JÜLICH
FORSCHUNGSZENTRUM

Simulation Laboratories at JSC

Paul Gibbon

Jülich Supercomputing Centre

Jülich Supercomputing Centre

Supercomputer operation for

- Centre – FZJ
- Regional – JARA
- Helmholtz & National – NIC, GCS
- Europe – PRACE, EU communities

Application support

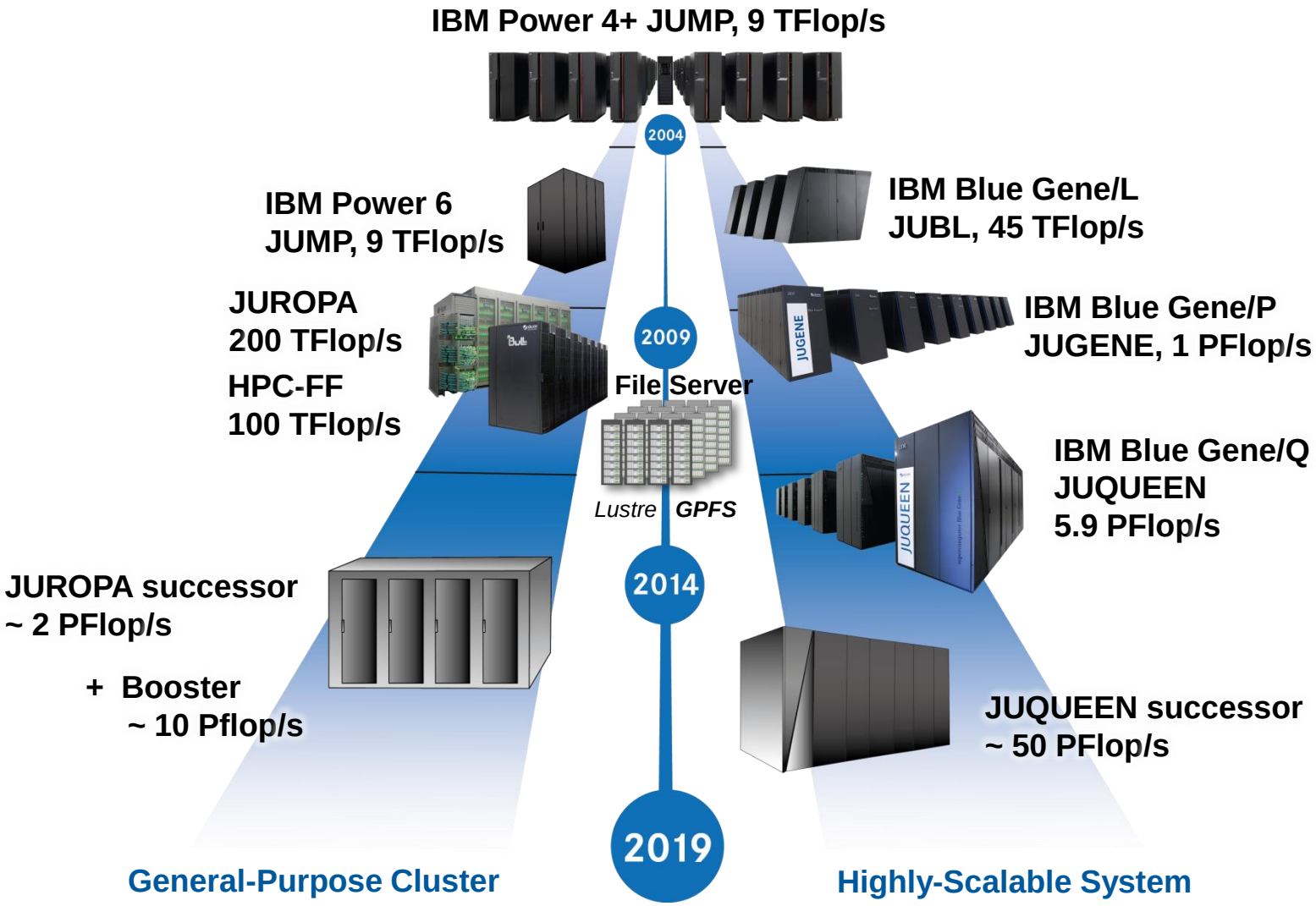
- **SimLabs**
- **Cross Sectional Groups**
- Peer review coordination

R&D work

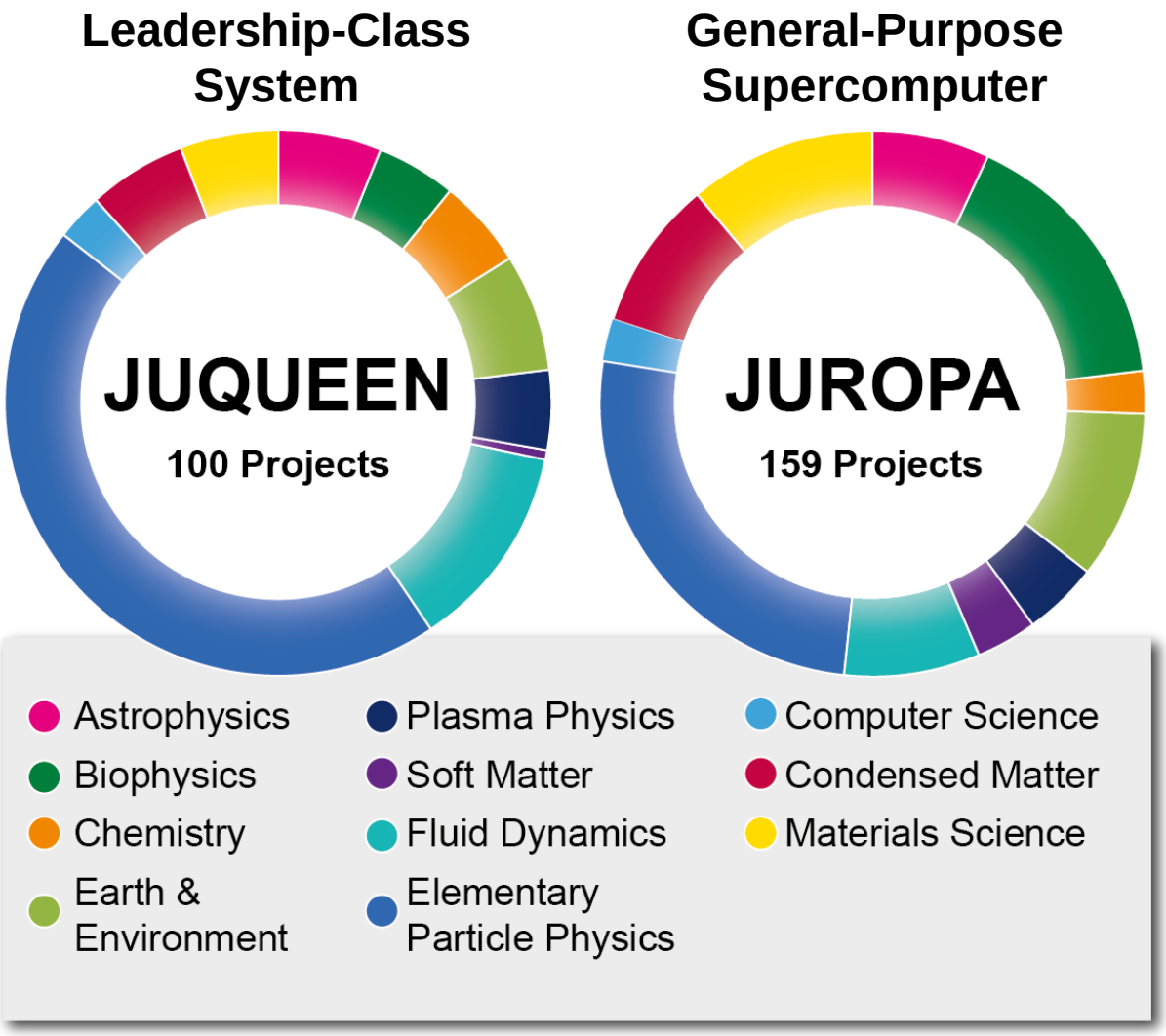
- Algorithms, performance analysis and tools
- Community data management service
- Novel computer architectures:
- Exascale Laboratories: EIC (IBM), ECL (Intel), NVIDIA

