JÜLICH
FORSCHUNGSZENTRUM

High Performance Computing Infrastructure at JSC

Paul Gibbon

Jülich Supercomputing Centre

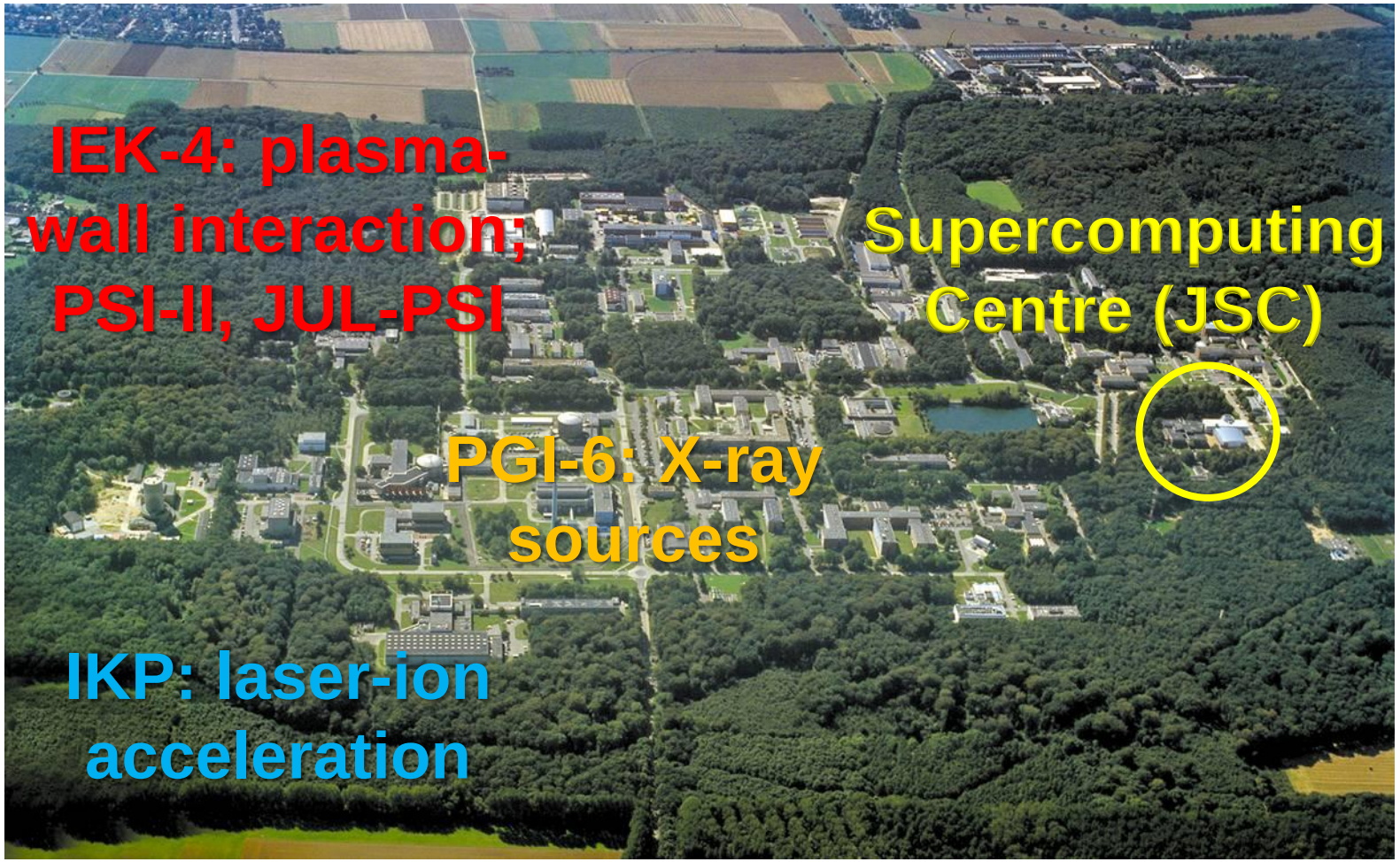
HELMHOLTZ
ASSOCIATION

Mission:

- Energy
- Climate
- Transport
- Health
- Key Technologies

FZ-Juelich:
5500 staff
2000 scientists
800 PhD students
Budget: 500M€

Plasma physics activity in Jülich



Jülich Supercomputing Centre

150 staff + 50 third party

Supercomputer operation for:

