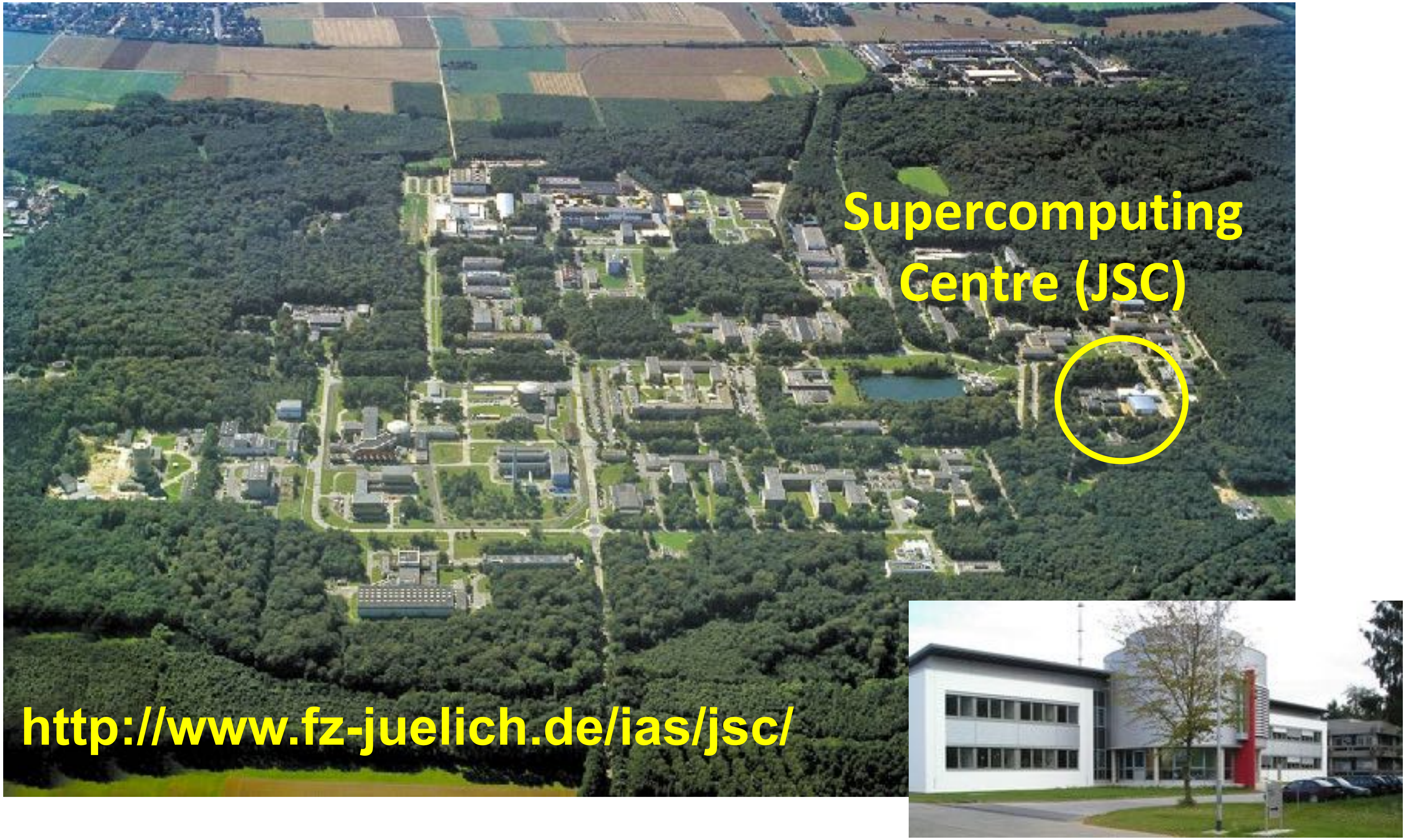
High-Performance Simulations at the Jülich Supercomputer Centre

Jülich Supercomputing Centre

Overview

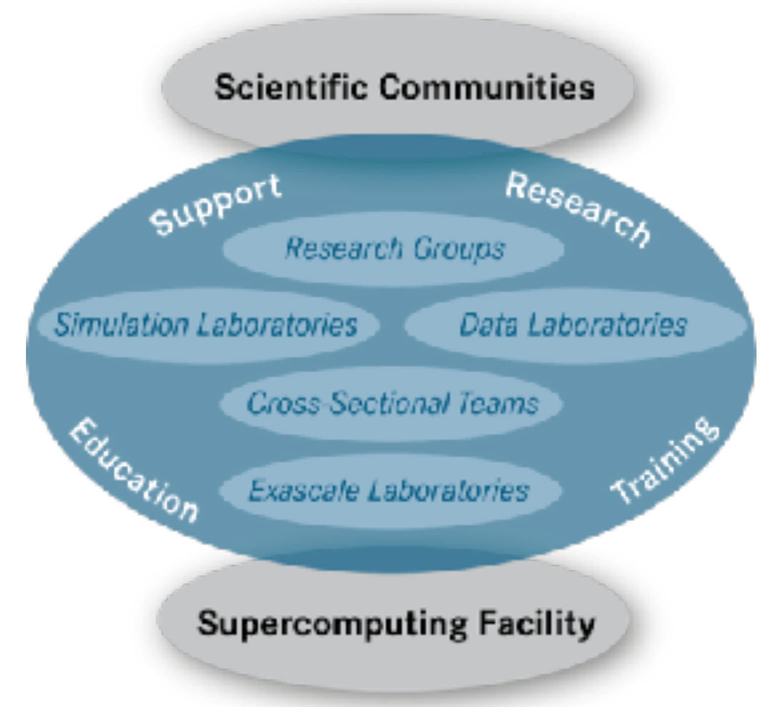
Jülich Supercomputing Centre



Jülich Supercomputing Centre

Supercomputer cycles for

- Centre – FZJ
- Region – RWTH Aachen University
- Germany – Gauss Centre for Supercomputing
  John von Neumann Institute for Computing
- Europe – PRACE, EU projects



Application support

- Unique support & research environment at JSC
- Peer review support and coordination

R&D work

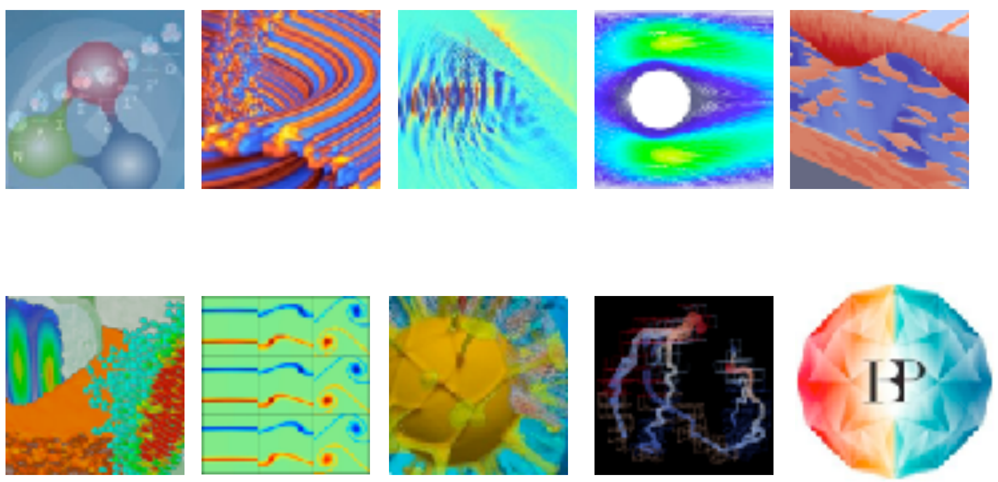
- Methods and algorithms, computational science, performance analysis and tools
- Scientific Big Data Analytics with HPC
- Computer architectures, Co-Design
  Exascale Labs together with IBM, Intel, NVIDIA

DEEP

Education and training

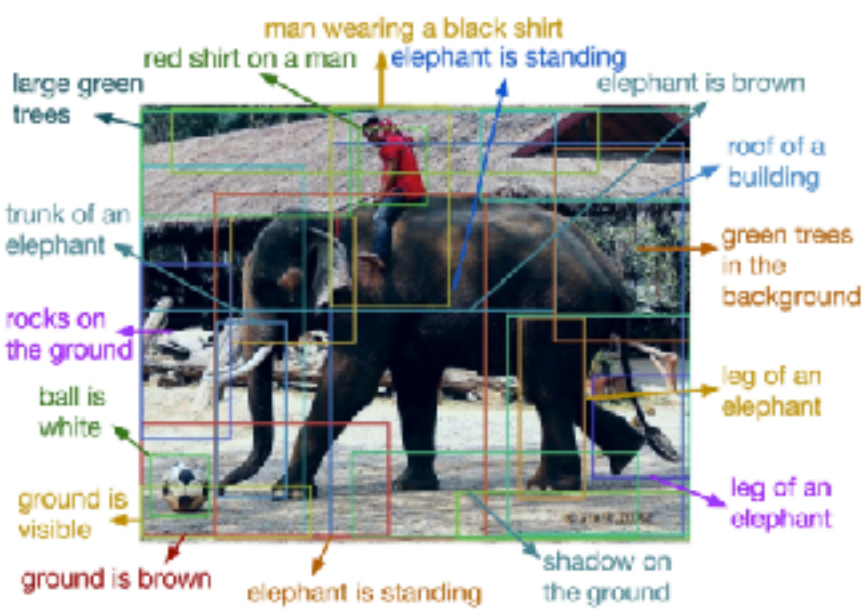
HPC has diverse challenges:

Extreme Scale Computing



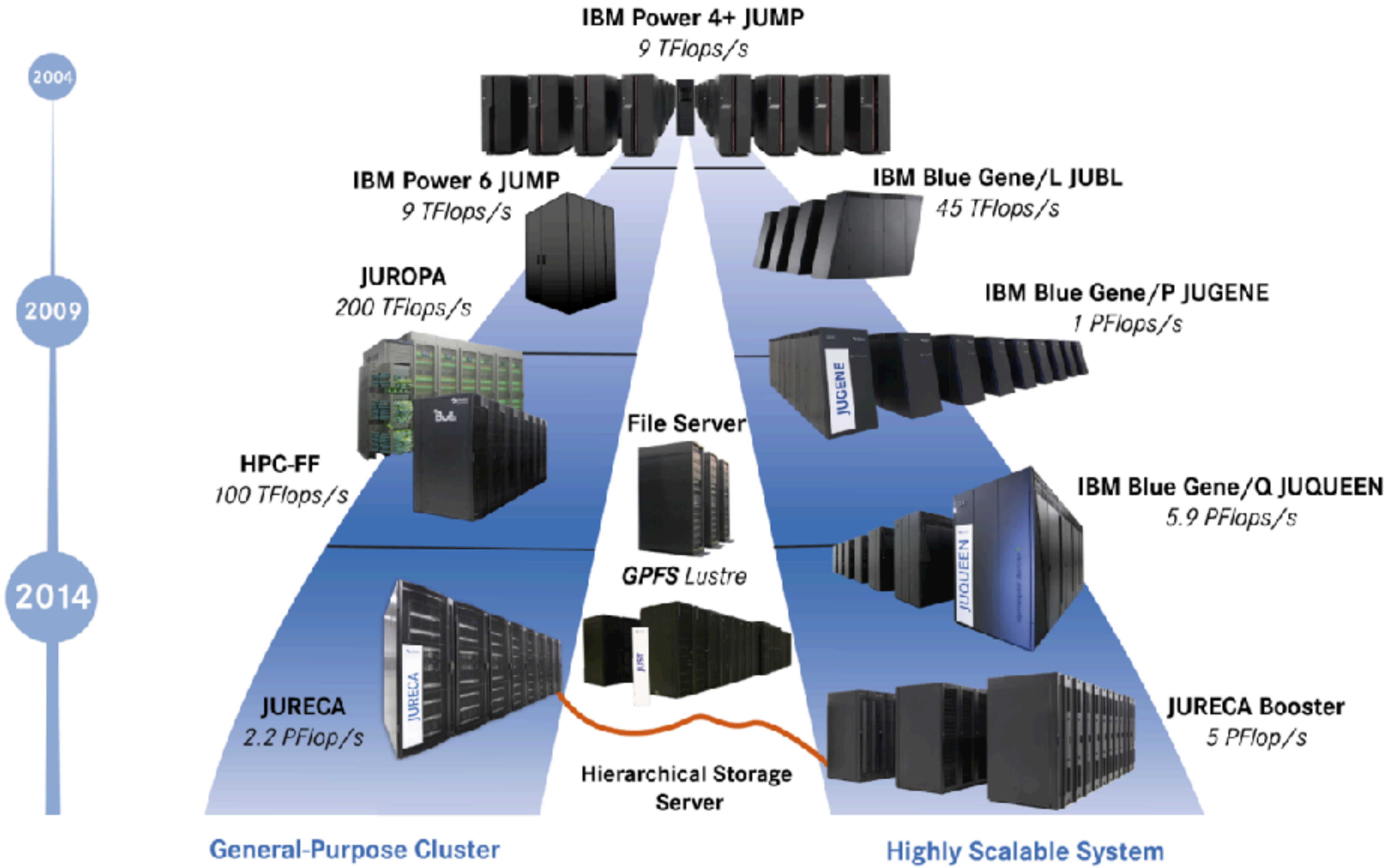
Big Data Analytics

Deep Learning

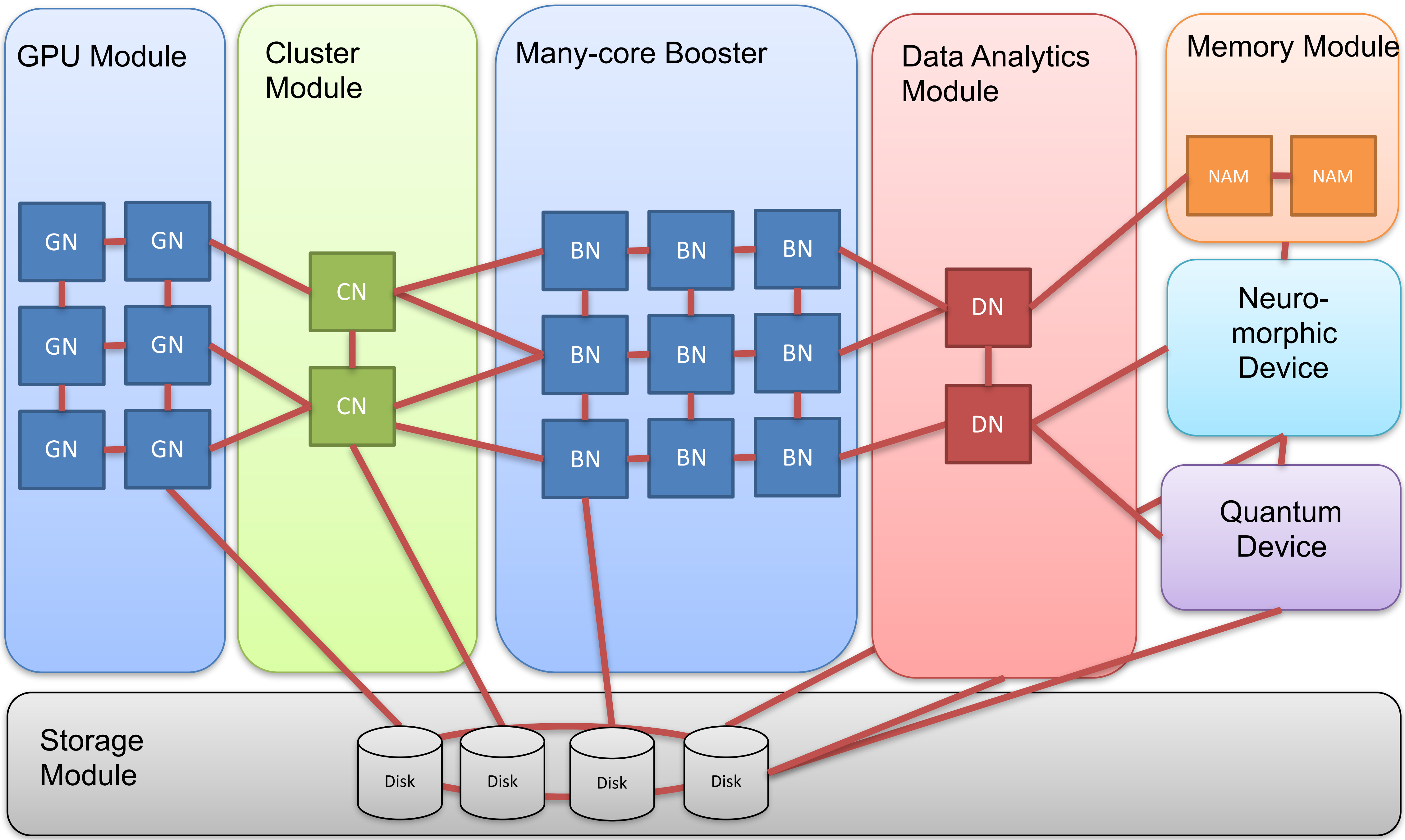


Interactivity

Dual Architecture Strategy at FZJ …



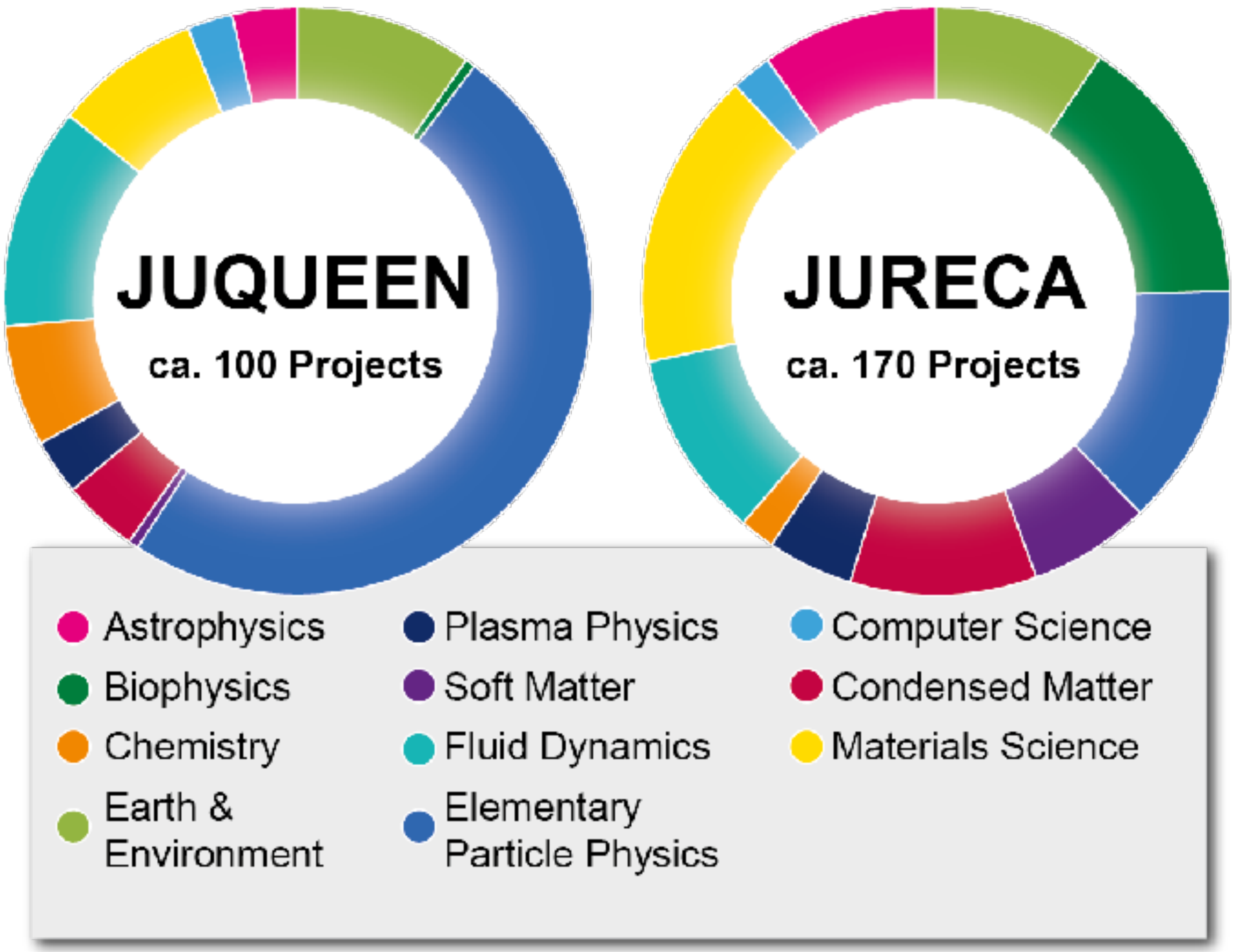
… and Evolution to Modular Supercomputing Architecture



Research Fields of Current Projects

Leadership-Class System

General-Purpose Supercomputer

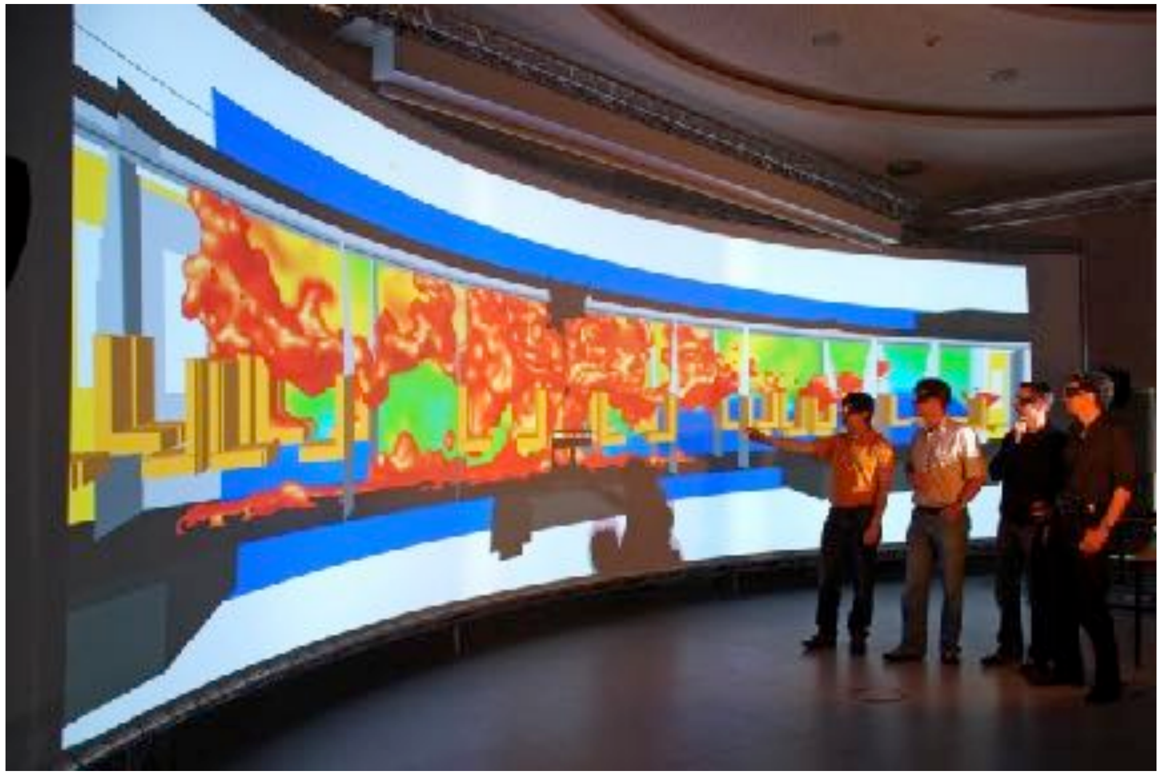


Computer simulations and applications in science

Seminar topics

Visualization

- Visualization of scientific data
- Big data visualization with parallel methods
- Coupling of visualization and HPC systems
- In situ visualization of running simulations

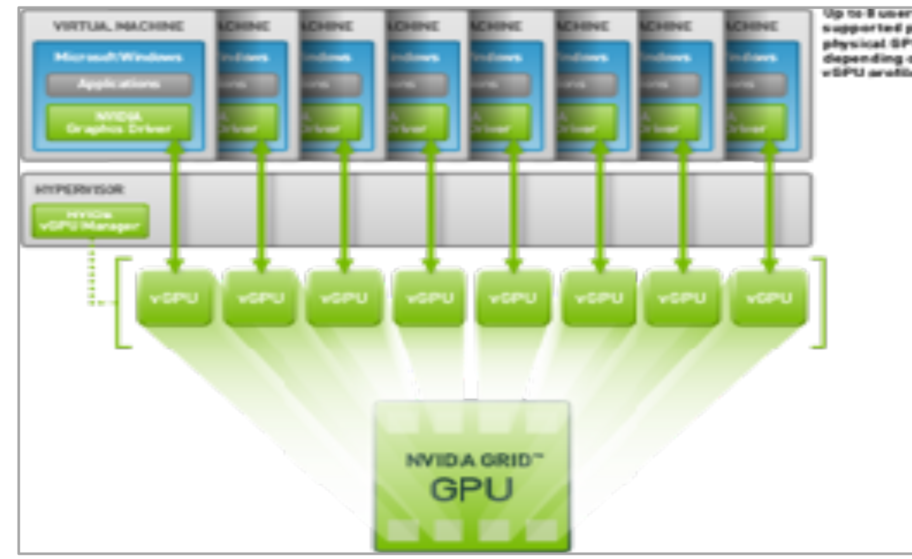


3D Visualization of Simulation Data on Large Screen Display

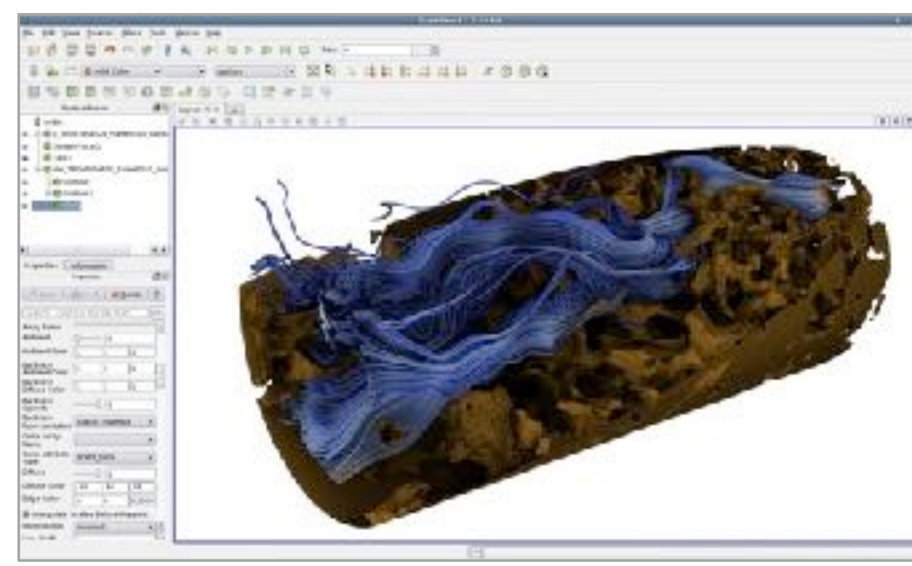
Contact: Jens Hendrik Goebbert (j.goebbert@fz-juelich.de)

