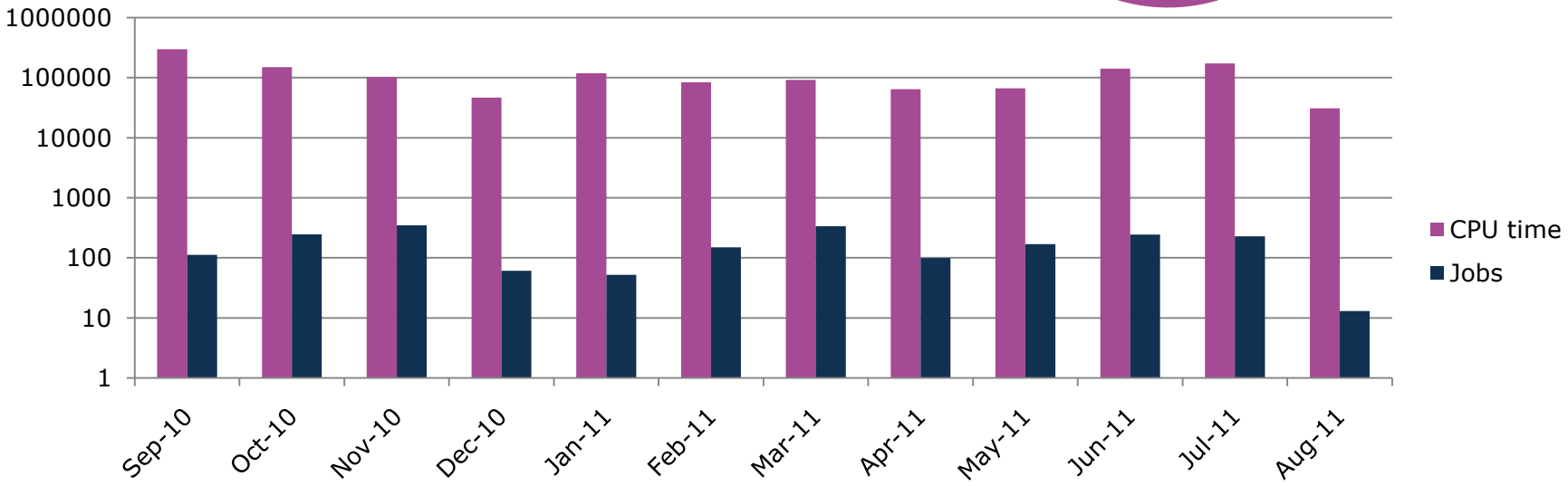


Accounting data



Job Number distribution per used cores





Key results: link to Southern Caucasus

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- Connecting South Caucasus to GÉANT
- 50% national contributions for link establishement
- Beneficiaries
  - Azerbaijan and Armenia, Georgia could not co-fund the link
- Operations of the decentralised virtual NOC in the Caucasus area from September 2011 until May 2013
  - Operational Procedures
  - Network Monitoring
  - Traffic Management
  - Security
  - Best Practices
  - Analysis of connectivity requirements of HPC users

Key results: software stack and technologies (1/2)

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- Study and improve the scalability of applications
  - Gathered the requirements of all applications in terms of software libraries and application codes.
  - Proposed guidelines for improving the scalability of applications via the efficient use of:
    - compilers
    - programming techniques and languages
    - libraries,
    - profiling
    - porting and optimization techniques

Key results: software stack and technologies (2/2)