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

Application support

- Primary support & Simulation Labs
- Peer review support & coordination

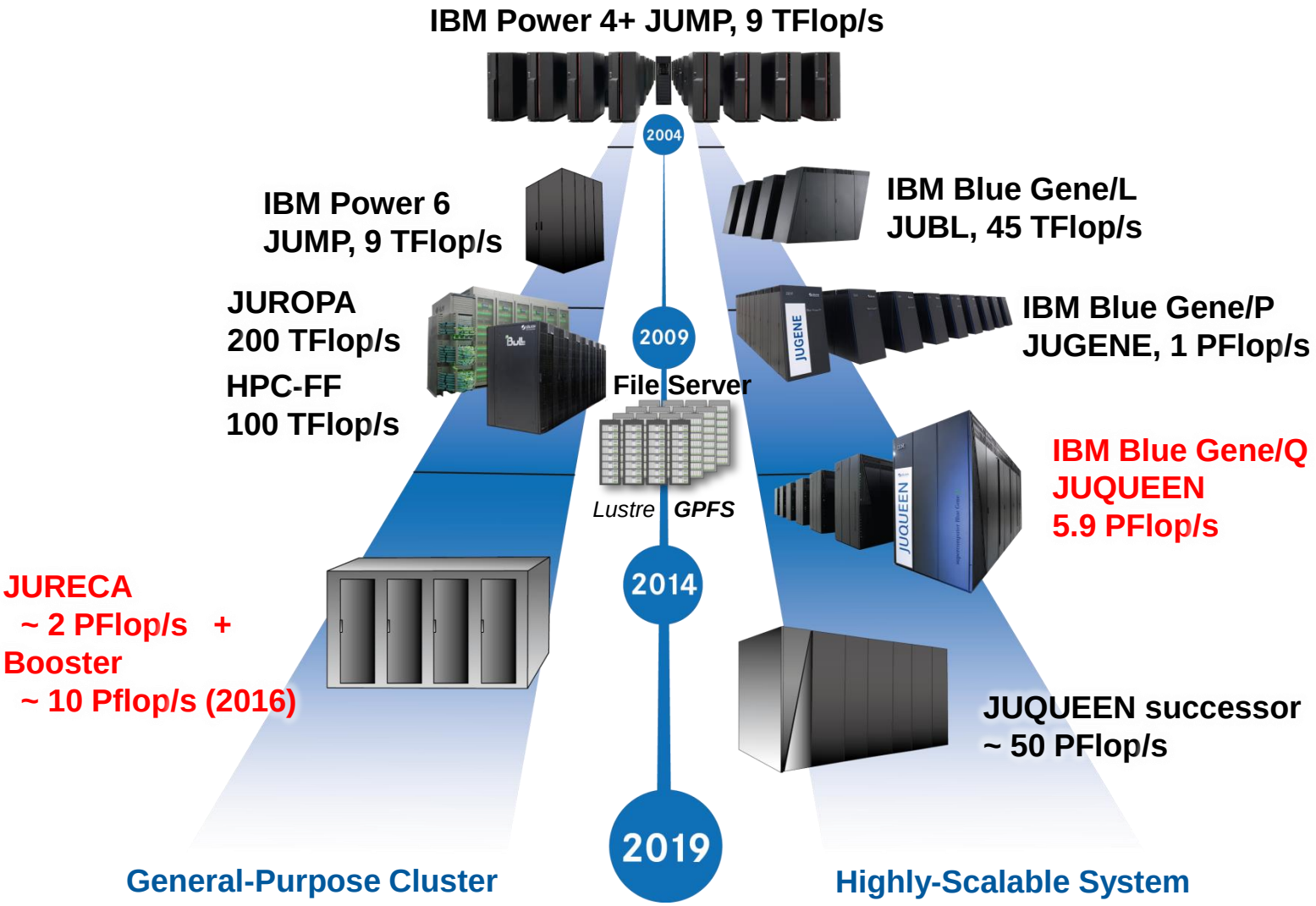
R&D work

- Methods and algorithms, performance tools
- Computer architectures,
  Exascale Laboratories: EIC, ECL, NVIDIA

Education and Training

- BSc, MSc MATSc
- Advanced courses PATC, CECAM

HPC Systems: Dual Architecture Strategy



JUQUEEN: Jülich's Scalable Petaflop System

IBM Blue Gene/Q JUQUEEN

- IBM PowerPC® A2 1.6 GHz,
  16 cores per node
- 28 racks, 458,752 cores
- 5,9 Petaflop/s peak
  5,0 Petaflop/s Linpack
- 448 TByte main memory
- connected to a Global Parallel File System (GPFS) with O(10) PByte online disk and O(50) PByte offline tape capacity
- 5D network
- Production start: Nov 5, 2012

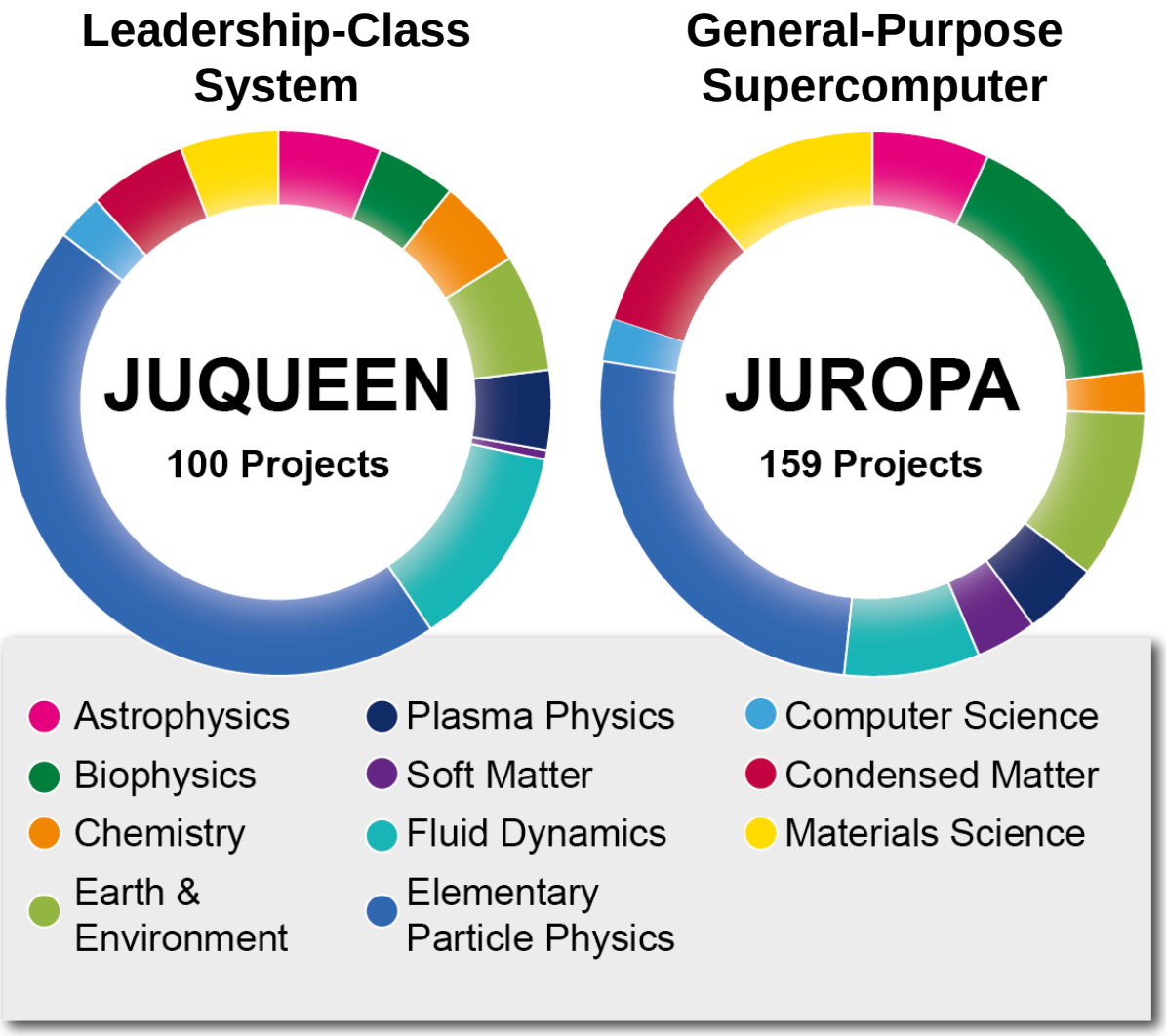
Nov 2014:
#2 in Europe
#8 worldwide
#40 in Green500