Seminar topics

- 3D visualization on remote desktops
  - Comparison of different concepts of 3D capable remote desktops
  - Usability study on some selected tools
  - Evaluation with particular emphasis on security aspects
- Modern ray tracing with OSPRay
  - Testing of OSPRay
  - Integration in visualization packages (ParaView, VisIt) using existing plugins
  - Performance measurements
  - Comparison with other ray tracers, e.g. OptiX from NVIDIA

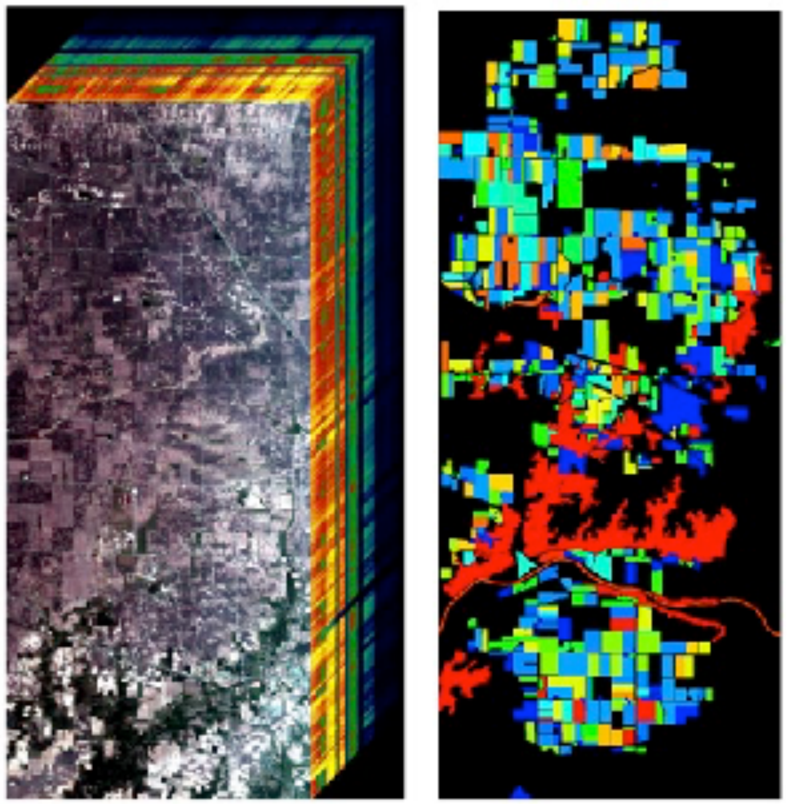


NVIDIA Virtual GPU Technology


OSPRay running inside ParaView

Learning from XXL Data

- Enables **Big Data Analytics** with parallel machine learning methods for XXL datasets from science, engineering, and industry 4.0
- Performs **classification, clustering**, and **regression** on scientific application data with high dimensions or large class numbers
- Develops scalable **Statistical Data Mining** methods in order to transform big data into smart data (e.g. dimensionality reduction, feature engineering, etc.)



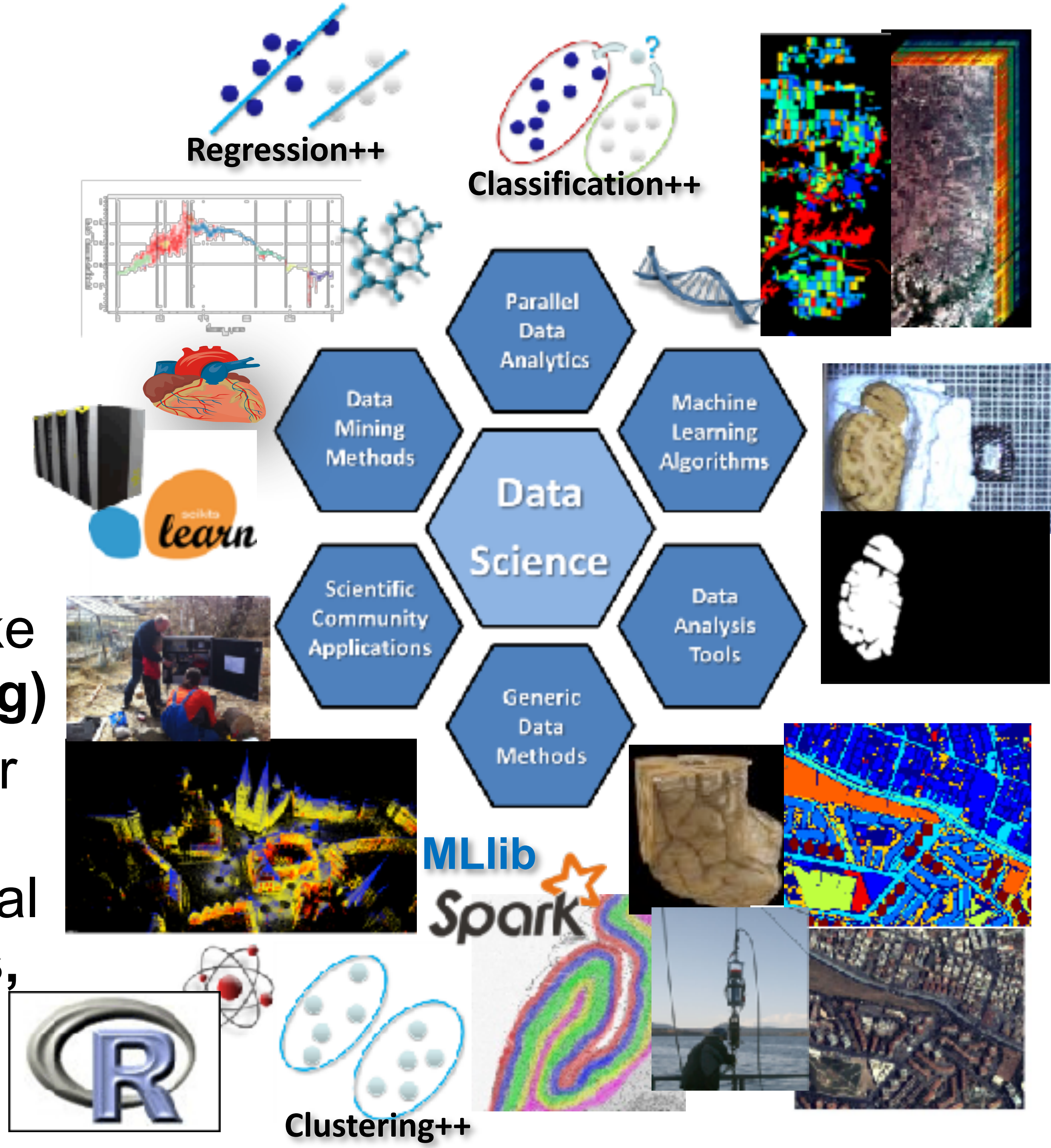
Speed-up classification method of satelite images into known 52 land cover classes using a parallel and scalable Support Vector Machine (SVM):

Research output: from ~9 hours to ~35 min

Contact: Morris Riedel (m.riedel@fz-juelich.de)

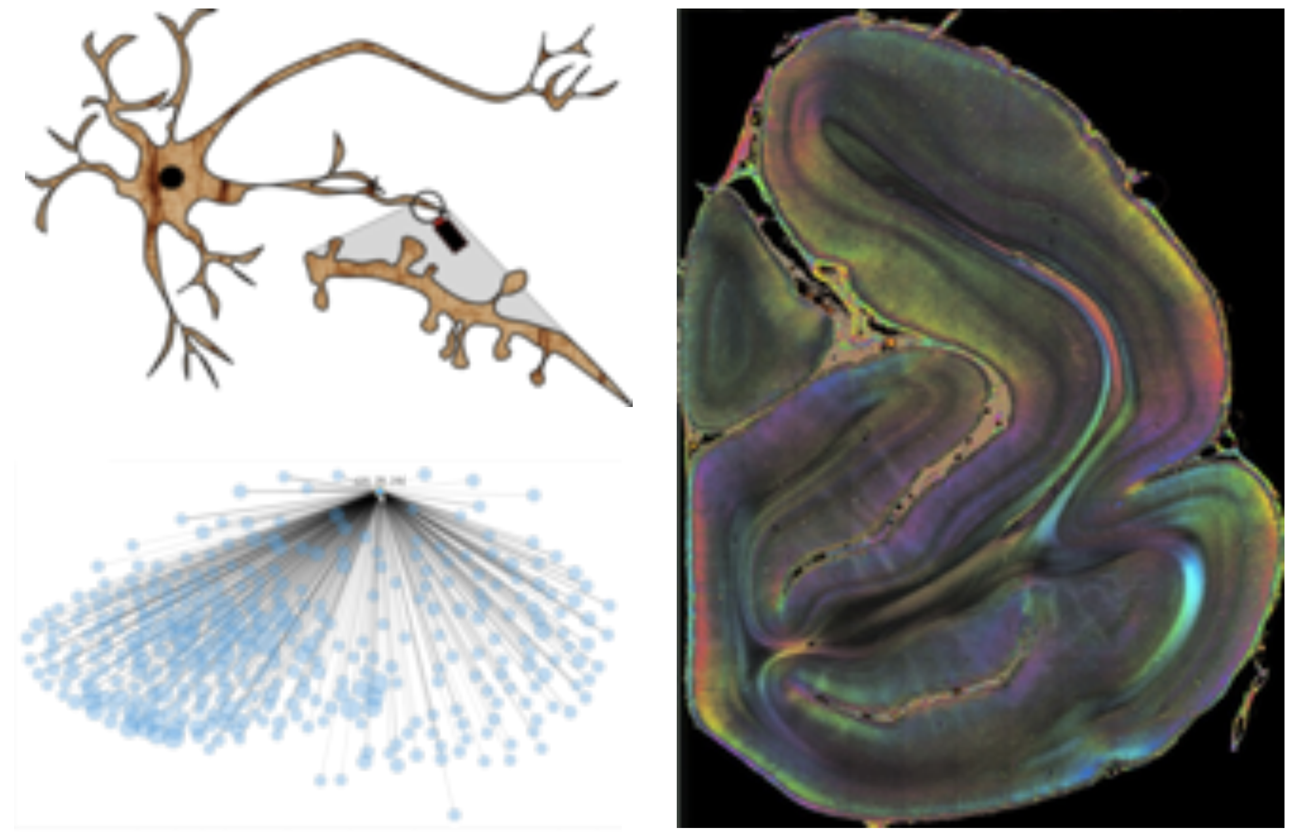
Seminar topics

- Perform big data analytics methods on extremely large **application domain datasets** (brain images, welds images, earth science data)
- Parallelize scalable machine learning algorithms using **map-reduce/Hadoop, MPI/OpenMP**, **GPGPUs, Spark,** or new tools like **Theano/Pylearn2 (deep learning)**
- Explore and create extensions for **R, Matlab, Weka, and/or scikit-learn** in order to perform statistical data mining on **supercomputers, distributed systems or clouds**



Simulation Lab Neuroscience

- Developing HPC simulation tools on multiple scales (biophysical neuron to whole brain)
- Developing and optimizing applications for functional and anatomical data analysis
- Establishing neuroimaging pipelines for HPC
- Neuromorphic computing

