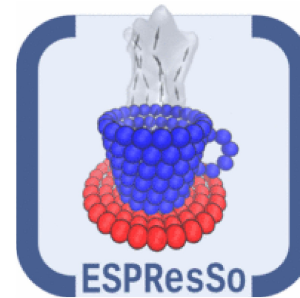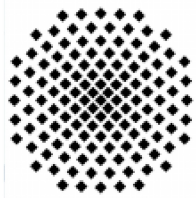# Recent and Future Developments of ESPResSo
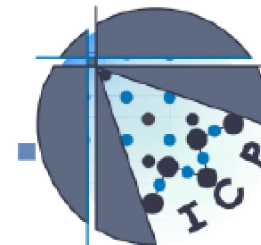
Olaf Lenz

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Stuttgart, Germany

New Publication

- New ESPResSo publication:

    Arnold, A.; Lenz, O.; Kesselheim, S.; Weeber, R.;
    Fahrenberger, F.; Röhm, D.; Košovan, P.; Holm, C.
    *ESPResSo 3.1 — Molecular Dynamics Software for
   Coarse-Grained Models*.
    Meshfree Methods for Partial Differential Equations VI;
    Griebel, M.; Schweitzer, M.A., Eds.
    Springer, 2013, Vol. 89, Lecture Notes in Computational
    Science and Engineering, pp. 1–23.

- Please cite it!

Releases

http://www.icp.uni-stuttgart.de

- 3.1.0: 8th March 2012
  (3.1.1: 2012-10-09; 3.1.2: 2013-03-08)

  - Analysis in the core

  - Dynamic bonding

  - Langevin per particle

  - Rhomboid constraint

  - ICC*

  - … and more

- 3.2.0: 10th May 2013

  - New potentials:
    HAT and GAUSSIAN

  - Simple reaction model

  - Rotation per particle

  - Functions to find particles of a type
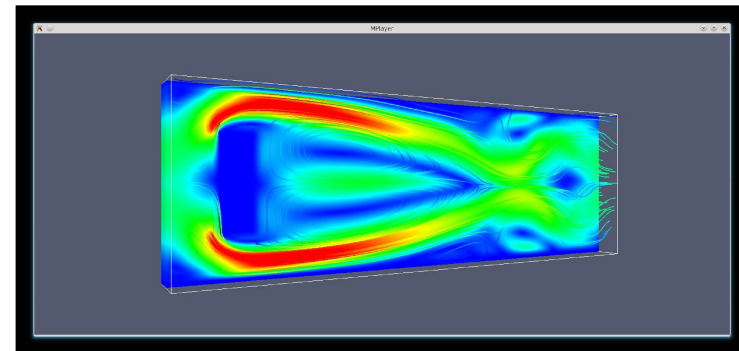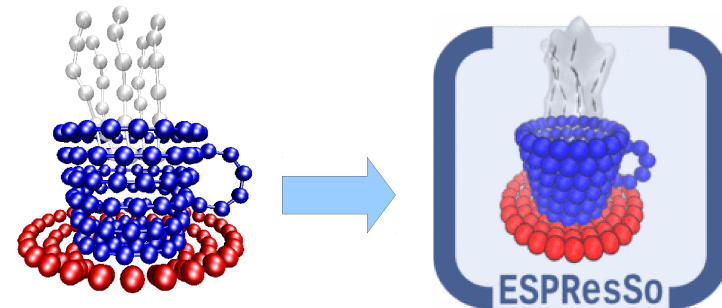
Recent Developments in Development Code

- New developments are only available in development version

- Get via git

  - From Github
    ```
    git clone \
      https://github.com/espressomd/espresso.git
    ```

  - From GNU Savannah
    ```
    git clone \
      git://git.savannah.nongnu.org/espressomd.git
    ```

- Compilation

  - Requires GNU autotools (autoconf, automake)

  - Requires one more step (in source directory!):
    ```
    ./bootstrap.sh
    ```

  - Afterwards
    ```
    configure; make; make check
    ```

- Check current state on Jenkins
  http://espressomd.org/jenkins/

Recent and Future Developments

- Already in the Development Code
  - Dielectric contrasts with MEMD (Florian Fahrenberger)
  - Two-phase flow a.k.a. Shan-Chen (Marcello Sega)
  - Immersed boundaries (a.k.a. "object-in-fluid" a.k.a. elastic objects)
    →**Iveta Jancingova**
  - Switch to C++ compiler (Olaf Lenz)
    - Allows to use C++ data structures (e.g. vector)
    - Allows to use classes; long-term goal: object-oriented refactoring
- In Progress
  - P3M on GPU (Florian Weik), Ewald on GPU (Sascha Erhardt)
  - Interface to ScaFaCoS (Olaf Lenz)
    - "**Sca**lable **Fa**st **Co**ulomb **S**olvers"
    - Library for electrostatics algorithms:
      FMM, P3M/P2NFFT, Multigrid solvers, Barnes-Hut-Tree
  - Polarizable Drude-Particles (Konrad Breitsprecher)
  - Electrokinetics →**Georg Rempfer**

Python Interface

- Nothing new has happened since 2012. :-(
- 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

http://www.icp.uni-stuttgart.de
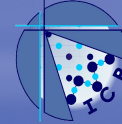
Coding Day

- You want to get involved?

- Irregular ESPResSo Coding Day!

  - Typically Friday

- On that day, developers at ICP work on the code

- You are invited to join!

  - Either in person

  - Or virtually

http://www.icp.uni-stuttgart.de