Education and Training

HPC Systems: Dual Architecture Strategy

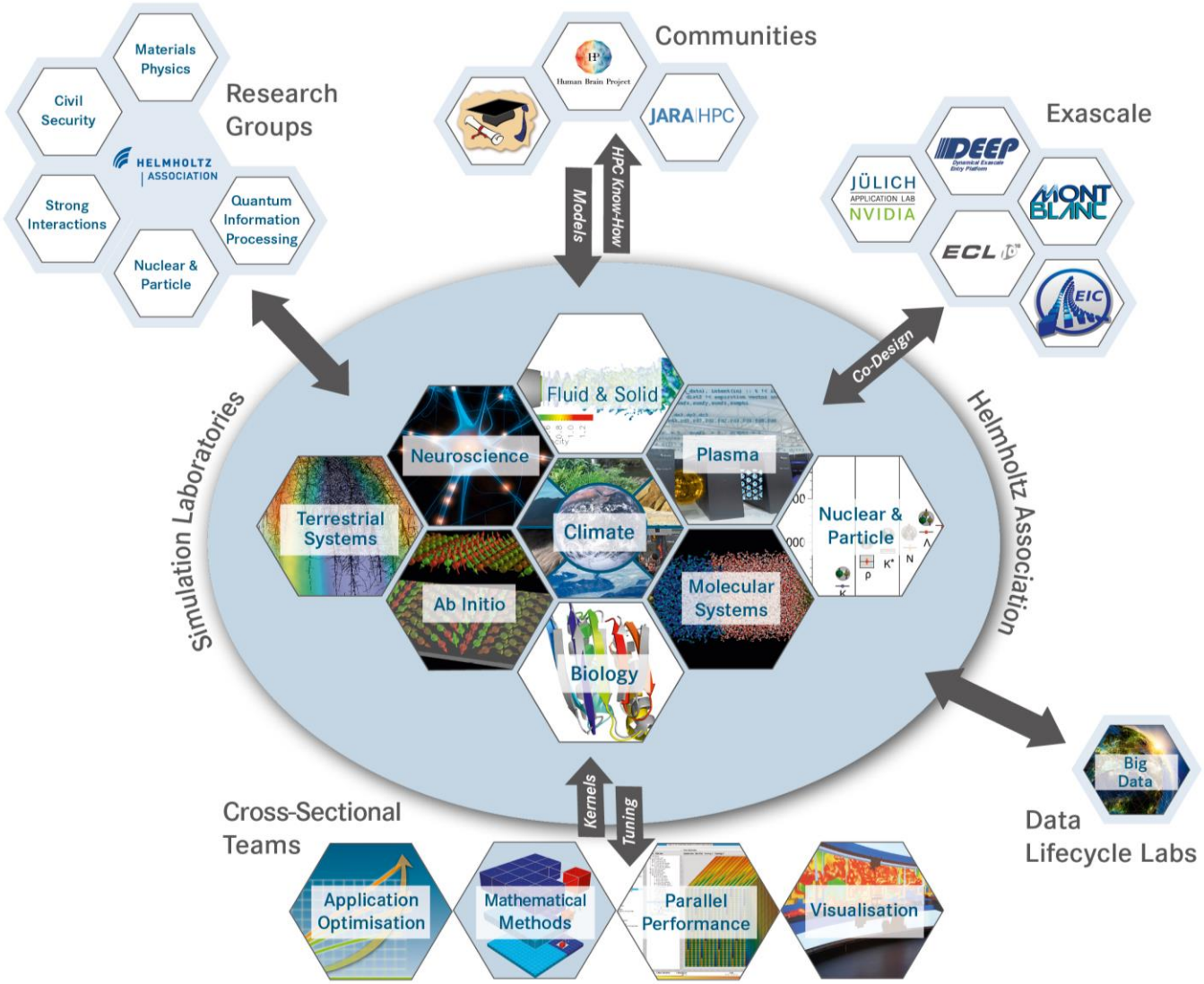


Research Fields of Current National Projects



Granting periods
11/2014 – 10/2015
05/2014 – 04/2015

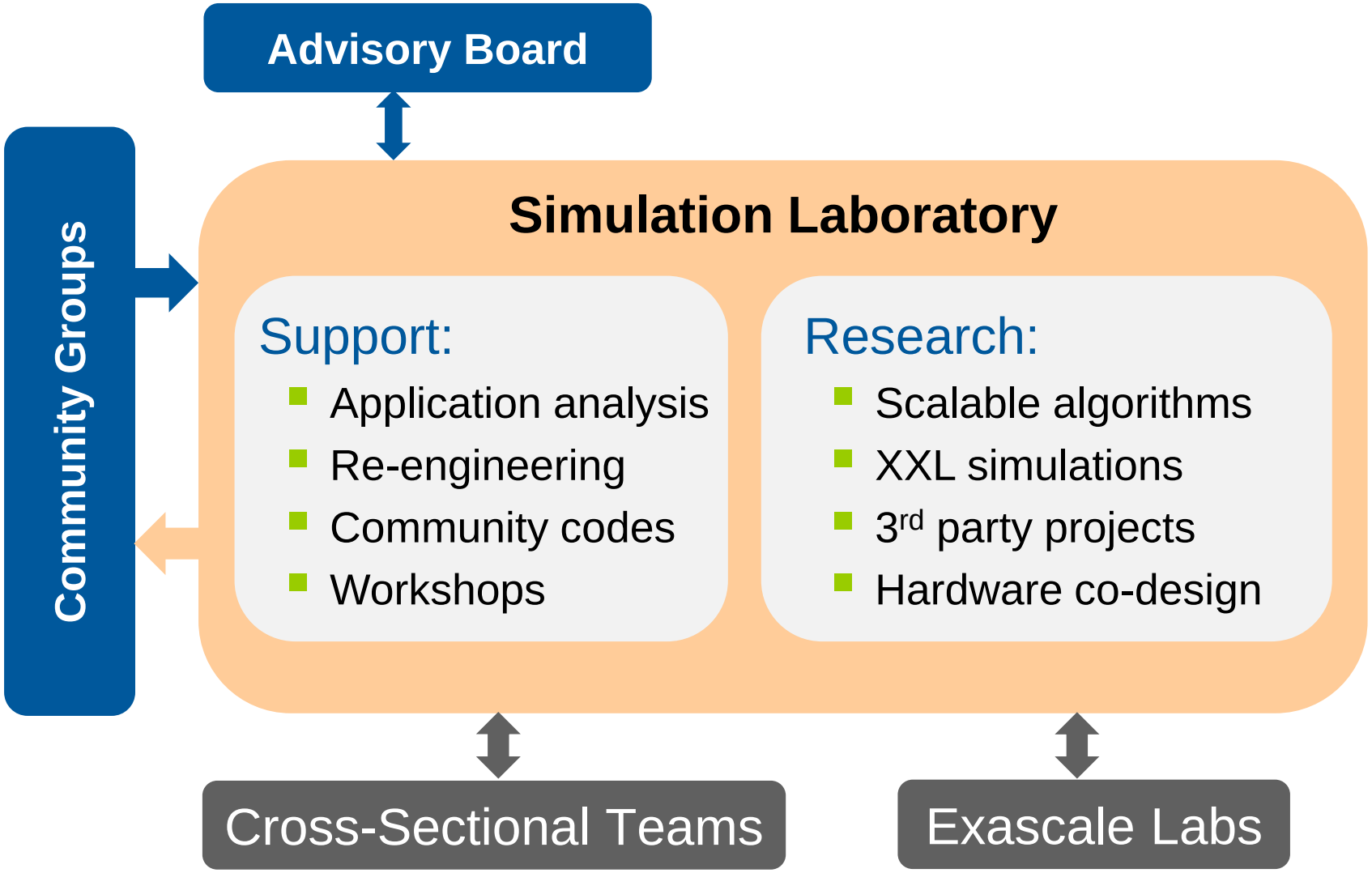
Domain-specific User Support and Research



Jülich Simulation Laboratory Concept

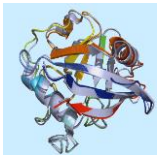
- **Staff (4-8 members)**
  - Senior scientist *recruited from field*
  - 1-2 postdocs + technical staff (informatics)
  - Jointly supervised PhD & MSc students
- **Support**
  - Porting & tuning (integral part of application advisory)
  - Algorithm scaling; code clinics (day-visits)
  - Workshops (BG/Q); schools (CECAM)
- **Research**
  - Common/generic methods
  - Scalable algorithms
  - 3rd party projects: FZJ, JARA, DFG, BMBF, EU, G8

The Simulation Laboratory as HPC Enabler



