



# HP-SEE Newsletter

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

## Flagship Applications Deployed in the HP-SEE infrastructure

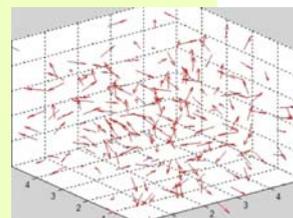
At the end of the first year of the project implementation, the HP-SEE infrastructure supports 22 target applications, while 4 more applications are supported on a best effort basis in terms of computational power and technical assistance. Nine applications have been deployed in the HP-SEE infrastructure and are now in the production stage. Among these, there are the three flagship applications designated by the Application Review Committee: FMD-PA (Computational Chemistry VRC), SIMPLE-TS 2D (Computational Physics VRC), and MDSCS (Life Sciences VRC).

### FMD-PA - Design of fullerene and metal-dithiolene-based materials for photonic applications

The overall project in which FMD-PA was developed involves the design of fullerene and M-dithiolene-based materials, where M = Ni, Pd, etc, for photonic applications. The key parameters for such a design are the nonlinear optical (NLO) properties. The increasing demand for faster data processing, storage and distribution can only be fulfilled by ongoing miniaturization of the basic electronic devices. The traditional silicon-based technologies used nowadays are approaching intrinsic limits in this respect, and new approaches are needed. Photonic technology, where light is used as information carrier instead of electrons, is considered to offer the answer. An important step towards this goal is the development of new photonic materials with large NLO properties by employing nano-derivatives.

The main scientific impact of the study is expected in the fields of:

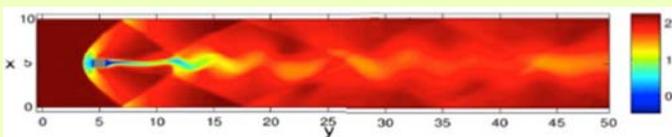
- The development of computational methods for the reasonably accurate determination of the linear and nonlinear optical properties of nano-systems.
- The investigation of a series of novel nano-systems with possible photonic applications.



### SIMPLE-TS 2D - Semi-Implicit Method for Pressure - Linked Equations - Time Step

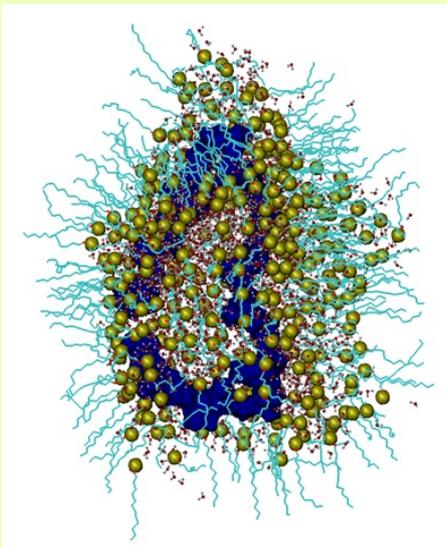
The application addresses the field of Computational Fluid Dynamics and simulates the internal and external gas flows in or around micro mechanical devices, which is important for their design. The gas flow is described through Navier-Stokes-Fourier compressible equations with diffusion coefficients determined by the first approximation of the Chapman-Enskog theory for low Knudsen numbers. The flows are characterized with areas of low Reynolds numbers, and can go from supersonic to very low speed regimes down to the incompressible limit. This made the pressure based numerical methods very suitable for simulations. The finite volume method SIMPLE-TS (a modification of SIMPLE created by K. S. Shterev and S. K. Stefanov) is used.

The investigation is expected to offer a better understanding of gas microflows, which are very important for the design of new Micro-Electro-Mechanical devices.



Horizontal velocity field calculated by parallel version of SIMPLE-TS

### MDSCS - Molecular Dynamics Study of Complex Systems



The snapshots from 15ns run point of inverse micelle with presence of polyampholyte at pH=9

Phospholipids and surfactant bilayers have been extensively investigated as model systems for biological membranes. During recent years molecular/atomic-level simulator applications and useful tools in the study of bilayers have been developed. The main targets of the proposed application are to simulate the cell model membranes, amphiphilic micelles, as well surfactant bilayers; computational experiments with the heterogeneous phospholipid membranes, consisting of multi-component phospholipid bilayer and proteins and amphiphilic micelles; to study the dynamical properties (molecular diffusion, membrane or micelle fusion, lipid rafts, etc) of complex systems. The successful research work requires the usage of HP-SEE massively parallel infrastructure. The application is based on NAMD and GROMACS packages.

Using atomic scale simulation we have investigated inverse micellar system with presence of polyampholyte at pH=9. Currently ~20ns parallel molecular dynamics (MD) simulation was carried out for a sodium dodecyl sulfate (SDS) /polyampholyte/toluene/pentanol/water system. The NAMD software code was applied. Analysis of the pre-results shows almost stable microdroplet during the whole simulation time, however additional run needs to reach equilibrium and compare to experimental findings. It is also planning to run the mentioned system at pH=4, which will make it possible to reveal the mechanism of droplet-droplet interactions in dependence on pH, as well give us information about the localization of polyampholyte. The system runs on the Armenian Grid Infrastructure and on the Bulgarian Supercomputer BlueGene/P using 512 cores.



