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 bio-molecules, 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

simulations and ab initio molecular dynamics for wet chemical reactions will be addressed as well to introduce the audience to the field. Within molecular dynamics special attention will be given to methods that are tailored to unravel solvation effects. Presentation of most recent developments in path integral simulation techniques will complement the lectures to cover the smallest scales on nuclear level, which are relevant in atomistic description of solvation.

The solution of large scale complex problems needs a direct link to high performance computing, which today includes the use of GPUs in addition to massively parallel CPU based systems. Recent developments and trends will be addressed in the School not only by providing lectures but also by including a hands-on practical tutorial on elementary GPU programming.

This IAS School is suited for highly motivated PhD students and PostDocs. Applications for participation can be sent until end of January 2015. Based on the required application documents about 50 participants will be selected by the organizers. Details about the School and the application process can be found at: http://www.fz-juelich.de/STL-2015 .

References

[1] For a list of past Schools, see: www.fz-juelich.de/ias/jsc/EN/Expertise/Workshops/Conferences/STL-2015/PastWorkshops/_node.html

[2] www.cecam.org

[3] CoE Ruhr Explores Solvation: www.ruhr-uni-bochum.de/solvation/

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3rd Workshop on Parallel-in-Time Integration Held at JSC

At the doorstep of the Exascale era, an urging demand for improved and new numerical algorithms arises. For time-dependent problems, the idea of concurrency in the time domain attracts more and more interest in many different communities. In order to overcome the serial dependence in the time direction and to enable integration of multiple time-steps simultaneously, time-parallel methods commonly introduce a space-time hierarchy, where integrators with different accuracies and costs are coupled in an iterative fashion. Serial dependencies are shifted to the coarsest level, allowing the computationally expensive parts on finer levels to be treated in parallel. Typical examples of this concept are Parareal and the "parallel full approximation scheme in space and time" (PFASST). The space-time hierarchy used in these approaches shows strong similarities to classical multigrid structures. For example, Parareal can be interpreted as two-grid algorithm in time. PFASST uses iterative spectral deferred corrections as smoother in time and employs a full approximation scheme, thus making it conceptually similar to spatial nonlinear multigrid methods.

From May 26 to 28, 2014, the 3rd Workshop on Parallel-in-Time Integration with special focus on parallel multilevel methods in space and time was held at Jülich Supercomputing Centre. It was jointly organized by Robert Speck (Forschungszentrum Jülich), Matthias Bolten (University of Wuppertal), Rolf Krause, and Daniel Ruprecht (both USI Lugano), and was supported by DFG via SPPEXA, the German Priority Programme 1648 "Software for Exascale Computing". With 42 participants from academia, research and industry coming from eleven different countries a broad spectrum of expertise was brought together to form a great ambiance for a successful exchange of ideas. The topics ranged from applied mathematics to climate and earth science as well as engineering and software development. With sufficient time for discussions and individual meetings, new collaborations were initiated and long-lasting contacts renewed.

This workshop was the third one in a series of workshops for a fast-growing community, following the events at Università della Svizzera italiana in 2011 and at the University of Manchester in 2013. In May 2015, the 4th workshop will be held at TU Dresden and further events are already envisaged for the following years.

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Figure 1: Participants of the 3rd Workshop on Parallel-in-Time Integration.