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 projects


## Application support

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

## R&D work

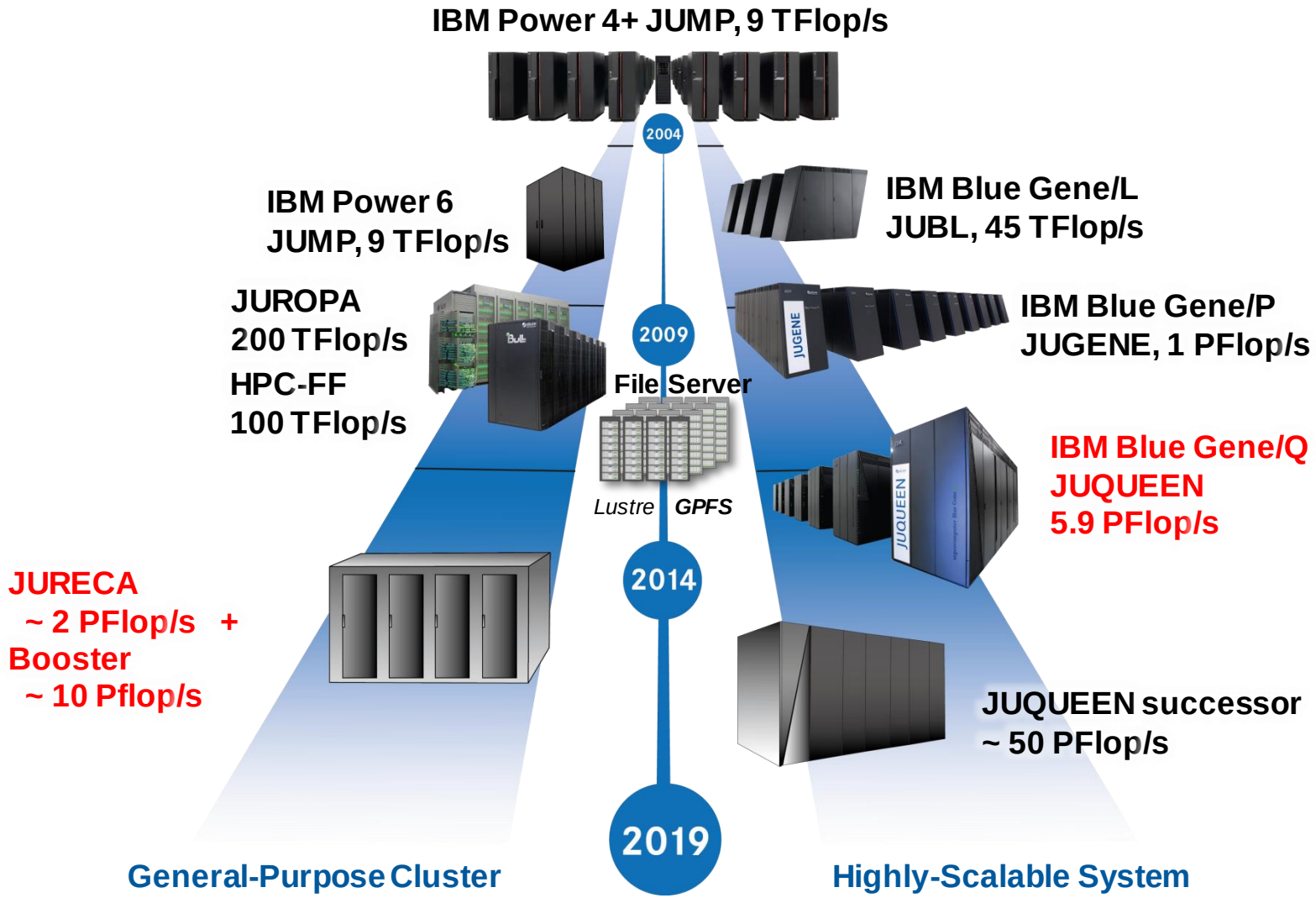
- Methods and algorithms, performance tools
- Computer architectures,
  Exascale Laboratories: EIC, ECL, NVIDIA