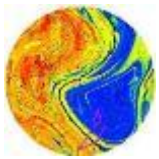
Active Simulation Labs @ JSC

Biology





Climate Science



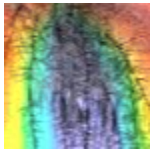



Molecular Systems

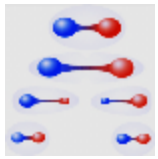




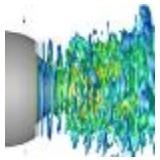

Terrestrial Systems



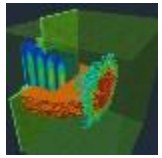

Nuclear & Particle




Fluid & Solid Eng.




Plasma Physics

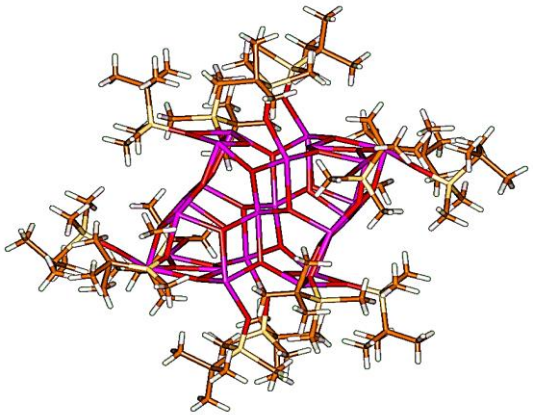



Ab Initio




Simulation Laboratory *Molecular Systems*

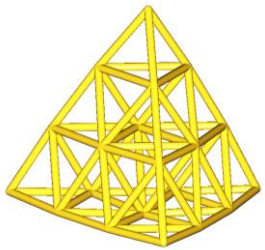
- TURBOMOLE: Parallel two-component DFT for large molecular clusters containing heavy elements [jointly implemented into



$[Bi_{22}O_{26}(OSiMe_2tBu)_{14}]$

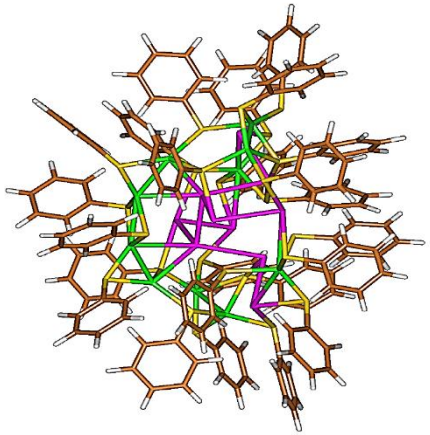
370 atoms, 3876 bfn
DHF-SVP-2c/BP86

realistic molecular transition metal clusters accessible on general purpose systems such as JUROPA



