JÜLICH
FORSCHUNGSZENTRUM

Simulation Laboratories at JSC

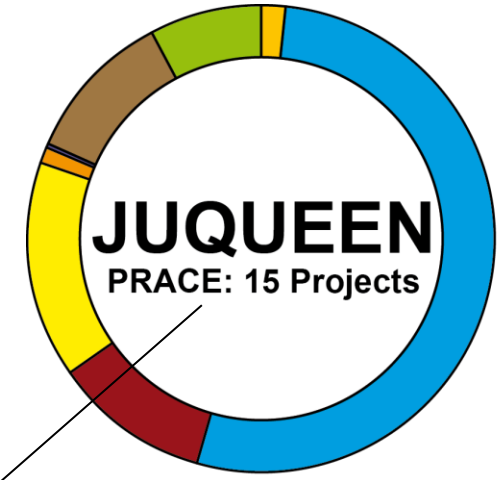
Paul Gibbon

Jülich Supercomputing Centre

2nd JUQUEEN Porting & Scaling Workshop, 3-5 February 2014

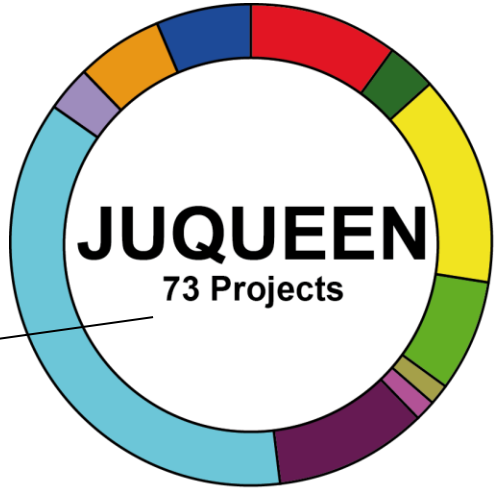
Projects in Europe and Germany

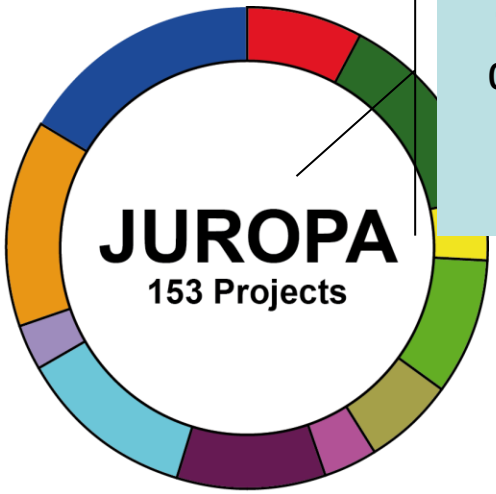
2012/13



- Social Sciences and Humanities
- Physical Sciences and Engineering
  - PE1 Mathematics
  - PE2 Fundamental constituents of matter
  - PE3 Condensed matter physics
  - PE4 Physical and analytical chemical sciences
  - PE5 Synthetic chemistry and materials
  - PE6 Computer science and informatics
  - PE7 Systems and communication engineering
  - PE8 Products and processes engineering
  - PE9 Universe sciences
  - PE10 Earth system science
- Medicine and Life Sciences

Few leading edge capability projects in EU
EU
PRACE





Capacity and data analytics
JARA
NIC

Large-scale national projects in
GCS

- Astrophysics
- Biophysics
- Chemistry
- Earth & Environment
- Plasma Physics
- Soft Matter
- Fluid Dynamics
- Elementary Particle Physics
- Computer Science
- Condensed Matter
- Materials Science

Jülich Simulation Laboratory Template

Staff

- Senior scientist *recruited from field*
- 1-2 postdocs + technical staff (informatics)
- Jointly supervised PhD & MSc students

