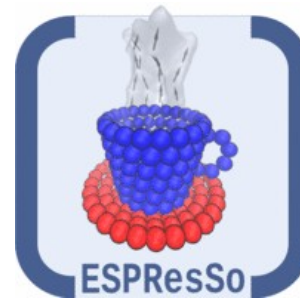
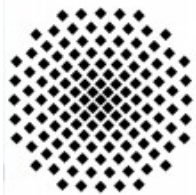


Recent and Future Developments of ESPResSo



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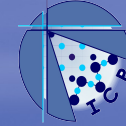


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PHYSICS

New Developments in Development Code

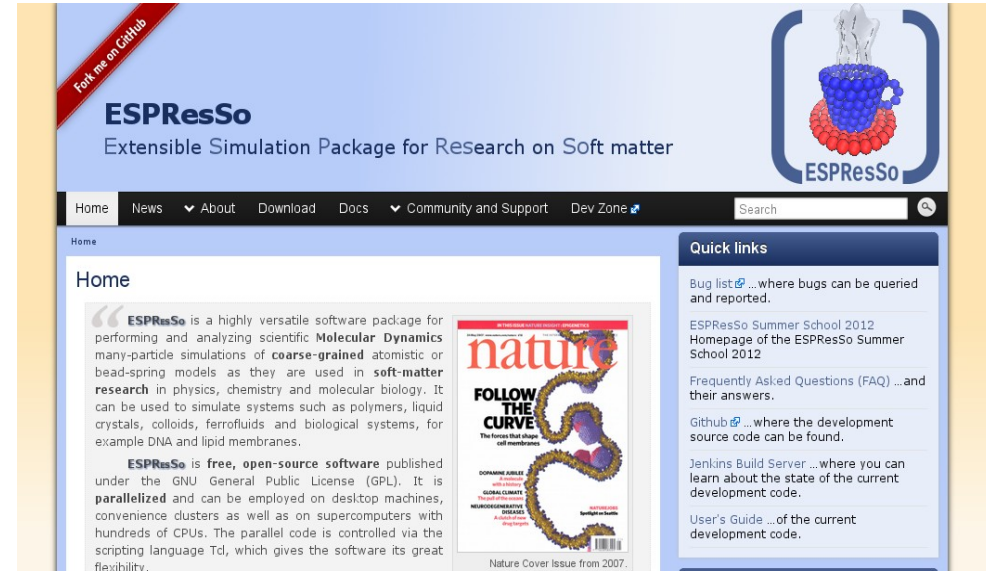
- New developments are only available in development version
- Get via git
`git clone git://git.savannah.nongnu.org/espressomd.git`
- Compilation requires one more step (in source directory):
`bootstrap`
- Requires GNU autotools (autoconf, automake)
- Afterwards
`configure`
`make`
`make check`



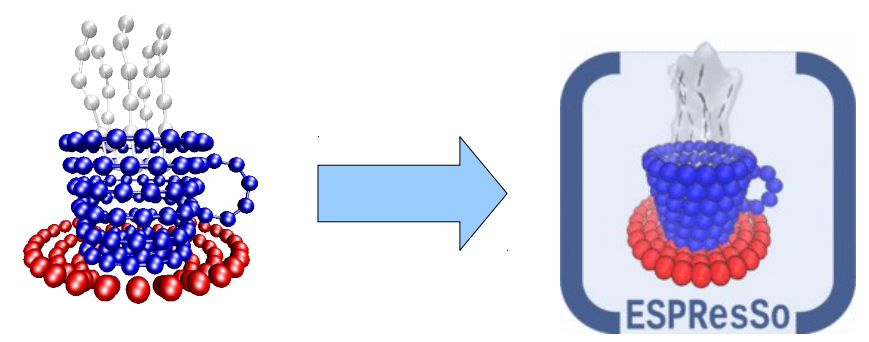


Logo & Website

- New website (Wordpress) since January (O. Lenz, K. Breitsprecher, ICP)

