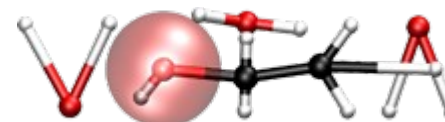
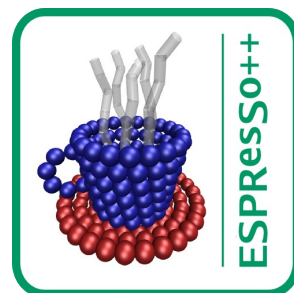
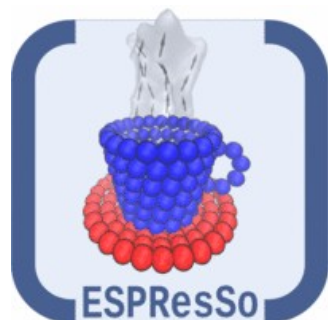


Welcome to the Summer School

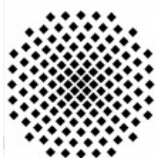
“Simulating Soft Matter with ESPResSo, ESPResSo++ and VOTCA”

8-12 October 2012

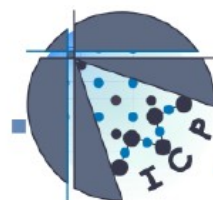


Olaf Lenz

Institut für Computerphysik, Universität Stuttgart, Germany



University of Stuttgart
Germany

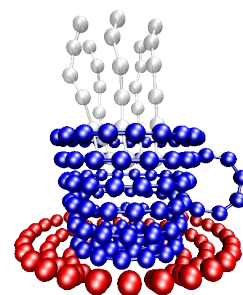


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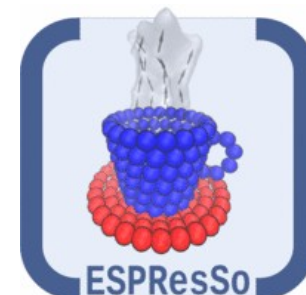


History of ESPResSo

- “**E**xtensible **S**imulation **P**ackage for **R**esearch on **S**oft 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



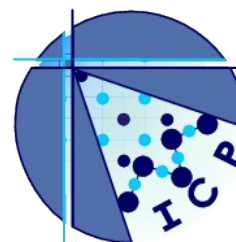
2003



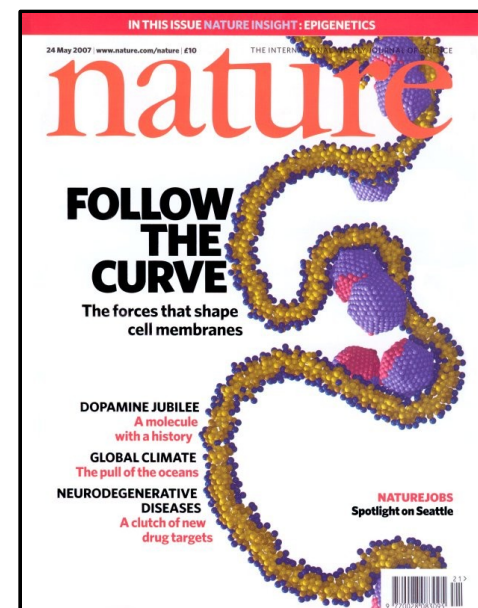
2012



2001



2010

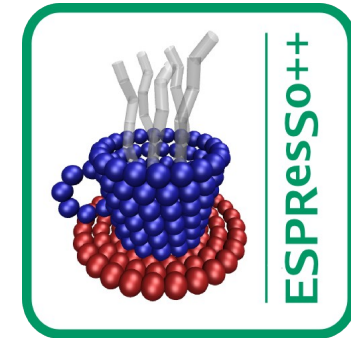


2007

2/11

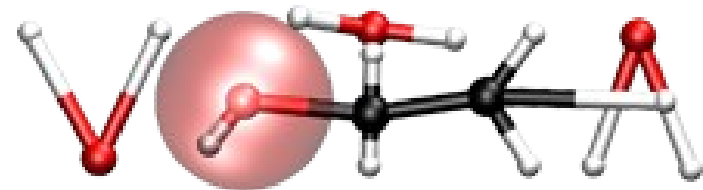
History of ESPResSo++

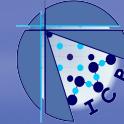
- Developed since 2008
- Rewrite of ESPResSo
- Joint project of Fraunhofer SCAI (Skt. Augustin) and MPIP (Mainz)
- Maintained and developed at MPIP
- Original project team:
Axel Arnold, Olaf Lenz, Torsten Stühn, Jonathan Halverson, Thomas Brandes; Supervisor: Dirk Reith
- Object-oriented C++ and Python
- 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