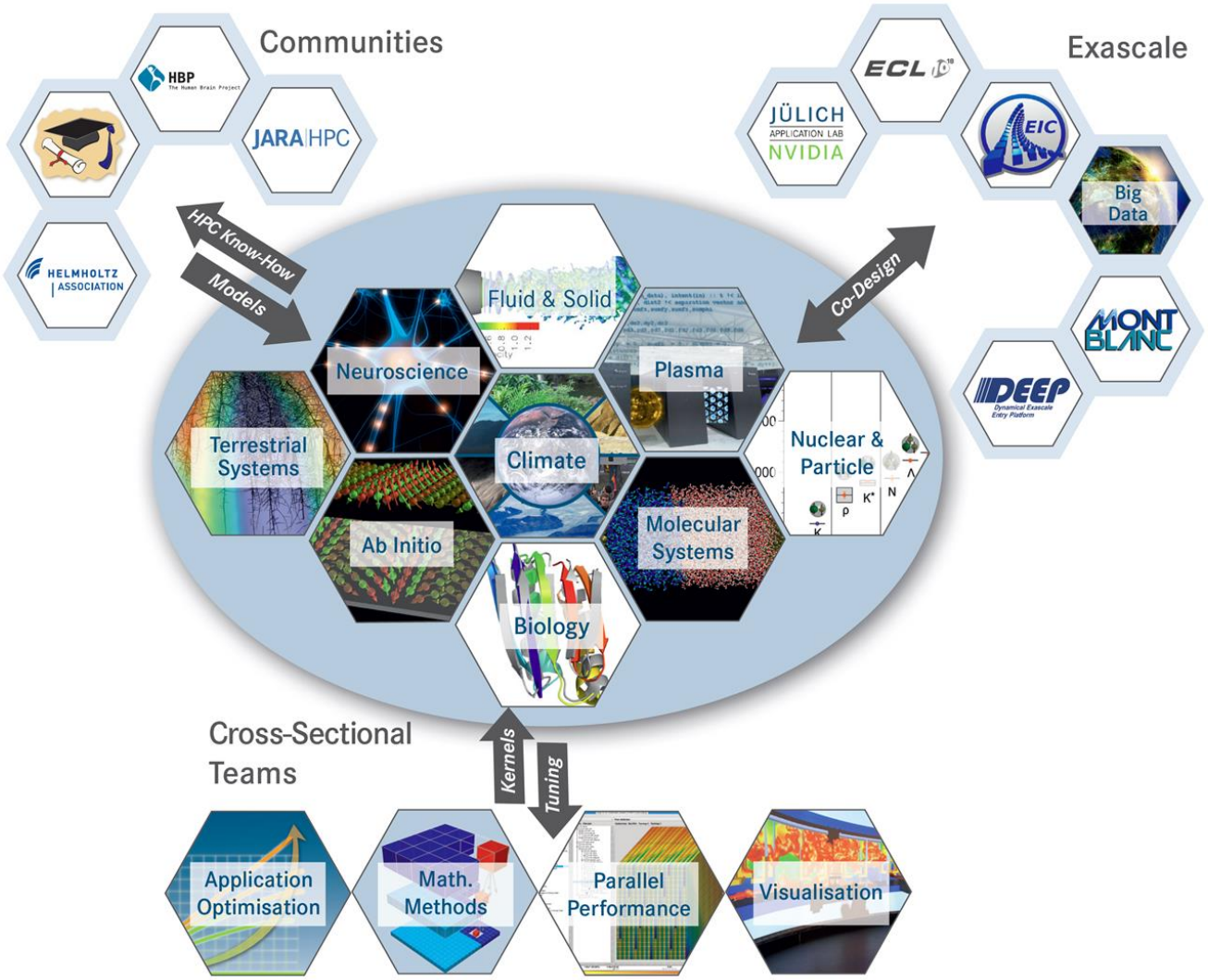
Support

- Porting/tuning/benchmarking
- Algorithm scaling; code clinics
- Workshops; schools