JURECA: Jülich Research on Exascale Cluster Architectures

JURECA: Intel, T-Platforms, ParTec

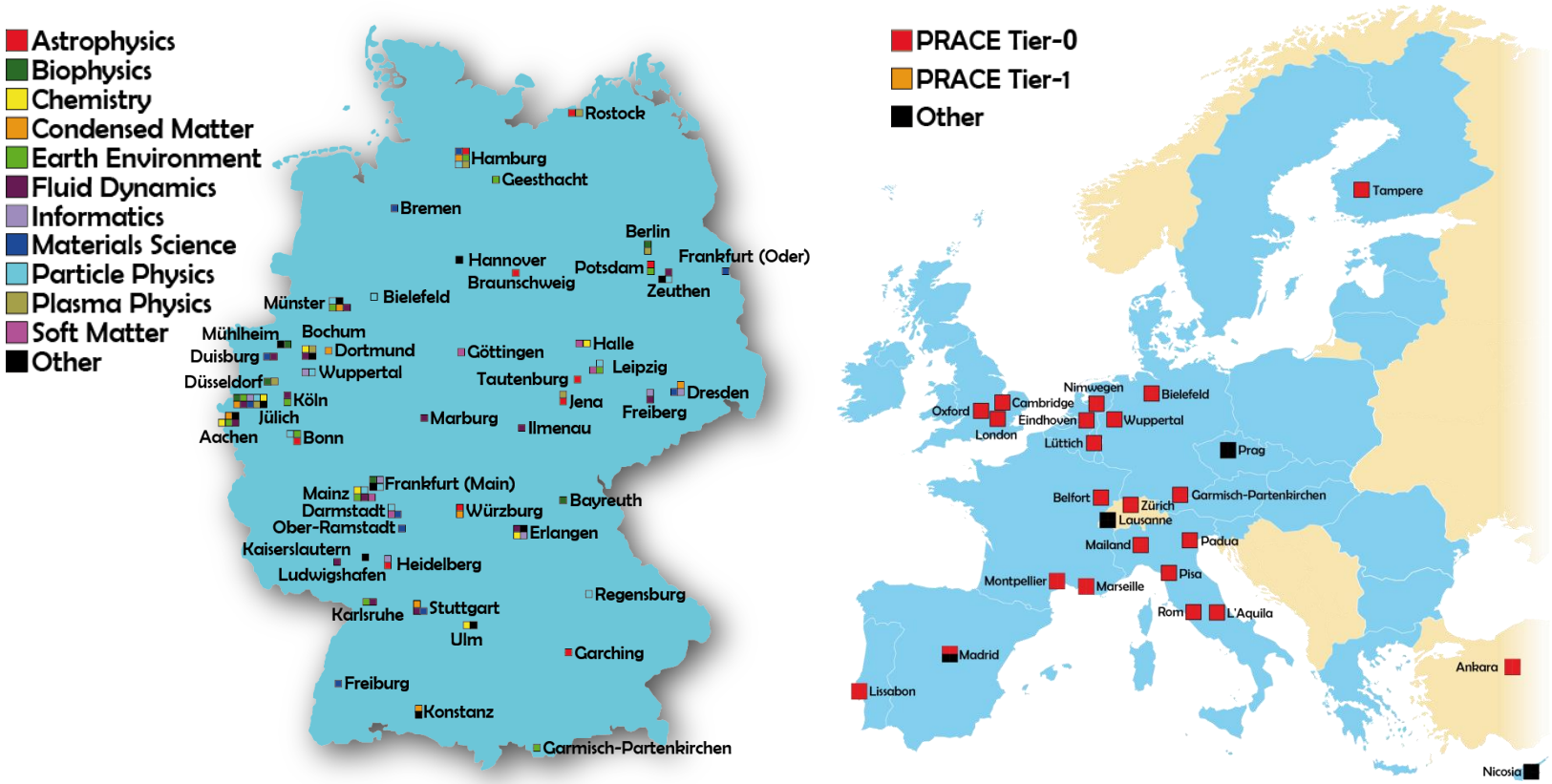
- 2 Intel Haswell CPUs per node
- 2x12 cores @ 2.5 GHz, SMT
- 1,872 compute nodes = 44928 cores
- Memory: 128-512 GB/node
- 12 visualization nodes
- 75 compute nodes with 2xNVIDIA K80 GPUs
- 1.8 (CPU) + 0.44 (GPU) Petaflop/s peak
- Mellanox Infiniband EDR with non-blocking Fat Tree topology
- 100 GB/s storage connection to JUST
- **http://www.fz-juelich.de/ias/jsc/jureca**