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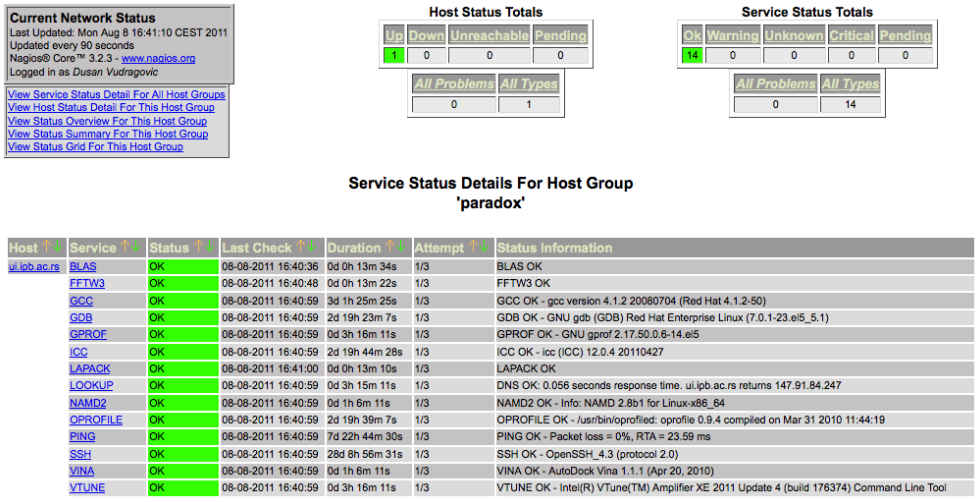
- Assess commonalities to facilitate usage of a heterogeneous infrastructure and foster transparent access to the integrated infrastructure
  - Developed tool for monitoring the software installed in the infrastructure (based on Nagios)
  - Defined metric to assess the level of HPC centers harmonization
  - Use of Grid middleware services for transparent access to the infrastructure as well as the modules framework
- Technology watch
  - Arranged meetings and information exchange with vendors to present and discuss new technology roadmaps for HPC systems of the future
- Deliverables produced
  - Software scalability analysis and interoperability issues assessment
  - Design of interoperability and scalability solutions



Current Network Status
Last Updated: Mon Aug 8 16:41:10 CEST 2011
Updated every 90 seconds
Nagios® Core™ 3.2.3 - www.nagios.org
Logged in as *Dusan Vudragovic*

View Service Status Detail For All Host Groups
View Host Status Detail For This Host Group
View Status Overview For This Host Group
View Status Summary For This Host Group
View Status Grid For This Host Group

Host Status Totals

Up	Down	Unreachable	Pending
1	0	0	0

All Problems	All Types
0	1

Service Status Totals

Ok	Warning	Unknown	Critical	Pending
14	0	0	0	0

All Problems	All Types
0	14

Service Status Details For Host Group 'paradox'

Host	Service	Status	Last Check	Duration	Attempt	Status Information
ui.ipb.ac.rs	BLAS	OK	08-08-2011 16:40:36	0d 0h 13m 34s	1/3	BLAS OK
	FFTW3	OK	08-08-2011 16:40:48	0d 0h 13m 22s	1/3	FFTW3 OK
	GCC	OK	08-08-2011 16:40:59	3d 1h 25m 25s	1/3	GCC OK - gcc version 4.1.2 20080704 (Red Hat 4.1.2-50)
	GDB	OK	08-08-2011 16:40:59	2d 19h 23m 7s	1/3	GDB OK - GNU gdb (GDB) Red Hat Enterprise Linux (7.0.1-23.el5_5.1)
	GPROF	OK	08-08-2011 16:40:59	0d 3h 16m 11s	1/3	GPROF OK - GNU gprof 2.17.50.0.6-14.el5
	ICC	OK	08-08-2011 16:40:59	2d 19h 44m 28s	1/3	ICC OK - icc (ICC) 12.0.4 20110427
	LAPACK	OK	08-08-2011 16:41:00	0d 0h 13m 10s	1/3	LAPACK OK
	LOOKUP	OK	08-08-2011 16:40:59	0d 3h 15m 11s	1/3	DNS OK: 0.056 seconds response time. ui.ipb.ac.rs returns 147.91.84.247
	NAMD2	OK	08-08-2011 16:40:59	0d 1h 6m 11s	1/3	NAMD2 OK - Info: NAMD 2.8b1 for Linux-x86_64
	OPROFILE	OK	08-08-2011 16:40:59	2d 19h 39m 7s	1/3	OPROFILE OK - /usr/bin/oprofiled: oprofile 0.9.4 compiled on Mar 31 2010 11:44:19
	PING	OK	08-08-2011 16:40:59	7d 22h 44m 30s	1/3	PING OK - Packet loss = 0%, RTA = 23.59 ms
	SSH	OK	08-08-2011 16:40:59	28d 8h 56m 31s	1/3	SSH OK - OpenSSH_4.3 (protocol 2.0)
	VINA	OK	08-08-2011 16:40:59	0d 1h 6m 11s	1/3	VINA OK - AutoDock Vina 1.1.1 (Apr 20, 2010)
	VTUNE	OK	08-08-2011 16:40:59	0d 3h 16m 11s	1/3	VTUNE OK - Intel(R) VTune(TM) Amplifier XE 2011 Update 4 (build 176374) Command Line Tool