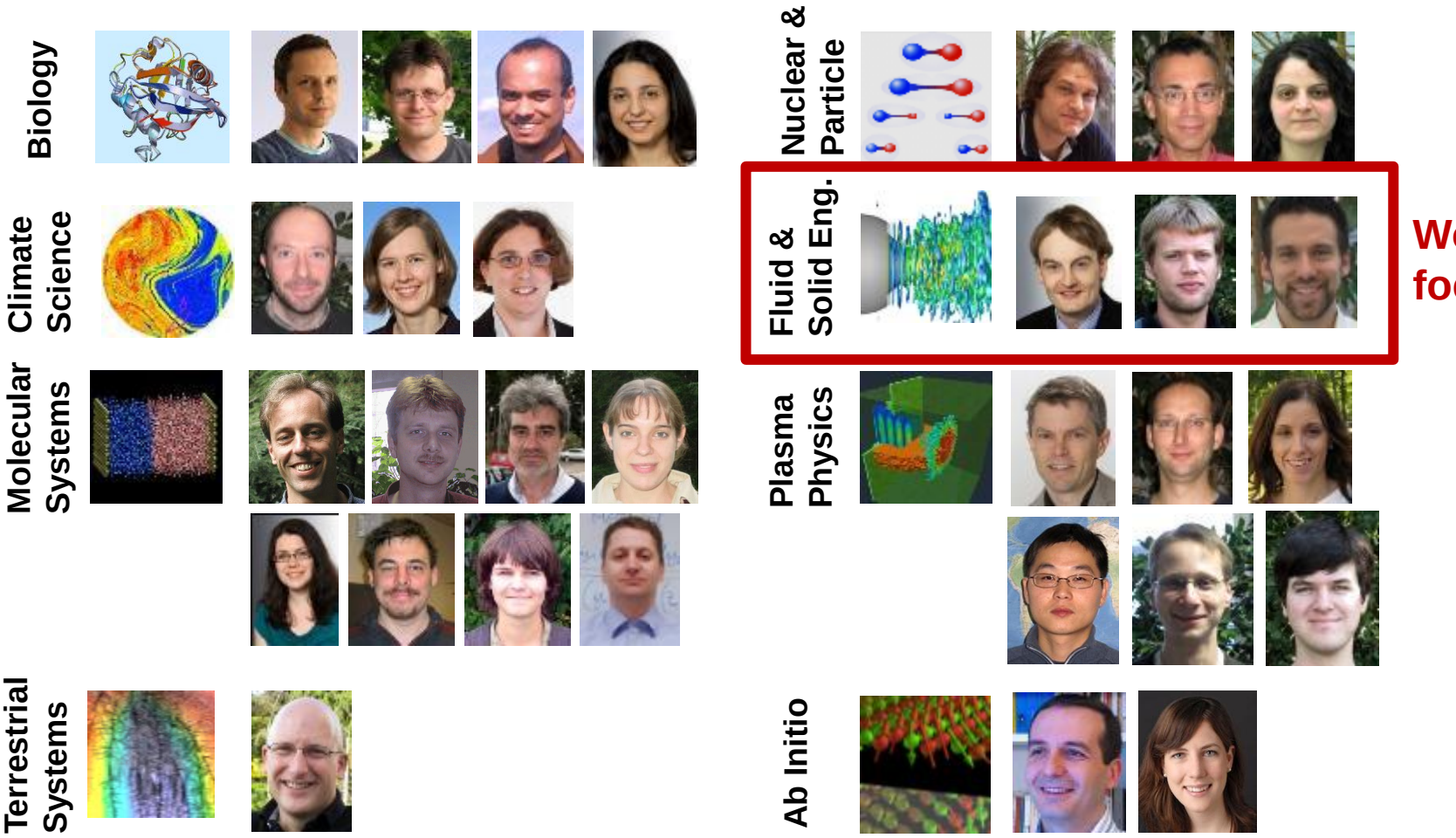
Research

- Common/generic methods
- Scalable algorithms
- 3rd party projects

Simulation Labs link simulation science communities to Exascale technology



Active Simulation Labs @ JSC

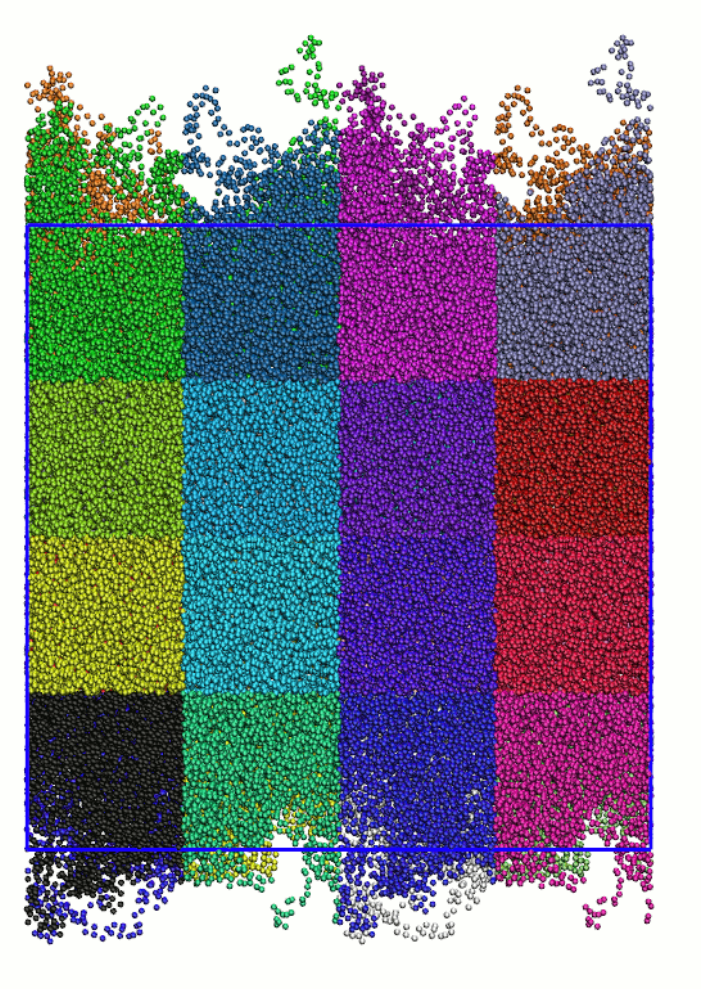


SimLab support and research activities

- **NIC/VSR advisory**
- **Code Clinics**
- **Training workshops**:
- **Advanced application support**
- **Research cooperations**