DEEP

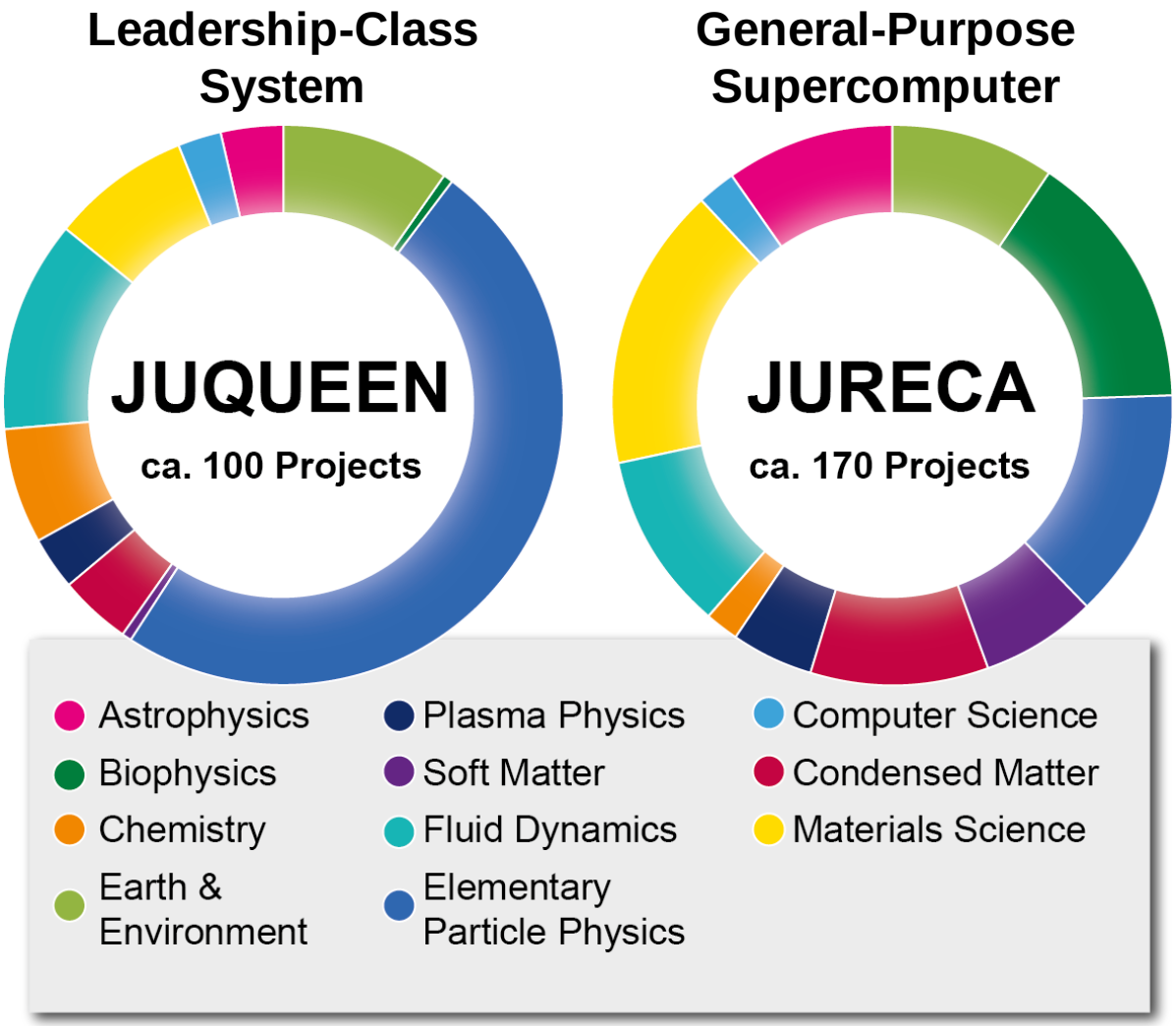
## Education and Training

- BSc, MSc MATSc
- Advanced courses PATC, CECAM

# HPC Systems: Dual Architecture Strategy



# Research Fields of Current National Projects



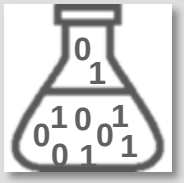
# Community-oriented support strategy

Research Communities

## Research Groups

Future-oriented research

## Simulation Labs




Advanced support & research

