



1. ESPResSo Workshop

FIAS, Frankfurt am Main

<http://www.uni-frankfurt.de/~simbio>

14 July 2006

- Funds by the Max-Planck-Institut für Polymerforschung in Mainz are gratefully acknowledged.
- Organized by Christian Holm and the SimBio Group at FIAS, Frankfurt.

Participants

1. ARNOLD, Axel (AMOLF Amsterdam, **invited speaker**)
2. QIAO, Bafou (FIAS Frankfurt)
3. CERDA, Juan J. (FIAS Frankfurt)
4. GRASS, Kai (FIAS Frankfurt)
5. HOLM, Christian (FIAS Frankfurt and MPI-P Mainz, **Organizer and Project Leader**)
6. KANTOROVICH, Sofia (FIAS Frankfurt, Ekaterinburg)
7. LENZ, Olaf (FIAS Frankfurt)
8. LIMBACH, Hans-Jörg (Nestlé Corporate Research Lausanne, **invited speaker**)
9. MANN, Bernward (BASF Germany, **invited speaker**)
10. QAMHIEH, Khawla (FIAS Frankfurt, and Al-Quds University Jerusalem)
11. REITH, Dirk (MPI-P Mainz)
12. REYNOLDS, Ben (MPI-P Mainz)
13. SAYAR, Mehmet (Koc University, Istanbul)
14. SCHILLER, Ulf (MPI-P Mainz, **invited speaker**)
15. SMIA TEK, Jens (Universität Bielefeld)
16. STUEHN, Torsten (MPI-P Mainz, **invited speaker**)
17. SÜZEN, Mehmet (FIAS Frankfurt)
18. TYAGI, Sandeep (FIAS Frankfurt)

Programme

Time	Event Title	Speaker(s)	Place
9:00	Registration/Coffee/Tea	all	2.210
9:15	ESPResSo structure data organization, parallelization, program structure (Tcl-C, I/O interface, module system, Integrator, force routine, electrostatics, analysis, etc.), scripting (general structure, tips und tricks), development (programming rules, CVS, tests und validation, despresso mailing list), Analysis, Checkpointing, Documentation, speed bottlenecks, limitations of the flexibility	Axel Arnold, Hans-Jörg Limbach and Bernward Mann	2.210
10:45	Coffee/Tea Break	all	2.210
11:00	Lattice-Boltzmann	Ulf Schiller	2.210
11:30	Open Problems FFTW, other machine architectures, further parallelization issues (OpenMP), parallelization of I/O and analysis routines, adaptive parallelization, checkpointing, discussion of all other open questions	Torsten Stühn	1.402
12:30	Lunch	all	FIZ
afterwards	Coffee/Tea	all	1.402
14:00	Atomistic features What is already implemented, what is missing?	Hans-Jörg Limbach	1.402
14:30	Future perspectives Changes in the user and development environment, resulting problems and possible solutions	Olaf Lenz	1.402
15:00	ESPResSo++ Reimplementation in C++, Co-development of ESPResSo and ESPResSo++	Axel Arnold	1.402
15:30	Open discussion / Closing session	all	
17:00	Core team discussion general strategy, development and documentation process, user model, usability, release policy, code distribution, QA, demo server, GUI, Homepage	only core team: CH, AA, HL, BM, TS, OL	1.402
afterwards	Dinner/Frankfurt-skyline at night	free to join	city