Simulation Laboratories at JSC: A Community-Oriented Software Support & Development Strategy for HPC
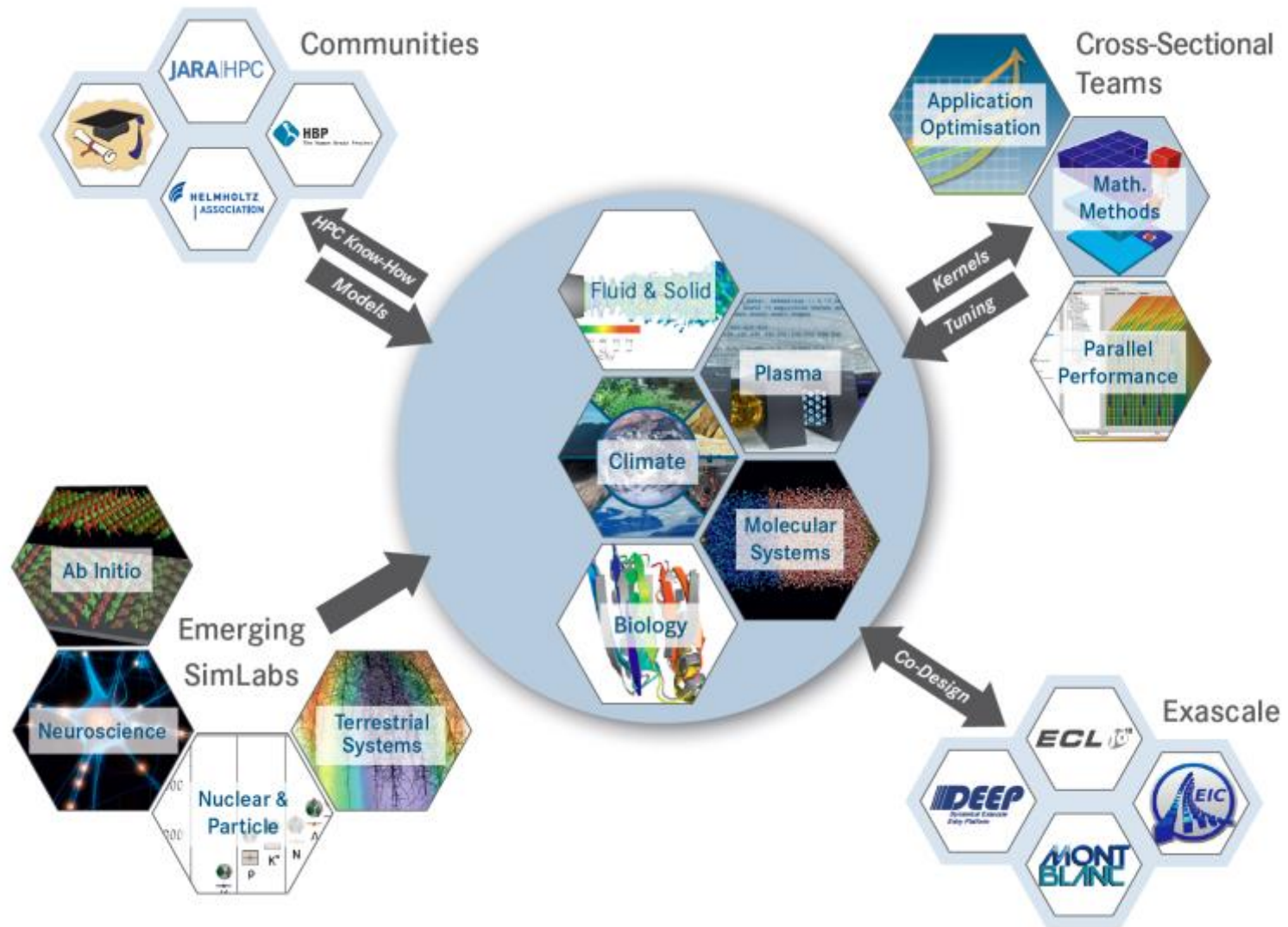
Paul Gibbon

