



## Eastern Europe Partnership Event: Policy-Makers & National Representatives from the Region Gathered to Deliberate on the Enhancement & Sustainability of E-Infrastructures in Eastern Europe

Politicians, civil servants, managers of National Research & Education Networks, R&D advisors and the e-Infrastructure experts from 22 countries in Eastern Europe and beyond gathered on November 7-8 in Bucharest to discuss the future perspectives of e-Infrastructures & services in Eastern Europe, and their relation to the pan European e-Infrastructure activities. The Eastern Europe Partnership event lasted 2 days - 1st day focused on the current status of network, Grid and HPC infrastructures at regional and European level, as well as on the need for further collaboration and support, in order to ensure their development and sustainability. On the 2nd day the status of e-Infrastructure in macro-regions was presented, key stakeholders of eInfrastructures were identified, and management organization and Sustainability of eInfrastructures was discussed in the last session. In his welcome address, the State Secretary & President of the ANCS Dragos Ciuparu, emphasized the significance of the

event, which brings together key players in the field of electronic infrastructures. Keynote speakers Kostas Glinos, director of the Unit GÉANT and E-Infrastructure at the European Commission, DANTE's John Chevers and GRNET's Ognjen Prnjat highlighted the importance of leveraging different aspects of the existing e-Infrastructures and services, thus ensuring the provision of advanced capabilities to the research and education communities in Europe and the region.



The event gave participants the opportunity to work together and agree on what is needed in order to achieve higher levels of collaboration and integration, as well as elaborate high-level national and regional policy issues concerning the development and sustainability of e-Infrastructures

for the benefit of the research and education communities in the targeted regions. The Eastern Europe Partnership event built on the significant impact of past and current well-coordinated EC co-funded projects in the field of e-Infrastructures and services.

"The decade-long collaboration of the countries in the region regarding e-Infrastructure issues has greatly helped support both the local scientists and technology/infrastructure providers, as well as the European Commission's vision of bridging the digital divide and supporting wider pan-European integrations of the region and beyond. I am confident that this collaboration will continue with full support of the beneficiary communities, the national governments, and the EC.", says Dr. Ognjen Prnjat, coordinator of SEERA-EI and HP-SEE projects.

The event was hosted by the National Authority for Scientific Research of Romania in collaboration with RoEduNet and the EC co-funded projects SEERA-EI, GÉANT, HP-SEE and CEENGINE.

### Inside this issue:

Eastern Europe Partnership Event: Policy-Makers & National Representatives from the Region Gathered to Deliberate on the Enhancement & Sustainability of E-Infrastructures in Eastern Europe	1
Successful 1st Quarter Of South Caucasus Interconnection to GÉANT In Higher Capacities, Through HP-SEE	1
Fullerene & metal-diothiolenel-based materials for photonic applications in HP-SEE Infrastructure	2
HP-SEE infrastructure extended with new supercomputers in Hungary	2
Extending HPC infrastructure in Bulgaria with GPU Computing Modules	2
HP-SEE project successfully passed its 1st review in October	3
HP-SEE training "Advanced Programming with MPI" took place in Sofia	3
HPC Centre Setup Cookbook	3

## Successful 1st Quarter Of South Caucasus Interconnection to GÉANT In Higher Capacities, Through HP-SEE

Two links which have been established by the HP-SEE project, and connect South Caucasus with the pan European GÉANT Network in higher capacities, have successfully completed the 1st quarter of operation. More specifically, the two links interconnect the National Research & Education Networks of Armenia (NAS RA) and Azerbaijan

(AzRENA); the connection capacity has been increased from 34 Mbps to 45 Mbps, and HP-SEE Network Operations Center (NOC) will operate these links for 24 Months. The establishment of the new improved links remodels the European map of e-Infrastructures, as the South East European infrastructure

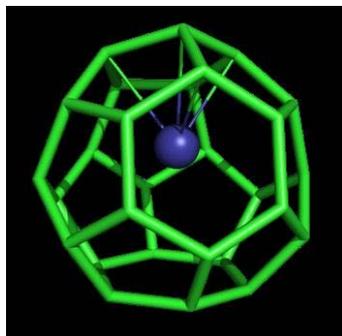
expands to serve new user communities. It also contributes to the fulfillment of the HP-SEE core objectives, by enabling collaboration and providing advanced capabilities to researchers of the beneficiary countries. The network usage statistics are now available on <http://network.hp-see.eu>.