## Cross-sectional Teams

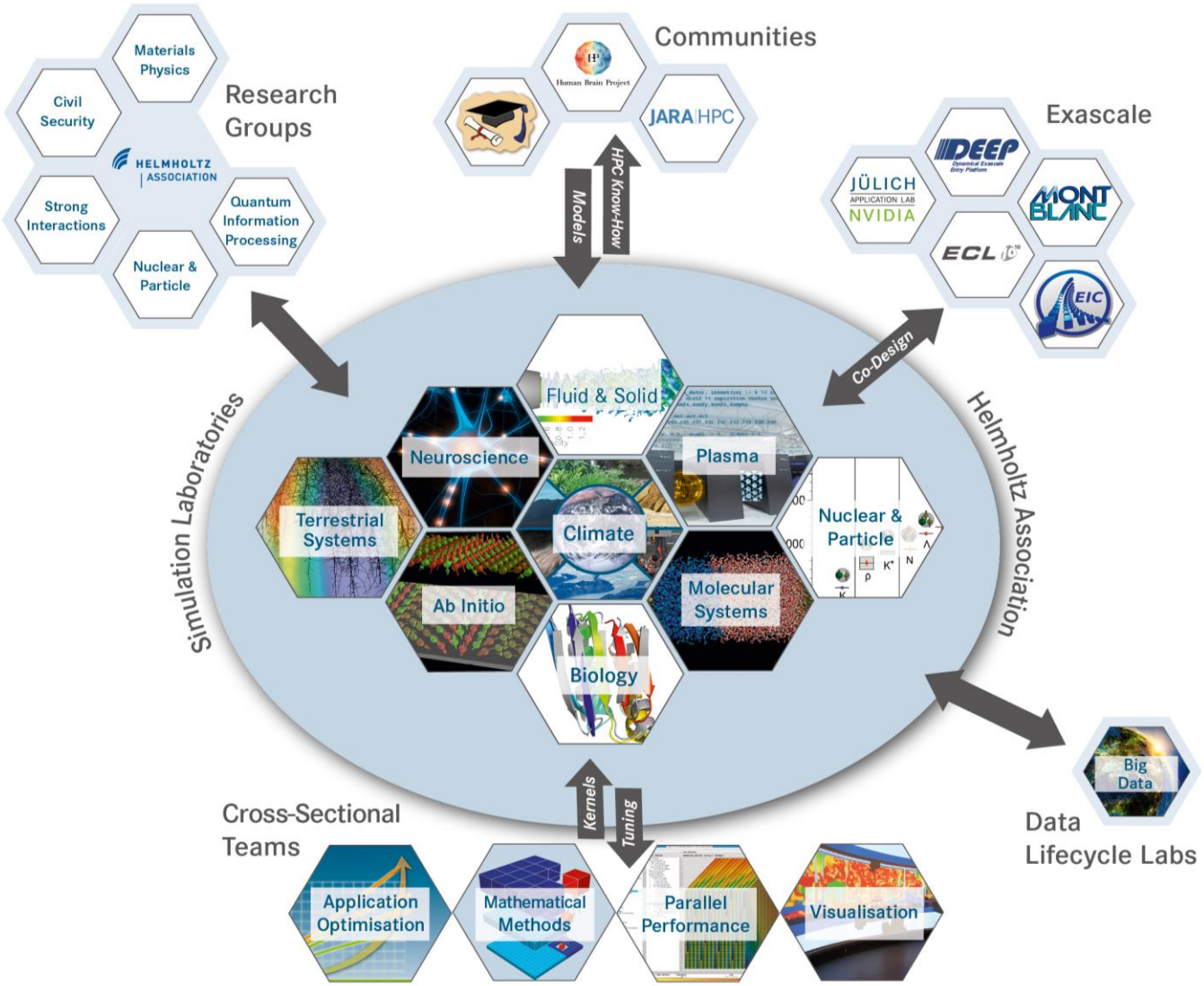
Generic HPC tools & methods

Exascale HPC Resources

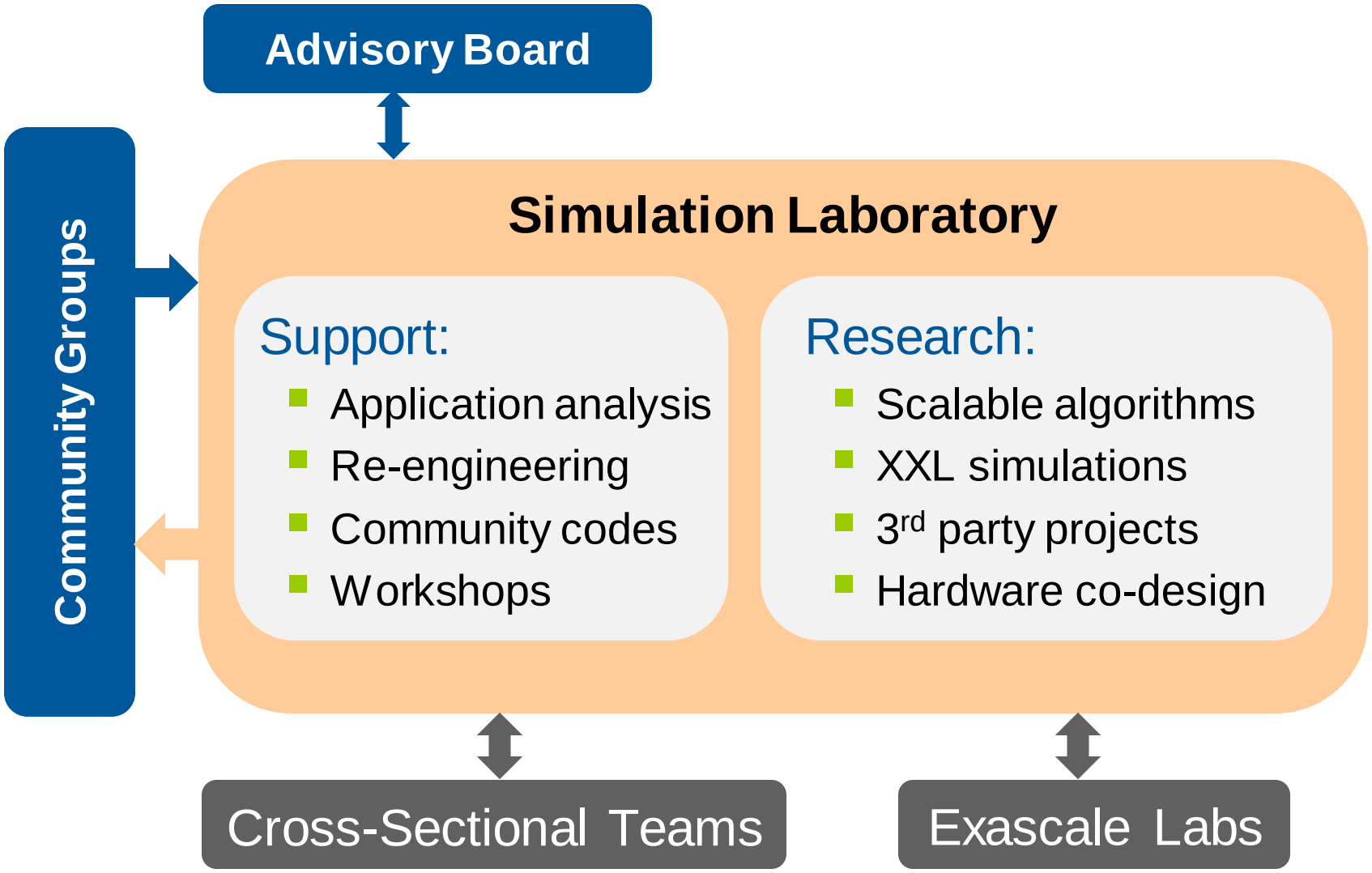
Natural & engineering sciences

Supercomputer science

# Domain-specific User Support and Research

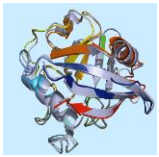


# The Simulation Laboratory as HPC Enabler



# Active Simulation Labs @ JSC

Biology



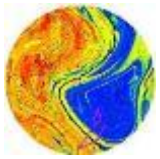


Molecular Systems

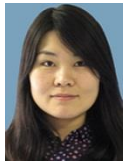




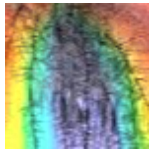
Climate Science





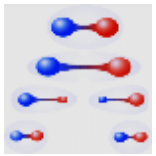




Terrestrial Systems

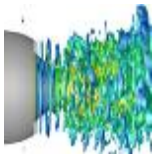





Nuclear & Particle

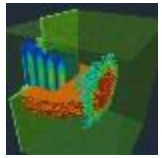



Fluid & Solid Eng.