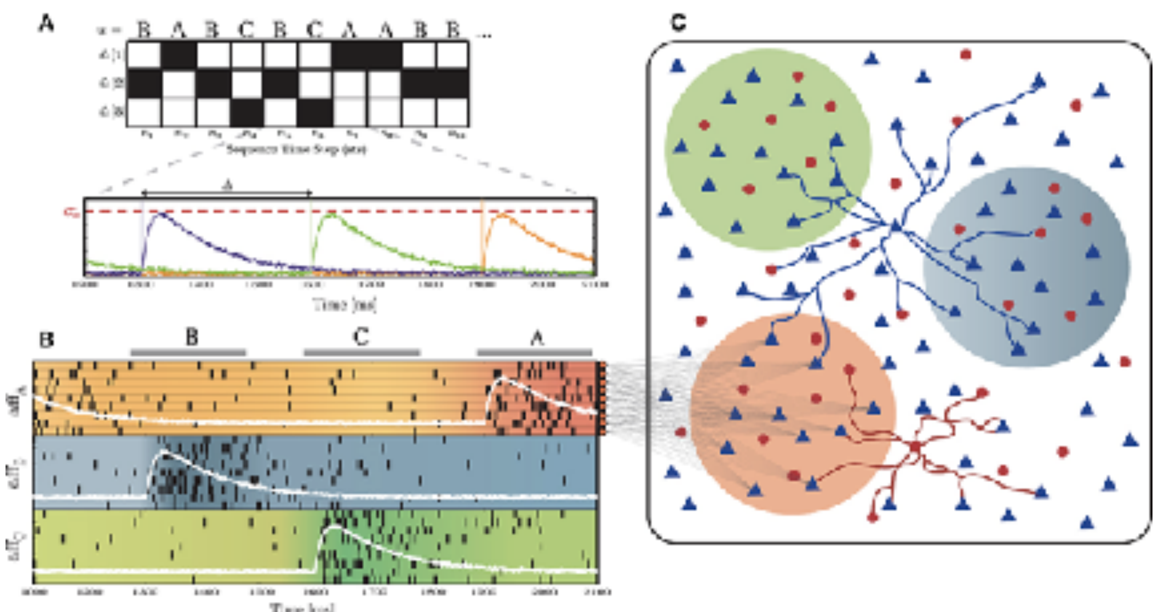


Typical applications in the SLNS: Structural plasticity modelling; Polarized Light Imaging pipeline; Graph visualization and analysis

Contacts: Abigail Morrison, Boris Orth (slns@fz-juelich.de)

Seminar topics

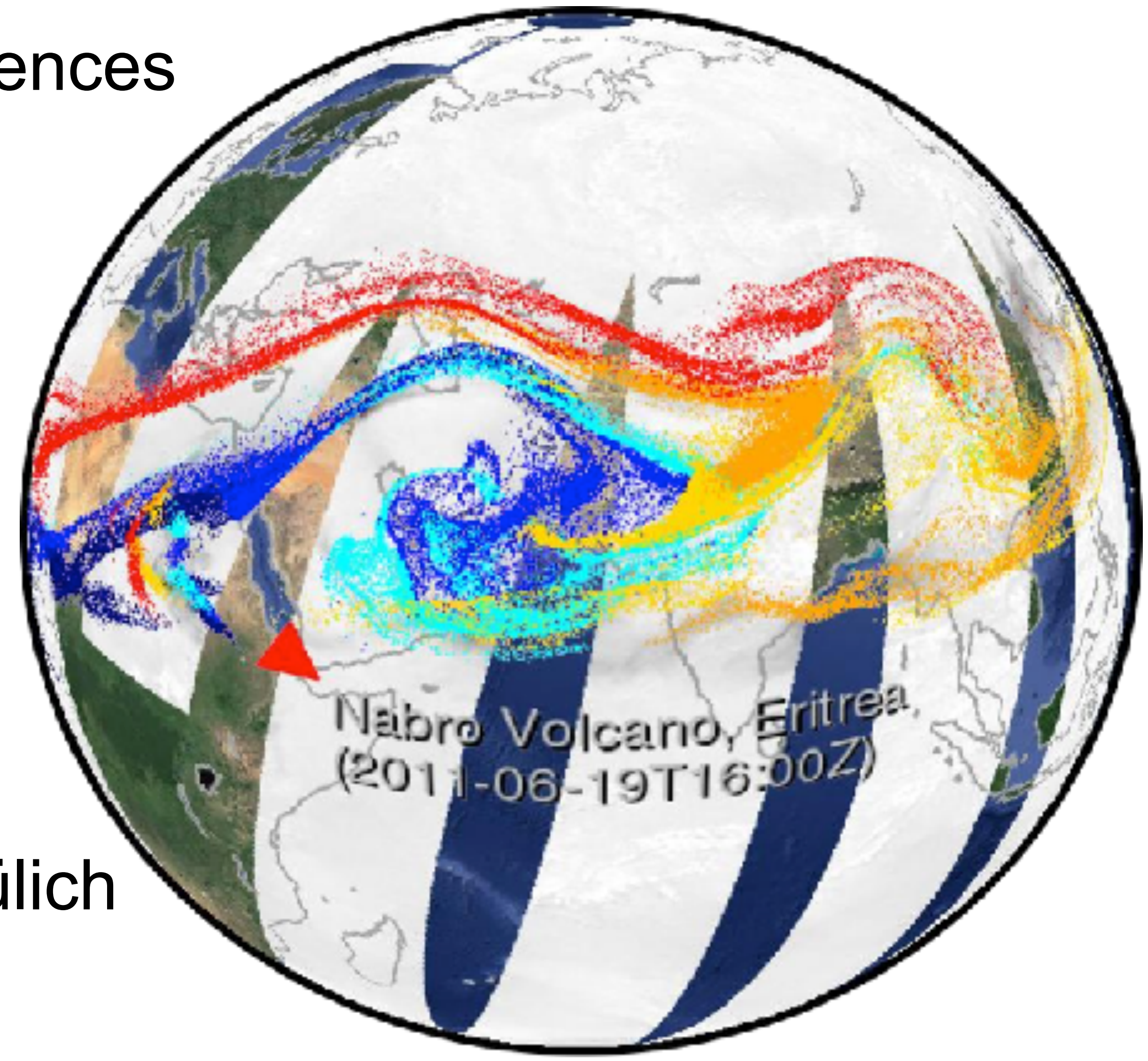
- Simulation approaches for the human brain
- Applications of machine learning to processing neuroimaging data
- Neuromorphic computing as a tool for neuroscience
- High-dimensional parameter optimization



Top: Simulation of a spiking neuronal network.
Bottom: The neuromorphic platform SpINNAker

Simulation Laboratory `Climate Science'

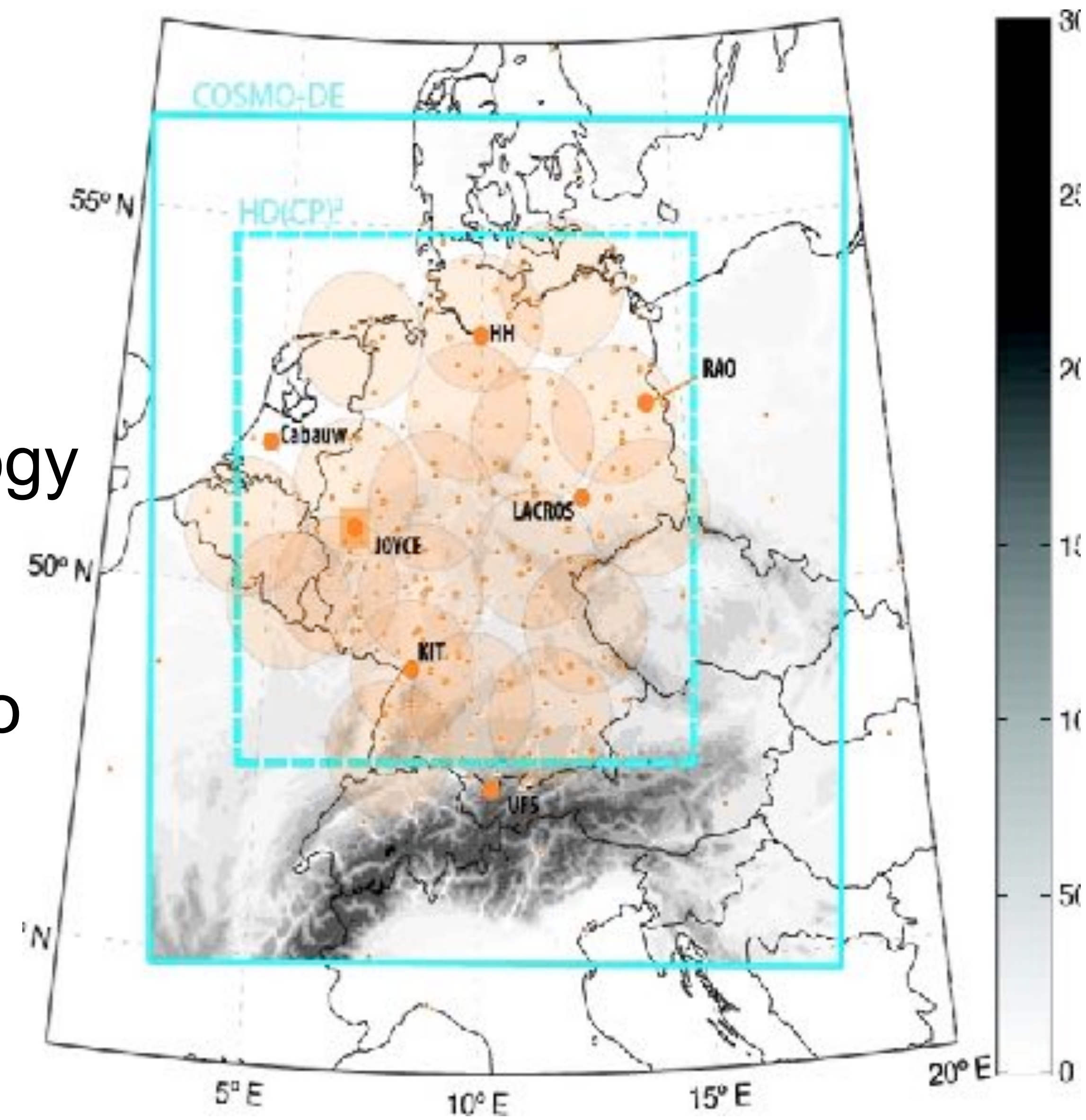
- research focus on atmospheric sciences
- earth system modeling and numerical weather prediction
- data analysis of remote sensing observations (e.g. ESA and NASA satellites)
- performance analysis and code optimization for HPC systems in Jülich



Contact: Lars Hoffmann (l.hoffmann@fz-juelich.de)

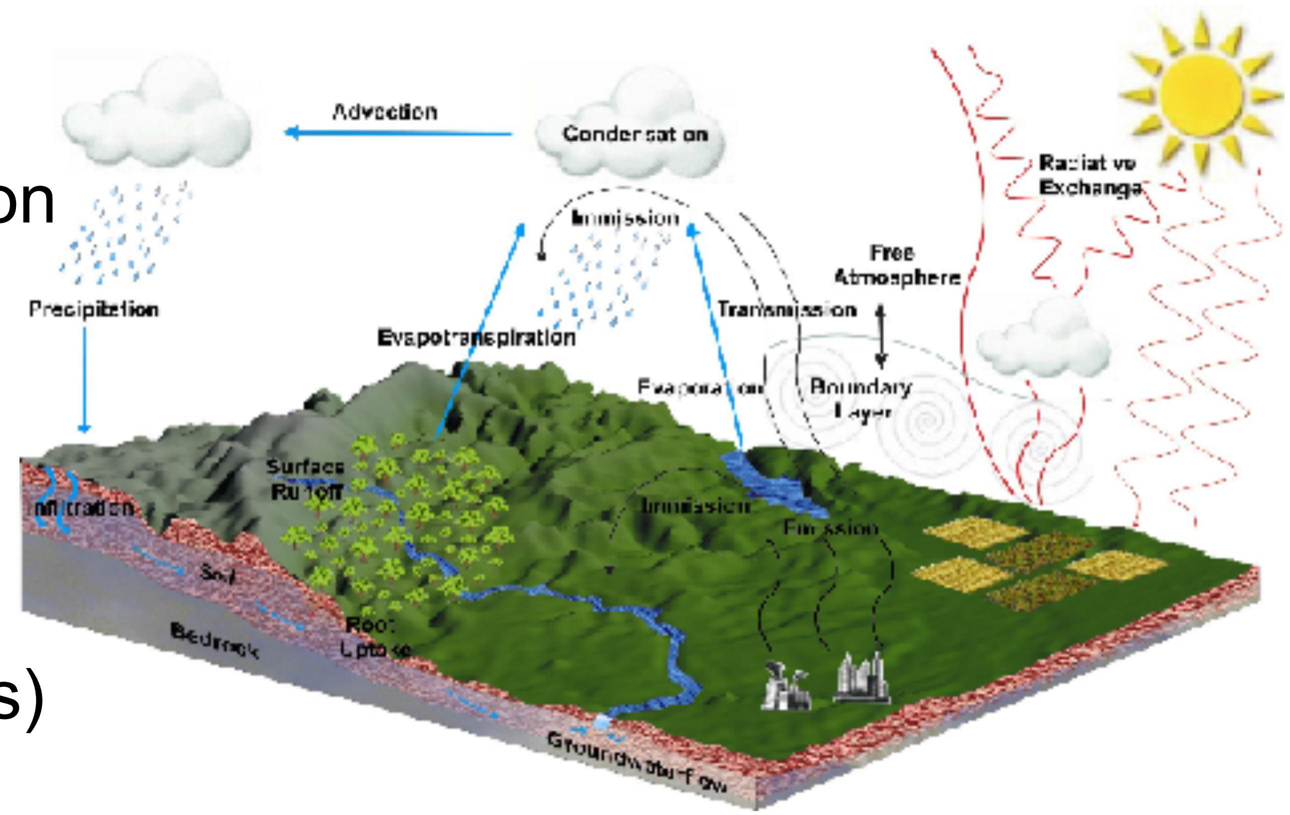
Seminar topic

- **Introduction to current numerical weather prediction techniques**
- Learn about the new ICON model developed by the German weather service DWD and MPI for Meteorology
- ICON is used in Jülich to perform simulations at ultra-high resolution to study clouds and precipitation (www.hdcp2.eu)