Research Fields of Current National Projects



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

National and European User Groups

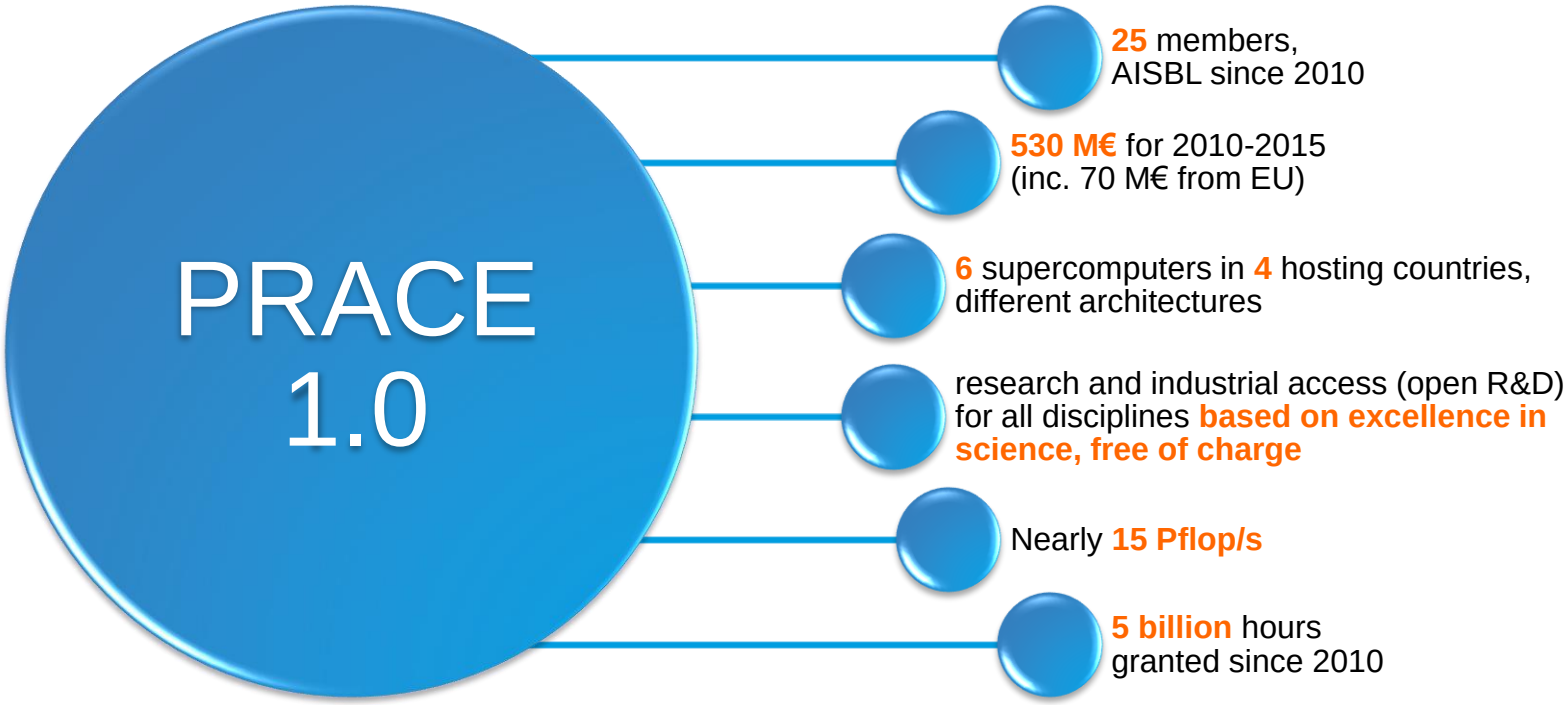


- Proposals for computer time accepted from Germany and Europe
- Peer review by international referees
- CPU time is granted by independent Scientific Councils

Access to Jülich HPC resources

1. PRACE
   - EU-wide access
   - Currently 5 participating facilities
   - Calls 2 x annually
2. GCS/NIC:
   - National projects, but exceptions possible
   - Deadlines 28 Feb or 31 Aug
3. Community access
   - Human Brain Project
   - Fusion (2009-2013)

PRACE - Partnership for Advanced Computing in Europe
The European HPC e-infrastructure (ESFRI)



PRACE 2.0 coming soon ….

Gauss Centre for Supercomputing (GCS)

GCS is the leading Tier-0 HPC centre in Europe

- Alliance of the *three German Tier-1 centres:*
- Jülich Supercomputing Centre (JSC),
- High Performance Computing Centre Stuttgart (HLRS),
- Leibniz Rechenzentrum (LRZ), Garching

