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SEMINAR

«AN ACADEMIA-INDUSTRY SUPERCOMPUTER CENTRE: DEVELOPMENT AND APPLICATIONS»

Prof. Maxim Fedorov

October 27, 2015

13.00 - 14.30

Room 148

TPOC-3

SEMINAR ABSTRACT:

The talk will briefly overview academic and industrial research activities of the West of Scotland Academia-Industry Supercomputer Centre (ARCHIE-WeST, www.archie-west.ac.uk) with a focus on several examples of applications of supercomputing techniques in energy and pharmaceutical sectors.

The ARCHIE-WeST Centre was established in 2012 as an EPSRC-supported Consortium of five universities located in the West of Scotland (Strathclyde, Glasgow, Glasgow Caledonian, West of Scotland, and Stirling Universities). The University of Strathclyde is the leading University of the Consortium that hosts the supercomputing facility. The main aims of the Centre are: (i) to support multi-disciplinary research in engineering and physical sciences, (ii) to reach out to other disciplines (arts, humanities, financials etc), (iii) to enable and encourage industrial usage and collaboration between academic and industrial partners.

Currently the Centre underpins a significant amount of the research base in the West of Scotland, particularly in such areas as Physics, Chemistry, Mechanical and Aerospace Engineering, Oil&Gas, Energy, Pharmaceutics, Chemical & Process Engineering, and Naval Architecture, Ocean & Marine Engineering. The Centre has established itself as a leading High-Performance Computing (HPC) centre in the UK in terms of real-world applications of this emergent technology. To-date the HPC-related initiatives supported by the Centre have delivered:

*More than 150 published peer-reviewed journal papers; the list of journals includes those with a very high impact factor such as those within the Nature family, Physical Review Letters, Chemical Reviews, etc.

*A multi-million portfolio of research and industrial grants.

*Underpinning of around 90 PhD projects.

The Centre has also expanded frontiers of HPC applications towards Financial & Social Sciences, Art & Humanities and Urbanistics.

Prof. Maxim Fedorov have been leading the Centre from its very beginning in 2012; in addition to the general overview of ARCHIE-WeST and its academic and industrial activities, he will also present several examples of his own research on supercomputing applications in electrochemical energy storage, oil&gas and pharmaceutics.

SPEAKER INTRODUCTION:

Professor Maxim Fedorov graduated from Voronezh State University in 1998 (Physics). He holds a PhD (Kandidat Nauk) in Physical and Mathematical Sciences (2002) and a DSc (Doktor Nauk) in Physical Chemistry (2007) degrees from the Russian Academy of Sciences.

As a Director of a regional-scale supercomputer centre he is actively involved in the development of sustainable large-scale e-infrastructure for Computational Science and Engineering.

His own research interests include computational chemical physics & physical chemistry and molecular biophysics with main focus on ionic liquids applications for electrochemical conversion and storage and ion & solvent effects on biomolecules and nanoparticles. A large part of this research is focused on energy-related applications covering a large range of topics from using molecular modelling methods for optimizing properties of ionic liquid-based super-capacitors to development of enhanced oil&gas recovery techniques.

His group actively works on scientific computing applications in molecular sciences and computational biophysics (ion/solvent effects on biomolecules and nanoparticles, solvation thermodynamics of bioactive molecules and modelling of complex electrolyte and biomolecular solutions at interfaces). Prof. Fedorov published over 80 peer-reviewed publications and presented over 100 invited talks and lectures on these subjects. Some of these publications were highlighted in international and national press; several became top 1% cited papers in corresponding areas. For his theoretical&computational works on thermodynamics of (bio)molecular solvation he was awarded the International Helmholtz Award in 2012 by IAPWS. He organized a dozen international conferences and workshops on biomolecule solvation, chemical physics, and physical chemistry of liquids and applications of high-performance computing in natural sciences and engineering.