Supercomputing in Geosciences

- Research focus on terrestrial water cycle, boundary layer meteorology, regional climate change impacts; multiscale interactions between hydro-, pedo-, bio-, and atmosphere
- Developments towards high resolution massively parallel coupled multi-physics earth system models (www.terrsysmp.org)
- Diverse experiment designs (process- and sensitivity studies, forecasts, climate change projections)
- Porting, optimization, scaling of applications on JSC HPC systems (within www.hpsc-terrsys.de)

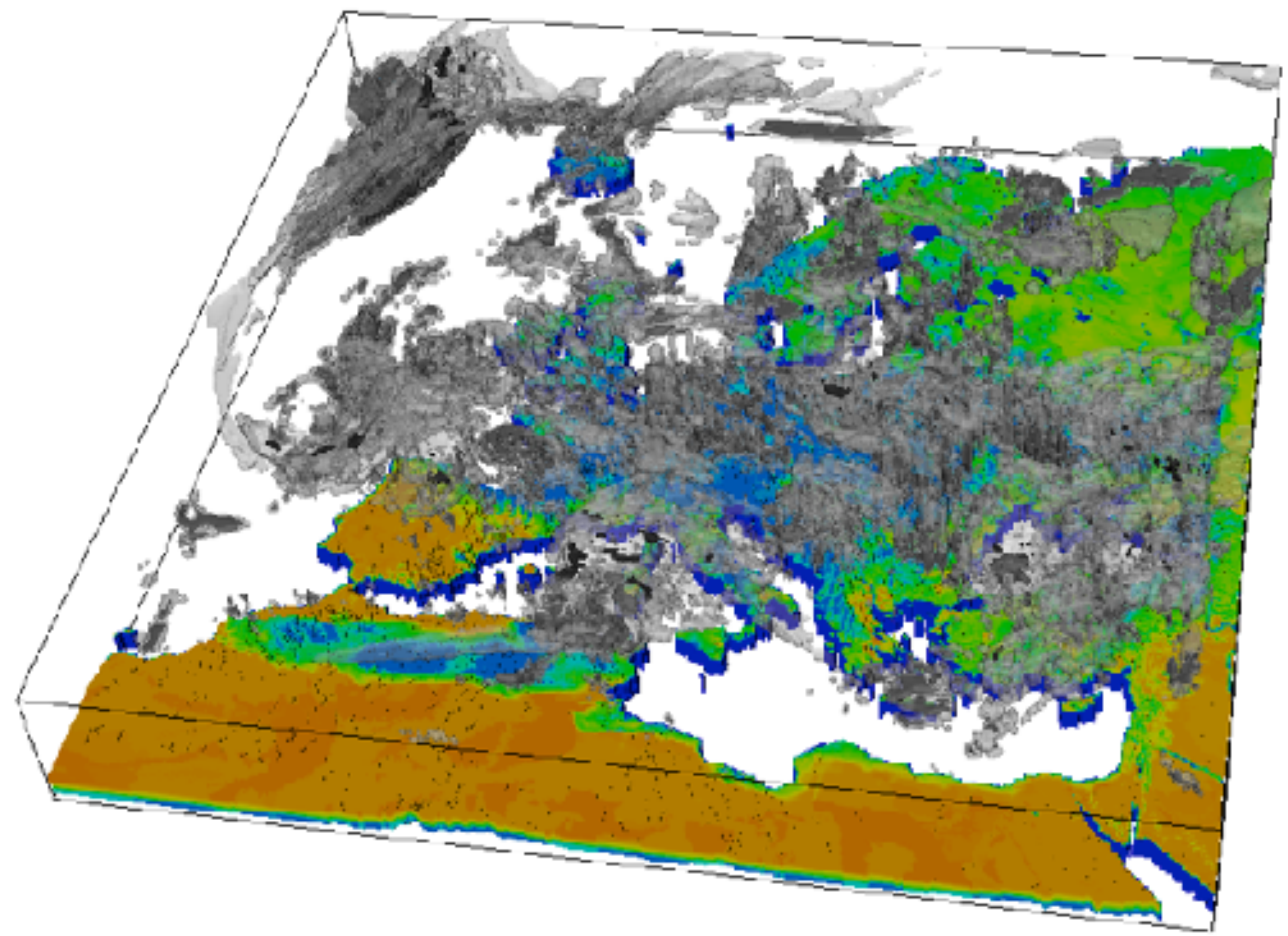


Schematic of interactions in TerrSysMP, resolving real world patterns; shown here is the NRW domain looking from North towards the Eifel

Contact: Slavko Brdar (s.brdar@fz-juelich.de)

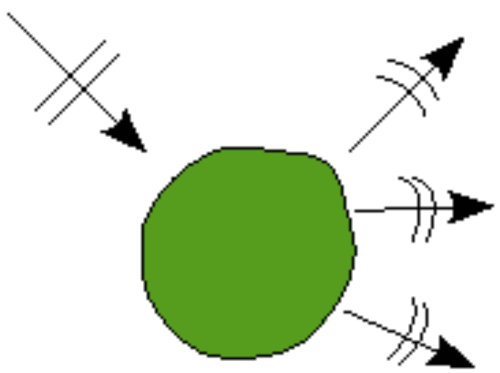
Seminar topics

- Terrestrial water cycle simulations with integrated TerrSysMP
- LSMs and parametrization schemes for convection permitting RCM runs (www.wrf-model.org)
- Very large high resolution continental RCM and HM simulations:
  - added value,
  - HPC and big data aspects (e.g., use of accelerators, mini-apps, in-situ processing) (www.parflow.org)



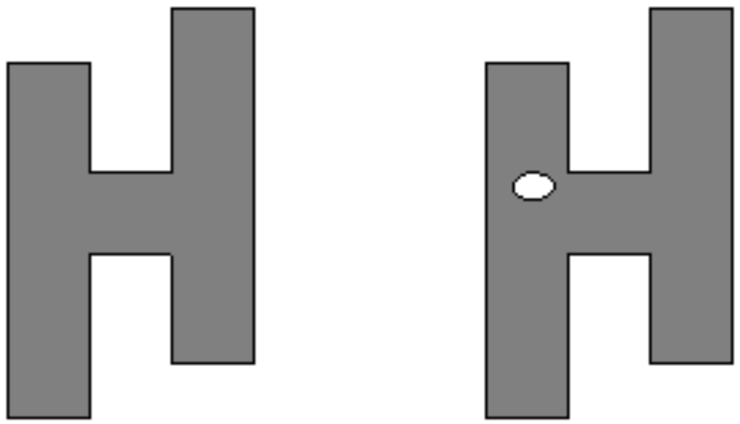
Example of fully integrated Terrestrial Systems Modelling Platform (TerrSysMP, COSMO NWP + CLM LSM + ParFlow HM + OASIS3-MCT) simulation over EURO-CORDEX EUR-11 12km model domain; soil moisture, cloud liquid water.

Interior transmission eigenvalues and nondestructive testing



Is there an incident wave that does not scatter?

Medical imaging



Interior transmission eigenvalues $k_1, k_2, k_3, \ldots$ for a homogeneous component are different from a component with an inhomogeneity.

Nondestructive testing

Contact: Andreas Kleefeld (a.kleefeld@fz-juelich.de)

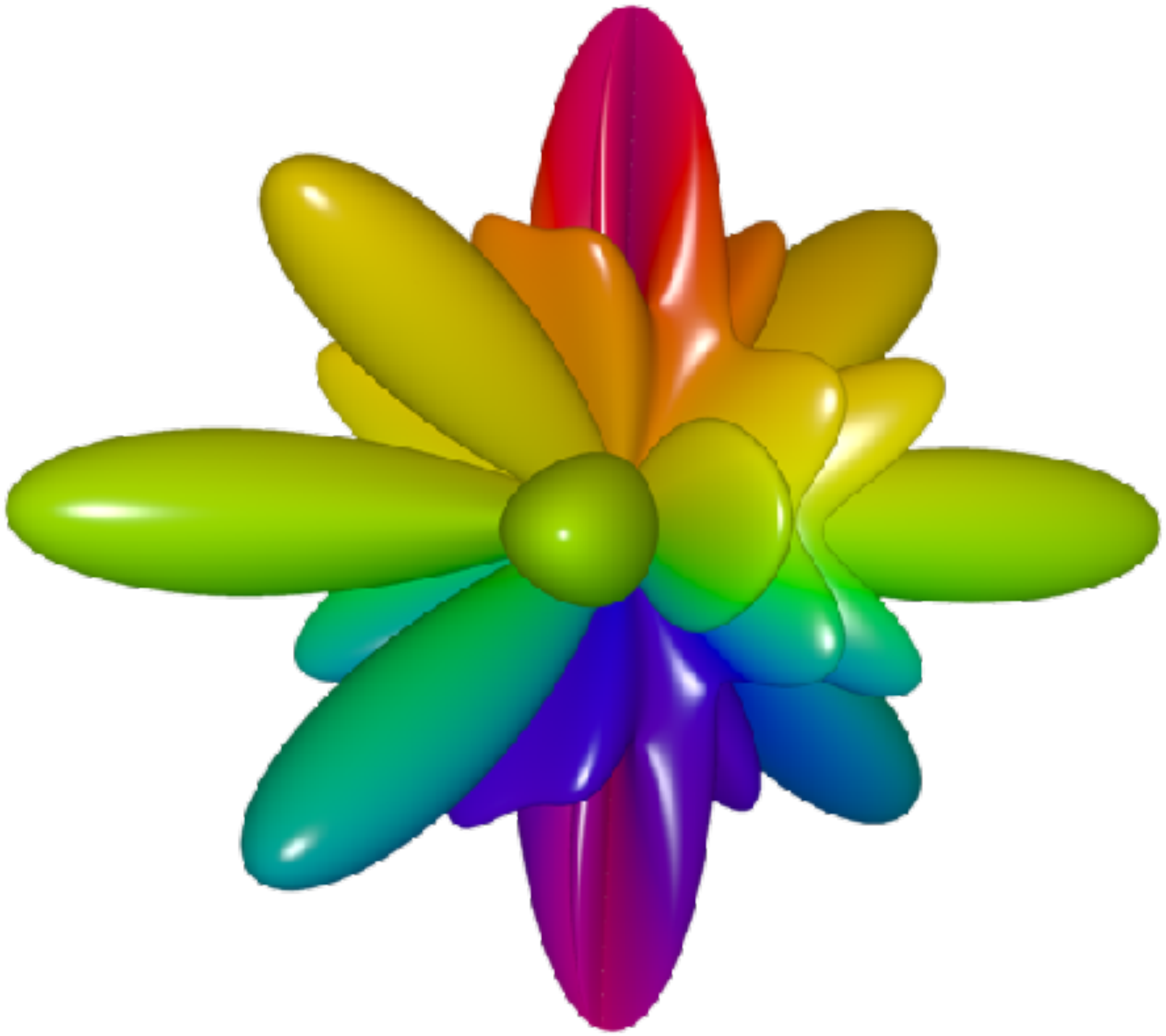
Seminar topics

- Numerical computation of interior acoustic transmission eigenvalues
- Algorithmic improvement
- Optimization for CPUs/GPUs
- Extension to electromagnetic and elastic scattering problem
- Development of imaging method to detect inhomogeneities inside an object using interior transmission eigenvalues

