

# HP-SEE User Forum 2012 Programme

National Library of Serbia, Belgrade, October 17-19, 2012

Wednesday, October 17, 2012	
08:15 – 09:00	Registration and welcome coffee
09:00 – 09:30	<b>Opening</b> Chair: <i>Ognjen PRNJAT</i> Speakers: <b>Ognjen PRNJAT</b> , HP-SEE Project Coordinator <b>Aleksandar BELIC</b> , Director of the Institute of Physics Belgrade <b>Representative of Ministry of Education, Research and Technology Development</b> , Republic of Serbia <b>Dejan RISTIC</b> , Acting Director of the National Library of Serbia
09:30 – 11:00	<b>Invited Session 1</b> Chair: <i>Aleksandar BELIC</i>
09:30	<b>Regional infrastructure Development for South East Europe's Research Communities</b> <i>Ioannis LIABOTIS</i> <i>(HP-SEE Technical Coordinator)</i>
10:15	<b>International HPC - Building bigger pyramid</b> <i>Richard KENWAY</i> , <i>(PRACE Scientific Steering Committee Chair)</i>
11:00 – 11:30	Coffee break
11:30 – 13:00	<b>Life Science Session 1</b> Chair: <i>Hrachya ASTSATRYAN</i>
11:30	A new microRNA target prediction tool identifies a novel interaction of a putative miRNA with CCND2 <i>Anastasis OULAS</i>
12:00	Quantum-Chemical Calculations for the Quantitative Estimations of the Processes in DNA <i>George MIKUCHADZE</i>
12:30	DNA muligene approach on HPC using RAxML software <i>Luka FILIPOVIC</i>
13:00 – 14:00	Lunch break
14:00 – 15:00	<b>Life Science Session 2</b> Chair: <i>Miklos KOZLOVSZKY</i>
14:00	Parallelizing computational models of memory function for the investigation of sustained activity in the prefrontal cortex <i>Anastasis OULAS</i>
14:30	Dynamical Features of Complex Systems: A Molecular Simulation Study <i>Hrachya ASTSATRYAN</i>

<b>15:00 – 16:00</b>	<b>Scientific Computing, HPC Systems and Network Operation Session 1</b> <i>Chair: Ioannis LIABOTIS</i>
15:00	Advanced Vulnerability Assessment Tool for Distributed Systems <i>Miklos Kozlovszky</i>
15:30	SCL Quantum Espresso Extensions <i>Dusan STANKOVIC</i>
<b>16:00 – 16:30</b>	Coffee Break
<b>16:30 – 18:30</b>	<b>Scientific Computing, HPC Systems and Network Operation Session 2</b> <i>Chair: Anastas Mishev</i>
16:30	On HPC for Hyperspectral Image Processing <i>Mihnea DULEA</i>
17:00	An Analysis of FFTW and FFTE Performance <i>Josip JAKIC</i>
17:30	Performance and scalability evaluation of short fragment sequence alignment applications <i>Gergely WINDISCH</i>
18:00	Number Theory Algorithms on GPU Cluster <i>Dobromir GEORGIEV</i> <i>Nikolai MANEV</i>
<b>Thursday, October 18, 2012</b>	
<b>09:00 – 11:15</b>	<b>Invited Session 2</b> <i>Chair: Mihnea DULEA</i>
09:00	LinkSCEEM2: Development of an HPC ecoSystem in the Eastern Mediterranean <i>Speaker: Jens WIEGAND</i> <i>(LinkSCEEM2 Project Coordinator)</i>
09:45	Numerical Study of Ultracold Quantum Gases: Formation of Faraday Patterns, Geometric Resonances, and Fragmentation <i>Speaker: Antun BALAZ</i> <i>(Institute of Physics Belgrade)</i>
10:30	Monte Carlo methods for Electron Transport: Scalability Study using HP-SEE infrastructure <i>Speaker: Aneta KARAIVANOVA</i> <i>(The Institute of Information and Communication Technologies at the Bulgarian Academy of Sciences)</i>
<b>11:15 – 11:45</b>	Coffee Break
<b>11:45 – 13:15</b>	<b>Computational Physics Session 1</b> <i>Chair: Emanouil ATANASSOV</i>
11:45	Using Structured Adaptive Computational Grid for Solving Multidimensional Computational Physics Tasks <i>Peter BOGATENCOV</i>
12:15	Computational approaches for electronic properties of semiconducting materials and nanostructures <i>Nenad VUKMIROVIC</i>
12:45	Reflections on Parallelization of Gravity Inversion <i>Neki FRASHERI</i>
<b>13:15 – 14:15</b>	Lunch Break