Applications: key results

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- Supported applications within **Virtual Research Communities**
- Computational Physics
  6 countries
  8 + 4 applications
- Computational Chemistry
  6 countries
  7 applications
- Life Sciences
  5 countries
  7 applications

Country	Physics	Chemistry	Life Sciences	TOTAL
Albania	2			**2**
Armenia			1	**1**
Bosnia-Herzegovina	1	1		**2**
Bulgaria	3	2		**5**
Georgia			1	**1**
Greee		1	2	**3**
Hungary			2	**2**
Moldova	1			**1**
Montenegro			1	**1**
FYR of Macedonia	1	1		**2**
Romania	3	1		**4**
Serbia	1	1		**2**
TOTAL	**12**	**7**	**7**	**26**

Computational Physics VRC

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- Applications Areas
  - High Energy and Particle Physics
  - Plasma Physics
  - Physics of Condensed Matter
  - Atomic Physics
  - Computational Fluid Dynamics
- Indicative Applications range
  - Nano-electronics
  - Micro-devices optimization and modeling of robotic devices for biomedicine
  - Feature detection in satellite images
  - Modeling of electron transport
  - Complex gas dynamics and convection

CP VRC – Selected Results (1/2)

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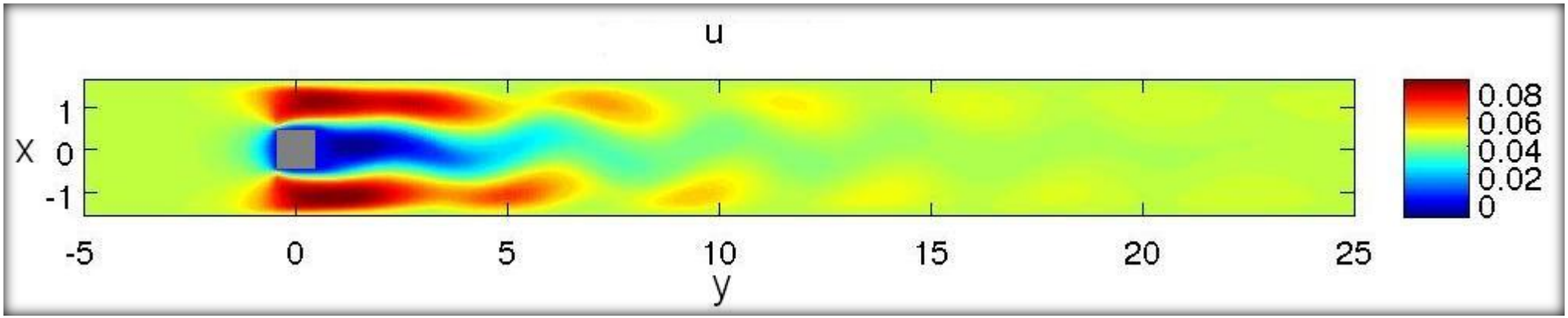
Finite Volume Method for calculation of 2D gas-microflows using standard MPI

- Simulation of internal and external gas flows in or around micro mechanical devices
- PUBLICATIONS

  2 papers

  Various presentations



Mach number 0.05, Knudsen number 0.001 (mean free path of molecules / square size)

CP VRC – Selected Results (2/2)

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Numerical study of ultra-cold quantum gases

- Study of parametric resonance effects in BEC due to harmonic modulation of the interaction strength

- PUBLICATIONS

  3 papers (PhysRev A, J.Stat.Mech.)