### Fullerene & metal-dithiolene-based materials for photonic applications in HP-SEE Infrastructure

The Computational Chemistry Group of the National Hellenic Research Foundation has worked on the design of novel photonic materials and the investigation of phenomena and factors, which may lead to unusual and interesting (hyper) polarizabilities. Two applications have been recently completed:

**The dipole moment and the (hyper)polarizabilities of C<sub>28</sub> and Ti@C<sub>28</sub>** have been computed by employing Hartree-Fock, DFT and MP2 [1]. The electronic and vibrational contributions to these properties have been presented. It has been found that: (i) Encapsulation of Ti in C<sub>28</sub> lowers the symmetry from T<sub>d</sub> to C<sub>3v</sub>, (ii) The endohedral complex is very stable; for Ti@C<sub>28</sub>, a binding energy of 181.3 kcal/mol has been computed at ROMP2/6-31G(d), (iii) The reduced symmetry of the fullerene cage, resulting from the encapsulation, is associated with larger diagonal components of the static electronic polarizability and second hyperpolarizability, as well as nonzero values of the dipole moment and the first hyperpolarizability, (iv) At the double harmonic approximation, the static vibrational average first hyperpolarizability is 5 times larger than its electronic counterpart (method of computation: B3LYP/6-31+G(d)), (v) The flat potential energy surface and the resulting very large anharmonic contribution to the first hyperpolarizability, indicate that the vibrational second hyperpolarizability may exceed the corresponding electronic property, if the anharmonicity is taken into account.



**Electronic ground state, stability and (hyper)polarizabilities of HXeOXeF and FXeOXeF.** The team has employed complete active space valence bond (CASVB), multi-state complete active space perturbation theory (MS-CASPT2) and coupled cluster methods [2]. It has been found that the inserted oxygen between the two Xe atoms has a significant effect on the ground state electronic configuration and the (hyper)polarizabilities of the resulting derivative. The dissociation channels of HXeOXeF and FXeOXeF have also been studied.

#### References:

1. B. Skwara, R. W. Gora, R. Zalesny, P. Lipkowsky, W. Bartkowiak, H. Reis, M. G. Papadopoulos, J. M. Luis, B. Kirtman, J. Phys. Chem. A, 115, 10370 (2011)
2. A. Avramopoulos, J. Li, N. Holzmann, G. frenking, M. G. Papadopoulos, J. Phys. Chem. A, 115, 10226 (2011)

### HP-SEE infrastructure extended with new supercomputers in Hungary

The NIIF Institute emphasizes its work on the improvement of computer networking infrastructure at academic and scientific levels. Recently the Institute provided 4 brand new supercomputers to execute computing tasks and store data for scientific purposes.

Amongst the beneficiaries of this extension are three universities and the NIIF itself. The universities of Debrecen and Pecs received SGI supercomputers while the University of Szeged and the NIIF HQ developed their computer infrastructure with fat-node HP cluster supercomput-

ers. Although two of the sites, i.e. Debrecen and Pecs, run SuSE Linux Enterprise as their main operating system platforms, the other two supercomputers at Szeged and Budapest both use RedHat. All supercomputers but the one in Pecs use Infiniband network for the internal high-performance communication. Designing these machines, modern, energy-efficient technologies were used, thus they are equipped with water-cooled racks.

All in all, a remarkable network of supercomputers were installed. The future HP-

SEE users could benefit from the remarkable power of the 5490 cores, the 19,9 TB memory and over 1 PB storage space, with approximately 50 Tflops of computing power. This infrastructure nurtures a breeding ground for research in the highest academic and scientific spheres.



