Coarse-grained Simulation of Biological Soft Matter Systems using ESPResSo

Scientific Report of the ESF Science Meeting 3569

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December 16, 2011

Contents

1. Summary

This is the scientific report for the ESF Science Meeting 3569, a tutorial workshop with the title "Coarse-grained Simulation of Biological Soft Matter Systems using ESPResSo", that was held on October 10–14, 2011 at the Institute for Computational Physics, Stuttgart University, Germany. It was very similar to the tutorial "Simulating Soft Matter with ESPResSo", that was held on October 11–15, 2010 (ESF Scientific Meeting 2979). It was organized as a part of the activity of the CECAM node Mainz–Darmstadt–Stuttgart and listed as a CECAM workshop [1]. Besides the funding received by the ESF, the workshop tutorial has been co-funded by the "SimTech Cluster of Excellence" of Stuttgart University.

The goal of the workshop was to teach the participants how to perform Molecular Dynamics simulations of coarse-grained systems as they are used in Soft Matter Research,

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[1] http://www.cecam.org/workshop-532.html

with a focus on biological systems, and how to use the open-source software ESPResSo and other related tools to do so.

The tutorial consisted of theoretical lectures in the morning, that introduced the algorithms and techniques used within ESPResSo, and practical hands-on sessions in the afternoon, where the participants could try out using the software themselves.

The speakers of the tutorial were mostly developers of ESPResSo, while the participants were typically users or users-to-be. Therefore, the tutorial also brought together the developers and users of the software, which was furthermore supported by a poster session in an informal atmosphere as well as a discussion session about the future of the software.

2. Scientific content

The first day of the tutorial was devoted to an introduction into the field and the software. In the first scientific lecture, Prof. Dr. Christian Holm (ICP, Stuttgart, Germany) gave a generic introduction to simulations in Soft Matter Research: Why are simulations used, how can one perform simulations of systems on mesoscopic scales using coarse-grained models (potentials, boundary conditions) and what are the problems (model development, parallelization, . . .). In the second lecture of the morning, Dr. Olaf Lenz (ICP, Stuttgart, Germany) the current maintainer of ESPResSo, gave an introduction to the concepts, methods and features of the software: Parallel simulation core in the C programming language, controlling the simulation from the Tcl scripting language, Introduction to Tcl, First simple simulation scripts (Lennard-Jones fluid, polymer melt).

In the afternoon of the first day, the hands-on session organized by Olaf Lenz gave the participants the opportunity to download, set up and compile the software and to write, run and visualize the first simple simulations (Lennard-Jones fluid, polymer melt).

The second day focussed on two topics. In the first lecture, JP Dr. Axel Arnold (ICP, Stuttgart, Germany), one of the initial developers of the software, gave a glance "under the hood" of the software, how the C-code of the parallelized core looks like and how the software is being developed. The second lecture, also held by JP Dr. Arnold, focussed on one of the strength of the software, namely long-range interactions. Besides giving an introduction on how they are used in the software, he also gave a profound insight into the algorithms and methods used to efficiently compute long-range interactions using Particle-Mesh-Ewald-Algorithms.

The hands-on session on the second day (Olaf Lenz) again handled the same subjects as the lectures in the morning. The participants where introduced to the versioning system `git` and the development platform Savannah, and it was demonstrated how a simple extension to ESPResSo could be developed. For their own experience, simulations of simple charged systems that requires long-ranged interactions (molten salt, polyelectrolyte) were explored.

In the evening, a poster session was held, where participants of the tutorial as well as members of the ICP in Stuttgart put up posters. The informal atmosphere of the session provided a good place for intense discussions between users and developers of

the software.

On Wednesday, 12th October, Dr. Ulf Schiller (FZ Jülich, Germany) talked about methods for simulating hydrodynamic interactions (DPD and Lattice-Boltzmann) in ESPRESSO, while in the second lecture, Mingyang Hu (Carnegie Mellon University, Pittsburgh, USA) presented the `mbtools` package within ESPRESSO that allows to set up and simulate coarse-grained lipid bilayers. The afternoon was devoted to corresponding hands-on sessions. Stefan Kesselheim (ICP, Stuttgart,Germany) gave the participants example codes that allowed them to use the Lattice-Boltzmann implementation within ESPRESSO, while Mingyang Hu gave practical examples for simulating membranes.

In the first lecture on Thursday, Dr. Denis Andrienko (MPIP, Mainz, Germany) talked about systematic coarse-graining and the software package VOTCA that can interoperate with ESPRESSO. Afterwards, Dr. Christoph Junghans (MPIP, Mainz, Germany) presented the ADResS method (**A**daptive **Res**olution **S**cheme), an advanced method for multiscale simulations that is implemented within ESPRESSO, and Dr. Torsten Stühn (MPIP, Mainz, Germany) talked about an offshoot of ESPRESSO called ESPRESSO ++. The hands-on sessions in the afternoon contained corresponding practical examples.