Support highlight: Re-engineering IBIsCO to study polymer surfaces (TU Darmstadt)

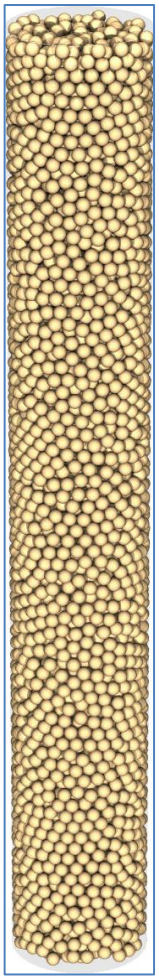
Viorel Chihaia, Rene Halver, SL Molecular Systems

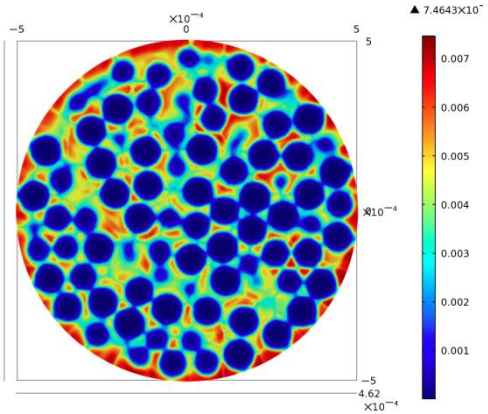


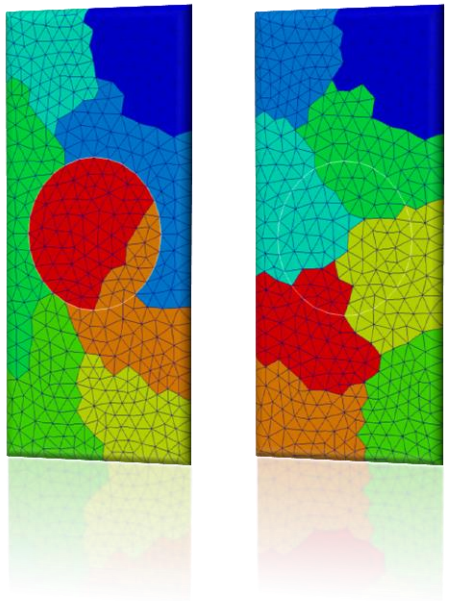
- Boundary conditions adapted for polymers
- 5x performance speed-up
- New NIC project
- Long-term cooperation

JARA SimLab Fluid & Solid Engineering: Packed-bed chromatography with XNS – IBT/FZJ