Fast Multipole Toolbox for MD Simulations

Developing HPC software with modern C++

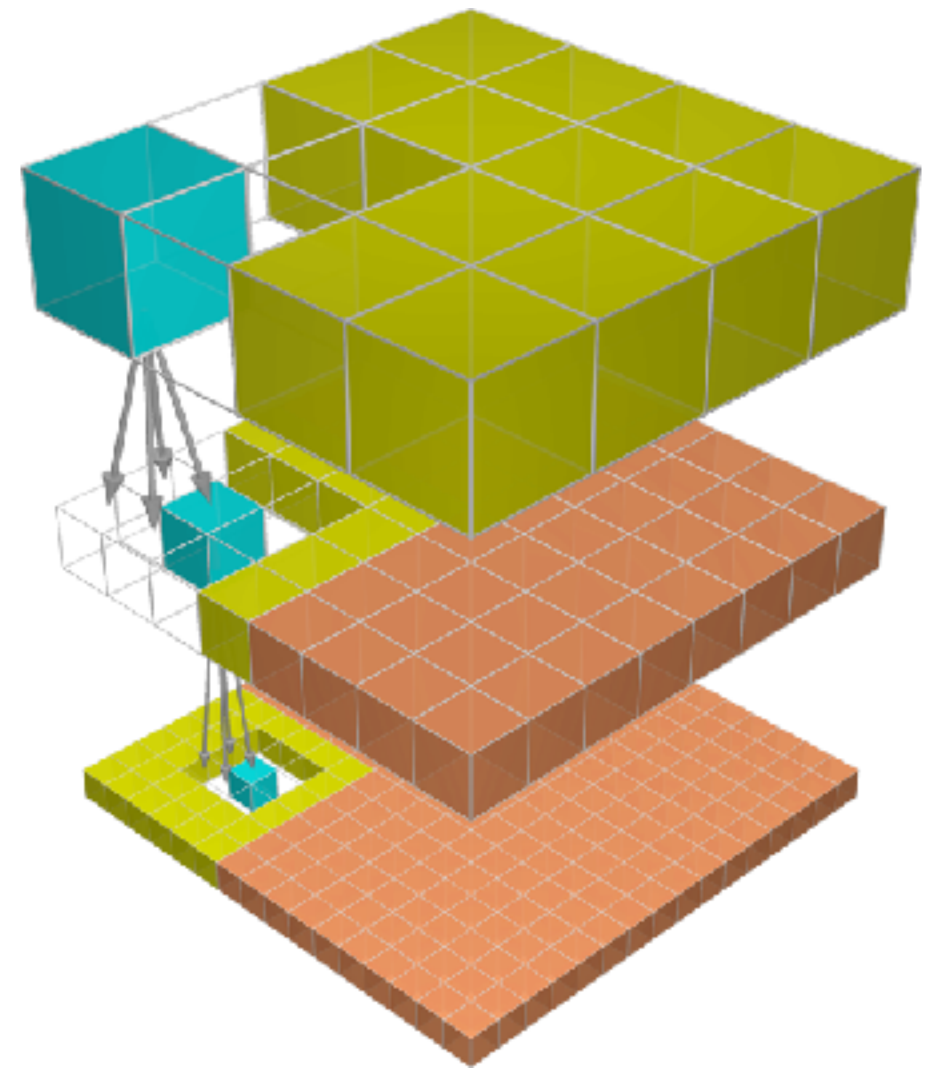
- Development of O(N) solver with a-priori error-control
- Extension of particle-based fast summation algorithms
- Improvement of electrostatics for real-world simulations
- Utilization of modern HPC hardware for the FMM
- Enhancement of open source MD code Gromacs



Contact: Ivo Kabadshow (i.kabadshow@fz-juelich.de)

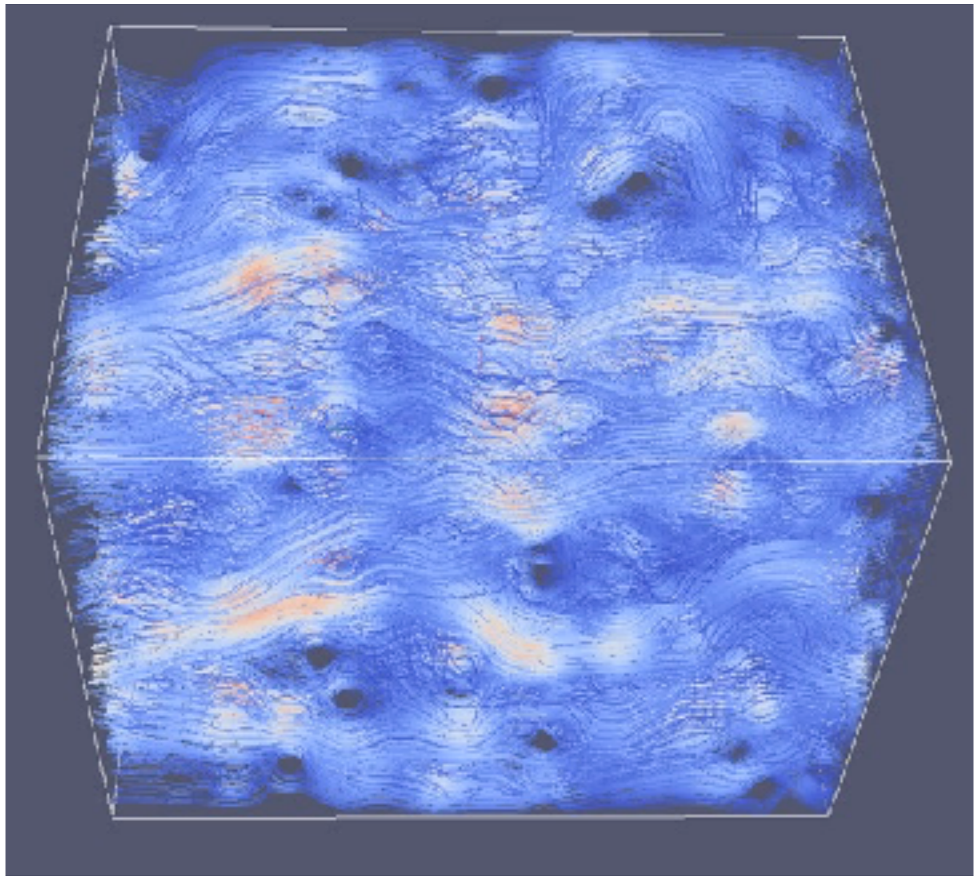
Seminar topics

- Comparison with competitors
- Performance benchmarks
- Visualization of the algorithm
- Algorithmic enhancements
- Optimization for CPUs/GPUs (SIMD/T)
- Graph-based load-balancing with MPI
- Extensions for GPUs & Intel Xeon Phi



Methods and Algorithms for Particle based Simulations in Complex Systems

- Parallel computing of large particle systems in
  - Statistical Physics
  - Soft Matter
  - Materials Science
- Fast Methods and algorithms to reduce memory, numerical complexity and CPU time
- Hybrid programming models
- Hierarchy of Methods
- Multi-scale and multi-level

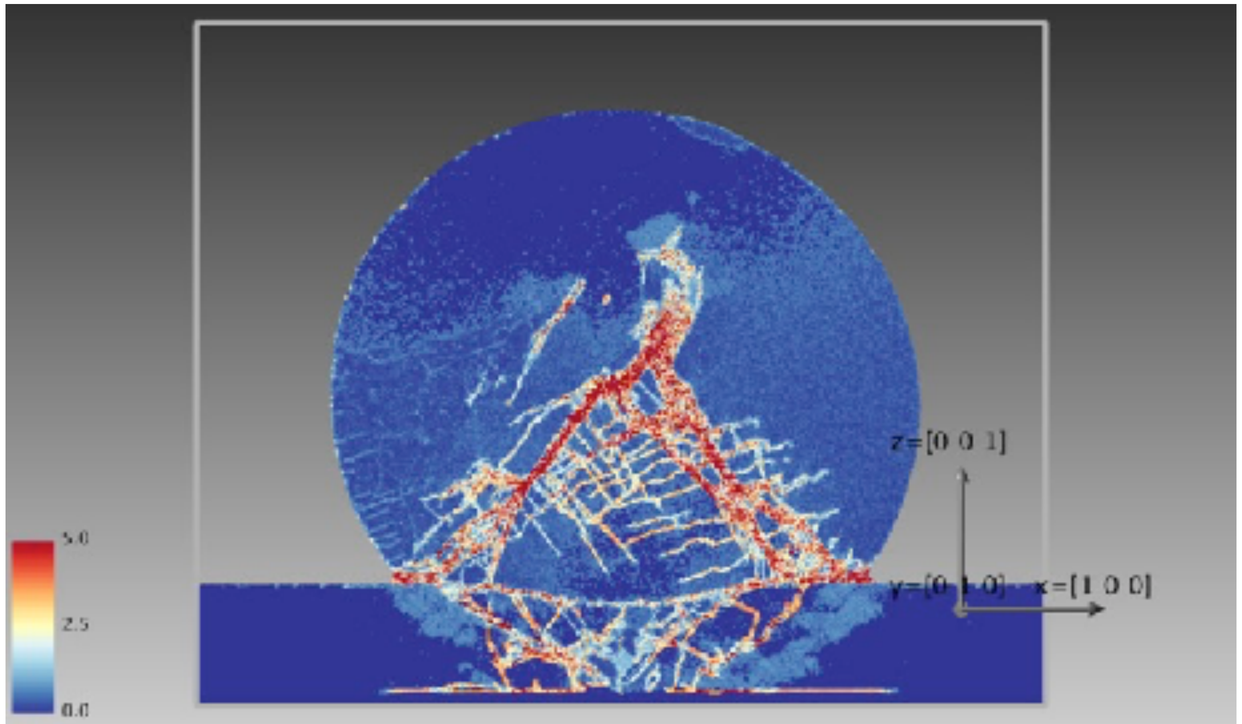


3d-view of a flow field in a gas diffusion layer (stochastic geometry) in a fuel cell. Hydrodynamics is modelled by a particle method. Calculations are done on several 100 processors.

Contact: Godehard Sutmann (g.sutmann@fz-juelich.de)

Seminar topics

- Load-balancing methods for particle simulations in hybrid programming models
- Restraint dynamics of large particle systems to speed up simulations
- Hybrid coupling of elastic-network models and force-field simulations in materials scienceAdaptive resolution simulations of complex systems
- Survey of particle based hydrodynamic methods



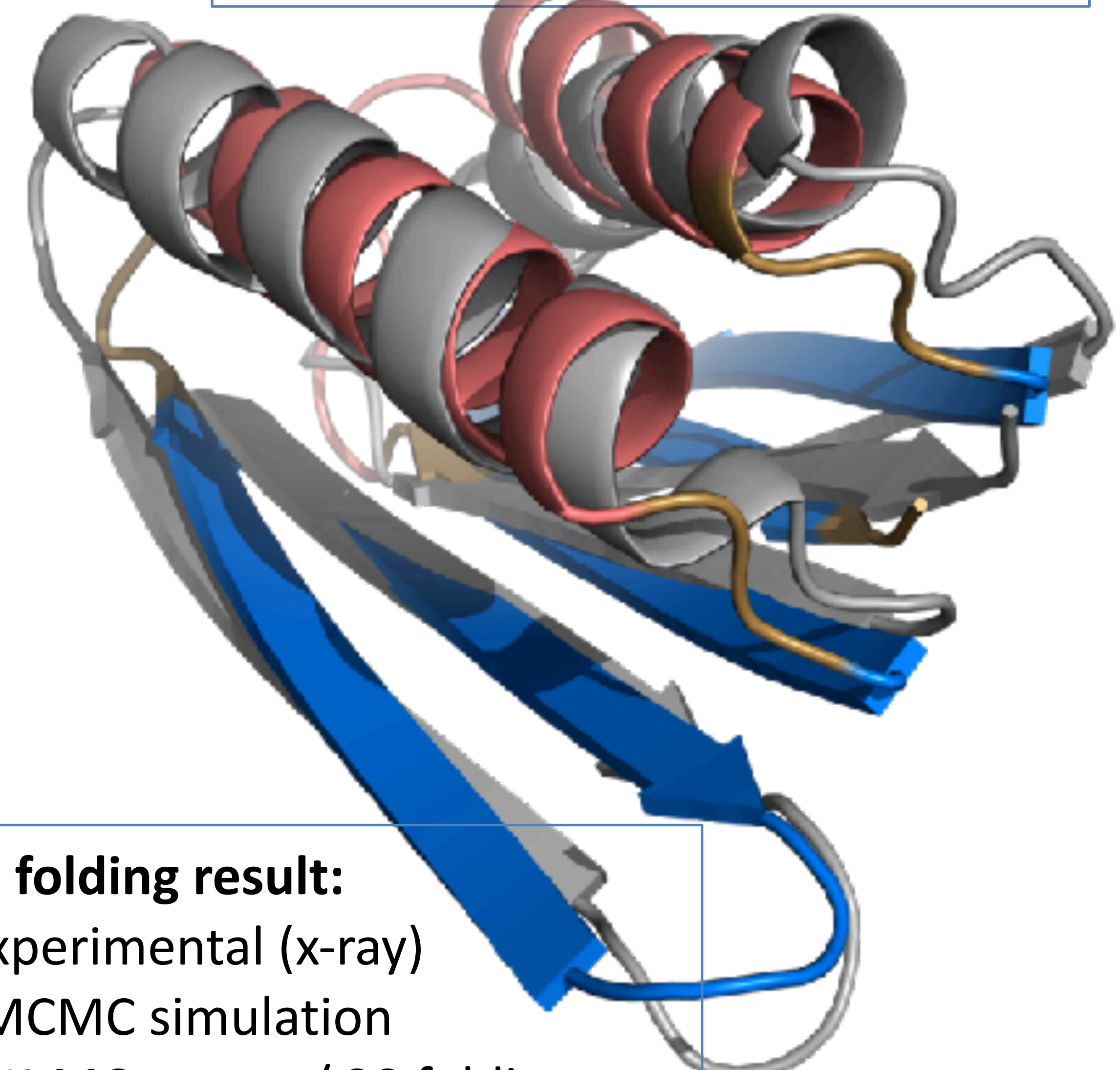
Molecular dynamics simulation of YSZ nano-particle deposition in a plasma spray experiment for thermal barrier coatings. Several million particles are simulated including long-range electrostatic interactions.