  4 presentations at conferences

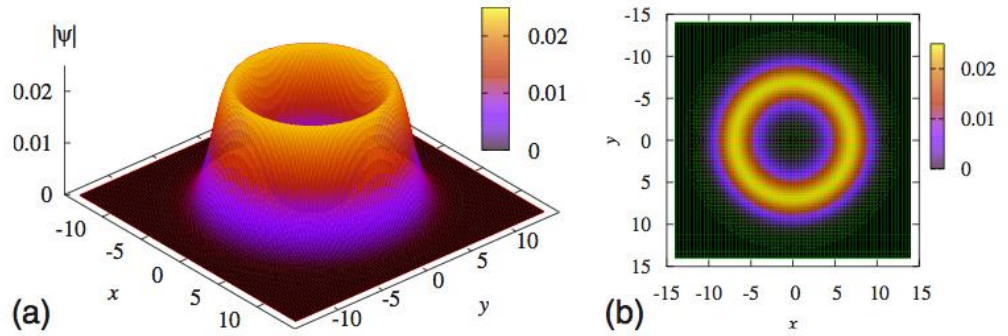

FIG. 6. (Color online) Ground state (as a three-dimensional plot on the left, and as a density plot on the right) of a rotating gas of ^{87}Rb atoms in a $d=2$ anharmonic trap obtained using $p=21$ effective action. The parameters are $r=1.05$, $g=g_{exp}$, $L=20$, $\Delta=0.25$, $t=0.2$.

Computational Chemistry VRC

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- Applications Areas
  - Molecular dynamics and simulations
  - Material science
- Indicative Applications range
  - Study of physicochemical properties of compounds
  - Molecular design of platinum complexes
  - Material design for photonic applications
  - Molecular-orbital simulations
  - Design of chemical reactors, burners, boilers
  - Quantum mechanical simulation of Condensed Phases

CC VRC – Selected Results (1/2)

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Design of fullerene and metal-diothiolene-based materials for photonic applications

- Development of computational methods for the reasonably accurate determination of the linear and nonlinear optical properties of nano-systems.
- The investigation of a series of novel nano-systems with possible photonic applications.
- Achieved Scalability: 512 cores

- PUBLICATIONS

  2 papers submitted for publications

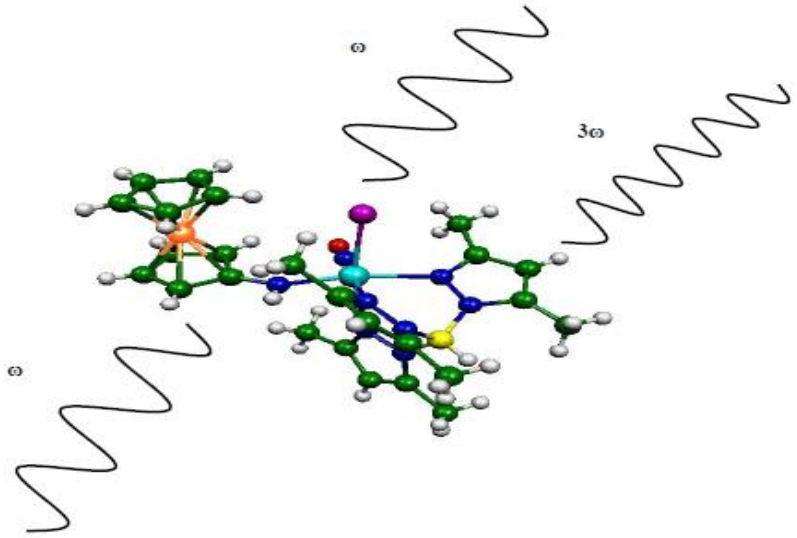

Figure. Third harmonic generation by a ferrocene derivative.

CC VRC – Selected Results (2/2)