On the last day (Friday, 14th October), the range of applications of the ESPRESSO software was demonstrated by a number of scientific talks on various subjects, given by Prof. Dr. F. Schmid (Universität Mainz, Germany), M. Hu (CMU, USA), Dr. U. Schiller (FZ Jülich, Germany) and S. Kesselheim (ICP, Stuttgart, Germany).

Concluding, we note that the tutorial gave an introduction to Molecular Dynamics simulations of coarse-grained models in Soft Matter Research in general, and a thourough insight into all aspects of the software packages ESPRESSO in particular.

3. Results

The tutorial primarily had an educational purpose, therefore no direct scientific results of the meeting were to be expected.

A. Speakers and Participants

A.1. Speakers

1. Dr. Denis Andrienko, MPIP Mainz, Germany

2. JP Dr. Axel Arnold, ICP, Stuttgart University, Germany

3. Mingyang Hu, Carnegie-Mellon University, Pittsburgh, United States of America

4. Prof. Dr. Christian Holm, ICP, Stuttgart University, Germany

5. Dr. Christoph Junghans, MPIP Mainz, Germany

6. Stefan Kesselheim, ICP, Stuttgart University, Germany

7. Dr. Olaf Lenz, ICP, Stuttgart University, Germany

8. Dr. Victor Rühle, MPIP Mainz, Germany

9. Dr. Ulf Schiller, FZ Jülich, Germany

10. Prof. Dr. Friederike Schmid, Mainz, Germany

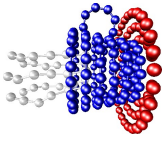11. Dr. Torsten Stühn, MPIP Mainz, Germany

A.2. Participants

1. Denis Antonov, Stuttgart, Germany

2. Muhammad Anwar, Luxembourg, Luxembourg

3. Ghosal Arkaprovo, Stuttgart, Germany

4. Konrad Breitsprecher, Stuttgart, Germany

5. Leonardo Darre, Montevideo, Urugua

6. Annalaura Del Regno, Manchester, UK

7. Farnoosh Farahpoor, Teheran, Iran

8. Andreas Irmler, Stuttgart, Germany

9. Benjamin Juhl, Stuttgart, Germany

10. Elena Minina, Ekatarinenburg, Russia

11. Davoud Puoladsaz, Chemnitz, Germany

12. Hauke Rabbel, Mainz, Germany

13. Jiajia Zhou, Mainz, Germany

14. Jitka Kuldova, Prague, Czech Republic

15. Karel Sindelka, Prague, Czech Republic

16. Marc Segovia, Montevideo, Uruguay

17. Martina Kieninger, Montevideo, Uruguay

18. Matias Machado, Montevideo, Uruguay

19. Mickael Lelimousin, Oxford, UK

20. Mohammad Karim Saeed Ghalati, Teheran, Iran

21. Pedro Sanchez, Germany, Stuttgart

22. Quy Vo Cam, Aachen, Germany

23. Rajarshi Chakrabarti, Stuttgart, Germany

24. Selina Nawaz, Manchester, UK

25. Armer Wafai, Stuttgart, Germany

26. Josh Berryman, Luxembourg, Luxembourg

27. Sebastian Fritsch, Mainz, Germany

B. Final Programme

The following pages contain an excerpt of the workshop's program that shows the final schedule of the event.
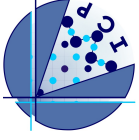
Monday, 10th October

8:00 - 9:00 Registration (*Foyer*)

9:00 - 10:30 Welcome (*Lecture hall*)
– *Dr. O. Lenz, Prof. Dr. C. Holm, ICP Stuttgart*

10:30 - 11:00 Coffee break (*Foyer*)

11:00 - 12:30 Introduction to ESPResSo (*Lecture hall*)
– *Dr. O. Lenz, ICP Stuttgart*

12:30 - 14:00 Lunch break (*Mensa*)

14:00 - 18:00 Hands-on: First steps with ESPResSo,
Compiling ESPResSo, Lennard-Jones liquid,
Visualization with VMD
(*Lecture hall, CIP Pools*)
– *Dr. O. Lenz, ICP Stuttgart*

In case of trouble, call O. Lenz on
his mobile phone:
+49.176.70531688

During the hands-on sessions, coffee, tea, drinks
and pastries are available in the reading room in
the ground floor.
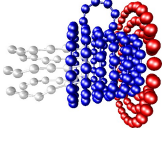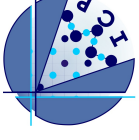
Tuesday, 11th October