Protein folding and structure predictions


PROTEINS
Folding of Top7 in unbiased all-atom Monte Carlo simulations
Sandipan Mohanty,* Jan H. Meinke, and Olav Zimmermann

Developing HPC methods for:

- **Simulation** of protein folding and peptide aggregation (Markov chain MC, Markov state models)
- **Prediction** of 3d protein structure from its sequence alone (machine learning, simulation)

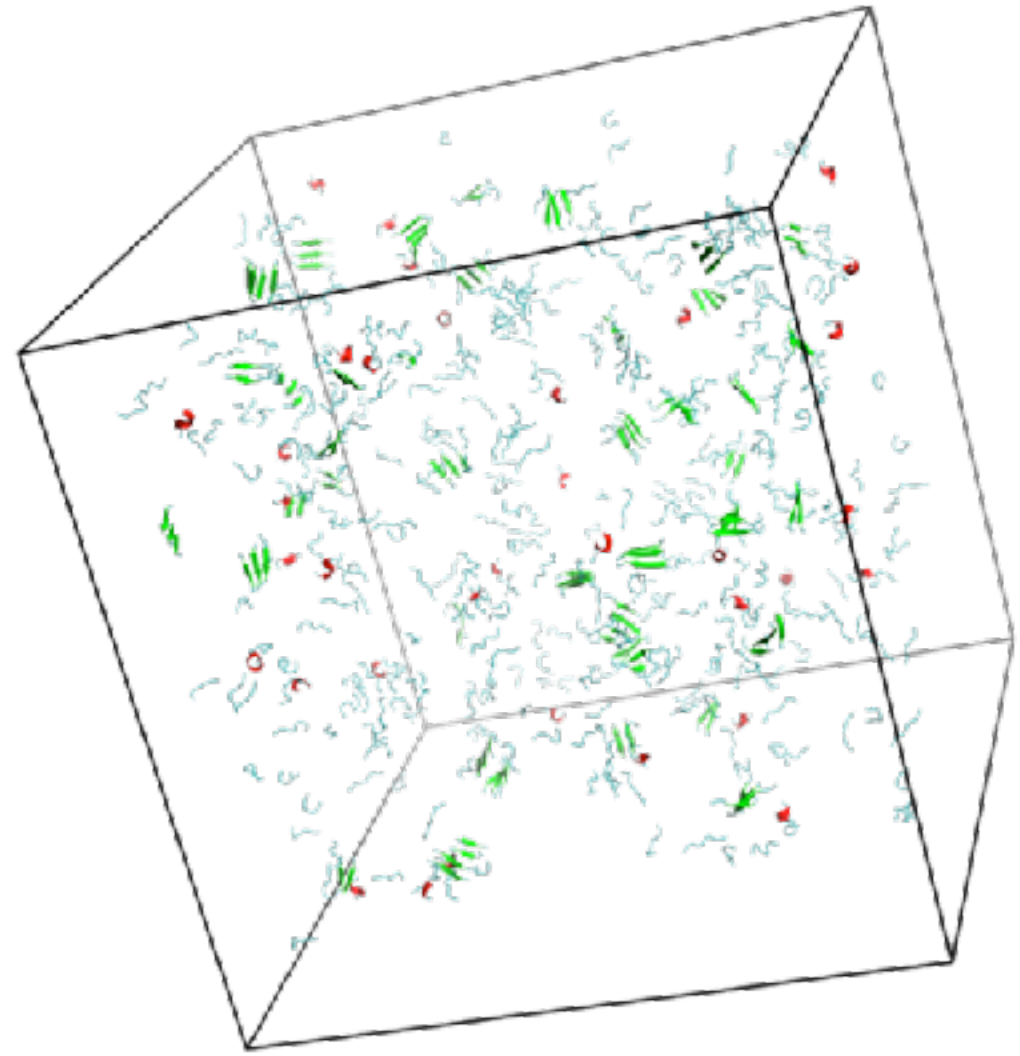


Protein folding result:
gray: experimental (x-ray)
color: MCMC simulation
1.4 · 10^{13} MC moves / 30 foldings

Contact: Olav Zimmermann (olav.zimmermann@fz-juelich.de)

Seminar topics

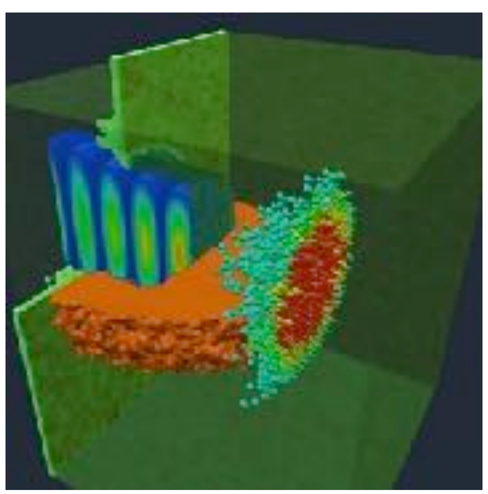
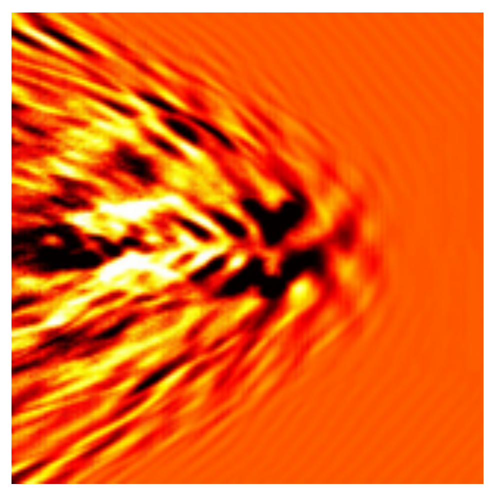
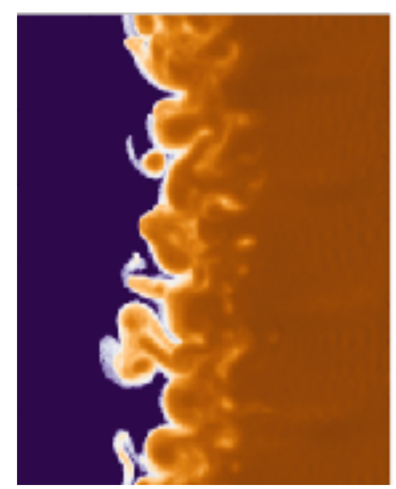
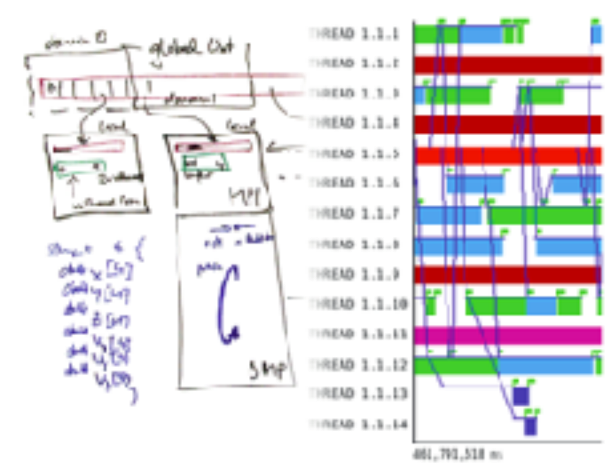
- Effect of pH on proteins (structure, stability, binding)
- Thermal vs chemical denaturation of proteins
- Systematic errors in the protein data bank (annotations, identification)
- Experimental results on protein folding dynamics (foldamers, speed, order, comparison to phi analysis)



Studying peptide aggregation (pot. linked to neurodegenerative disease):
Large scale MCMC simulation
(500 chains, -> full aggregation
5.4 · 10^{13} MC moves / 1000 runs

Computational Plasma Physics

- Particle acceleration with high-power lasers
- Advanced light sources (THz to x-ray)
- Dynamics of plasma boundary layers (eg in fusion devices)
- Novel particle-based algorithms

Contact: Dirk Brömmel (d.broemmel@fz-juelich.de)

JÜLICH
FORSCHUNGSZENTRUM

Seminar topics

1. Survey of laser-based ion acceleration
2. Attosecond light sources
3. Interactive particle simulation with Python
4. Tree codes in astro- and plasma physics
5. Load balancing and over-decomposition in Particle-in-Cell codes

Quantum Information Processing

Gate-based quantum computing & quantum annealing

Simulator for large-scale multi-qubit systems

Machine learning for single-event "quantum" experiments

QIP JSC

48 qubit Pen- and Paper Quantum computer: world record in 2018

Study of environmental effects on operation of ideal quantum computer

Testing quantum fault tolerance protocols

Simulation on and of quantum computers and quantum annealers for benchmarking purposes and for testing applications

Quantum algorithms

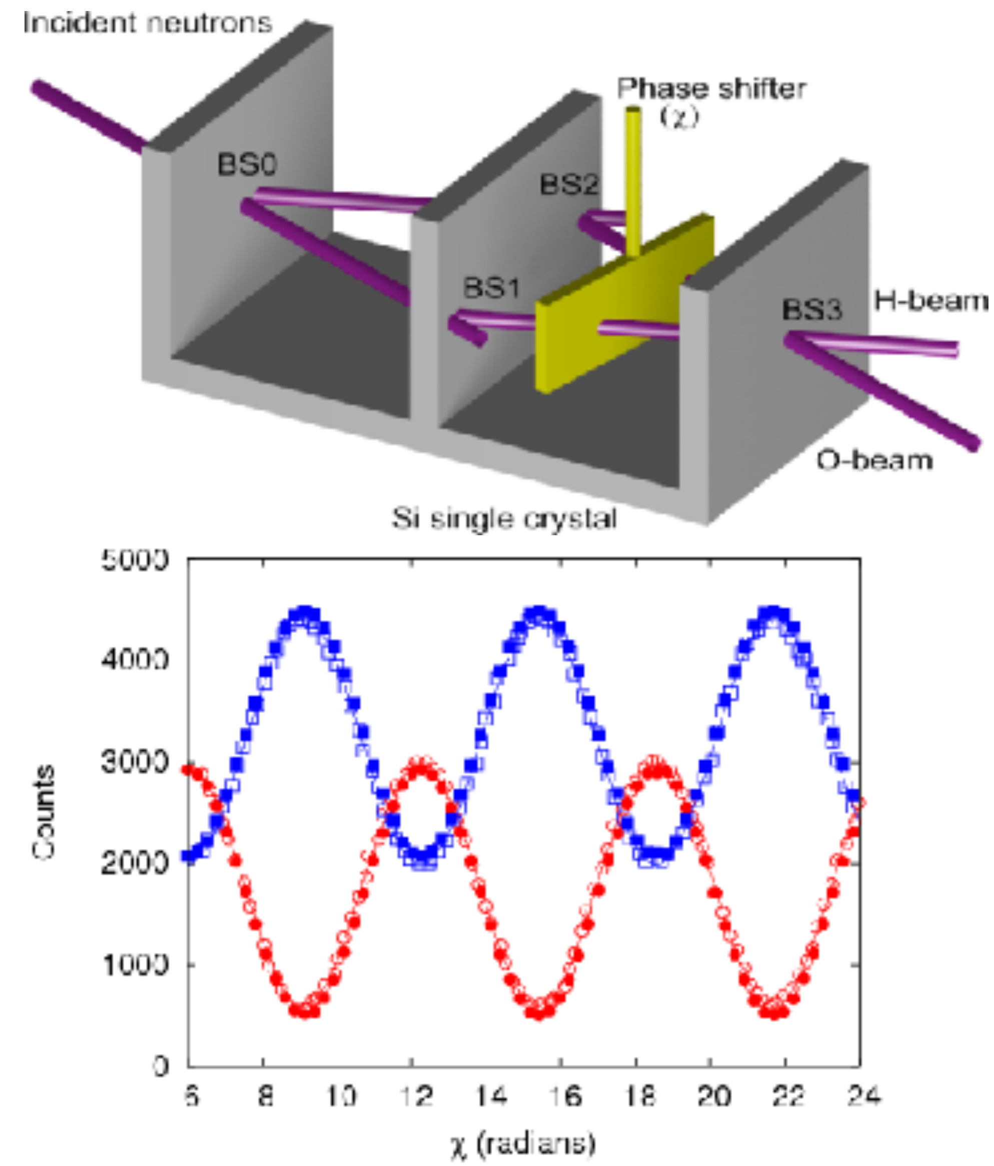
Reproduces the statistical distributions of quantum theory by modeling physical phenomena as a chronological sequence of single events