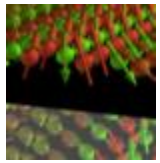


Plasma Physics

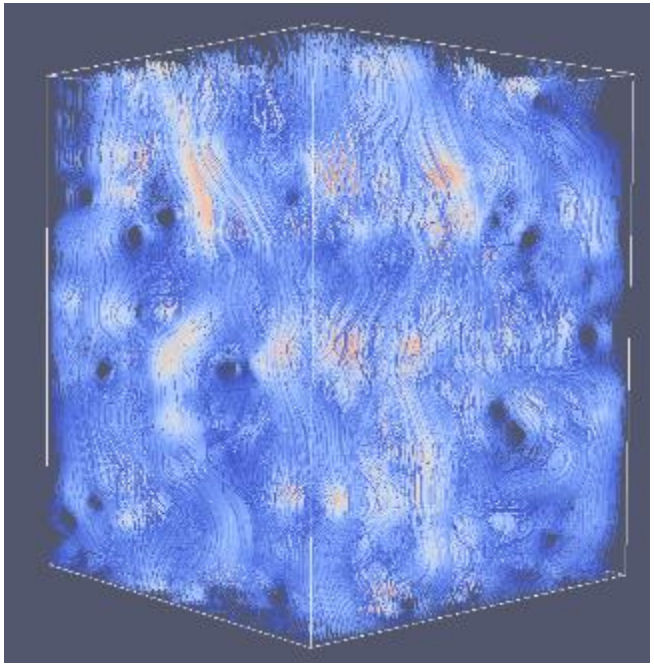


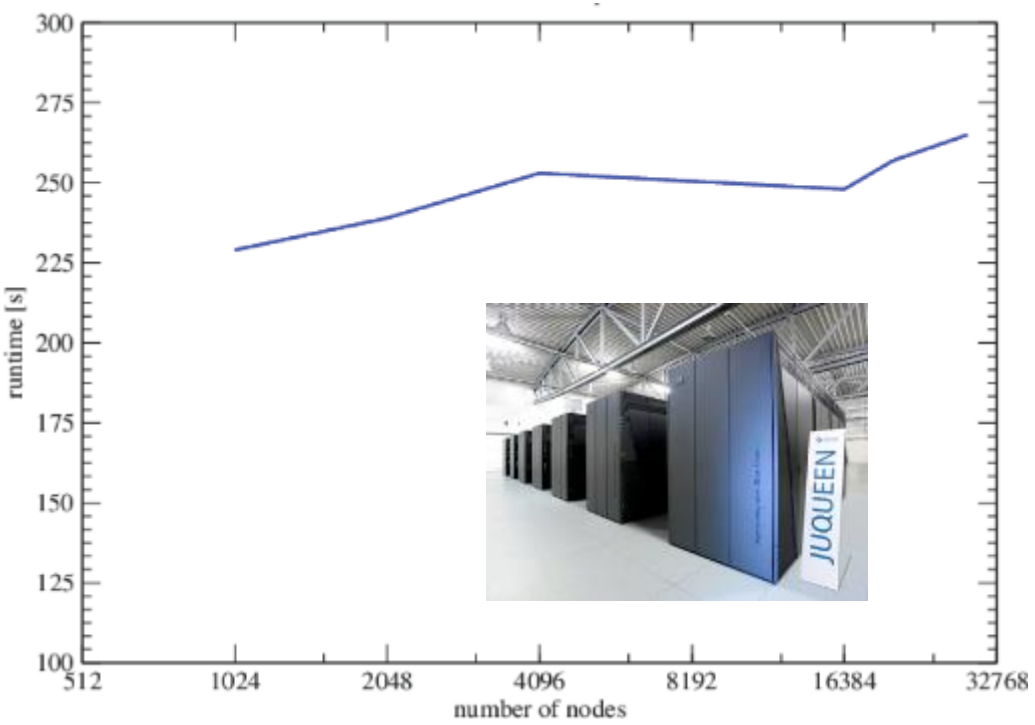


Ab Initio



# Sim Lab *Molecular Systems:*
# MP2C - innovative particle-based hydrodynamics

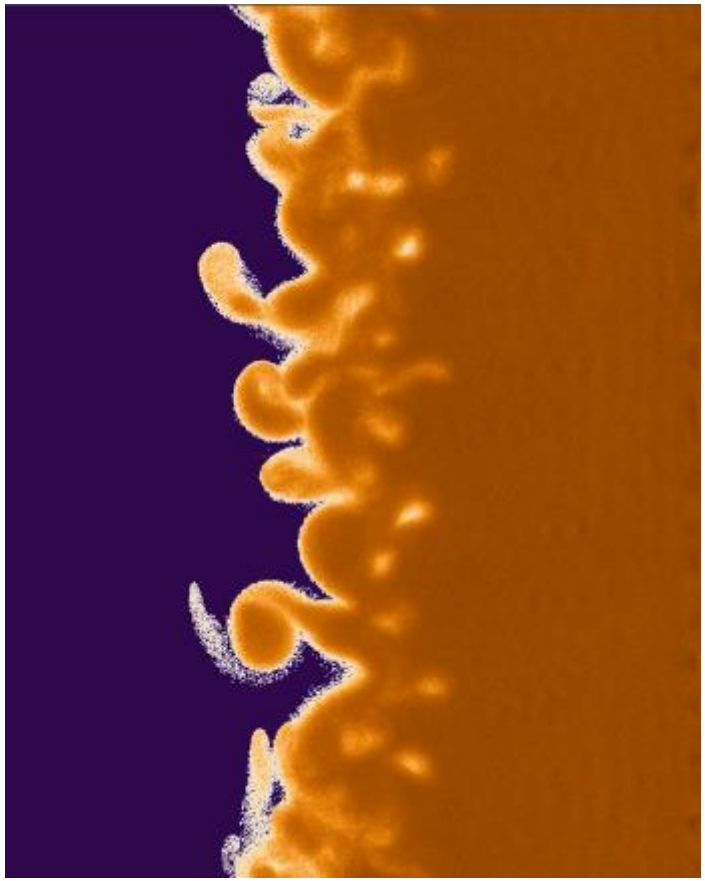