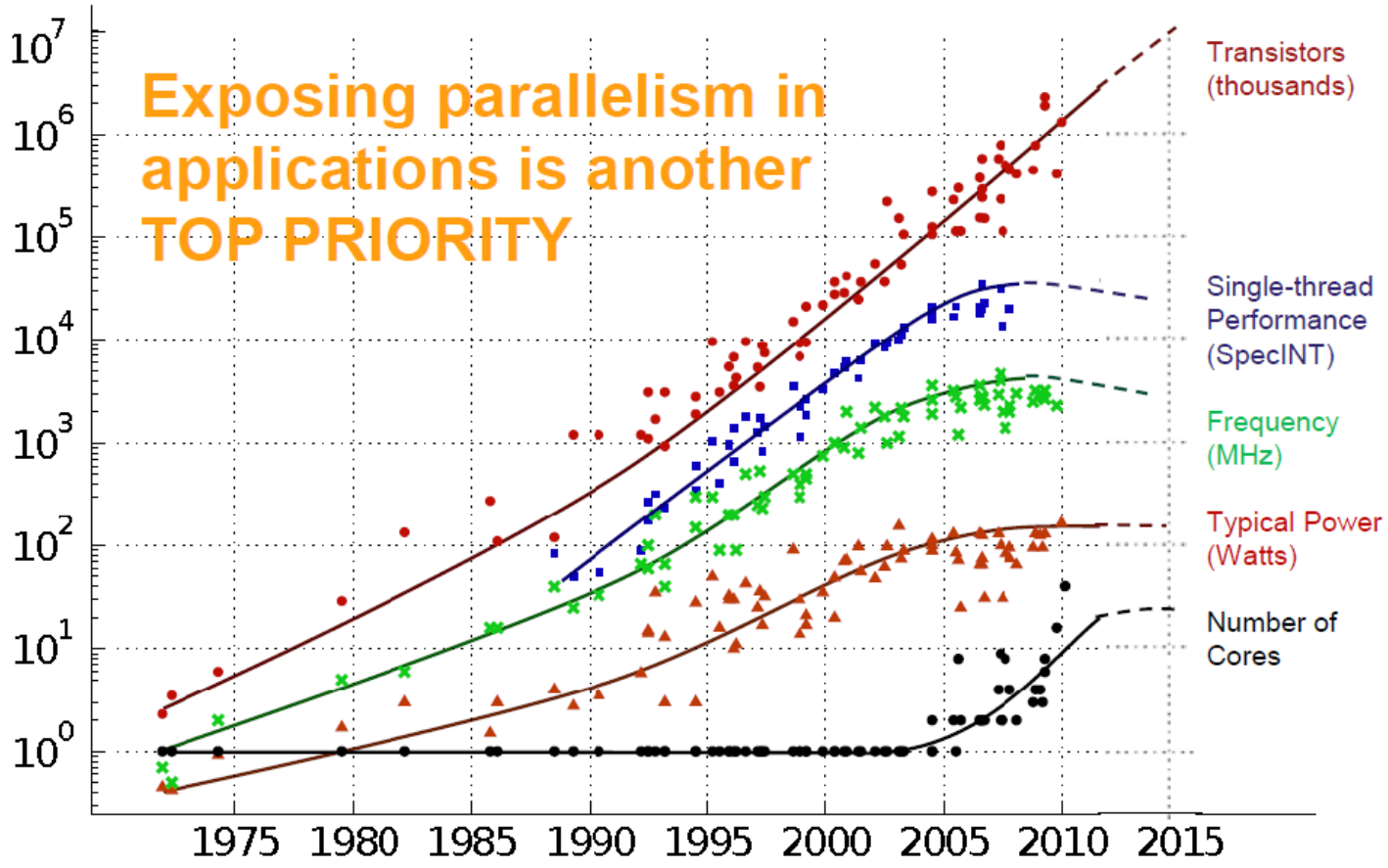
Key Facts

- Since its inception at least two systems in TOP 10
- To date in sum more than 10 Petaflops (continuously expanding)
- 400 people for Operation, HPC-research, Services, Training
- Extensive know-how in key scientific fields

The theoretician's view of HPC…

- Just wait until next year for next processor – it'll be faster.
- I'll keep my code the way it is – the next compiler will be smart enough to decifer it.
- Someone will come up with an architecture that's easier to program.

35 Years of Microprocessor Trend Tata



Original data collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond and C. Batten
Dotted line extrapolations by C. Moore

Source: C. Moore's talk at Salishan, April 201

The Exascale computer

Metric	2020	Today's technology
System peak	1 Eflop/s	
System memory	10 PB	
Node performance	1-10 Tflop/s	
Node memory bandwidth	200-400 GB/s	
Node concurrency	O(1000)	
Interconnect bandwidth	50 GB/s	
System size (nodes)	100,000-1,000,000	
Total concurrency	O(1,000,000,000)	92,000,000
Storage	300 PB	
IO	20 TB/s	
Power	**~20 MW**	

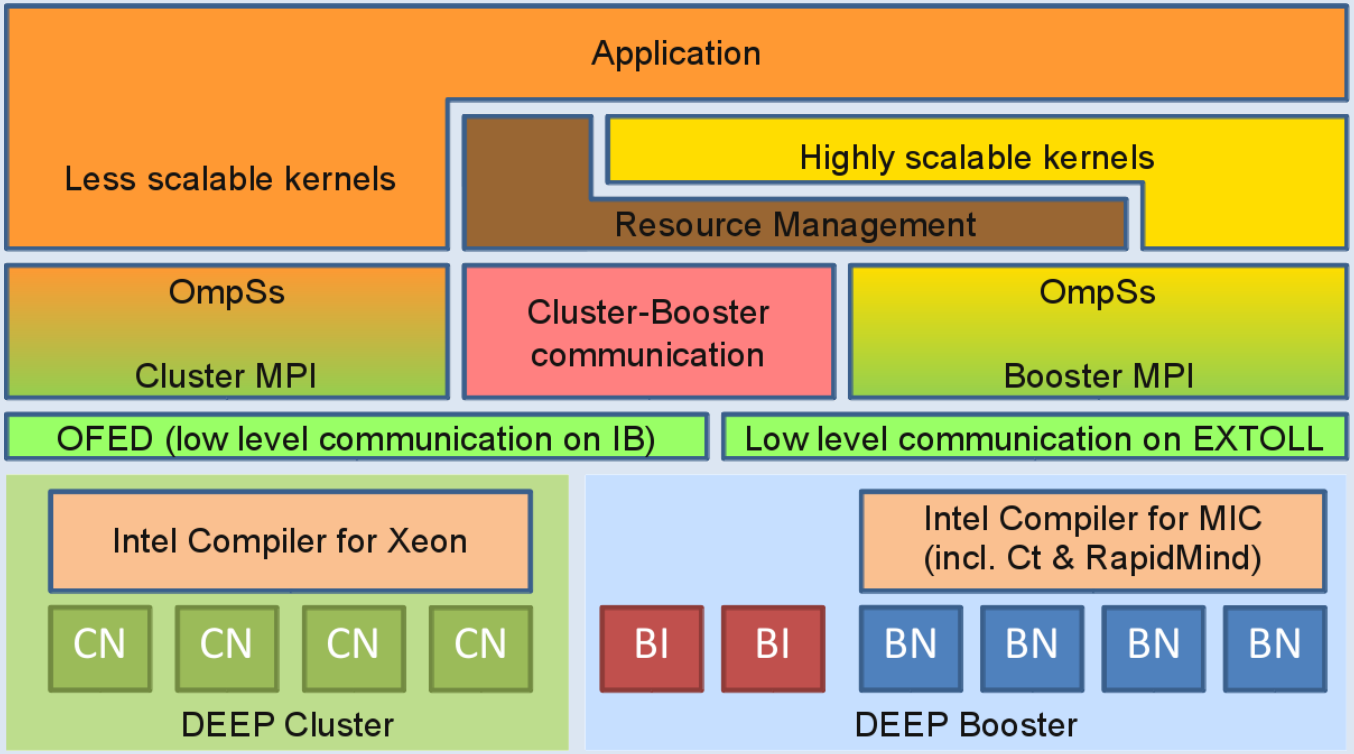
Technology Development: Co-Design → Exascale Labs

- Exascale Innovation Centre
  - IBM
  - Blue Gene Active Storage (BGAS)
  - Application Scaling
  - Open Power Engagement
- Exacluster Lab
  - Intel, ParTec
  - EU Exascale projects DEEP and DEEP-ER
- NVIDIA Application Lab
  - NVIDIA
  - Application Porting and Optimization

Hardware Architecture

Software Architecture

- Basic strategy to port applications:
  - Highly scalable kernels offloaded to the Booster part
  - Less scalable kernels executed on the Cluster part



