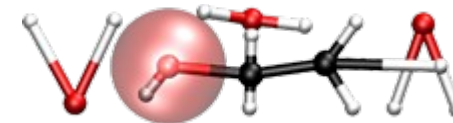
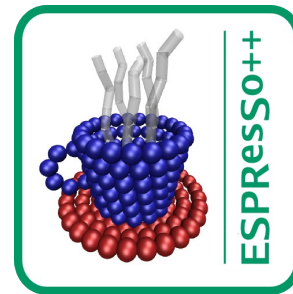




Welcome to the Summer School

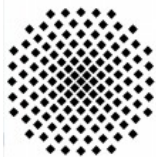
“Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA”

7-11 October 2013

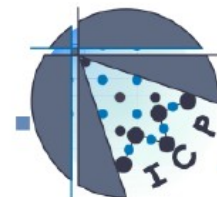


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University of Stuttgart
Germany



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PHYSICS





Thanks go to...



...for the publicity.

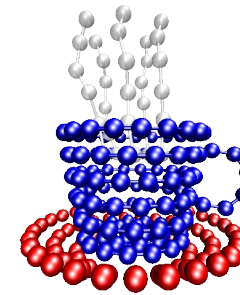


...for financial support.

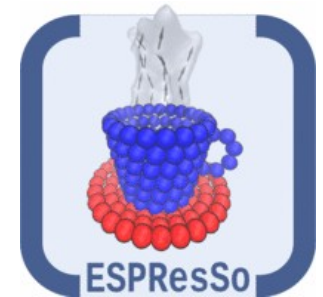
DFG Sonderforschungsbereich 716:
“Dynamische Simulation von Systemen
mit großen Teilchenzahlen”

History of ESPResSo

- “**Extensible Simulation Package for Research on Soft matter systems**”
- Software for Coarse-Grained Simulations
- Developed since 2001
(first commit 13 Nov 2001 by AA)
- Created by 3 PhD students at the Max-Planck-Institute for Polymer Research in Mainz (MPIP):
Axel Arnold, Bernward Mann († 2006), Hanjo Limbach; Supervisor: Christian Holm
- Written in C and Tcl
- Initially used mostly at MPIP
- 2007: Nature cover issue
- Since 2010: Maintained and developed at ICP



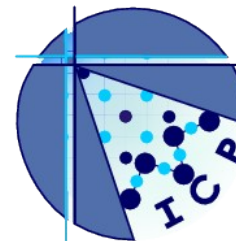
2003



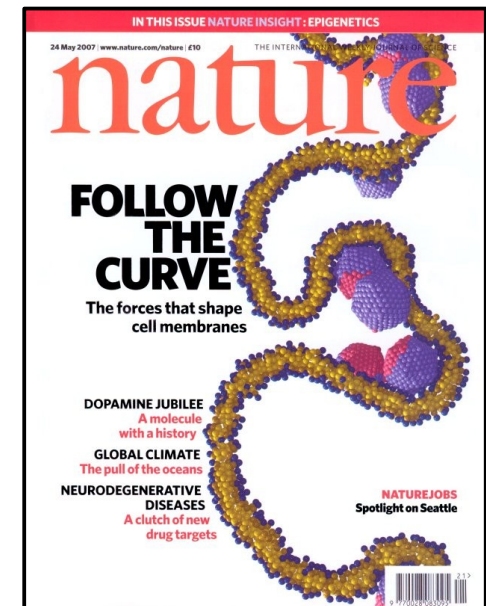
2012



2001



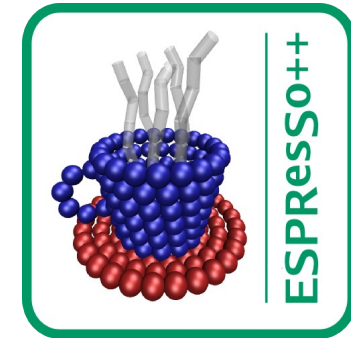
2010



2007

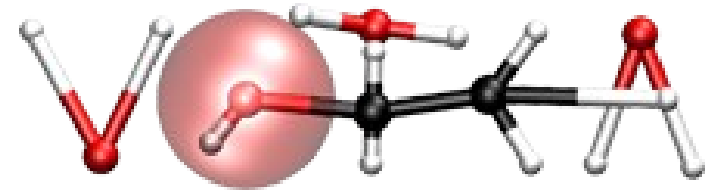
History of ESPResSo++

- Developed since 2008
- Rewrite of ESPResSo
- Joint project of Fraunhofer SCAI (Skt. Augustin) and MPIP (Mainz)
- Maintained and developed at MPIP
- Original project team:
Axel Arnold, Olaf Lenz, Torsten Stühn, Jonathan Halverson, Thomas Brandes; Supervisor: Dirk Reith
- Object-oriented C++ and Python
- Cleaner code
- Currently not as many features as ESPResSo
- Good implementation of ADResS (Adaptive Resolution Scheme)
- ESPResSo is now adapting some of ESPResSo++'s features (e.g. Python)
→ Merge in the future?