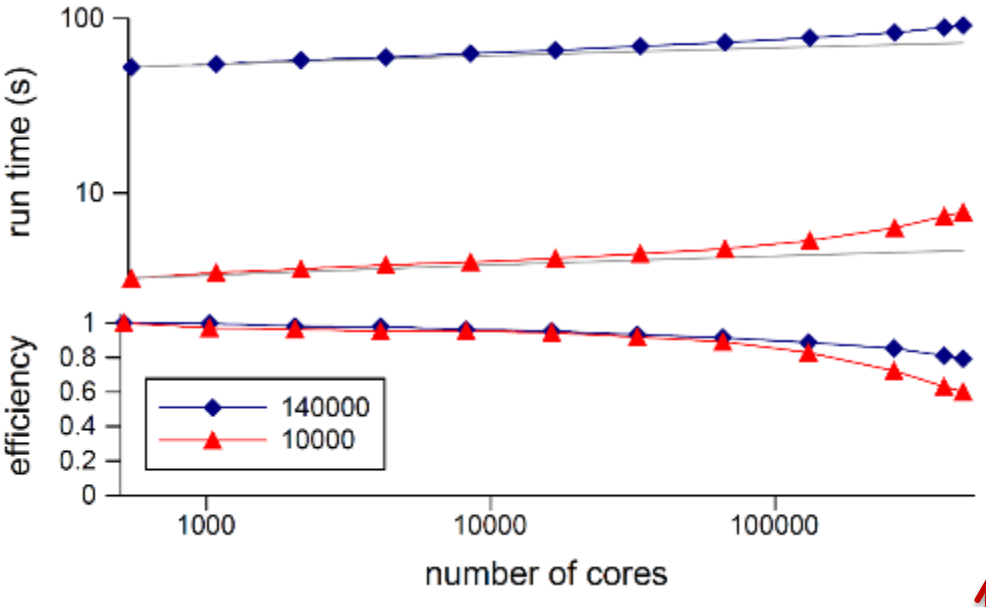



- Flow field in a gas diffusion membrane
- With stochastic geometry

- Weak scaling on full JUQUEEN

# SimLab *Plasma Physics*: Mesh-free plasma boundary modelling

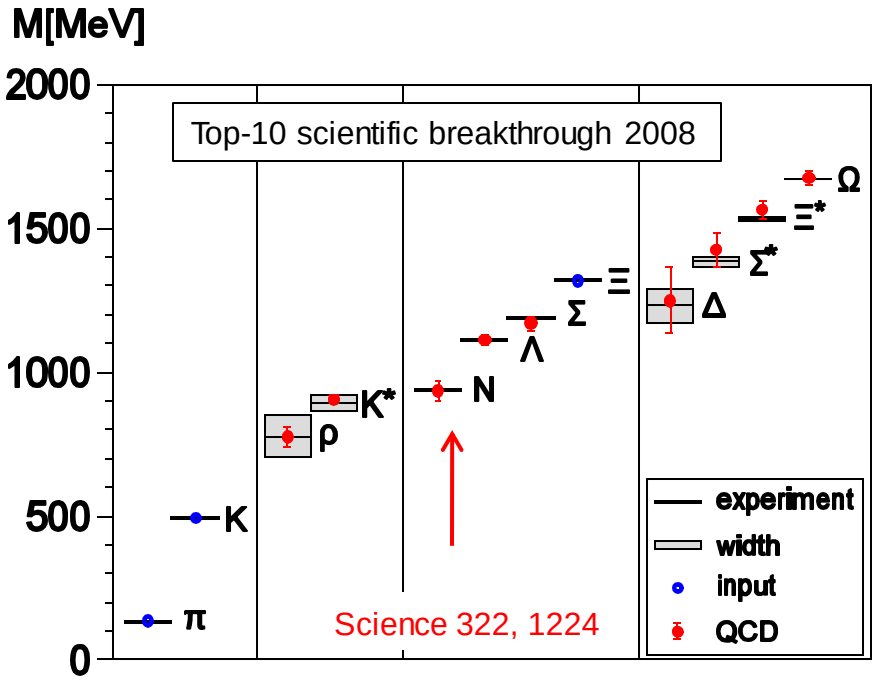





458752
(64 x $10^9$ particles)