Jülich Supercomputing Centre

1st Jülich-Daresbury Workshop, Jülich, 7-8 May 2013

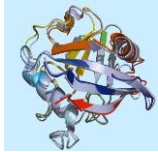# Simulation laboratory infrastructure
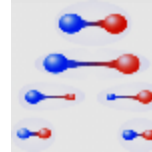
Simulation Labs: Structure

- **Staff**
  - Senior scientist recruited from field
  - 1-2 postdocs
  - 1 technical staff (informatics)
  - Jointly supervised PhD & MSc students
- **Support**
  - Porting/tuning/benchmarking; code hosting
  - Algorithm scaling; code clinics
  - Workshops; schools
- **Research**
  - Common/generic simulation methods
  - Scalable algorithms
  - Project work with SL partners
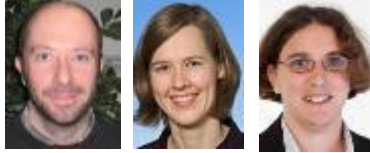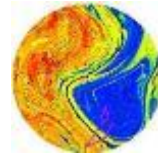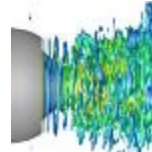
Active Simulation Labs @ JSC

Biology

Climate Science

Molecular Systems

Terrestrial Systems

Nuclear & Particle

Fluid & Solid Eng.
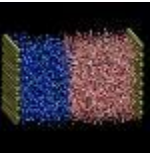
Plasma Physics

Ab Initio

SimLab Activities

1. **NIC/VSR advisory**
   - Project mentoring; Parateam; technical & scientific reviews

2. **Code Clinics**
   - Short visits to JSC: hands-on performance checks & tuning

3. **Training workshops**:
   - 1st Porting Workshop, June 2010; Heraeus Summer School, Sept 2010
   - CECAM Workshops: September 2011, March & Sept 2012
   - BlueGene/Q Workshop, February 2013

4. **Advanced application support**
   - http://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/2ndSupportCall
   - Source-code tuning, redesign, refactoring, scaling

5. **Research cooperations**
   - Research groups: FZJ, JARA, DE, EU, RoW
   - 3rd party projects; HGF, BMBF, DFG, EU, G8
   - Exascale labs EIC, ECL, Nvidia – ***co-design***

Advanced Support Pilot Project 2010/11

- 1st Call issued October 2010
- SimLabs involved:
    - Biology
    - Molecular Systems
    - Plasma Physics
    - Climate Research
- 23 applications; 18 accepted (~ 4 per SimLab)
- Report:

http://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/2ndSupportCall/1stSupportCallReport.pdf

Support highlight: seeking finite-time singularities in CFD with *racoon* (U. Bochum)

- Scaling enhancement: 2 racks ⇨ 32 racks on BG/P: increase in resolution leads to *transformative advance in physical insight*