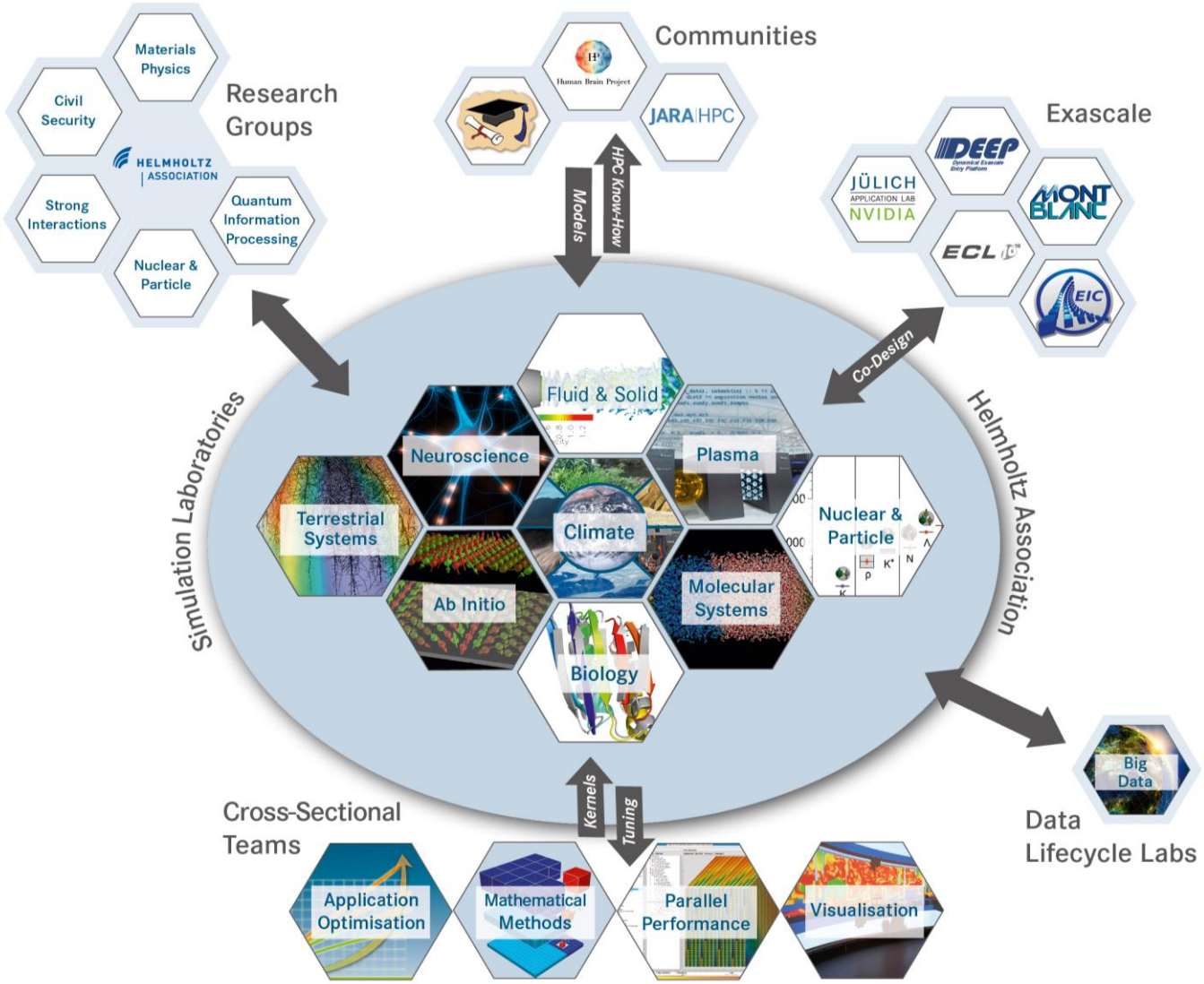
The challenge

- Concurrency: hybrid/multi-level algorithms
- Energy efficiency: avoid data movement

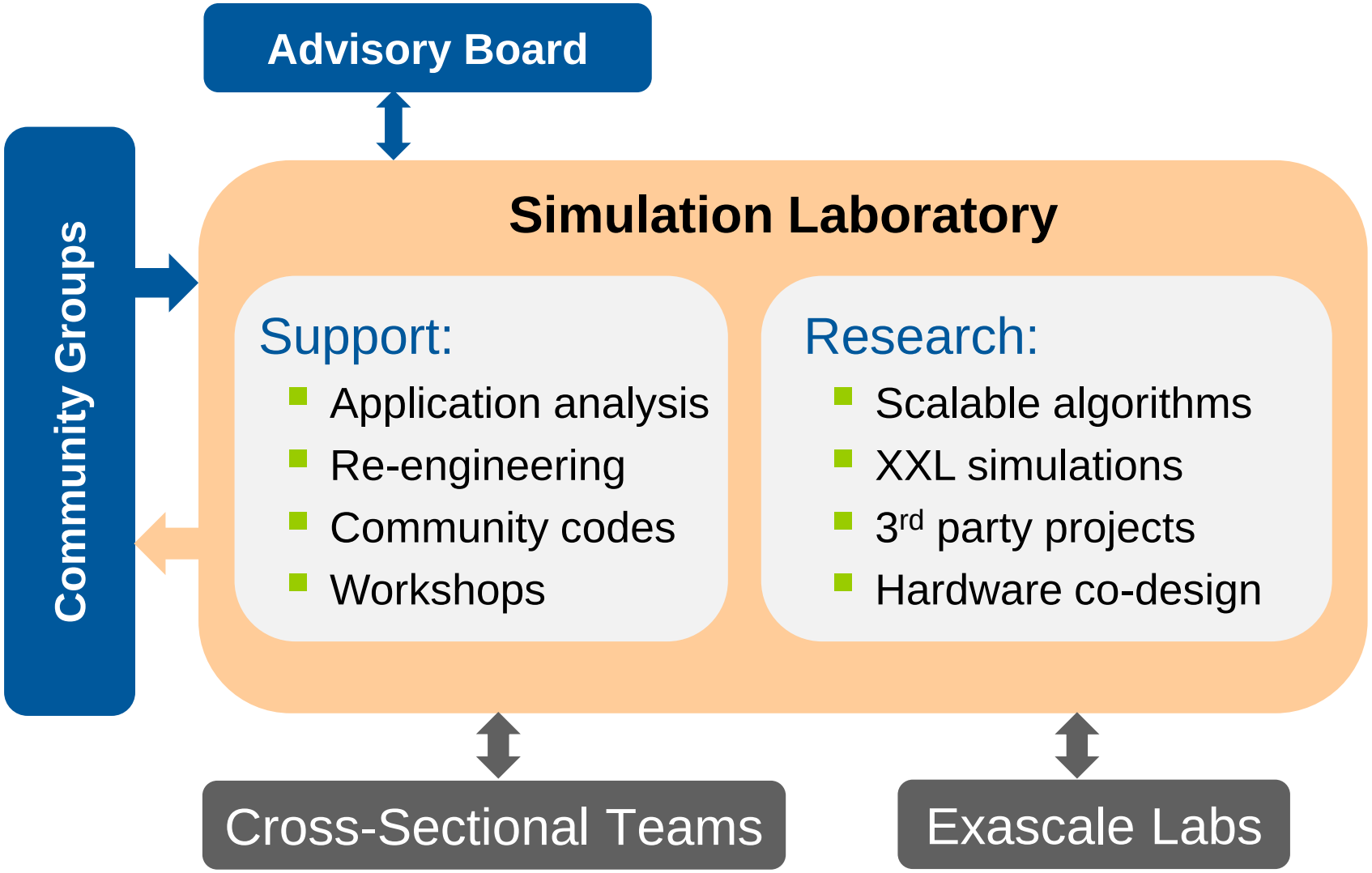
- Implementing numerical algorithms is getting *harder*, not easier:
  - in-depth knowledge of algorithm
  - computer-science know-how
  - community readiness to abandon legacy code