Mike Nicolai, Eric von Lieres





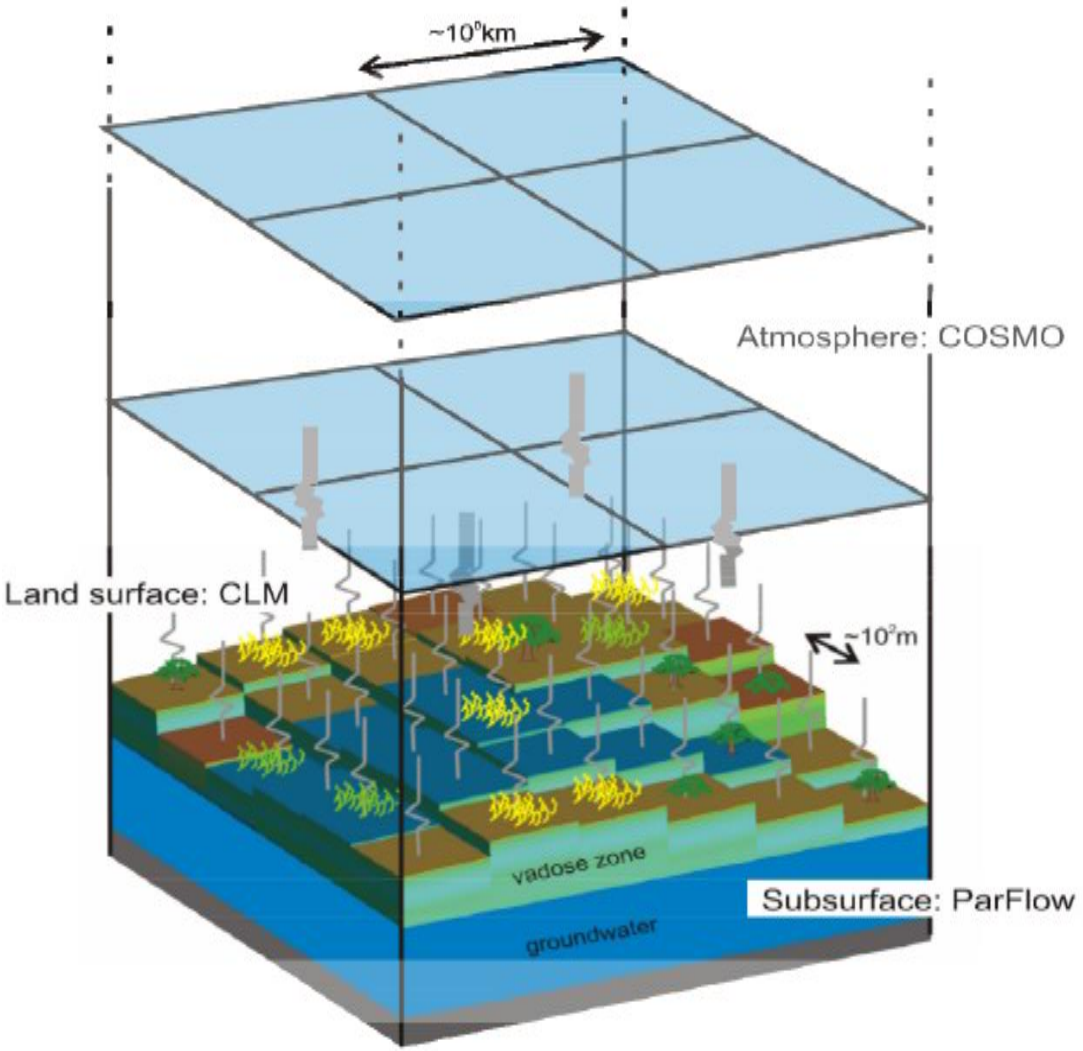


- Effort: ~ 1 core/bead
- Lab-scale column: 10^7 beads
- No scalable commercial code available

