Mitglied der Helmholtz-Gemeinschaft

# Jülich Supercomputing Centre

**CHANGES**

**CHinese-AmericaN-German cyberinfrastructure and E-Science workshop**

**3-9-2012**

# Supercomputing @ Jülich: Mission and Objectives

## Mission

Enable scientists and engineers to solve grand challenge problems of highest complexity in science and engineering in collaborative infrastructures by means of supercomputing and Grid technologies

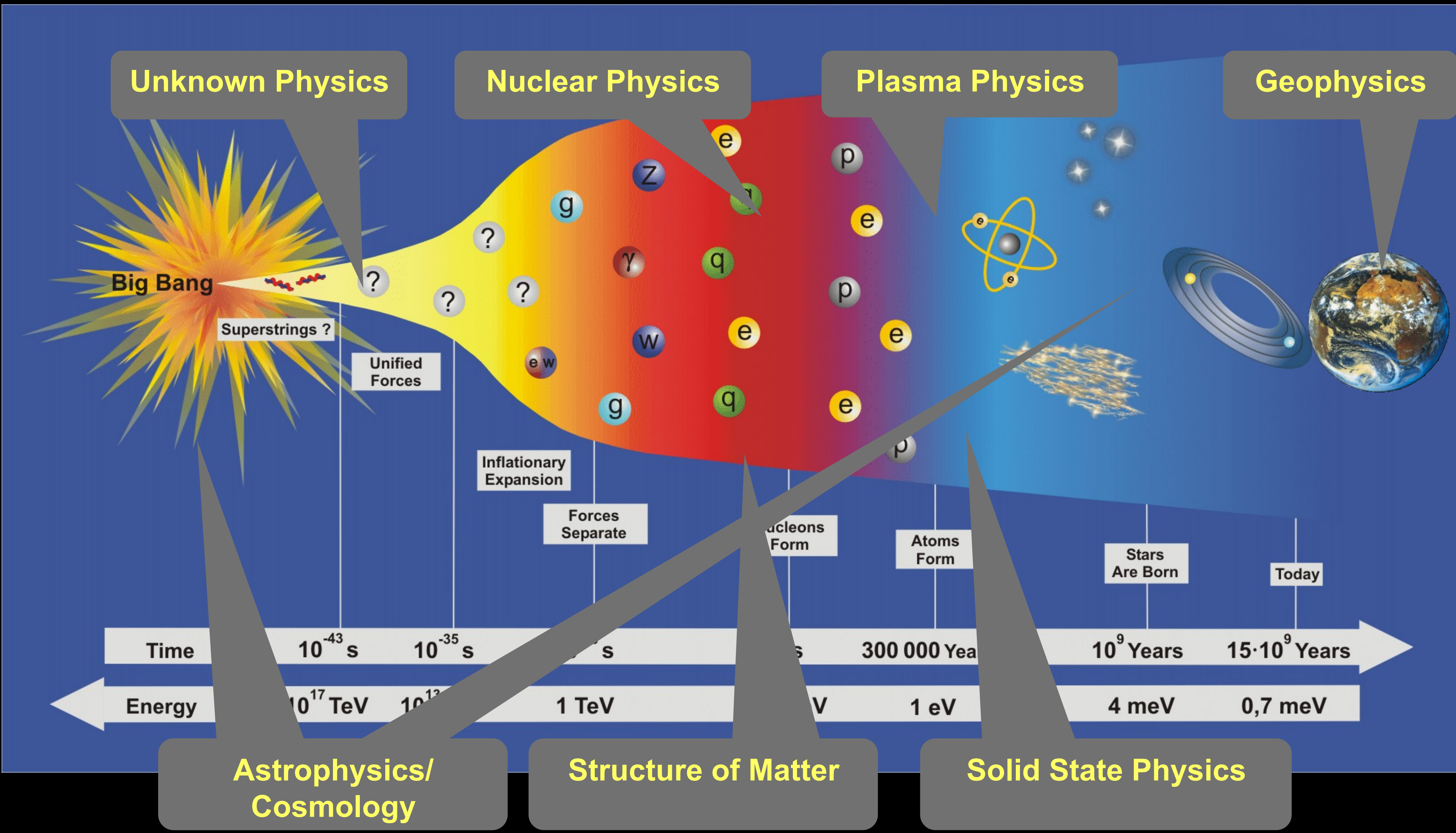
## Objectives

Provide supercomputer resources of the highest performance class and enable their most effective usage