- But help is at hand …

Domain-specific User Support and Research

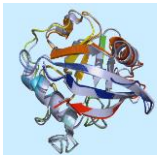


The Simulation Laboratory as HPC Enabler



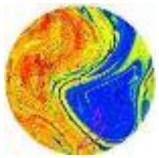
Active Simulation Labs @ JSC

Biology





Climate Science



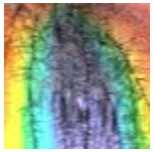



Molecular Systems

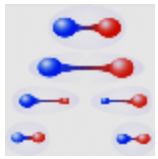




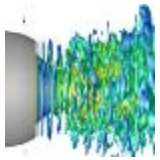

Terrestrial Systems




Nuclear & Particle

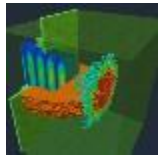



Fluid & Solid Eng.

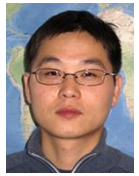




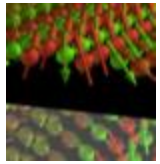
Plasma Physics







Ab Initio




Simulation Lab *Terrestrial Systems*

- TerrSysMP:
- Fully integrated groundwater-vegetation-atmosphere simulation platform; earth system models at regional scale
- Water cycle processes and variability across scales
- Climate and land use impacts

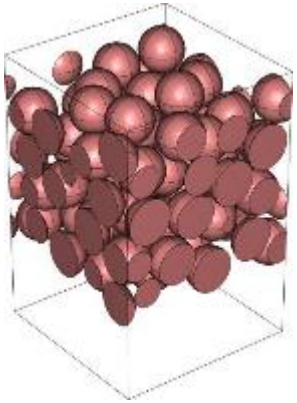
- Scalasca performance analysis
- Refactoring of OASIS-MCT coupling interface to remove scaling bottleneck
- Scaling now to 32k cores:
  64x increased problem size!

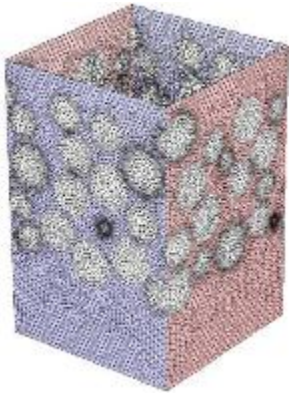
HPSC TerrSys

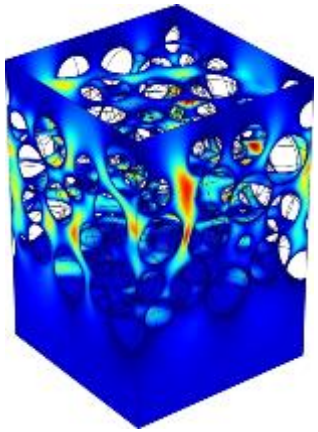
geoverbund
aachen bonn köln jülich

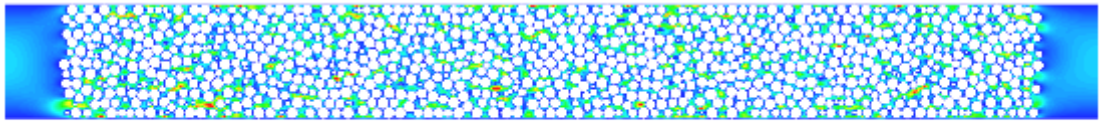
JARA-SimLab *Fluids and Solid Engineering*

- Fluid flow and porous media mixed simulations using FEM.