9:00 – 9:30 Developers' infrastructure (*Lecture room*)
– *Dr. O. Lenz, ICP Stuttgart*

9:30 - 10:30 Advanced Usage (*Lecture hall*)
– *JP Dr. A. Arnold, ICP Stuttgart*

10:30 - 11:00 Coffee break (*Foyer*)

11:00 - 12:30 Long-range interactions (*Lecture hall*)
– *JP Dr. A. Arnold, ICP Stuttgart*

12:30 - 14:00 Lunch break (*Mensa*)

14:00 - 17:00 Hands-on: Code development, Simulating
charged systems (*Lecture hall, CIP Pools*)
– *Dr. O. Lenz, F. Fahrenberger, ICP Stuttgart*

17:00 - ??? *Poster Session, Dinner (maybe BBQ) (Foyer)*

To enter the computer rooms (i.e. CIP-Pools) in
the basement use your login at the entrance.

In the basement (and maybe on the ground
floor), WLAN is accessible for participants:

SSID: espresso
WPA2-Key: es-ws2011
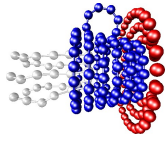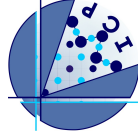
Wednesday, 12th October

9:00 - 10:30 Hydrodynamics: Lattice-Boltzmann and DPD *(Lecture hall)*
– *Dr. U. Schiller, FZ Jülich, Germany*

10:30 - 11:00 Coffee break *(Foyer)*

11:00 - 12:30 Simulating Membranes *(Lecture hall)*
– *M. Hu, CMU, Pittsburgh, USA*

12:30 - 14:00 Lunch break *(Mensa)*

14:00 - 17:00 Hands-on: Hydrodynamics *(CIP Pool 1)*
– *Stefan Kesselheim, ICP Stuttgart*
Hands-on: Membranes *(CIP Pool 2)*
– *M. Hu, CMU, Pittsburgh, USA*

17:00 - 19:00 Discussion: Future of ESPResSo
– *Participants and Developers*

19:00 Common departure from ICP to Stuttgart center

from 19:30 Conference dinner at the *Trollinger Weinstube in Stuttgart center*
http://www.trollingerstubn.de
Rotebühlstraße 50, 70178 Stuttgart
Local train S1/S2/S3, leave at "Feuersee"
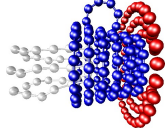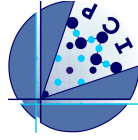
Thursday, 13th October

9:00 - 10:30 Systematic Coarse-Graining with VOTCA *(Lecture hall)*
– *D. Andrienko, MPI for Polymer Research*

10:30 - 11:00 Coffee break *(Foyer)*

11:00 - 11:45 AdResS: The Adaptive Resolution Scheme *(Lecture hall)*
– *C. Junghans, MPI for Polymer Research*

11:45 - 12:30 ESPResSo++ *(Lecture hall)*
– *T. Stühn, MPI for Polymer Research*

12:30 - 14:00 Lunch break *(Mensa)*

14:00 - 18:00 Hands-on: VOTCA *(CIP Pool 1)*
– *C. Junghans, S. Fritsch, V. Rühle;*
Hands-on: ESPResSo++ *(CIP Pool 2)*
– *T. Stühn, MPI for Polymer Research*

Lecture slides and hands-on material is available on the homepage (http://www.cecam.org/workshop-532.html). Extended paper tutorials will be available in the source code some time after the workshop.
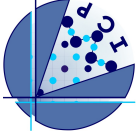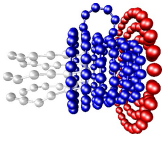
Friday, 14th October

9:00 - 9:45   Simulation of Electroosmotic Flow and
Electrophoresis in Microfluidics
(Lecture hall)
– *Prof. Dr. F. Schmid, Uni Mainz*

9:45 - 10:30   Determining the Gaussian Bending Modulus of
Lipid Membranes in Simulations
(Lecture hall)
– *Dr. M. Hu, CMU, Pittsburgh, USA*

10:30 - 11:00   Coffee break *(Foyer)*

11:00 - 11:45   Modeling Deformable Particles: Red Blood
Cells *(Lecture hall)*
– *Dr. U. Schiller, FZ Jülich, Germany*

11:45 - 12:30   Correlations and Dielectric Boundaries
(Lecture hall)
– *S. Kesselheim, ICP Stuttgart*

12:30 - 13:00   Closing remarks
– *Dr. O. Lenz, JP Dr. A. Arnold; ICP Stuttgart*

from 13:00   Lunch *(Mensa)* and departure