$[Au_{20}]^-$

20 atoms, 1400 bfn
DHF-TZVP-2c/TPSS

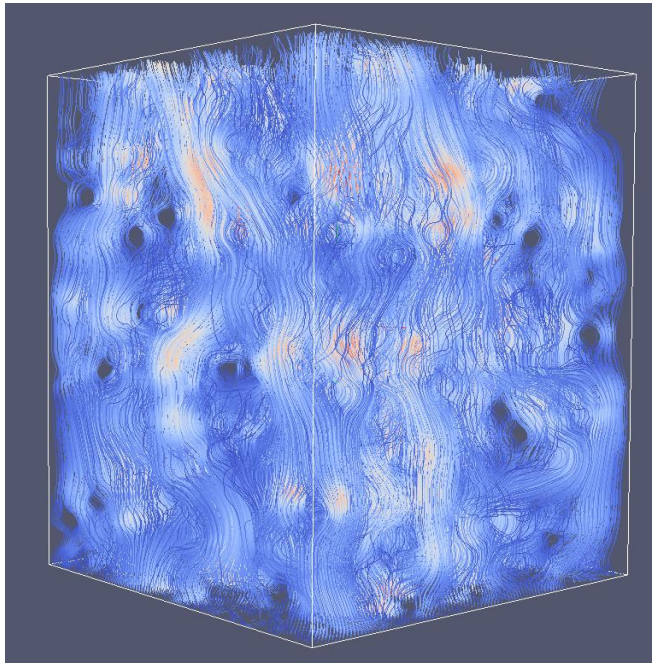


$Bi_{10}Cu_{10}(SPh)_{24}]^{2-}$

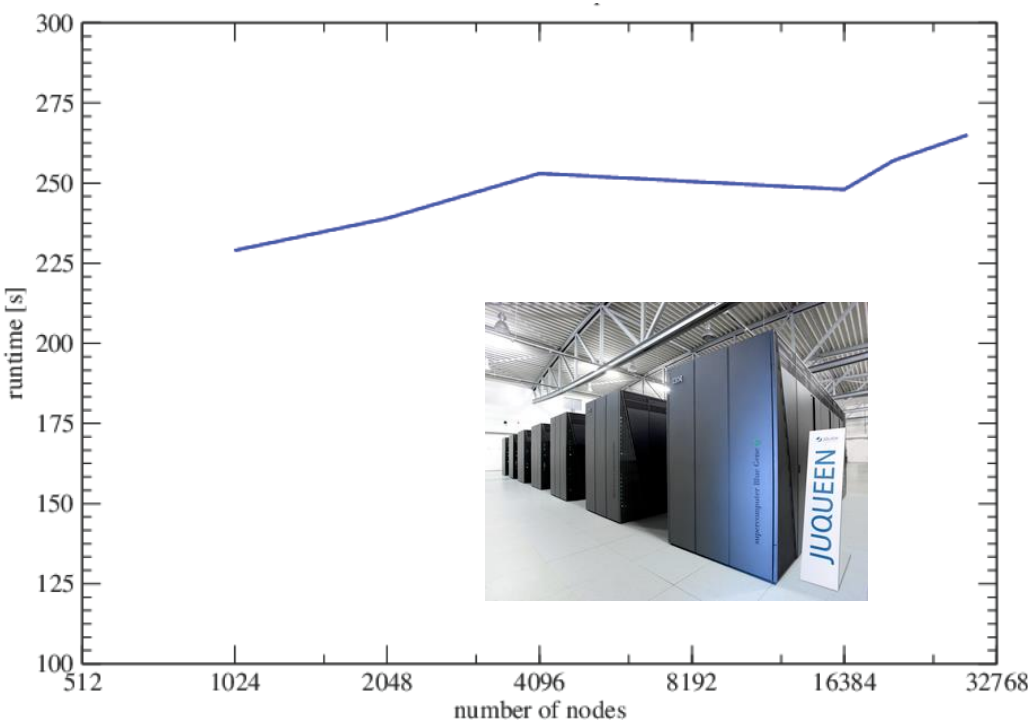
308 atoms,7162 bfn
DHF-TZVP-2c/BP86

Simulation Laboratory *Molecular Systems*

- MP2C: particle-based hydrodynamics

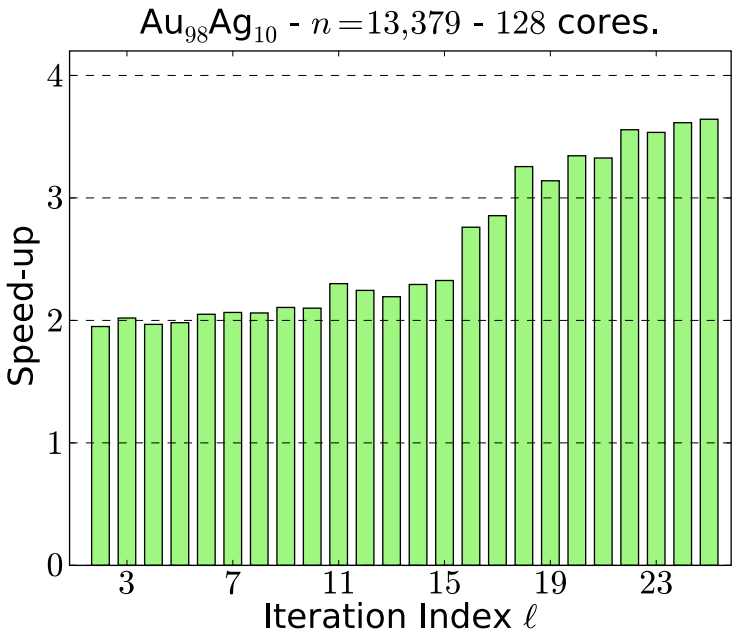


- Flow field in a gas diffusion membrane
- With stochastic geometry

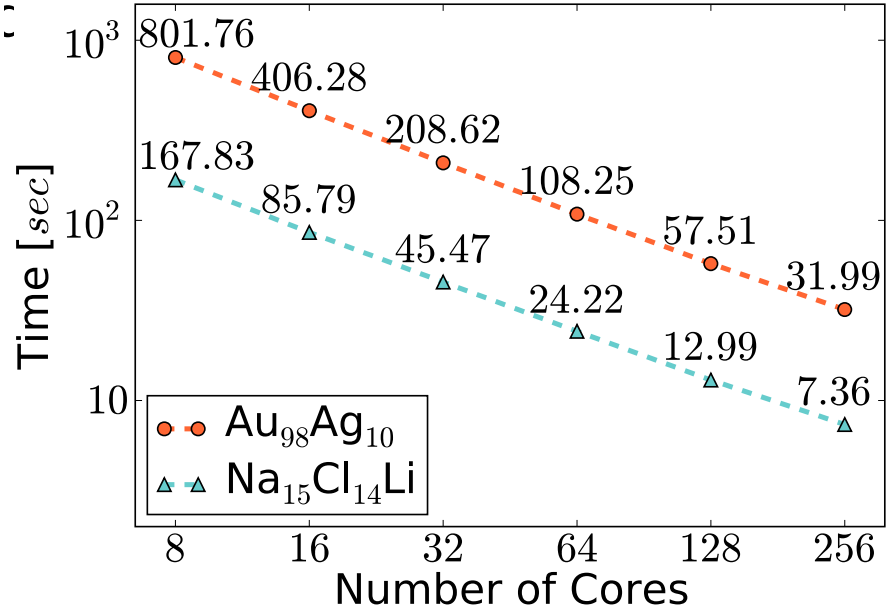


- Weak scaling on full JUQUEEN

Simulation Laboratory *ab initio Methods*



Speed-up when inputing the eigensolver approximate solutions vs random vectors



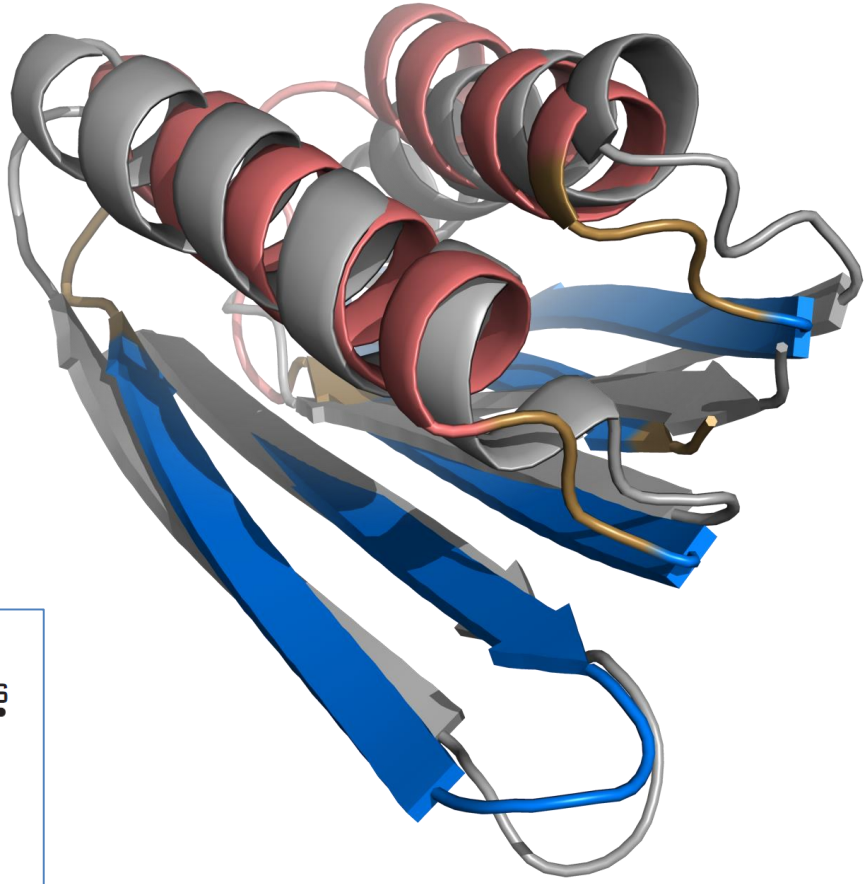