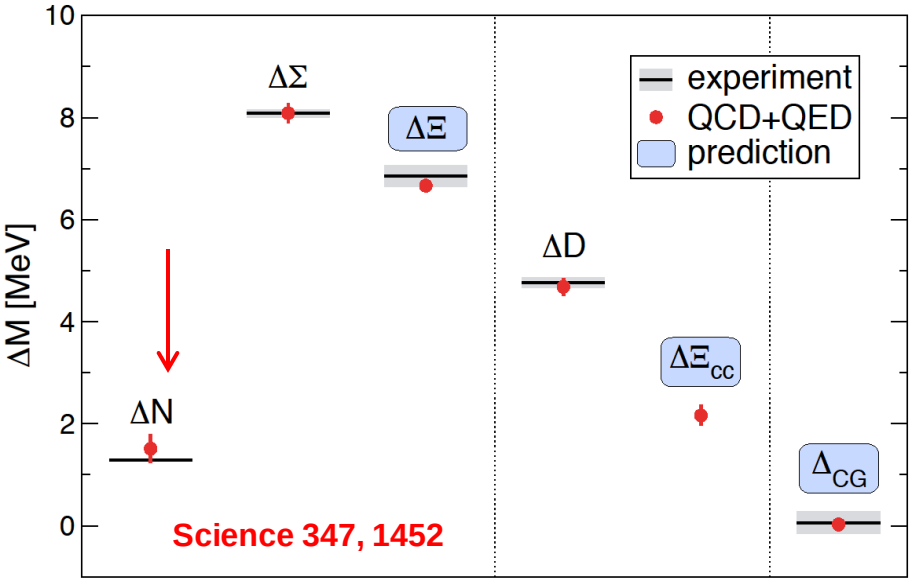
# SimLab *Nuclear and Particle Physics*

- Proton/neutron mass




*Mass of ordinary matter:* over 99% due to nucleons, 95% of which are 'dynamical'

- Lattice QCD including QED

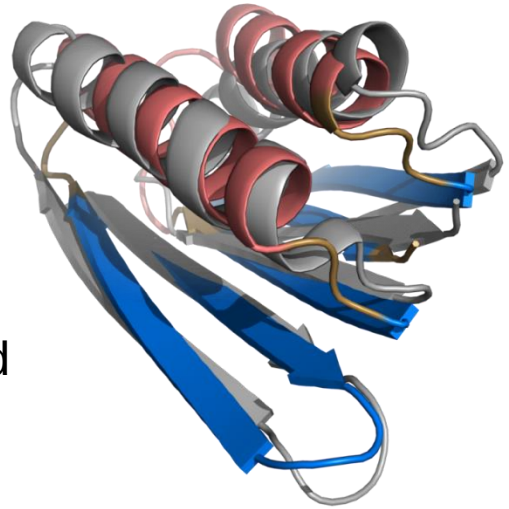



*Stability of ordinary matter:* Neutron-Proton and other mass-splittings of octet baryons

# Simulation Laboratory *Biology*

## Research Focus:

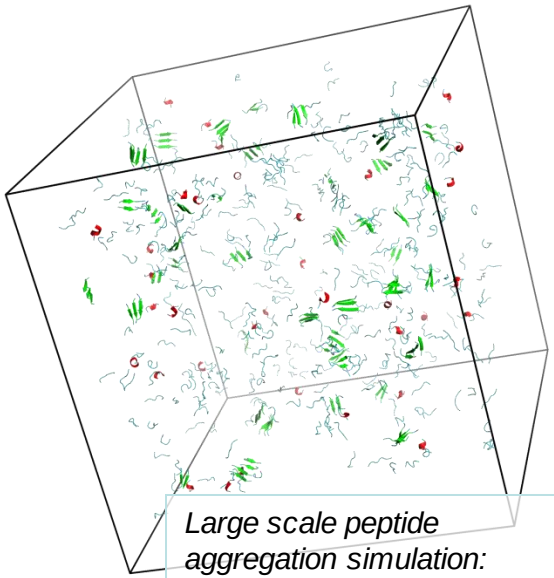
- *HPC Monte Carlo simulations* of macromolecules for protein folding and peptide aggregation beyond the millisecond **(ProFASi)**:
- Combination of machine learning and MC simulation
- Optimization in Bioinformatic workflow systems