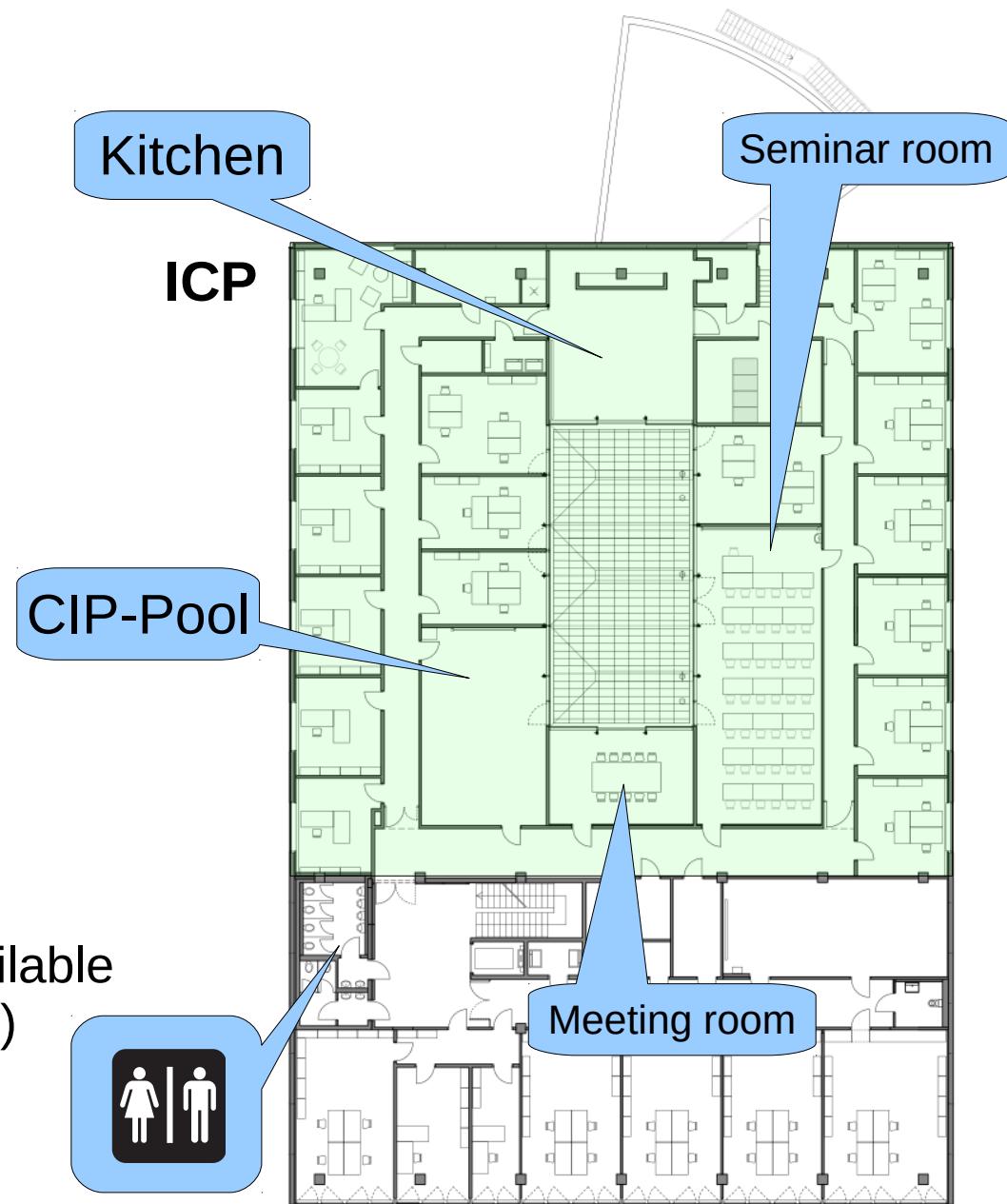
VOTCA

- “**V**ersatile **O**bject-oriented **T**oolkit for **C**oarse-graining **A**pplications”
- Tool for systematic coarse-graining
- Can work together with ESPResSo, ESPResSo++ or GROMACS
- Developed since 2008
- Maintained and developed at MPIP
- Main developers:
Victor Rühle, Christoph Junghans;
Supervisor: Denis Andrienko



Locations

- Seminar room:
Common Talks, Track 1
- CIP-Pool 1.033: Track 2
- Meeting room: Track 3
(Monday only)
- Kitchen:
Coffee breaks;
Coffee, Tea, Drinks,
Brezels, Pastries
available at all times
- WLAN everywhere
(SSID: "ess2013",
WPA2-Key: "Ess@I.C.P.")
- Some ICP computers are available
(Accounts at registration desk)
- Lunch at Mensa
(follow the crowd at 12:30!)





Programme

- Mornings (9:00-12:30)
 - 2 Lectures, 1½ h each; ½ h Coffee break
 - Sometimes 2 tracks
- Afternoon (14:00-17:30)
 - Hands-on Sessions
 - Up to 4 tutorials per session
 - Handouts, not instructed, but tutors are available for questions
- Lightning Talk Session on Monday, 17:00-18:00: Contact Olaf
- Poster Session and BBQ on Tuesday
 - Posters can stay mounted the whole week
- Conference Dinner on Wednesday
 - “Trollinger” in City center
 - Pay yourself for participants
 - ~20€ for food and drinks