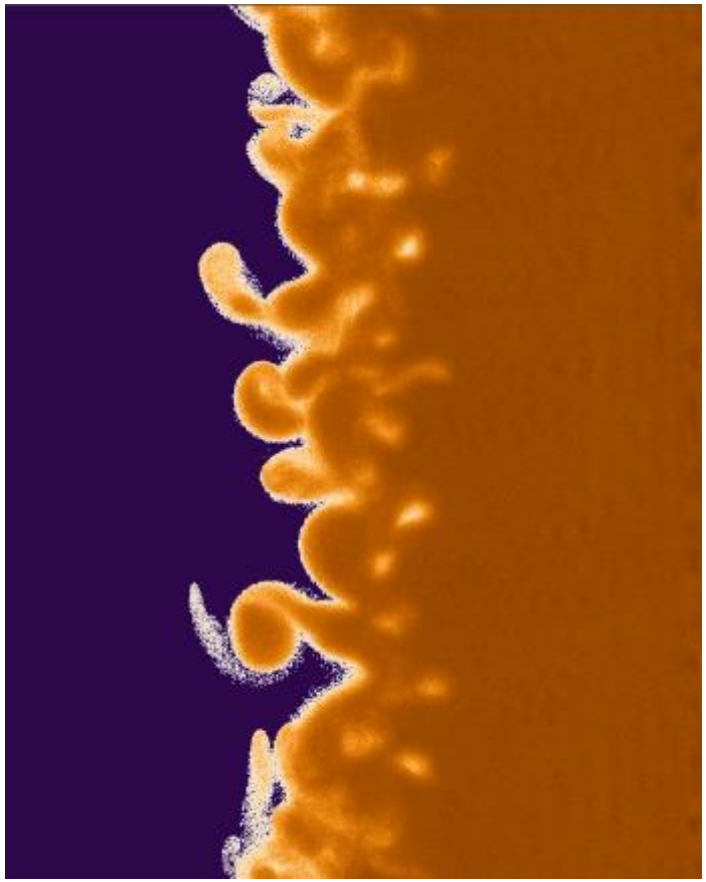


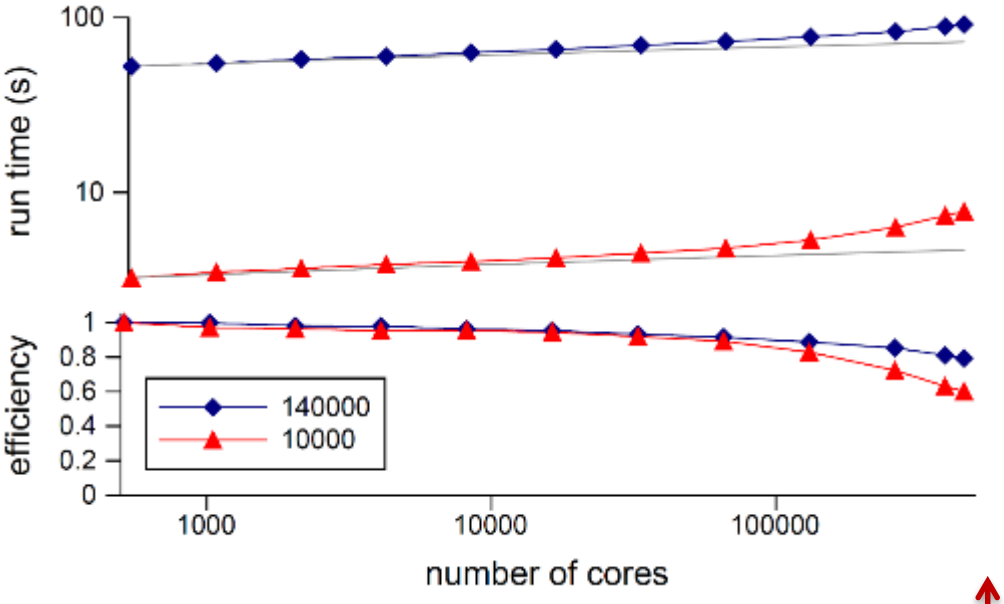


- 2011 Simulations with commercial code COMSOL.
- Largest chromatography simulations with 750 beads take **days**.

- 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

SL *Plasma Physics*: Mesh-free plasma boundary modelling



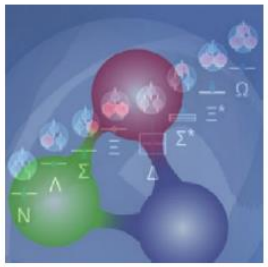
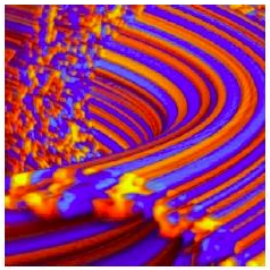
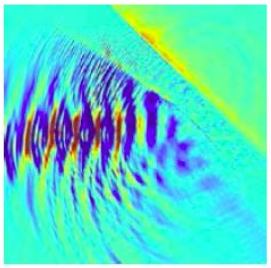
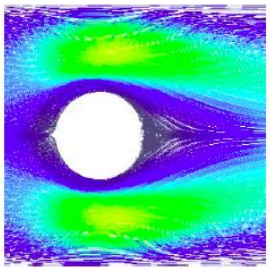
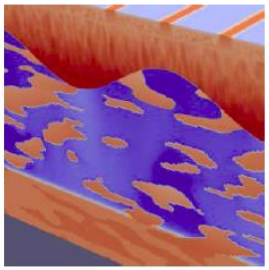
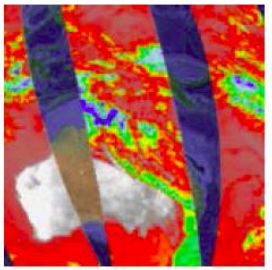


458752
(64 x 10^9 particles)

High-Q Club: Exascale-Ready Applications on JUQUEEN

JÜLICH FORSCHUNGSZENTRUM

HiQ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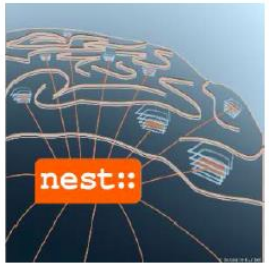	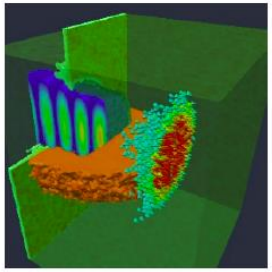	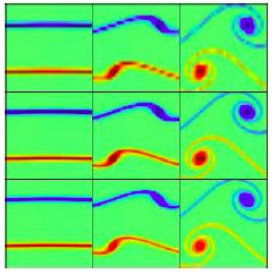	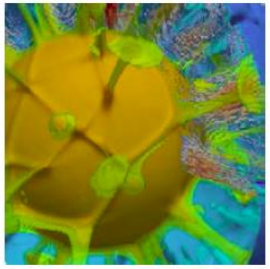	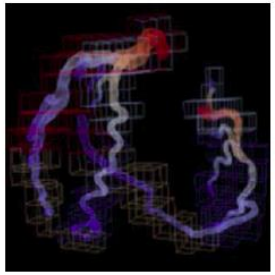	
NEST	PEPC	PMG+PFASST	TerraNeo	WaLBerla	OpenTBL

- 25 diverse applications scaling to entire BlueGene/Q (0.5M cores)

JUQUEEN Porting, Tuning, and Scaling Workshop

2–6 February 2015

- A total of 25 participants for the workshop(s)
- 7 teams invited to (im)prove their application scalability with 30 hours of dedicated access to the entire JUQUEEN system
- Expert assistance provided by JSC Simulation Laboratories (SimLabs) and Cross-sectional teams, with IBM and JUQUEEN technical support
- All 7 teams within 24 hours successfully run their codes using the full system, preparing for entry to the High-Q Club
- Additional experience gained about effectively exploiting extremely scalable computer systems