Strong scalability on Juropa showing the potential for simulating larger crystals

SL *Biology*: protein folding highlight

results

- 92-residue
- complex topology
- Estimated folding time: few ms
- ProFASi w. parallel tempering
- 32 independent simulations
- Free energy minimum at 3.5 Å
- ~ 19.000 CPU-h/folding event

- Experimental folding time: 1 s



PROTEINS
STRUCTURE | FUNCTION | BIOINFORMATICS

Folding of Top7 in unbiased all-atom Monte Carlo simulations

Sandipan Mohanty,* Jan H. Meinke, and Olav Zimmermann

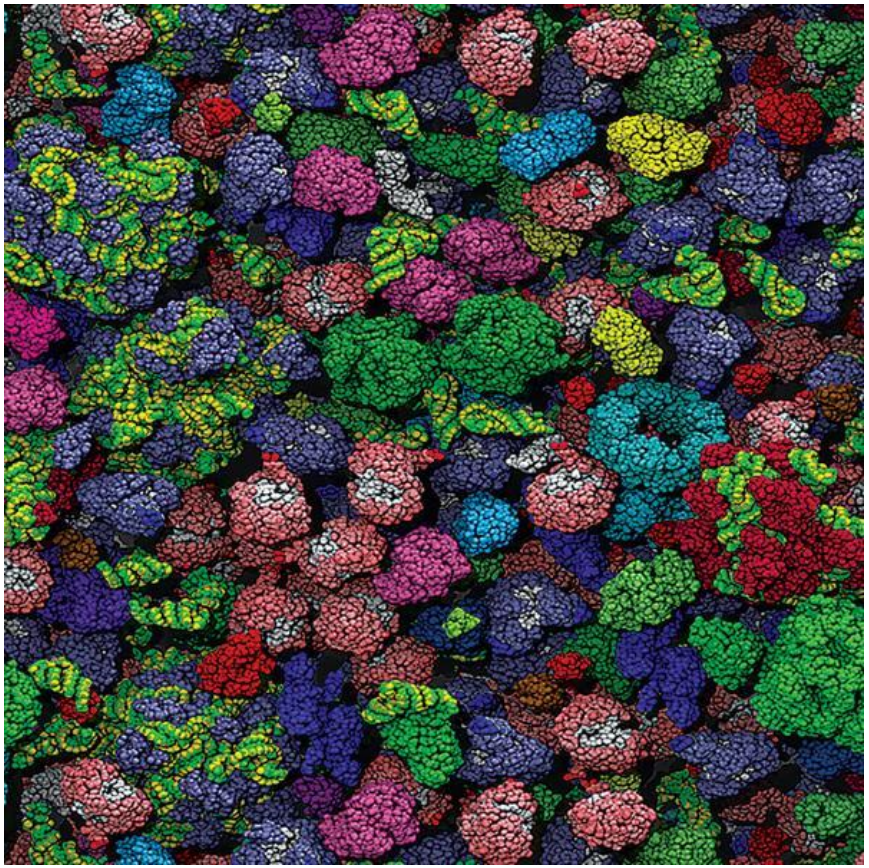
Jülich Supercomputing Centre, Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