multigrid solver @ 131072 cores BG/P
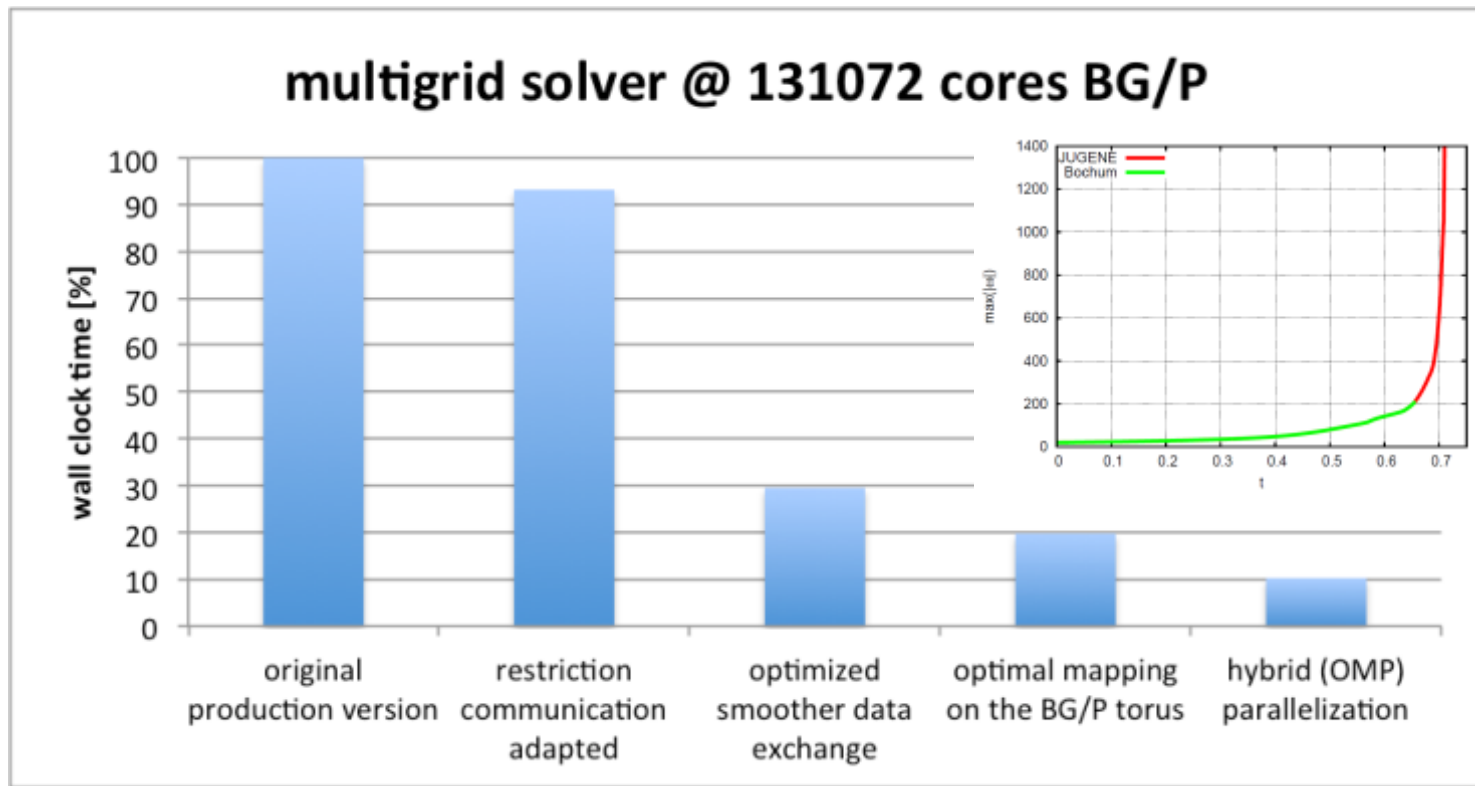
Re-engineering IBIsCO to study surface properties of polymers (TU Darmstadt)
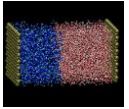
Viorel Chihaia, Rene Halver

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

Advanced Support Initiative: lessons learned
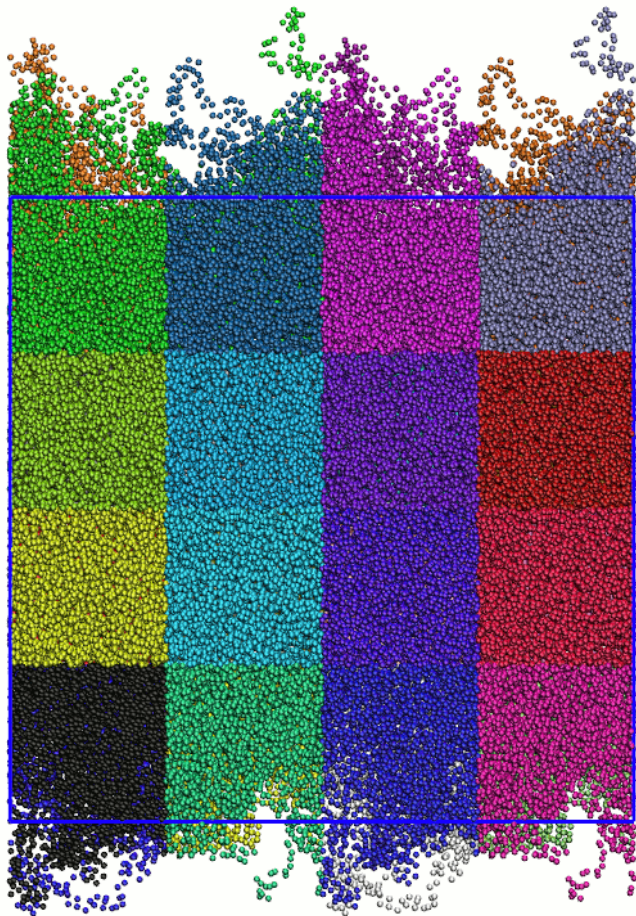
Outcomes:

- 1-2 PMs effort (from JSC) per proposal; variable in-kind
- Enhanced scaling in 50% of apps
- Follow-ups: i) proposals for computing time ii) 3rd-party projects iii) joint publications
- Report available here:

http://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/2ndSupportCall

Conclusions:

- Better project vetting to sift out non-starters
- Closer connection to established NIC/VSR projects
- Selected ‚priority' projects (6PMs) to encourage joint dissemination

SimLab Activities

1. **NIC/VSR advisory**
    - Project mentoring; Parateam; technical & scientific reviews
2. **Code Clinics**
    - Short visits to JSC: hands-on performance checks & tuning
3. **Training workshops**:
    - 1st Porting Workshop, June 2010; Heraeus Summer School, Sept 2010
   - CECAM Workshops: September 2011, March & Sept 2012
4. **Advanced application support**
    - http://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/2ndSupportCall
    - Source-code tuning, redesign, refactoring, scaling
5. **Research cooperations**
    - Research groups: FZJ, JARA, DE, EU, RoW
    - 3rd party projects; HGF, BMBF, DFG, EU, G8
    - Exascale labs EIC, ECL, Nvidia – ***co-design***
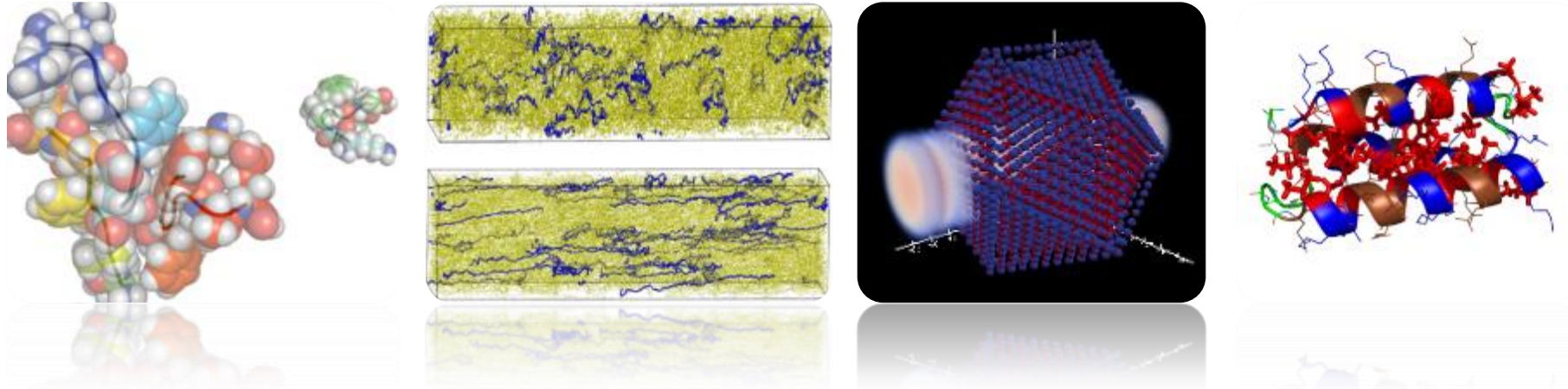
ScaFaCoS: BMBF project 2009-2012
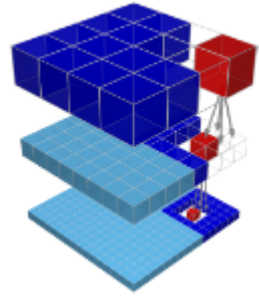
- Fast Electrostatics Library