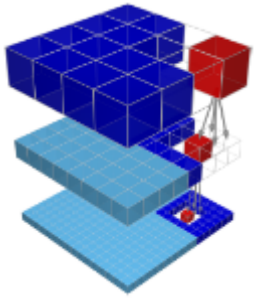
SimLab Terrestrial Systems

Klaus Görgen, Stefan Kollet

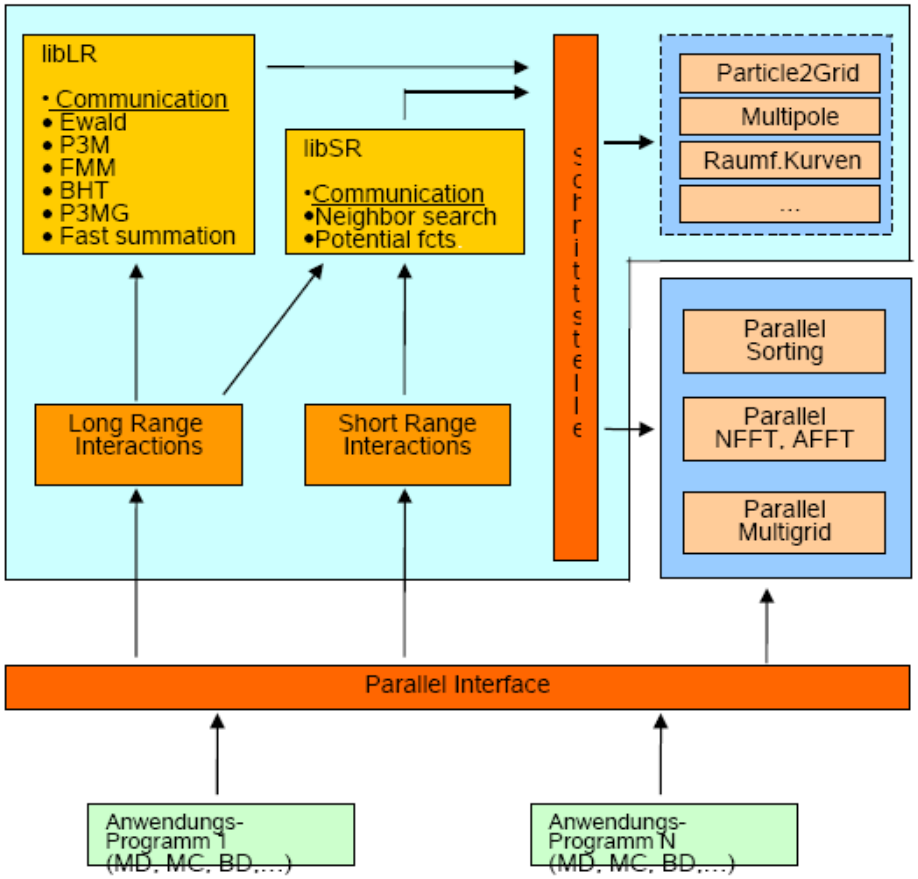
- TerrSysMP (code coupling framework OASIS3)
- Parflow (hydrology)
- CLM (surface)
- COSMO (weather)
- WRF/ARM (climate)



ScaFaCoS: BMBF project 2009-2012



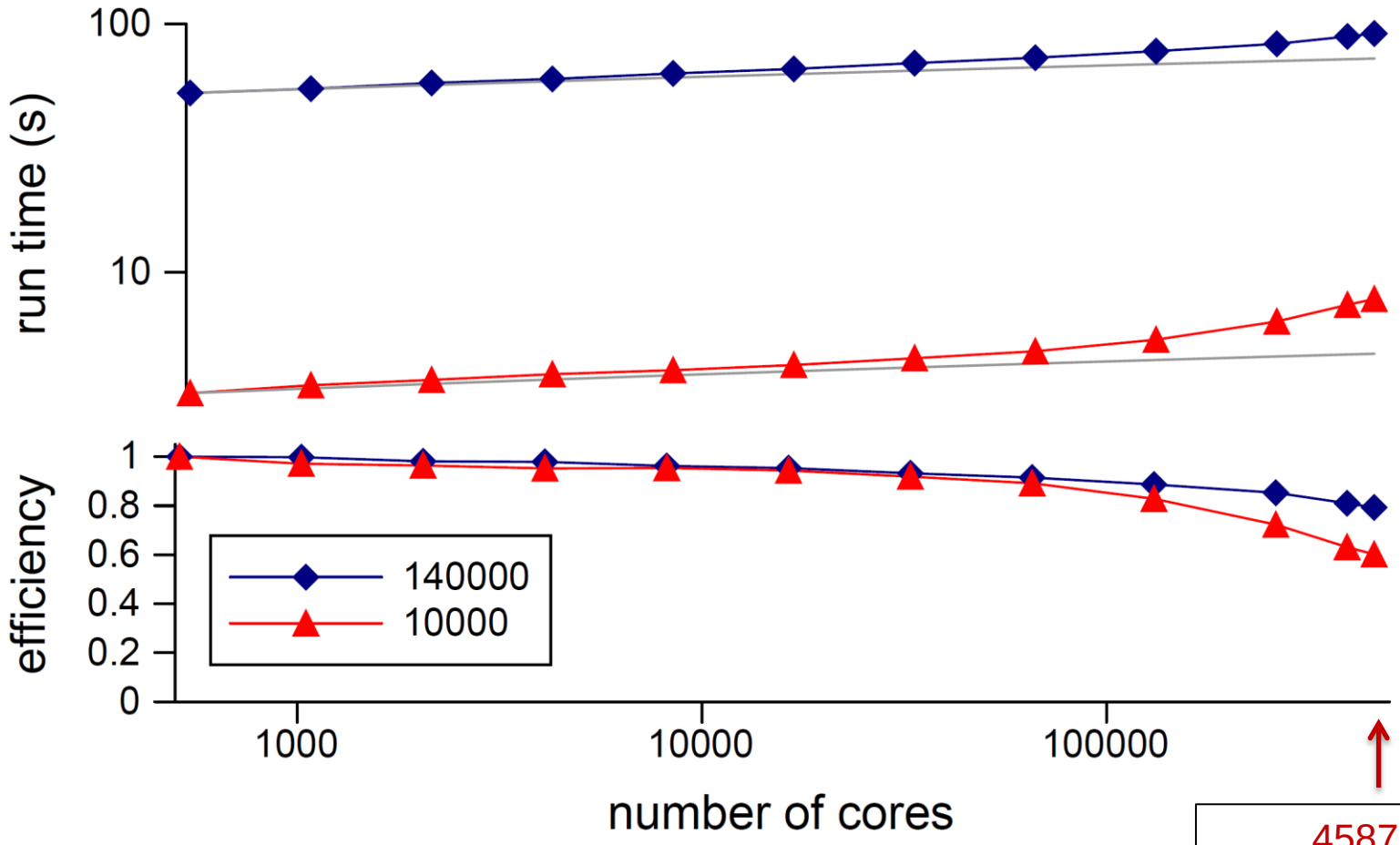
- Fast Electrostatics Library
  - Unified parallel library for various methods of long range interactions
  - Multiple boundary conditions: open, 1d-,2d-,3d-periodic
  - Error control
  - OpenSource distribution under LGPL license