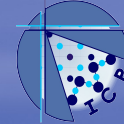
- “**V**ersatile **O**bject-oriented **T**oolkit for **C**oarse-graining **A**pplications”
- Tool for systematic coarse-graining
- Can work together with ESPResSo, ESPResSo++ or GROMACS
- Developed since 2008
- Maintained and developed at MPIP
- Main developers:
Victor Rühle, Christoph Junghans;
Supervisor: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





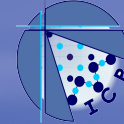
Programme

- 2 Tracks
 - 3½ h per Session, including ½ h Coffee Break
 - Morning session 9:00-12:30, afternoon session 14:00-17:30
 - Sessions contain lectures and hands-on exercises
- Some ICP computers are available (Accounts at registration desk)
- WLAN everywhere (SSID: “ess2012”, WPA2-Key: “Ess@I.C.P.”)
- Brezels, Pastry, Coffee, Tea, Water available at all times
- Lightning Talk Session on Monday
 - Contact me (Olaf)
- Poster Session and BBQ on Tuesday
- Conference Dinner on Wednesday
 - “Trollinger” in City center
 - Pay yourself for participants
 - ~20€ for food and drinks
 - Please sign up *today* at registration desk



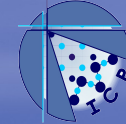
Monday, 8th October

9:00 – 9:30	“Welcome” – O. Lenz (ICP)	
	<i>Track 1</i>	<i>Track 2</i>
9:30 – 12:30	“Introduction to Soft Matter Simulations” – C. Holm, O. Lenz (ICP)	“ESPresSo: Under the hood” – A. Arnold (ICP)
12:30 – 14:00	Lunch Break	
14:00 – 17:00	“Introduction to Tcl” - P. Sanchez (ICP)	“Introduction to Python” - S. Kesselheim, T. Steinle (ICP)
17:00 – 18:00	Lightning Talks	



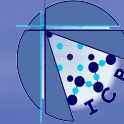
Tuesday, 9th October

	Track 1	Track 2
9:00 – 12:30	“Introduction to ESPResSo” - <i>O. Lenz (ICP)</i>	“Introduction to ESPResSo++” - <i>T. Stühn (MPIP)</i>
12:30 – 14:00	Lunch Break	
14:00 – 17:30	“Recent and Future Developments of ESPResSo” - <i>O. Lenz,</i> <i>S. Kesselheim,</i> <i>R. Weeber,</i> <i>P. Kosovan (ICP)</i>	“ESPResSo++ and AdResS” - <i>T. Stühn (MPIP),</i> <i>C. Junghans (LANL, USA),</i> <i>S. Bevc (NIC, Slovenia)</i>
17:30 -	Poster Session and BBQ	



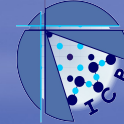
Wednesday, 10th October

9:00 – 12:30	“Data Analysis and Visualization” <i>- Gaël Varoquaux (INRIA, France)</i>	
12:30 – 14:00	Lunch Break	
	<i>Track 1</i>	<i>Track 2</i>
14:00 – 17:30	“Electrostatic Interactions in ESPResSo” <i>- A. Arnold (ICP)</i>	“Systematic Coarse-Graining with VOTCA” <i>- V. Rühle (Cambridge, UK), C. Junghans (LANL, USA)</i>
17:30-	Conference Dinner	



Thursday, 11th October

	Track 1	Track 2
9:00 – 12:30	“Hydrodynamics in ESPResSo” - U. Schiller (FZ Jülich), J. Smiatek (ICP)	“Systematic Coarse-Graining with VOTCA 2” - V. Rühle (Cambridge, UK), C. Junghans (LANL, USA)
12:30 – 14:00	Lunch Break	
14:00 – 17:30	“Simulating Membranes in ESPResSo” - M. Hu, P. Diggins (CMU, USA)	“Rare event sampling with FRESHS” - K. Kratzer (ICP)



Friday, 12th October

9:00 – 9:45	“Magnetic Soft Matter: A Simulational Approach” - <i>C. Holm (ICP)</i>
9:45 – 10:30	“Determining the Gaussian curvature modulus of lipid membranes in simulations: A comparative study via global shape transformations and local stress distributions” - <i>M. Hu (Carnegie-Mellon University, USA)</i>
10:30 – 11:00	Coffee Break
11:00 – 11:45	“Agglomeration of nano- and micron-sized particles” - <i>A. Kronenburg (Institut für Technische Verbrennung, Universität Stuttgart, Germany)</i>
11:45 – 12:30	“Tracer diffusion in polymers and gels” - <i>P. Kosovan (ICP)</i>
12:30 – 13:00	Wrap-up - <i>O. Lenz, A. Arnold, C. Holm (ICP)</i>

Locations

- Seminar room 1.079:
Common Talks, Track 1
- CIP-Pool 1.033:
Track 2
- Kitchen:
Coffee breaks;
Coffee, Tea, Drinks,
Brezels, Pastry
- Atrium: No-go
- Mensa: Lunch
(follow the crowd at 12:30!)

