fibres and is nowadays one of the most challenging tasks in neuroscience. The application of the UNICORE workflow system for this particular use case resulted in minimizing user interaction and time to completion of the scientific workflow. The next presentations highlighted current state, new ideas and concepts for the future development of the UNICORE portal [5], experiences with certificate-free user-friendly HPC access based on LDAP with UNICORE and UNITY [6], perspectives for REST services in the UNICORE environment, integration of UNICORE services in a private cloud computing platform and resource scheduling algorithms in distributed problem-oriented environments. Finally, the UNICORE roadmap and future developments were discussed by the attendees from Germany, Poland, Russia, and the United States.

The slides to the presentations can be found on the web at http://www.unicore.eu/summit/2014/schedule.php

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"Bernstein Network – Simulation Lab Neuroscience" HPC Workshop

Neuroscience today is attacking problems of increasing complexity and scale as exemplified by projects like the Human Brain Project, which require computationally intensive simulations and the analysis of large data sets. However, many projects currently using local clusters for these purposes have not yet adapted their software and theoretical approaches to take advantage of HPC systems such as those available at the Jülich Supercomputing Centre (JSC).

The "Bernstein Network – Simulation Lab Neuroscience" HPC Workshop on June 4th and 5th at the JSC brought together Jülich computational neuroscientists and HPC experts with neuroscience domain experts from across Germany who are interested in developing petascale simulations and analyses. An important goal of this meeting was to find ways for the neuroscience community to fully exploit available JSC resources by catalyzing collaborations and adapting tools to supercomputer scales.

A total of 32 participants shared their perspectives on HPC in neuroscience. Members of the SimLab Neuroscience [1] and the JSC's HPC in Neuroscience Division delivered presentations covering a range of issues regarding the use of computing facilities at the JSC, in addition to describing work being currently done by the SimLab which leverages these resources such as structural plasticity modeling in the visual cortex using the NEST simulator [2].

Figure 1: Participants of the "Bernstein Network – Simulation Lab Neuroscience" HPC Workshop.

Other experts from the JSC and Jülich's Institute of Neuroscience and Medicine (INM) explained the compute-time grant-writing process, as well as showing a variety of projects that already leverage JSC resources including large-scale neuronal network simulations on the JUQUEEN supercomputer and "Big Data" approaches to experimental electrophysiological analyses.

Fifteen external neuroscientists from the Bernstein Network [3] presented projects which they hoped to bring to the JSC supercomputers, ranging from macroscopic models of whole brain functions through neuronal network self-organization and down to ion flows in dendritic spines. Discussions regarding how to directly port these projects as well as how to further extend them so as to maximize parallelization for supercomputing architectures should lead to a new generation of neuroscience projects at the JSC.

Further details on the program are available at:

http://www.fz-juelich.de/SharedDocs/Termine/IAS/JSC/EN/events/2014/bernstein-hpc-2014.html

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Jülich School on Computational Trends in Solvation and Transport in Liquids

From 23 to 27 March 2015 the IAS School on "Computational Trends in Solvation and Transport in Liquids" will take place at Jülich Supercomputing Centre. This event is part of a series of Schools in Computational Science, which are regularly organized at Jülich since more than 15 years [1]. More than 20 renowned scientists from seven countries will present lectures on modern methods and algorithms for treating solvents most efficiently on different length and time scales. The School is part of the activities of the Jülich CECAM node [2] and is co-supported by the Cluster of Excellence RESOLV [3].

"Solvation Science" is increasingly recognized as an interdisciplinary field akin to "Materials Science" or "Neuroscience" addressing a variety of different computational and simulation methods, appropriate for hierarchies of time- and length-scales, which provide a challenge to be solved. Since solvation and transport problems are apparent in a broad field, ranging from fundamental questions in chemistry or soft matter physics to industrial applications, the field is highly interdisciplinary. This calls for meetings bringing experts together from various directions and triggering exchange of ideas between disciplines. The IAS School 2015 will focus on the computational trends, multi-method approaches and modeling in this interdisciplinary field. It covers the field from large-scale coarse grain modeling down to fully quantum-mechanical simulations of liquids at the level of electrons and nuclei. Not only bulk liquids and homogeneous solutions will be discussed, but also heterogeneous systems such as liquid/solid interfaces as well as solvated (bio)molecules. In particular, recent advances in adaptive resolution methods both in the realm of finite element modeling and of interfacing atomistic and coarse-grain descriptions of liquids will be covered. Moreover, a variety of hybrid methods, such as QM/MM approaches for solvated biomolecules, continuum solvation and lattice Boltzmann techniques, will be part of the program. Coarse graining in many distinct flavors certainly is an important approach to describe transport in liquids and solvation of increasing complex systems. This includes methods such as Brownian dynamics for biomolecular recognition, mesoscale particle methods for hydrodynamics to model particle-fluid interactions or neural network potentials to describe reactive water.

The recent revival of liquid-state integral equation methods in combination with molecular dynamics and electronic structure theory is acknowledged in the program as well as new developments in molecular density functional theory of aqueous solutions. Well-established techniques such as force field molecular dynamics for large-scale