SL Biology: whole cell simulation

BMBF project

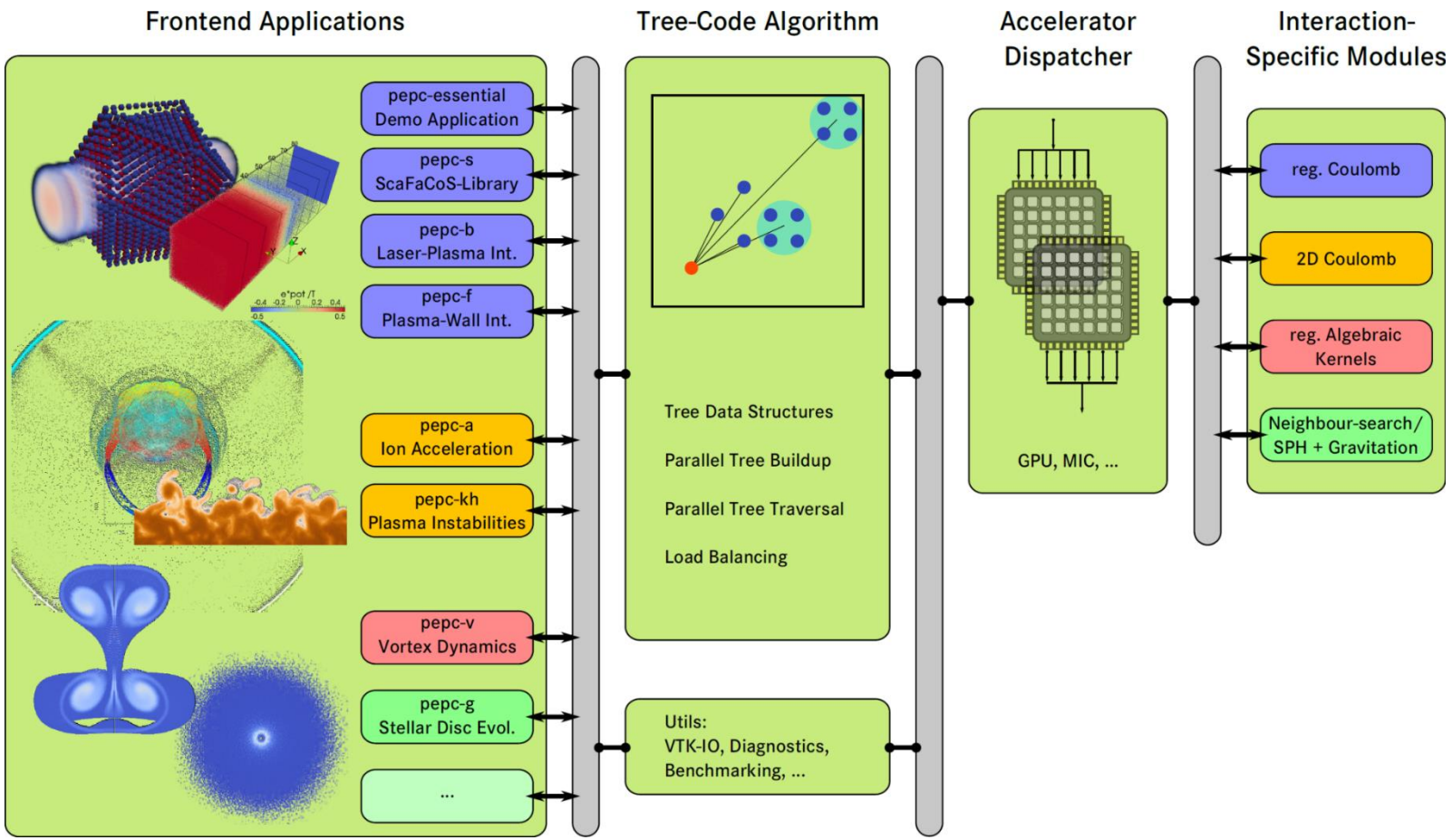
- PI: Eric v. Lieres (IBG-1)
- PostDoc: Slavko Kondrat
- Multiscale simulation
- Combining BD + CA +PDE

- Main focus:
- What quantitative effect has the spatial inhomogeneous distribution of proteins on the metabolic network level
- Challenges: many!!