### Extending HPC infrastructure in Bulgaria with GPU Computing Modules

Following the National Roadmap for Research Infrastructures the HPCG cluster located at IICT-BAS in Sofia was upgraded with an HP SL390s G7 4U Lft Half Tray Server with four NVIDIA Tesla M2090 6GB Modules, included in Pro-

Liant SL6500 Scalable System Rack. The GPU cards have 2048 CUDA cores. The peak GPU computing performance exceeds the value of 2.66 Tflops in double precision or 5.32 Tflops in single precision. The GPU computing modules

are connected to the HPCG blade cluster with QDR InfiniBand cards. The Lustre file system of the cluster has been expanded significantly to 96 TB total with the inclusion of 48 TB of SAN storage in a P2000 G3 FC system.



## HP-SEE project successfully passed its 1st review in October

The HP-SEE project progress during 1st year of implementation has proven to be excellent, according to the results of the review meeting that took place in Belgrade at the end of October.

More specifically, the project has contributed to the state of the art in developing

the use of HPC resources in the SEE region, and already several peer reviewed scientific papers have been produced, showing that the project has had a real impact of enabling & supporting collaborative scientific research in SEE.

Thanks to the project effective manage-

ment and the excellent collaboration of all partners, the work done has adhered well to the workplan, and financial & human resources have been used effectively & efficiently.

## HP-SEE training "Advanced Programming with MPI" took place in Sofia

The HP-SEE training "Advanced Programming with MPI" was held on December 1st, 2011, in Sofia, Bulgaria, in the building of the Institute of Information and Communication Technologies – Bulgarian Academy of Sciences (IICT-BAS), Acad. G. Bonchev Str. 25 A. The training included lectures and hands-on sessions on advanced programming with MPI and using high-performance computing. It started

with an introduction to the principles and methods of advanced programming with MPI and continued with more complex questions, regarding the performance analysis, optimization and improvement of parallel applications scaling.

*More information:* <http://indico.ipb.ac.rs/conferenceDisplay.py?confid=255>



## HPC Centre Setup Cookbook

Deliverable 2.3 "HPC Centre Setup Cookbook" defines the guidelines for the setup of a HPC center with the required equipment. It provides detailed technical considerations for the procurement & construction of HPC systems in the region, including all the relevant components of the HPC system itself, as well as the hosting data center components.

The document first introduces the topic of HPC facility and equipment setup, and identifies its scope by giving generic HPC design guidelines. The subsequent sections go through different aspects of HPC site design, beginning with data center construction topics, followed by a sum-

mary of hardware related issues, such as CPU, memory, storage, and network subsystems. Software related aspects, such as operating systems, and software stacks are detailed, followed by a section on benchmarking and testing.

The conclusions are summarized in the following:

The setup of an HPC site requires the implementation a wide range of actions: collection of user requirements, site design, site description, site acquisition & procurement, vendor contract, site delivery and installation, benchmarking and testing, site inauguration and continuous refinement, provision of HPC services.

Design and implementation of all components that facilitate the provision of and HPC system has to be carefully performed. The main such components that are described in the deliverable are: Electrical systems, cooling systems, physical security related devices, CPUs, GPUs, memory, storage, networking components, monitoring devices, software components and benchmarks.

The HPC Centre Setup Cookbook is available on the project website:

[http://www.hp-see.eu/documents/doc\\_download/54-hpsee-wp2-niifi-005-d23-d-2011-11-18](http://www.hp-see.eu/documents/doc_download/54-hpsee-wp2-niifi-005-d23-d-2011-11-18)

[www.hp-see.eu](http://www.hp-see.eu)

## Contact

HP SEE Project Management Office  
56 Mesogion Av  
GR 115 27  
Athens Greece

Phone: +30 210 7474254  
Fax: +30 210 7474490  
E-mail: [hp-see-pmo@hp-see.eu](mailto:hp-see-pmo@hp-see.eu)

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

**Communities works across strategic lines of action** to link existing and upcoming HPC facilities in South East Europe in a common infrastructure, and to provide operational solutions for it, as well as HPC user and applications support. As a complementary action, the project has established and maintains two GÉANT links for Southern Caucasus. The initiative will open the South East European HPC infrastructure 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, computational chemistry and life sciences.

HP-SEE receives EC support through FP7 under the "Research Infrastructures" action.