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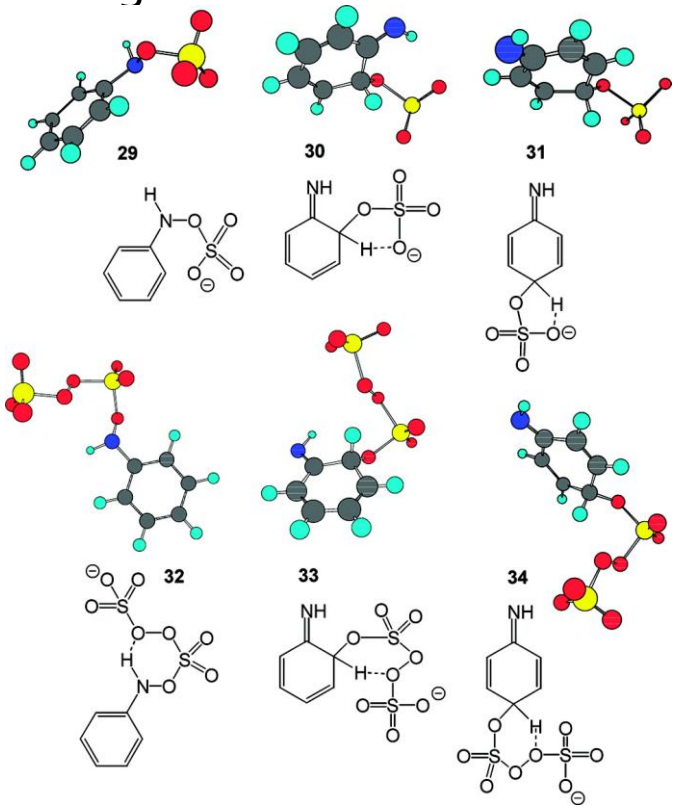
Quantum Mechanical, Molecular Mechanics, and Molecular Dynamics computation in chemistry

- Developing of new medicines on the rational way including recognition of target (enzyme, protein) that causes a specific physiological disorder and developing of molecules that could modify those targets in a manner which attenuate symptoms or cure the illness.

- PUBLICATIONS

  3 publications



Life Sciences VRC

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- Applications Areas
  - Neuroscience
  - Proteomics
  - Genomics and DNA sequence analysis
- Indicative Applications range
  - Network models of short and long term memory
  - Identification of novel miRNA genes
  - Genomics / sequence analysis
  - Molecular Dynamics
  - Synthesis of nucleotide bases

LS VRC – Selected Results (1/2)

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Molecular Dynamics Study of Complex Systems

- Parallel molecular dynamics simulation of Sodium dodecylsulfate (SDS) – polymer systems (inverse micellar and lamellar) depending on the temperature and the polymer concentration.
- Scalability Achieved: 4096 cores

- PUBLICATIONS

  1 publications

  2 in preparation

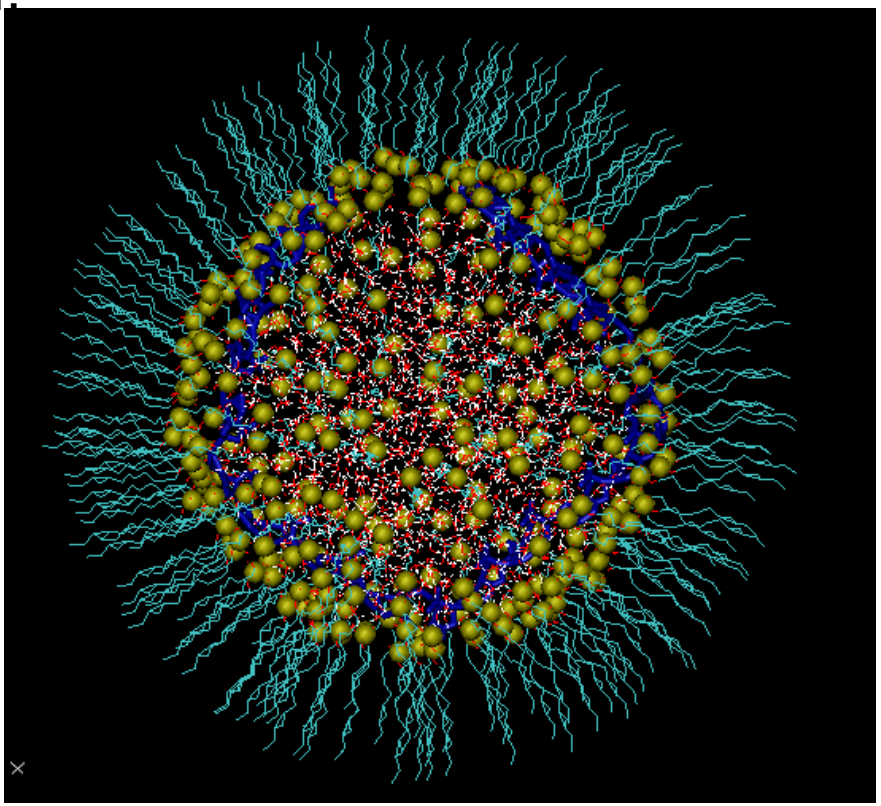

Figure - Sodium dodecyl sulfate (SDS)/PalH/ water system in oil solute

LS VRC – Selected Results (2/2)

