

Modeling and Optimization in Science and Technologies

Volume 2

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

Results of the HP-SEE User Forum 2012

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Heraklion, Crete
Greece

Ognjen Prnjat
GRNET S.A.
Greek Research and Technology Network
Athens
Greece

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Preface

High-Performance Computing (HPC) is one of the key enablers of scientific research and of the development of Information Society in Europe. Enabling large-scale innovative research to be conducted through collaboration of distributed teams of scientists across the European Research Area paves the way towards a long-term vision of a sustainable, transparent, ubiquitous electronic infrastructure open to a wide range of scientific user communities. European Commission sees “strategic nature of High-Performance Computing as a crucial asset for the EU’s innovation capacity, and calls on Member States, industry and the scientific communities, in cooperation with the Commission, to step up joint efforts to ensure European leadership in the supply and use of HPC systems and services by 2020.” Pan-European PRACE infrastructure supports this strategy and currently provides the core of High-Performance Computing power for European research. In this context, the inclusion of less-developed regions of Europe, which suffer from the digital divide and brain-drain in all fields and especially high-technology, into the wider European Research Area is an aim closely aligned to this vision. HP-SEE project, co-funded by Framework Programme 7 of the European Commission, is currently advancing the computing infrastructures in South-East Europe (SEE), activating new user communities and enabling collaborative research across a number of fields, and thus contributes to closing the existing technological and scientific gap, and following the wider European HPC strategy.

The HP-SEE User Forum took place in Belgrade on October 17-19, 2012, at premises of National Library of Serbia and hosted by the Institutes of Physics Belgrade: this scientific conference gathered 65 participants from 16 countries in the region and beyond, with main focus on the fields of Computational Physics, Computational Chemistry, Life Sciences, Scientific Computing and HPC Systems and Network Operations. Conference programme comprised of seven invited lectures, both from related e-Infrastructure projects and HP-SEE scientific community, 26 contributed oral presentations and a poster session featuring 11 poster presentations. This edition of papers from the User Forum is comprised of 20 peer-reviewed papers: 7 from Computational Physics applications in HPC, 5 from Computational Chemistry, 3 from Life Sciences, and 5 from Scientific computing and HPC operations. The project as well as the wider SEE community has benefited greatly from the exchange of experiences of leading scientists in

the region in their use of High-Performance Computing technology to empower their research.

In my role of HP-SEE project manager, I would like to thank the authors, reviewers, editors, programme and organization committees and guest speakers for their contributions to this event.

April 2013

Dr. Ognjen Prnjat
HP-SEE Project Manager

Conference Topics

- Computational Physics
- Computational Chemistry
- Life Sciences
- Scientific Computing
- HPC Systems and Network Operation

Keynote Speakers

Regional eInfrastructure Development for South East Europe's Research Communities
Ioannis Liabotis, GRNET, Greece

International HPC - Building bigger pyramids
Richard Kenway, NeSC, UK

LinkSCEEM2: Development of an HPC ecoSystem in the Eastern Mediterranean
Jens Wiegand, CaSToRC, Cyprus

The impact of GISELA Science Gateway (GSG) on the supported Latin America VRC's
Jesus Cruz Guzman, UNAM, Mexico

Numerical Study of Ultracold Quantum Gases: Formation of Faraday Patterns, Geometric Resonances, and Fragmentation
Antun Balaž, IPB, Serbia

Monte Carlo methods for Electron Transport: Scalability Study using HP-SEE infrastructure
Aneta Karaivanova, IICT-BAS, Bulgaria

Use of High Performance Computing in (Bio)Chemistry
Ivan Juranić, FCUB, Serbia

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The Editors and the HP-SEE project would like to acknowledge valuable help and support by the National Library of Serbia which hosted the conference.

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