*TOP7: Largest ab initio folding simulation to date (92 aa, 30k CPU-hrs/folding, ~1000 ms natural folding time)*

## Support & Cooperation Projects

- Biotechnology/Systems Biology
- Genomics
- Big Data
  - Data mining and analysis for large-scale Monte Carlo simulation data = $10^6$-$10^8$ independent conformations
  - SDIL Medicine (evaluating)



*Large scale peptide aggregation simulation: (500 chains, -> full aggregation $5.4 \cdot 10^{13}$ MC moves )*

# 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!

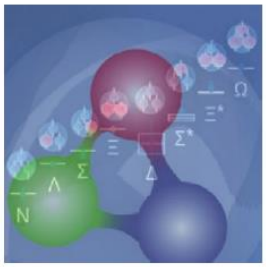
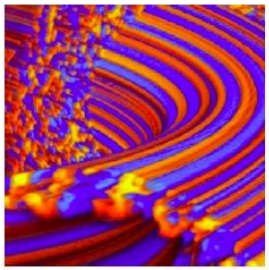
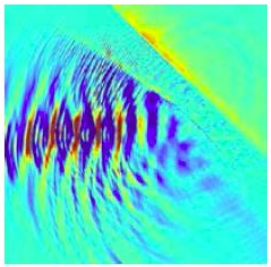
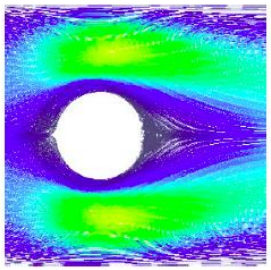
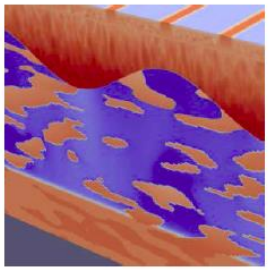
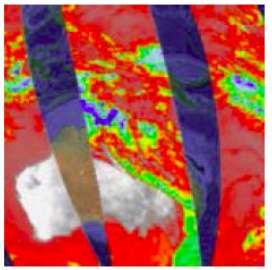
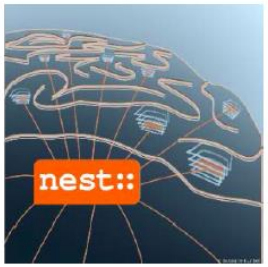
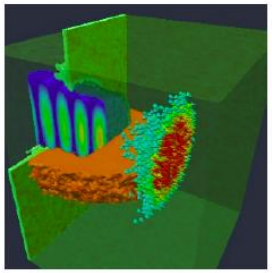
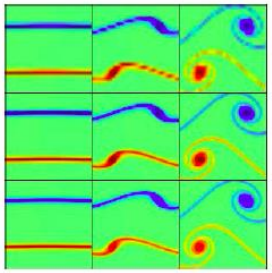
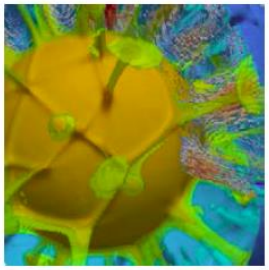
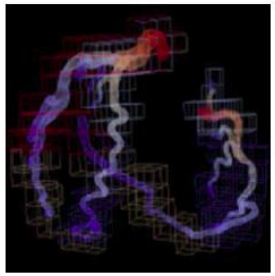
HPSC TerrSys

geoverbund
aachen bonn köln jülich

# High-Q Club: Exascale-Ready Applications on JUQUEEN

JÜLICH FORSCHUNGSZENTRUM

HiQ

| | | | | | |
|---|---|---|---|---|---|
|  |  |  |  |  |  |
| dynQCD | GYSELA | JuSPIC | MP2C | muPhi | JURASSIC |
|   |  |  |  |  |  |
| NEST | PEPC | PMG+PFASST | TerraNeo | WaLBerla | OpenTBL |

- >30 applications scaling to entire BlueGene/Q (0.5M cores)

# Repair Shop

| SYMPTOM | REMEDY | CONTACT |
|---|---|---|
| Serial Code | MPI/OpenMP course | SimLabs, App Support |
| Slow I/O | I/O course, SIONlib | App Support |
| Code doesn't scale | Perf. Analysis tool (Scalasca, Score-P) | Parallel Perf. Team |
| Code uses old libraries | Replace lib | Math Methods Team |
| Algorithm scales in theory but not in my code | Perf. Analysis; Benchmarking | SimLabs, Perf Team |
| Accelerator slows code down | Memory transport analysis/opt | SimLabs, Exascale Lab, (Nvidia, Intel) |
| Code behaving oddly | | JUST ASK! |