  - 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
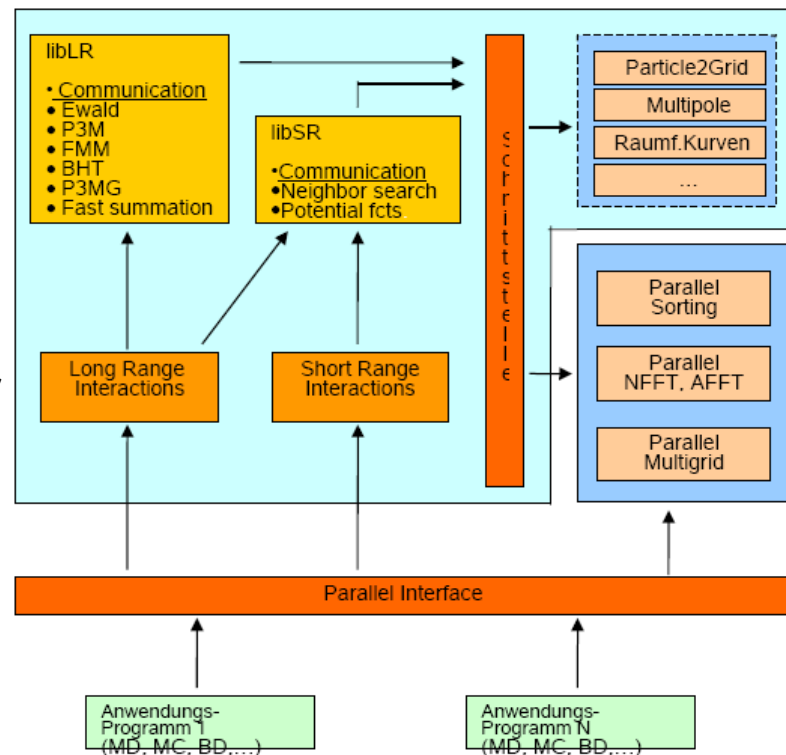
Exascale Lab support

- JSC contributions:
  - Tools: Scalasca
  - Applications: SMMP, MP2C, PEPC, ProFASI
- JSC (SimLab) participants:
  - Dirk Broemmel, Thomas Fieseler, Paul Gibbon, Rene Halver, Daniel Lorenz, Jan Meinke, Sandipan Mohanty, Bernd Mohr, Annika Schiller, Mark Schlütter, Godehard Sutmann, Olav Zimmermann

Scalability of JSC Codes on JUGENE (BG/P)

- **Quantum Computing Simulator**

  42 Qbits on 262,144 cores

- **Tree code PEPC**

  2 billion particles + load-balancing on 294,912 cores

- **Fast Multipole Method**

  3 011 561 968 121 particles on 294,912 cores;
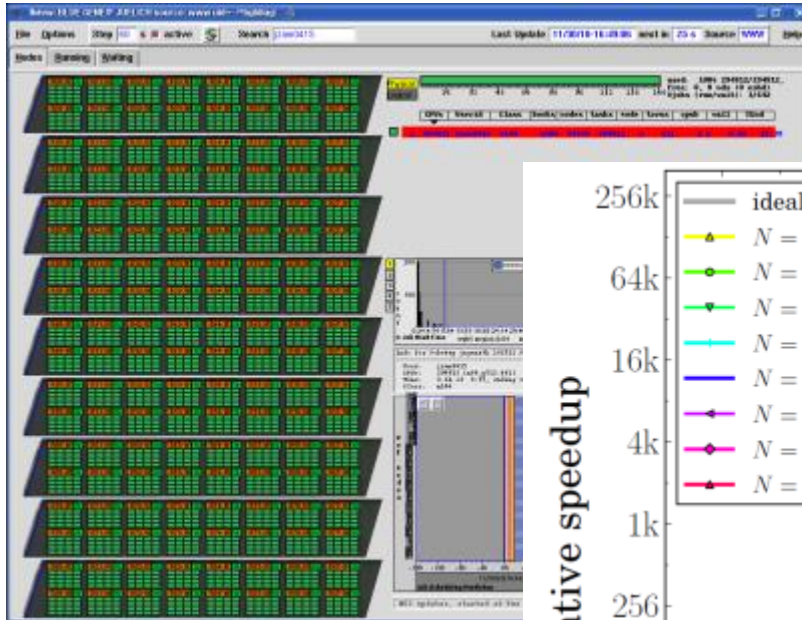
  44.16 bytes/particle; runtime: 715s