<b>14:15 – 15:45</b>	<b>Computational Physics Session 2</b> <i>Chair: Antun BALAZ</i>
14:15	Numerical Simulations of the Structure and Transport Properties of the Complex Networks <i>Igor STANKOVIC</i>
14:45	Emergence of resonant waves in cigar-shaped Bose-Einstein condensates <i>Alexandru NICOLIN</i>
15:15	Iterative Perturbative Method for a Study of Disordered Strongly Correlated Systems <i>Jaksa VUCICEVIC</i>
<b>15:45 – 17:00</b>	<b>Poster session</b>
	<ul style="list-style-type: none"> <li>• EagleEye: Feature Extraction from Satellite Images Using a Hybrid Computing Architecture <i>Razvan DOBRE</i></li> <li>• Evolution of an gravitational bound n-body system with DLA (Diffusion Limited Aggregation) initial mass distribution using GPU parallel computing <i>Bogdan Alexandru DUMITRU</i></li> <li>• Formation of Faraday and Resonant Waves in Driven High-Density Bose-Einstein Condensates <i>Mihaela Carina RAPORTARU</i></li> <li>• GPAW optimisations <i>Petar JOVANOVIC</i></li> <li>• Generalization of the parallel HPC implementation for solving differential equations <i>Dragan JAKIMOVSKI</i></li> <li>• Quenched Hadron Spectroscopy Using FermiQCD <i>Rudina ZEQRILLARI</i></li> <li>• Some aspects of the comparative study of semi-empirical combustion models on FLUENT and OpenFOAM codes <i>Sreten LEKIC</i></li> <li>• Using Parallel Computing to Calculate Quark-Antiquark Potential from LatticeQCD <i>Dafina XHAKO</i></li> <li>• Self-avoiding Hamiltonian Walks Counting in Parallel processing mode <i>Sreten LEKIC</i></li> <li>• Data analysis in high energy physics using CUDA and OpenCL <i>Alexandru Bogdan DUMITRU</i></li> <li>• Conformational Analysis of Kyotorphin Analogues Containing Unnatural Amino Acids <i>Emanouil ATANASSOV</i></li> </ul>
<b>17:00 – 18:00</b>	<b>Computational Physics Session 3</b> <i>Chair: Alexandru NICOLIN</i>
17:00	Determination of zone of flow instability in a gas flow past a square particle in a narrow microchannel <i>Kiril SHTEREV</i>
17:30	Electronic Structure and Lattice Dynamics Calculations of FeSb <sub>2</sub> and CoSb <sub>2</sub> <i>Milos M.RADONJIC</i>

## Friday, October 19, 2012

<b>09:00 – 10:30</b>	<b>Invited Session 3</b> <i>Chair: Aneta KARAIIVANOVA</i>
09:00	Use of High Performance Computing in (Bio)Chemistry <i>Speaker: Ivan JURANIC</i> <i>(University of Belgrade, Faculty of Chemistry)</i>
09:45	The impact of GISELA Science Gateway (GSG) on the supported Latin America VRC's <i>Speaker: Jesus CRUZ GUZMAN</i> <i>(Universidad Nacional Autonoma de Mexico UNAM)</i>
<b>10:30 – 11:30</b>	<b>Computational Chemistry Session 1</b> <i>Chair: Aneta KARAIIVANOVA</i>
10:30	Dynamics of uninhibited and covalently inhibited cysteine protease on non-physiological pH <i>Branko J. DRAKULIC</i>
11:00	Development of a Hybrid Statistical Physics – Quantum Mechanical Methodology for Computer Simulations of Condensed Phases and its Implementation on High-Performance Computing Systems <i>Ljupco PEJOV</i>
<b>11:30 – 12:00</b>	Coffee/Tea break
<b>12:00 – 14:30</b>	<b>Computational Chemistry Session 2</b> <i>Chair: Nenad Vukmirovic</i>
12:00	Design of novel nano-photonics materials <i>Manthos PAPADOPOULOS</i>
12:30	Efficient Parallel Simulations of Large-Ring Cyclodextrins on HPC cluster <i>Emanouil ATANASSOV</i>
13:00	Free-energy surfaces of 2-[(carboxymethyl)sulfanyl]-4-oxo-4-arylbutanoic acids. Molecular dynamics study in explicit solvents. <i>Branko J. DRAKULIC</i>
13:30	Investigations of biomolecular systems within the ISyMAB simulation framework <i>Ionut VASILE</i>
14:00	In the search of the HDAC-1 inhibitors: The preliminary results of ligand based virtual screening. <i>Ilija N. CVIJETIC</i>
<b>14:30</b>	<b>Closing</b>