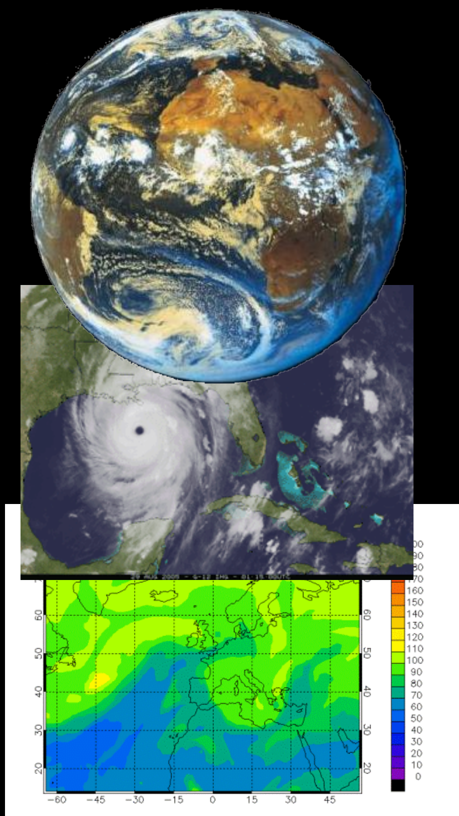
Provide large-scale data resources and services of the highest quality worldwide

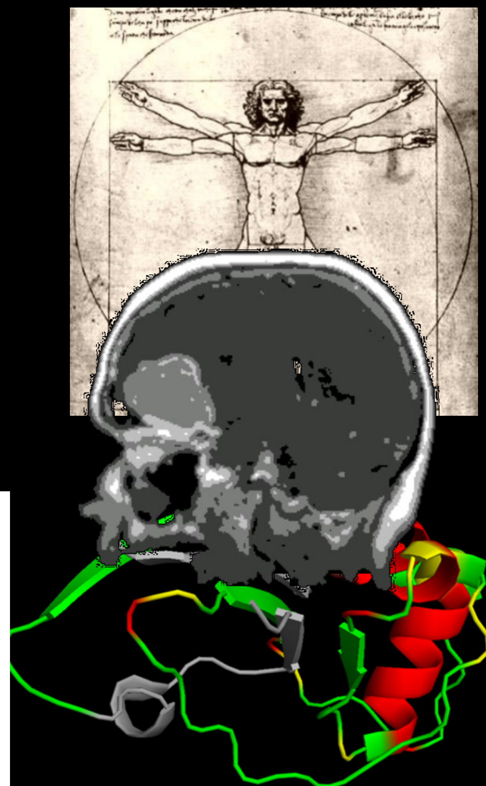
Develop leading European supercomputing centre as user facility with broad horizontal profile (since 2010)

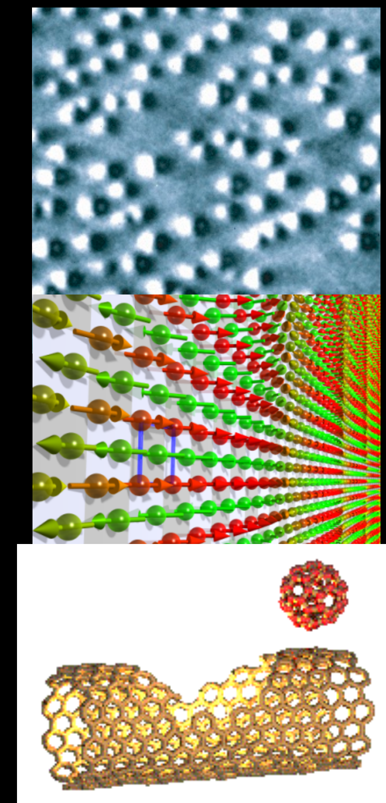
# Computational Challenges in Fundamental Sciences