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Searching for novel miRNA genes and their targets tems

- Prediction of miRNA genes and their targets.
- Aiming to introduce of a publicly available new miRNA gene and target perdition tool with improved prediction accuracy and significantly faster computational analyses time.

Prediction algorithm	Number of predicted targets mapped to Refseq	Number of targets measured by pSILAC	Number of down-regulated targets (log2FC <-0.1)	Fraction of down-regulated targets (log2FC <-0.1)
TargetScanS	2842	622	381	61.25%
PicTar	3289	629	386	61.37%
rna22 on 3'UTRs	4112	723	255	35.27%
rna22 on 5'UTRs	607	79	20	25.32%
PITA to 600	3000	325	139	42.77%
PITA top 1000	5000	572	226	39.51%
miRbase	3347	658	288	43.77%
miRanda	8605	1533	715	46.64%
Diana-MicroT 3.0	1678	294	194	65.99%
TargetProfiler	1879	290	194	66.90%

- PUBLICATIONS

  3 publications

Key results: dissemination

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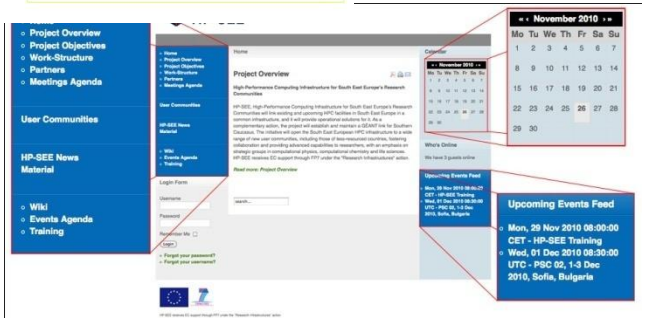
- Dissemination Event Agenda:
  - http://indico.hp-see.eu/categoryDisplay.py?categId=13

- Core promotional material
- Additional brochures and posters

- Newsletters & Media Presence
- HP-SEE Newsletter, Issue No1, March 2011
- HP-SEE Newsletter, Issue No2, August 201
- Press releases (1)
- TV (2)
- Newspapers (6)
- Scientific papers (45+)



Key results: training

- Training community established
  - 21 accredited HP-SEE trainers
  - Trainers expertise captured trough questionnaire
- Training infrastructure established
  - 152 heterogeneous nodes available at 8 sites with 5400 cores in total
- Standardized training material available at the HP-SEE Training Centre
  - Presentations and additional material covering all HPC topics relevant to HP-SEE users
- Trainings agenda available
  - Contains detailed timetable, presented slides, relevant links, additional training material and documents
- HP-SEE Training centre
  - http://wiki.hp-see.eu/index.php/HP-SEE_Training_Center

Key results: HPC Initiatives

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- HPC Centre Setup Cookbook – guidelines for set-up of HPC centers with required equipment (D2.3)
- Support the setup of national HPC task forces or their incorporation in existing structures
  - National HPC initiatives guidelines provided
  - Governance, organizational, operational, training and dissemination guidelines provided
  - D2.2: National HPC task-force modeling and organizational guidelines
- Guidelines for HPC centers procurement provided
  - Legal, procedural, technical and planning guidelines provided
  - D2.1: Procurement guidelines analysis
- Regional collaboration models in definition: Draft resource sharing MoU in place.
- Liaison with PRACE, other pan-European activities, and world-wide initiatives

Long-term Vision

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- Being on the technological par with the rest of Europe
- Enabling local scientists to use their potential
- Integrating the region into pan-European HPC landscape
- Role-model for regional developments
- Leading the way in wider contexts