Applications: interference, entanglement, quantum cryptography, …

Contact: Kristel Michielsen (k.michielsen@fz-juelich.de)

Seminar topics

- Simulation of gate-based quantum computer & quantum annealer
- Quantum algorithms
- Simulations on gate-based quantum computers (e.g. IBM Quantum Experience)
- Simulations on the D-Wave quantum annealer (optimization, machine learning)
- Machine learning for single-event "quantum" experiments: Simple rules define discrete-event processes that may lead to the behavior observed in experiments such as e.g. single neutron experiments (see figure on the right)

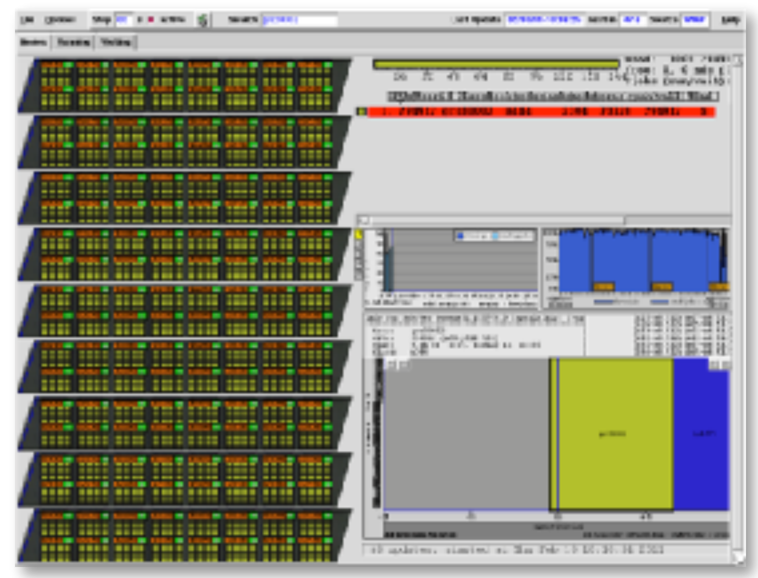


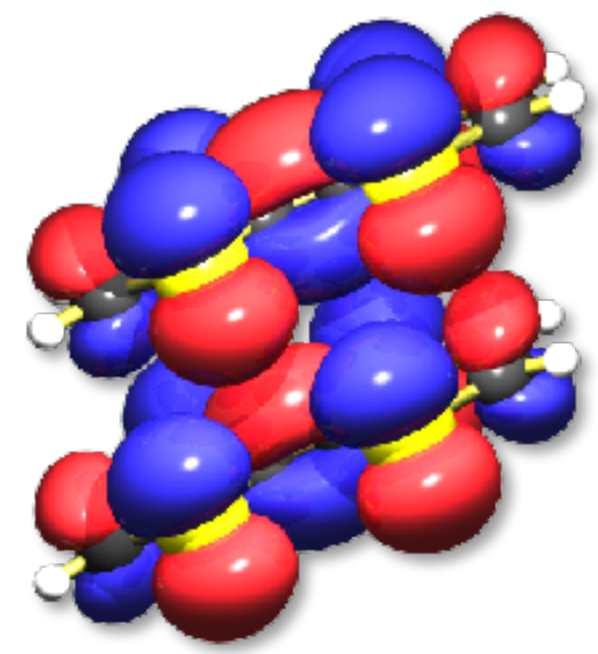
Example: Single-neutron interferometry experiment

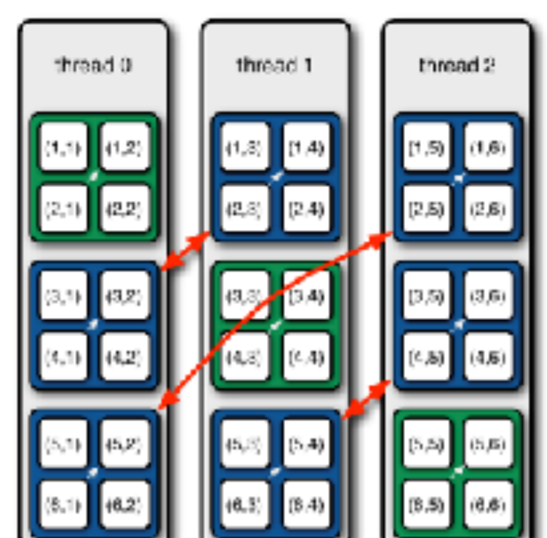
*Circles: O-beam, squares: H-beam. Solid symbols: **simulation results**; open symbols: **experimental data***

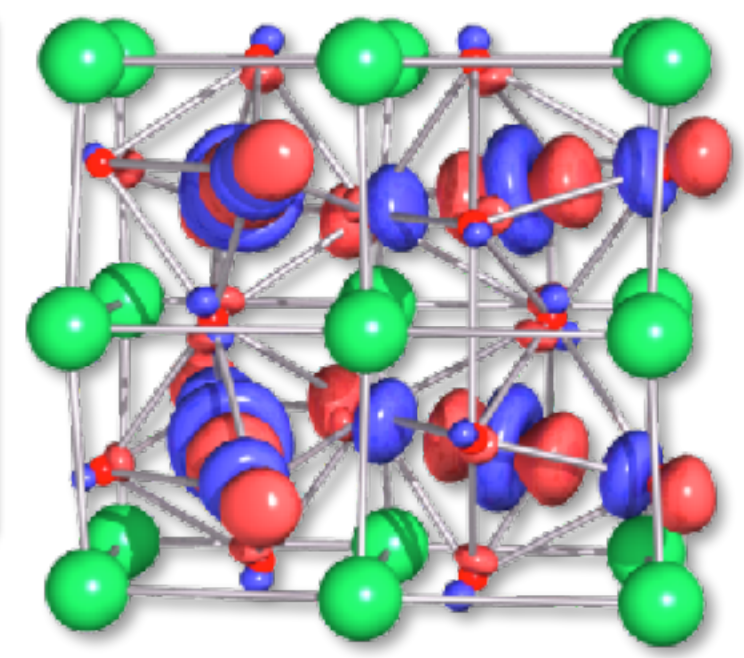
Computational Materials Science

- Understanding materials properties & design
- Modeling of real materials: as simple as possible, as complex as necessary
- The Many-Body Problem: computational complexity, emergent properties
- Massively parallel simulations, understanding of mechanisms





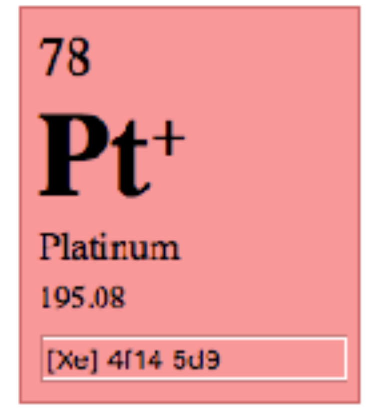


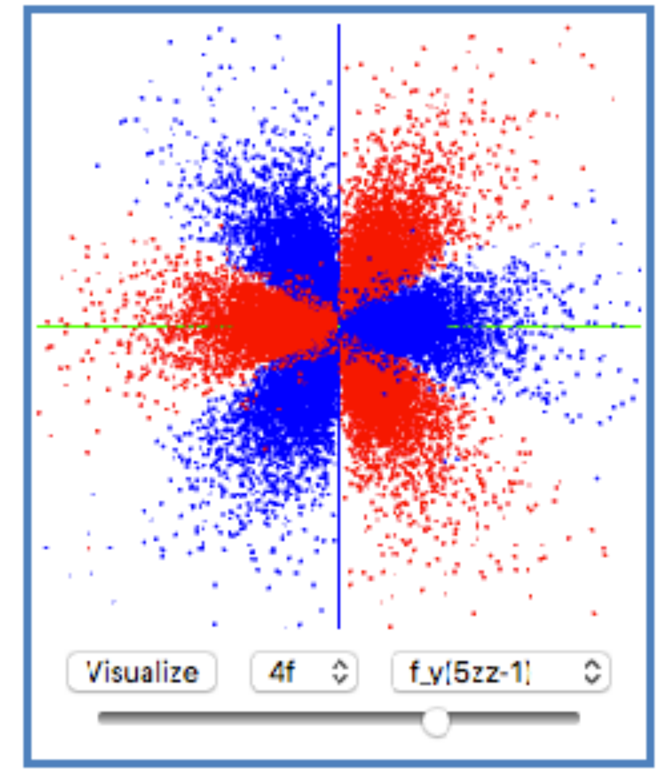


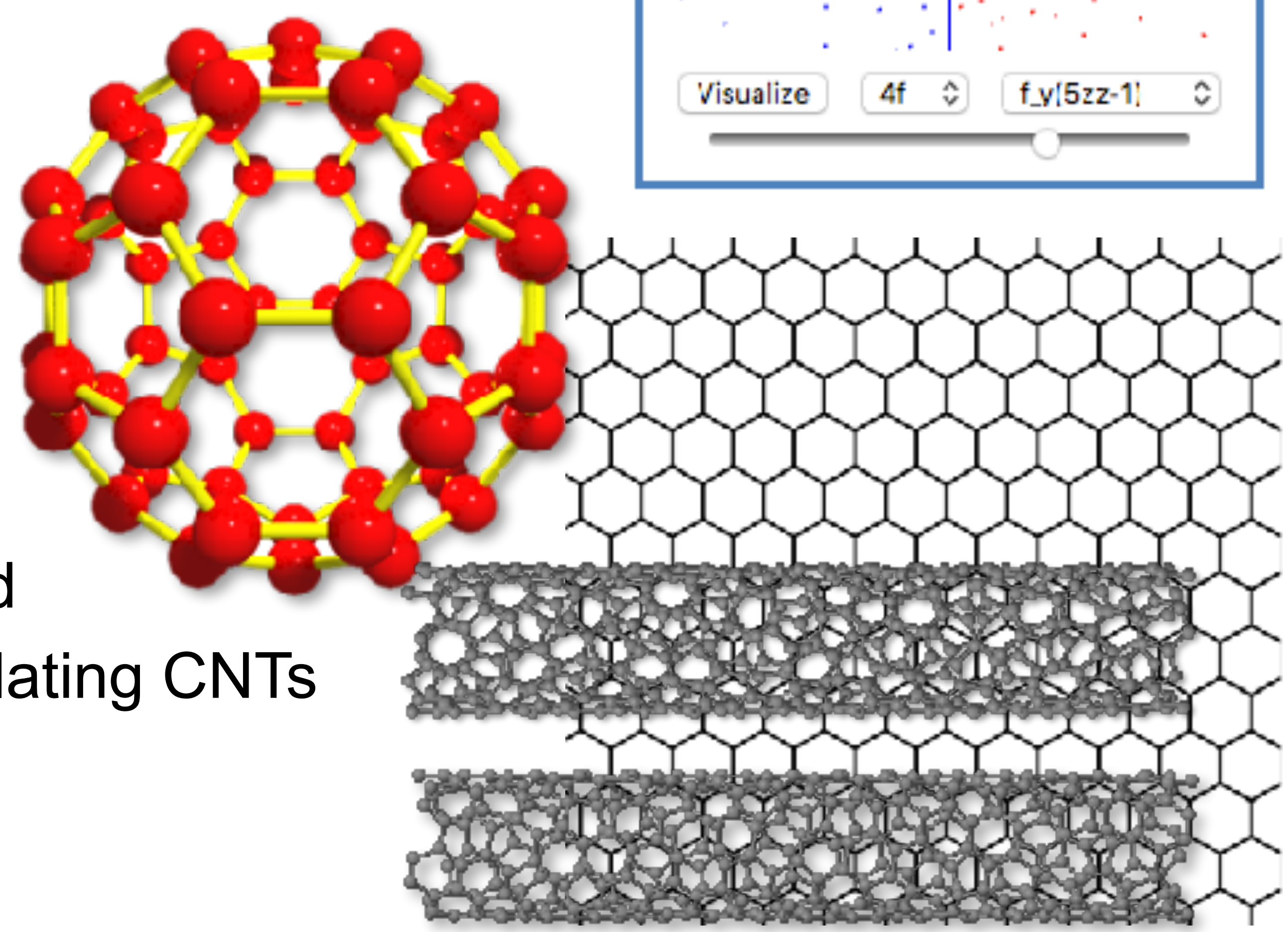
Contact: Erik Koch (e.koch@fz-juelich.de)

Seminar topics

- Atomic structure in DFT: self-consistent calculations
  - Integrate Schrödinger equation
  - Self-consistent electrostatic Hartree potential
  - Exchange-Correlation terms
- Bonding in carbon structures
  - Hückel method
  - Hamiltonian matrix
  - Buckminsterfullerenes, graphene, carbon nanotubes, graphite, diamond
  - How to distinguish metallic from insulating CNTs







www.fz-juelich.de/ias/jsc/gsp

GUEST STUDENT PROGRAMME 2019

JÜLICH SUPERCOMPUTING CENTRE

5 August 2019 – 11 October 2019

Closing Date 24 March 2019

YOUR ASSIGNMENT

Join our scientists for a 10 week programme and get in touch with cutting-edge research on world-leading supercomputers in the fields of