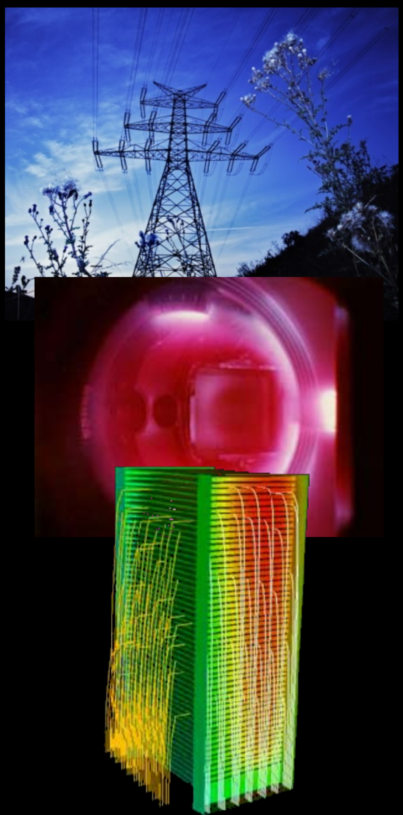


# Challenges in Applied Sciences









**Environment**
Climatology
Pollution

**Aging Society**
Medicine
Biology

**Materials**
Spintronics
Nano-Technology

**Energy**
Plasma Physics
Batteries

# Helmholtz Programme Supercomputing: Strategic Significance of Supercomputing

## Computational Science and Engineering

- New ways of insight and evolution for scientific research
- Give boost to industrial innovation

## Simulation

- Understanding the most complex scientific and eng. phenomena
- Anticipation of the future, fighting uncertainties

## Supercomputers

- Most powerful locomotives of simulation science
- Challenging from design, procurement, operation to exploitation

## Grid Technologies and Infrastructures

- Integrate the full supercomputing and data ecosystem
- Create collaborative environments for simulation science

# Programme Structure

## Topic 1

**Computational Science and Mathematical Methods**

## Topic 2

**Grid Technologies and Infrastructures**

## Large Scale Facility

**Supercomputer development, procurement, operation, technical support and training**

# Large Scale Facility: Supercomputer

## Supercomputer Operation for


- **Centre** – FZJ,
- **Regional** – JARA
- **Helmholtz & National** – NIC – GCS
- **Europe** – PRACE, European Communities (CECAM, EFDA, HBP...)

## Interconnects / Networks

- **FZJ, D-Grid, DEISA, PRACE, HBP**


## Application Support

  - User support; coordination with SimLabs
  - Scientific Visualization
  - Peer review support and coordination

## Technology Development


  - Community data management service
  - Exascale Laboratories:
    EIC and ECL → EU Project DEEP

# Computational Science and Mathematical Methods

## Simulation Laboratories

- Biology
- Molecular Systems
- Plasma Physics
- Climate Science
- Fluid & Solid Engineering
- (Nuclear and Particle Physics)

## Cross-Sectional Teams

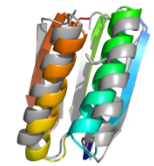
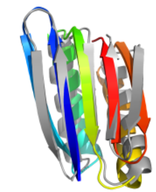
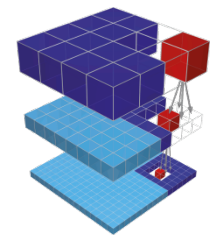
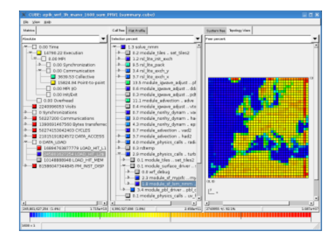
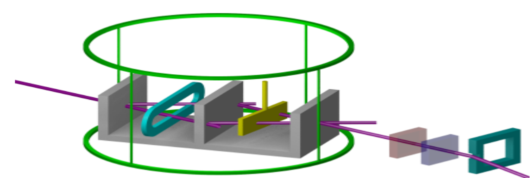
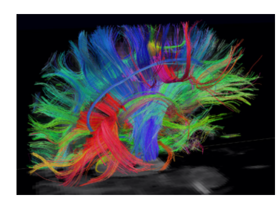
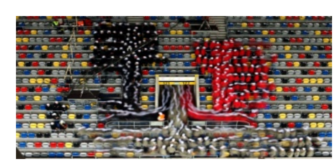
- Mathematical Methods & Algorithms
- Application Optimization
- Parallel Performance Analysis

