

Retrospective of International Jülich CECAM School on Computational Trends in Solvation and Transport in Liquids

The Jülich CECAM School [1], organized this year at JSC continued a series of Schools which started in 2000 and which takes place in bi- or triennial periods [2]. It has entered the CECAM [3] event calendar since 2012 and addresses a larger audience interested in computational science and parallelization of algorithms in various fields of application. This year the focus of the School was on Computational Trends in Solvation and Transport in Liquids, partially motivated by the Cluster of Excellence RESOLV, coordinated at Ruhr-University Bochum, which also co-sponsored the School financially [4].

The participants, 43 young scientists from 8 countries (Europe and overseas), proved a broad interest in the topic, which covers both Soft Matter Physics and Solvation Chemistry. The well balanced topics of the lectures made it possible to present both topics as coupled together. The 23 lecturers from 7 countries (also Europe and overseas) were highly renowned scientists who presented latest developments of research embedded in a broad overview over the field.



The topics of the School were grouped into several blocks, covering Atomistic Methods, Coarse Grain and Continuum Methods, Hybrid Methods, Mesoscale Fluid Methods as well as Numerical Methods and Hardware. It is the mix of topical blocks, which has proven to be most efficient in addressing the audience, having sometimes a very diverse background but profiting highly of the introductory character of the lectures spiced with advanced topics which gives a perspective of research in the various fields.

An essential part of the School is the provision of Lecture Notes to the audience on the first day of the School, which makes it even more accessible to follow the courses and refresh the knowledge during and after the School. The Lecture Notes have been published as volume 28 of the IAS series, which is available either as hard copy or as PDF file on the web [5]. Although the topics were well structured in blocks in the Lecture Notes, during the School topics were intentionally scattered over the whole week to provide a broad spectrum of topics to the whole audience and to avoid topic selected days, which would have reduced the number of participants during School days. As a practical aspect of the School, a hands-on session for computing on graphical processing units (GPU) was organized, providing a code oriented approach for first steps in GPU computing.

To stimulate discussion between participants and lecturers, 4 evening events were organized, containing a get-together during the first evening, 2 poster sessions and an excursion of the whole group to the brown coal open cast mining in the close neighbor-

hood of Jülich together with a dinner. The positive feedback from participants and lecturers provides strong motivation to further organize Computational Science oriented Schools in a similar scheme.

References

- [1] www.fz-juelich.de/stl-2015
- [2] For a list of past Schools, see: www.fz-juelich.de/ias/jsc/EN/Expertise/Workshops/Conferences/STL-2015/PastWorkshops/_node.html
- [3] www.cecarn.org
- [4] CoE Ruhr Explores Solvation: www.ruhr-uni-bochum.de/solvation/
- [5] IAS Series, Vol. 28: <https://user.fz-juelich.de/record/188877/files/IAS-Band-28-V2.pdf>

- Godehard Sutmann¹
- Johannes Gritendorst¹
- Gerhard Gompper
- Dominik Marx²

¹ Jülich Supercomputing Centre (JSC), Germany

² Ruhr-University Bonn, Germany