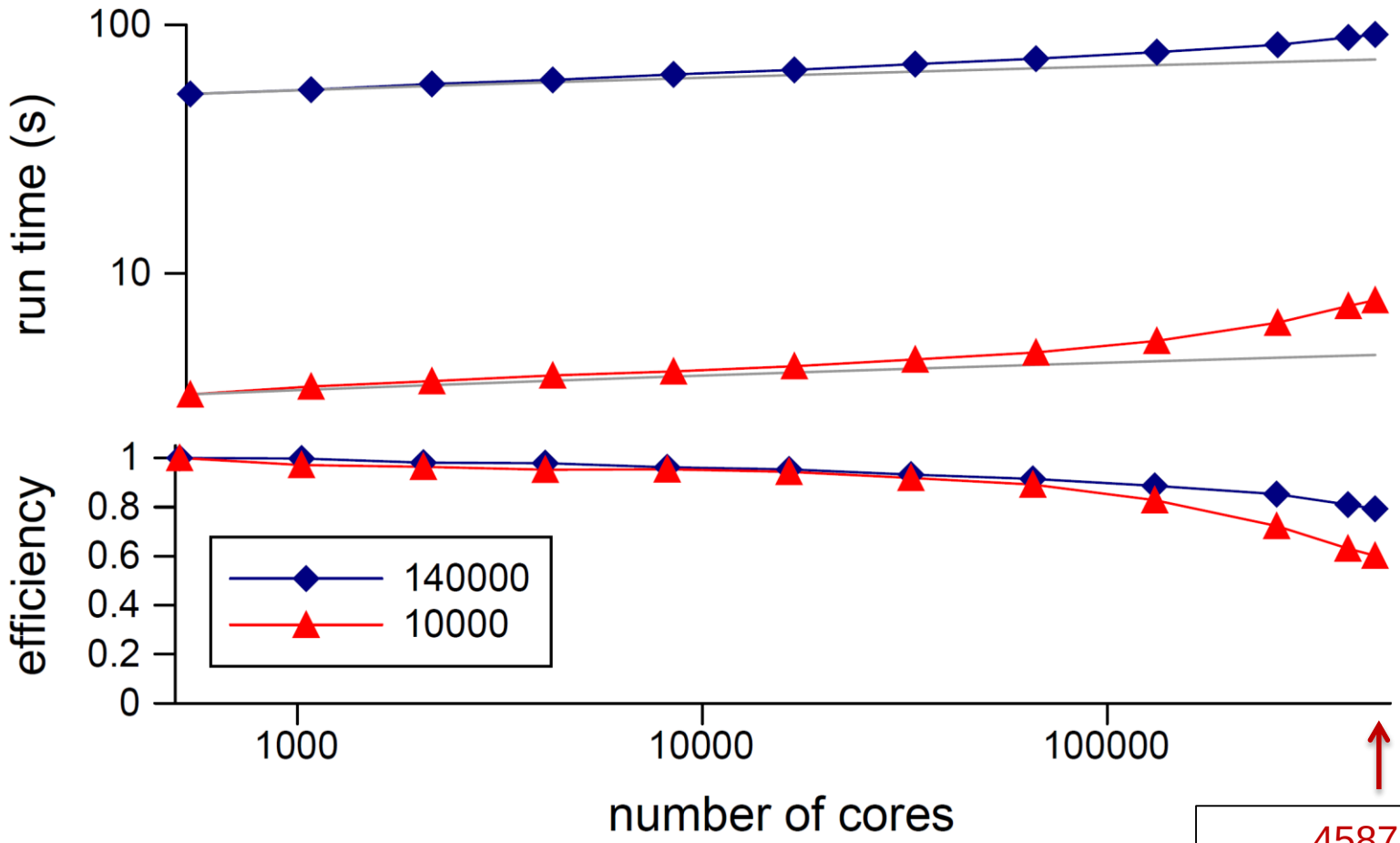


(graphics taken from work of A. Elcock)

SimLab *Plasma Physics*
Parallel tree code development (PEPC)

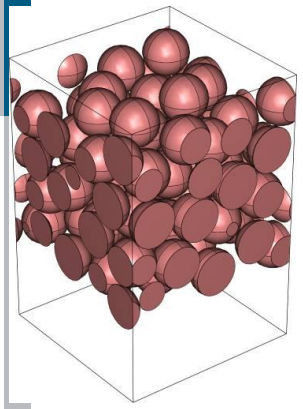


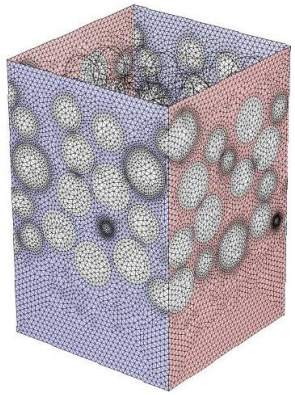
SL *Plasma*: tree-code on JUQUEEN

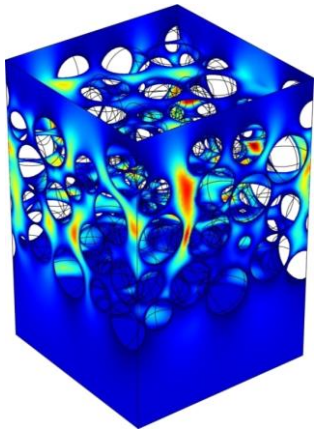


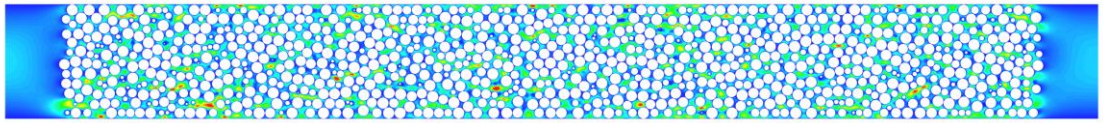
SL *Fluids and Solid Engineering*

- Fluid flow and porous media mixed simulations using FEM.







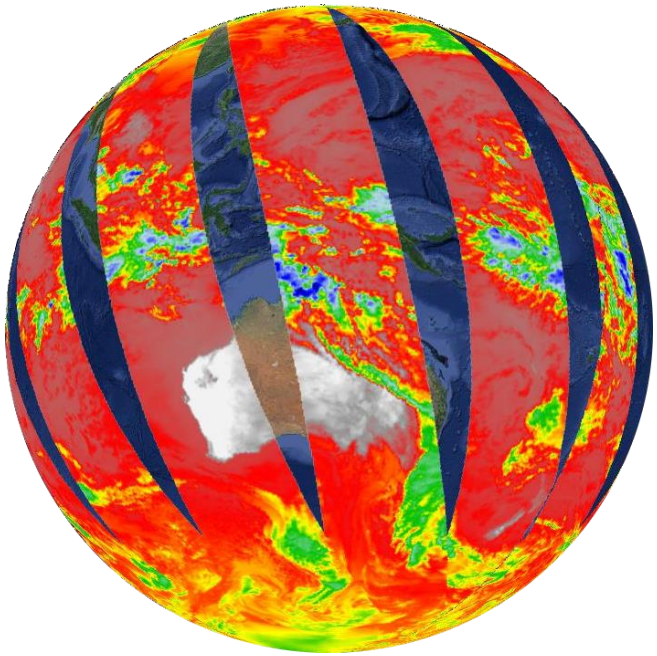


- 2011 Simulations with commercial code COMSOL.
- Largest chromatography simulations with 750 beads take **days**.

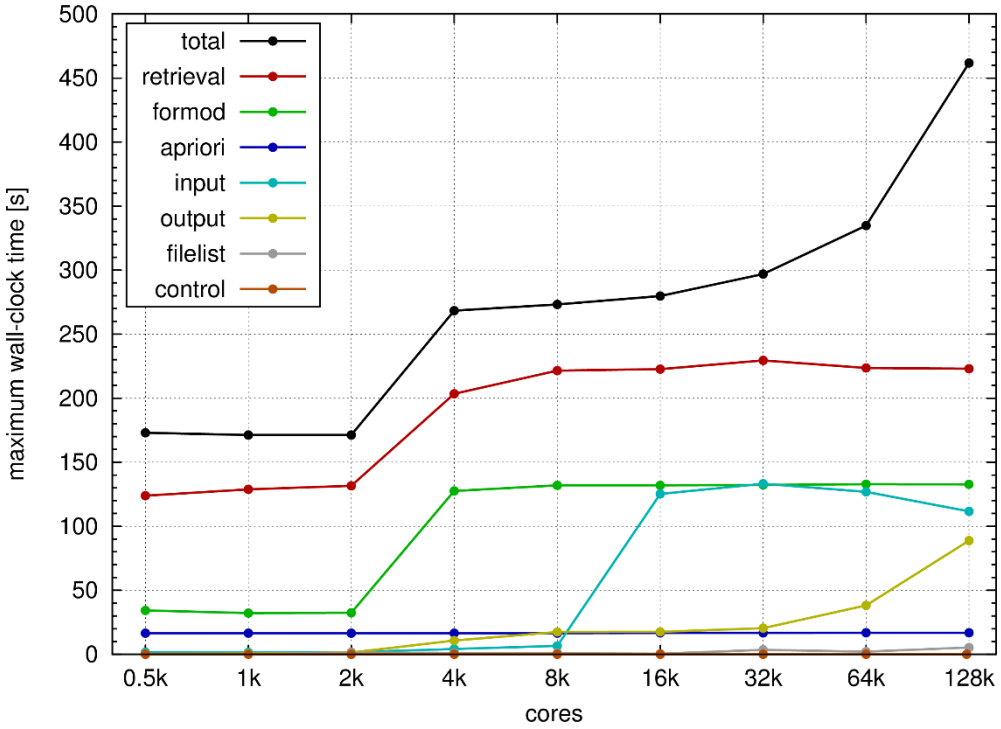
- 2013 Modelling with with RWTH/JSC research code XNS.
- Simulation up with 7681 beads can be done easily in under one hour on 4096 cores of JUQUEEN.
- GOAL: full-sized columns with millions of beads