## Research Groups

- Quantum Information Processing
- Materials Physics (NIC Group)

## HGF Portfolio Topics

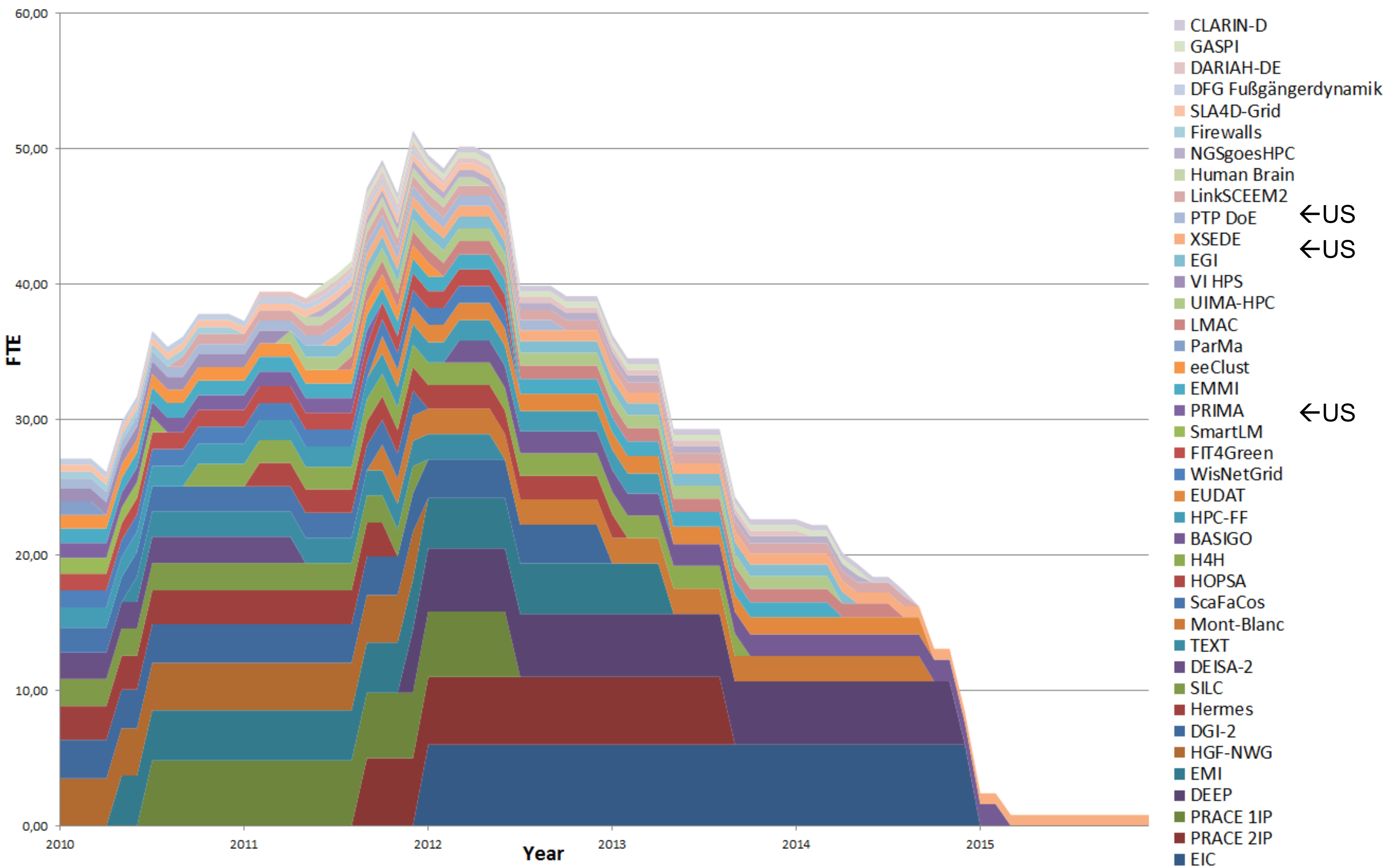
- Supercomputing and Modelling for the Human Brain
- Safety Research