- **MD code MP2C**
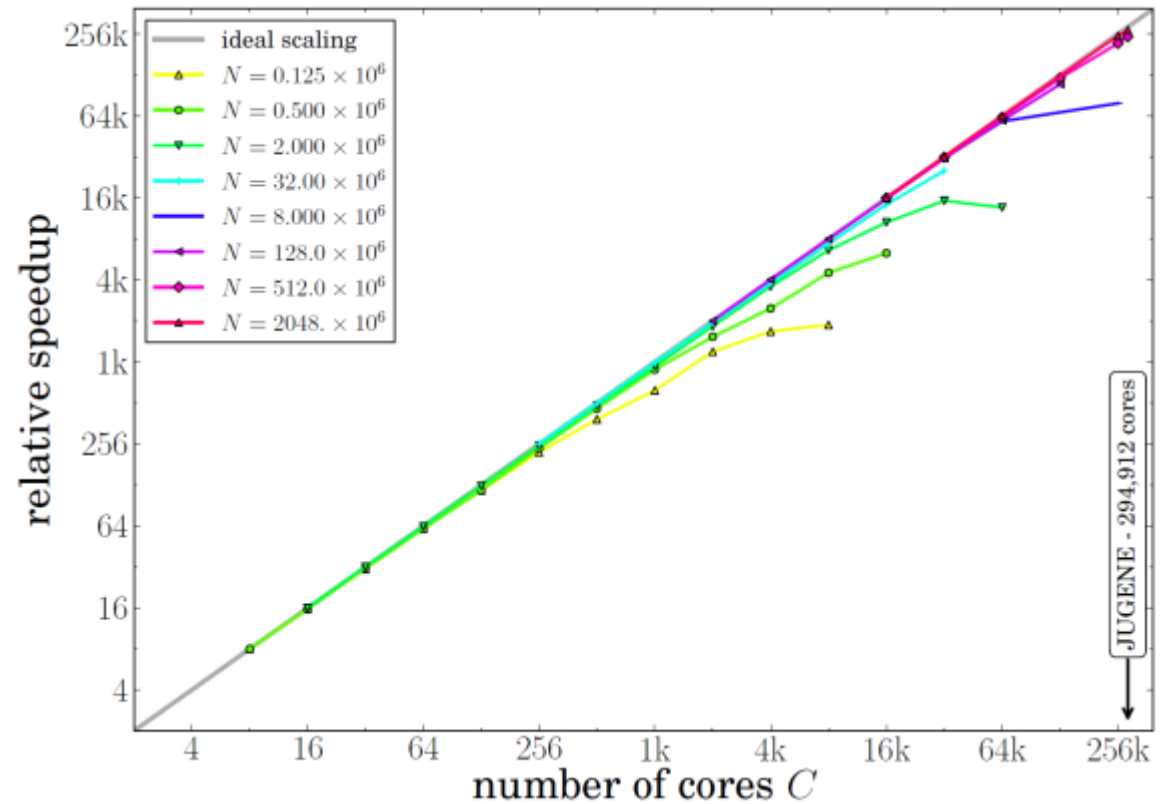
  Full scalability on 294,912 cores

- **HMC-QCD**

  342 TFlop/s (38% peak) on 294,912 cores

Scaling things up: tree code world record (2010)

2x10^9 particles on 294 912 tasks of BlueGene/P, load-balanced

M. Winkel et al., Comp. Phys. Commun. **187**, 880 (2012)

Simulation Labs: Action items 2012/13

- Sept. 2012: Open call for advanced support:
http://www.fz-juelich.de/ias/jsc/EN/Expertise/SimLab/2ndSupportCall

- Feb. 2013: BG/Q porting workshop 2012/13

- Sept. 2013: CECAM Tutorial on Fast Coulomb Algorithms

- Engagement with Exascale projects

Extending the SimLab Blueprint

- **JARA-HPC**:
  - Fluid & Solid Engineering
  - Ab Initio Methods in Physics & Chemistry
  - Terrestrial Systems (Geoverbund ABC/J)

- **Helmholtz Association**:
  - Climate Science/Earth & Environment + KIT
  - Neuroscience: Bernstein Facility (new SL > 1/2013)
  - HSL: white paper on 16 potential SimLabs in HGF ⇨ PoF III