Simulation Laboratory Climate Science: Highlight

- JURASSIC: fast infrared radiative transfer calculations



- AIRS/Aqua satellite observation
  - of atmospheric composition



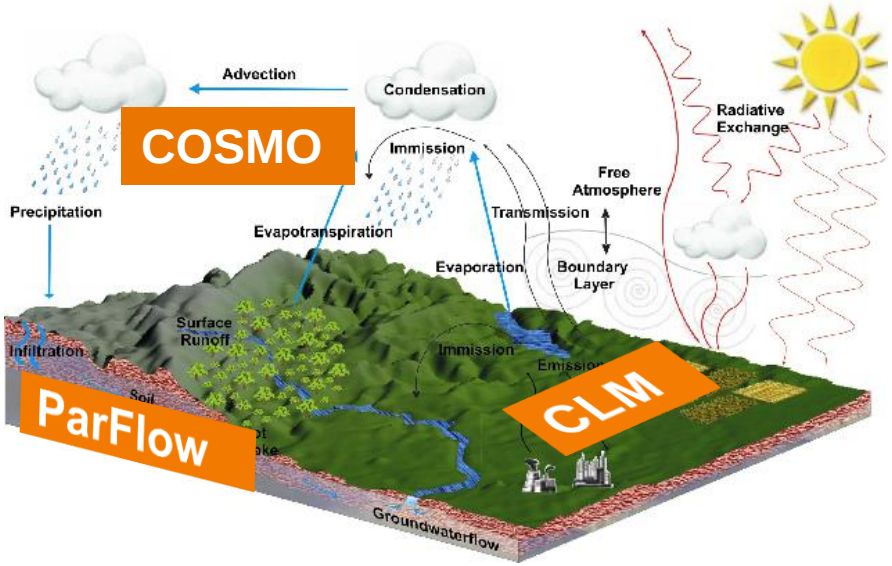
- Weak scaling of AIRS temperature retrieval
  - with JURASSIC on JUQUEEN

Simulation Lab *Terrestrial Systems*

Klaus Görgen, Stefan Kollet

TerrSysMP:

- Fully integrated groundwater-vegetation-atmosphere simulation platform; earth system models at regional scale
- Water cycle processes and variability across scales



use impacts

- Scalasca performance analysis
- Refactoring of OASIS-MCT coupling interface to remove scaling bottleneck
- Scaling now to 32k cores:
  64x increased problem size!

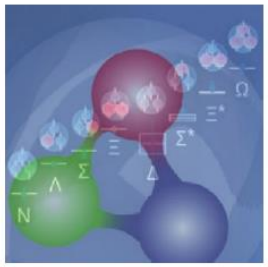
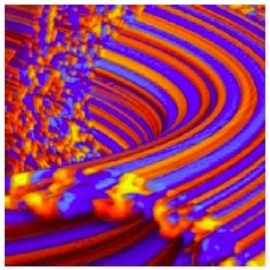
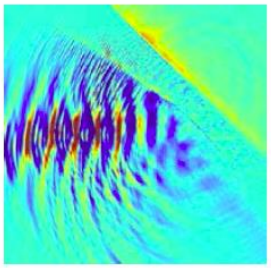
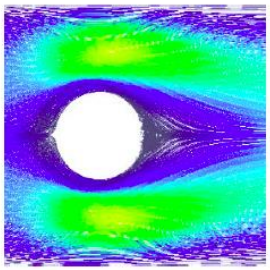
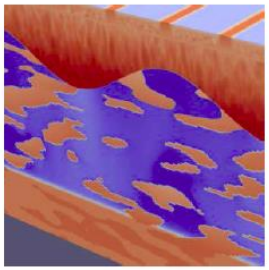
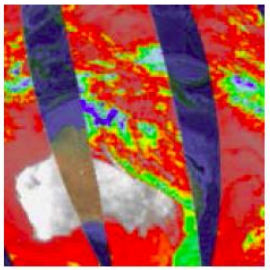
HPSC TerrSys

A B C/J geoverbund aachen bonn köln jülich

High-Q Club: Exascale-Ready Applications on JUQUEEN

JÜLICH FORSCHUNGSZENTRUM

HiQ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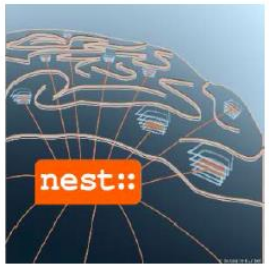	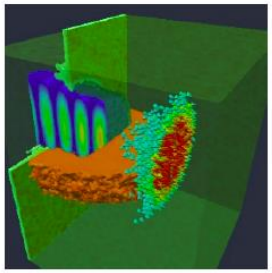	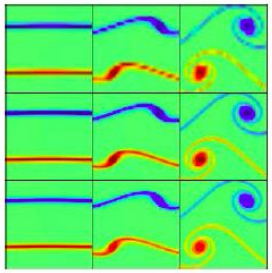	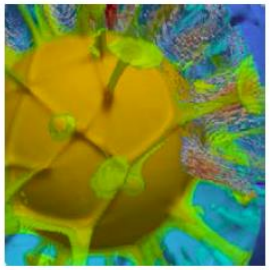	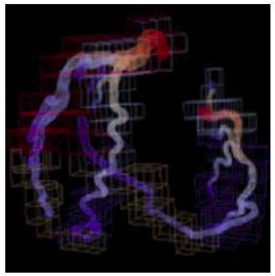	
NEST	PEPC	PMG+PFASST	TerraNeo	WaLBerla	OpenTBL

12+ codes scaling across 458,752 JUQUEEN cores

WWW: http://www.fz-juelich.de/ias/jsc/EN/Expertise/High-Q-Club/_node.html