Spin off: DFG SPPEXA 'GROMEX' project to couple Gromacs to FMM

Weak scaling on JUQUEEN

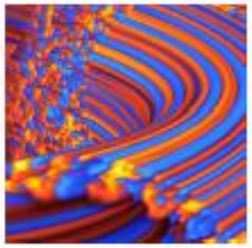
Bendikt Steinbusch (SL Plasma)



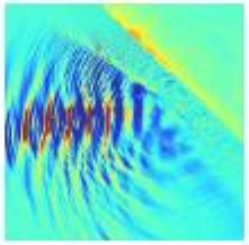
High-Q Club

Members

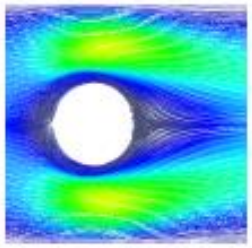
dynQCD



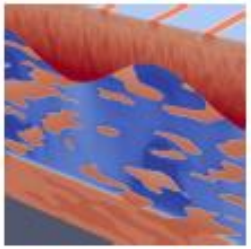
Gysela



JuSPIC



MP2C



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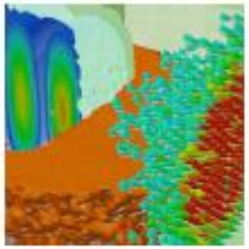
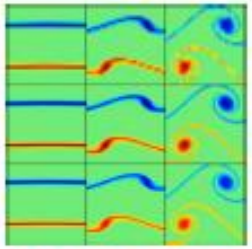
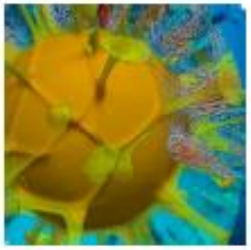
NEST



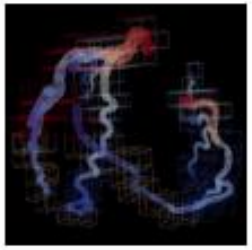
PEPC



PMG+PFASST



Terra-Neo



waLBerla

Currently 10 applications from several fields

Applications from JSC

The Simulation Lab Mission

- **Programming supercomputers is getting harder:**
  - *Many-core/accelerators*
  - *Hybrid programming models*
  - *Memory management*
  - *I/O; Big Data: how much storage is necessary?*

- **Algorithm research:**
  - *Goal to replace legacy code (climate, engineering, chemistry) with scalable algorithms*
  - *Anticipate architecture trends: design choices*
  - *Co-design: give software authors a say in next-generation supercomputers!*