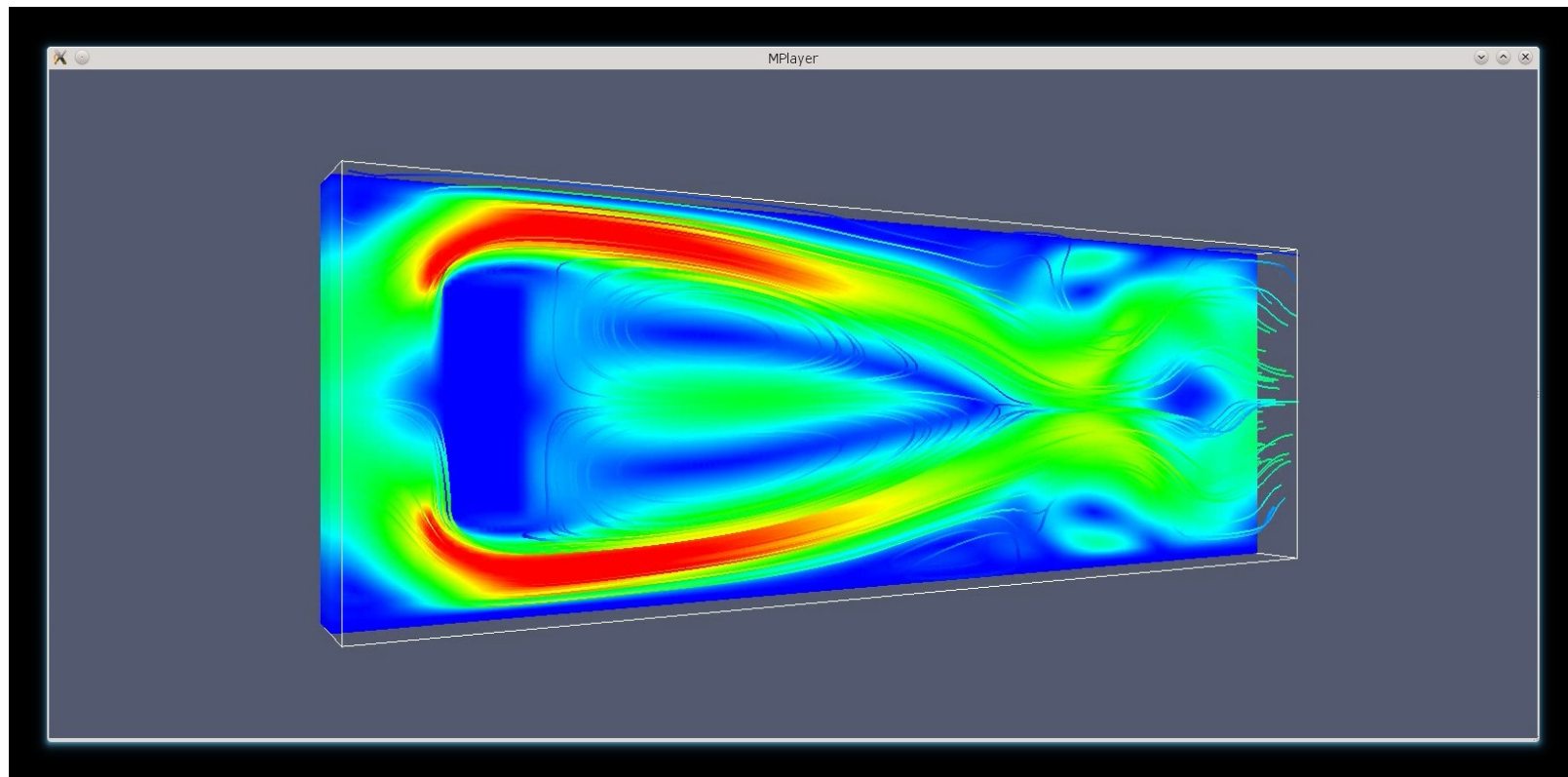


- New logo since June (O. Lenz, ICP)