## Joint HP-SEE, LinkSCEEM-2 and PRACE HPC Summer Training took place in Athens

The HPC Summer Training, jointly organized by HP-SEE, LinkSCEEM-2 and PRACE, was held on 13-15 June in Athens, Greece. It gathered 55 researchers from 15 countries and working in the wide variety of scientific disciplines, including computational physics, life sciences, computational chemistry, engineering, computer science, earth sciences etc. The main goals of the training were to enhance the knowledge of current HPC users, and to engage new user communities in the use of HPC infrastructure.

During the three days course the participants learned about methods and tools that are necessary for developing highly efficient



HPC applications and optimal usage of the available computing resources. The main subjects that were covered in the training sessions were advanced modules in MPI, OpenMP, Hybrid Programming, CUDA Programming, Profiling Optimization and Benchmarking. Every module was accompanied with the hands-on sessions where participants had the chance to try out the HPC resources provided by IPB and IICT-BAS through a series of examples and exercises.

The training was complemented with the Introduction to IBM Blue Gene and WS-PGRADE/gUSE, and it was preceded by the LinkSCEEM-2 session where the project, its user support system, sites, users and activities were presented.



## HP-SEE releases "National HPC task-force modeling and organizational guidelines"

WP2 of the HP-SEE project released in June 2011 the "National HPC task-force modeling and organizational guidelines". The document defines the guidelines for the set-up of national HPC task forces and their organizational model. It identifies and addresses all topics that have to be considered, collects and analyzes experiences from several European and SEE countries, and

uses them to provide guidelines to the countries from the region in setting up their national HPC initiatives. The analysis presented in the document, addresses the following issues:

- Governance models for HPC initiatives: coordination of national HPC activities, MoU, national-level projects and funding issues.
- Peer review and scientific

assessment for HPC access proposals

- Coordination of HPC centers, including technical support, system management, training and dissemination activities, European coordination and interoperability, and user support.

The document can be found at: <http://goo.gl/KcDm7>

## News from partners

### Inauguration of new HPC cluster in Skopje in September

As a result of the initiative of the Ministry of Education to invest 60M EUR in new research and scientific laboratories, a new HPC cluster (1.1 M EUR) will be inaugurated during September 2011. The HPC cluster, which is in the phase of setup and installation, is manufactured by HP. It consists of 1008 CPU cores with Hyper-

threading, based on Intel Xeon L5640 low power processors, with 2GB RAM per core. The interconnectivity is realized using QDR Infiniband technology, delivering non-blocking communication using fat tree. SAS based storage with total of 30TB storage space is connected to the cluster's management nodes. The whole system is enclosed with integrated chassis cooling system, delivering large number of CPU

cores on a very small footprint. The Faculty of Computer Science and Engineering, University Ss Cyril and Methodius in Skopje will manage this HPC installation, which will be used by researchers throughout the country. It will also be used regionally, in the framework of the HP-SEE project and will be part of the MARGI grid infrastructure.

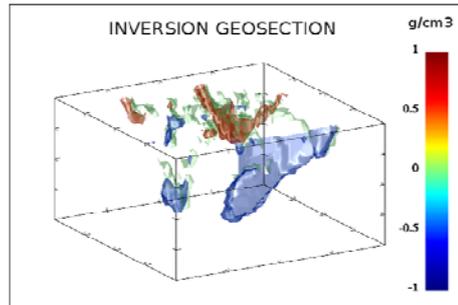
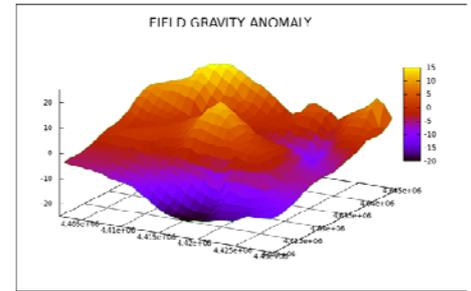


## News from partners

### GIM Application

The team of the Polytechnic University of Tirana, Faculty of Information Technology, is working on the GIM application for the calculation of gravity inversion in geophysics. The first suite of tests for the convergence rate of the algorithm was completed using OpenMP in 16 cores in the HPC cluster in Sofia, and the first paper was submitted in the ICT Innovations 2011 Conference, Skopje, that will take place on 14-16 September 2011. Further tests were done to analyze in depth the process of convergence, and the first test with field data was completed. A second paper with recently obtained results is in preparation for the Workshop on High Performance Computing with Applications in Environ-

ment, that will take place in Timisoara, Romania, on September 26 - 29, 2011.



*Field gravity anomaly and the geosection obtained from the inversion, showing the difference between the average density and the density of anomalous bodies. The field anomaly data is obtained from Academy of Sciences of Albania.*



**HP-SEE**  
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HP-SEE, High-Performance Computing Infrastructure for South East Europe's Research Communities will link existing and upcoming HPC facilities in South East Europe in a common infrastructure, and it will provide operational solutions for it. As a complementary action, the project will establish and maintain a GÉANT link 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.