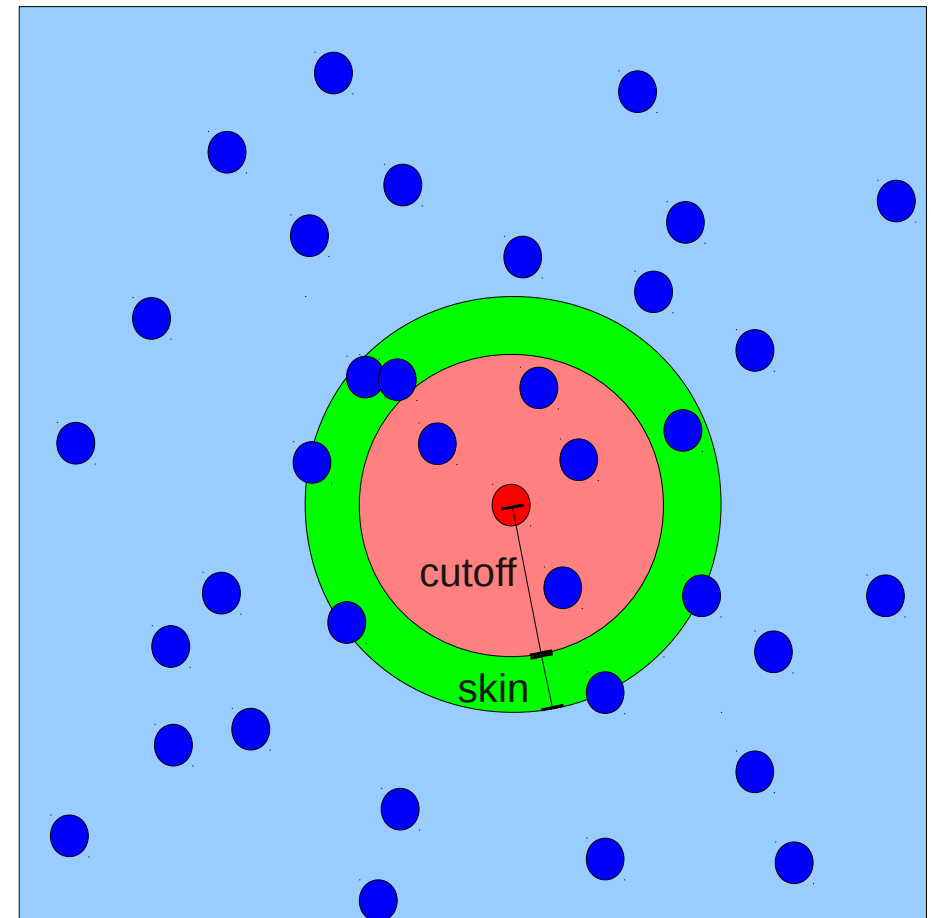
New constraint: Rhomboid

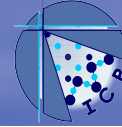
- Since June (G. Rempfer, ICP)
- Basic building block for arbitrary shapes



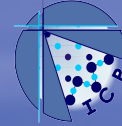
Verlet list optimization

- Since January (A. Arnold, G. Inci, ICP)
- So far, particle pairs within the maximal interaction range were in the list
- Independent of actual interaction
- Now, only pairs within interactions cutoff are included
- Very useful for asymmetric mixtures or non-interacting particles





And now for more serious developments...



Future Developments

Coding Week in January 2013! Join, if you like!

- Efficient constraints
 - From Toronto, Canada, Group of G. Slater
 - So far, constraints are computed for all particles
 - Cell list structure also include constraints
 - Useful for systems with a lot of constraints
 - Mostly ready, but not well-integrated
 - → Coding week?
- Interface to ScaFaCoS library
 - “Scalable Fast Coulomb Solver”
 - Library for electrostatic algorithms:
 - FMM
 - P3M / P2NFFT
 - Multigrid solvers
 - Barnes Hut Tree
 - → End of the year?

Python interface

- First signs in master: Split off the Tcl interface from the C-code
- Branch cython in git repo
- Based on Cython
- Simple Python interface is already running
- Work on actual interface can start