# Grid Technologies and Infrastructures

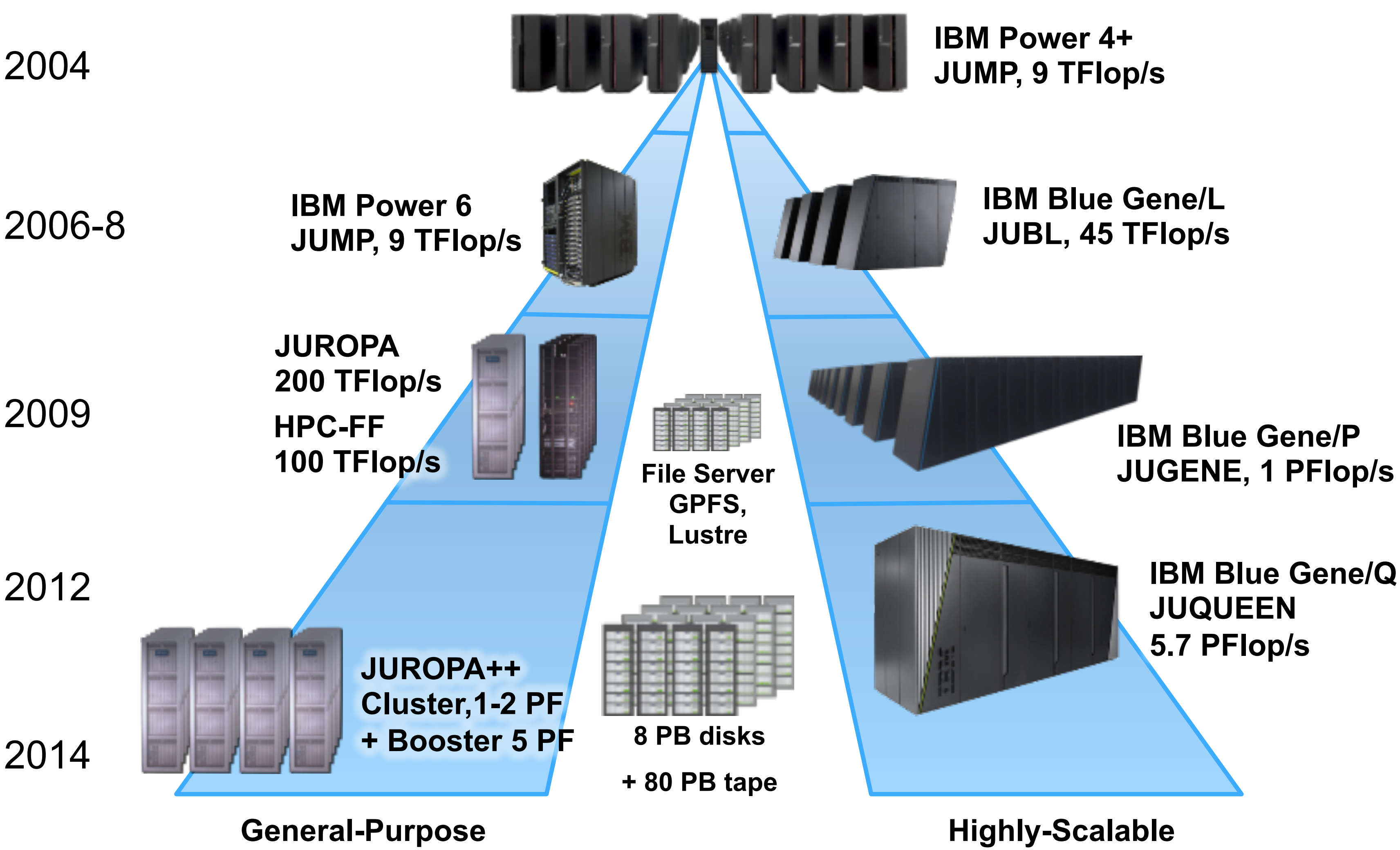
- Middleware Development: UNICORE
- Interoperability through open standards
- Application support and advancement
- e-Infrastructure operations and support
- Data management, access, transfer, control, and governance
- Distributed systems research
- Dissemination, education, and training

# 3rd Party Funded Projects (Head Count)



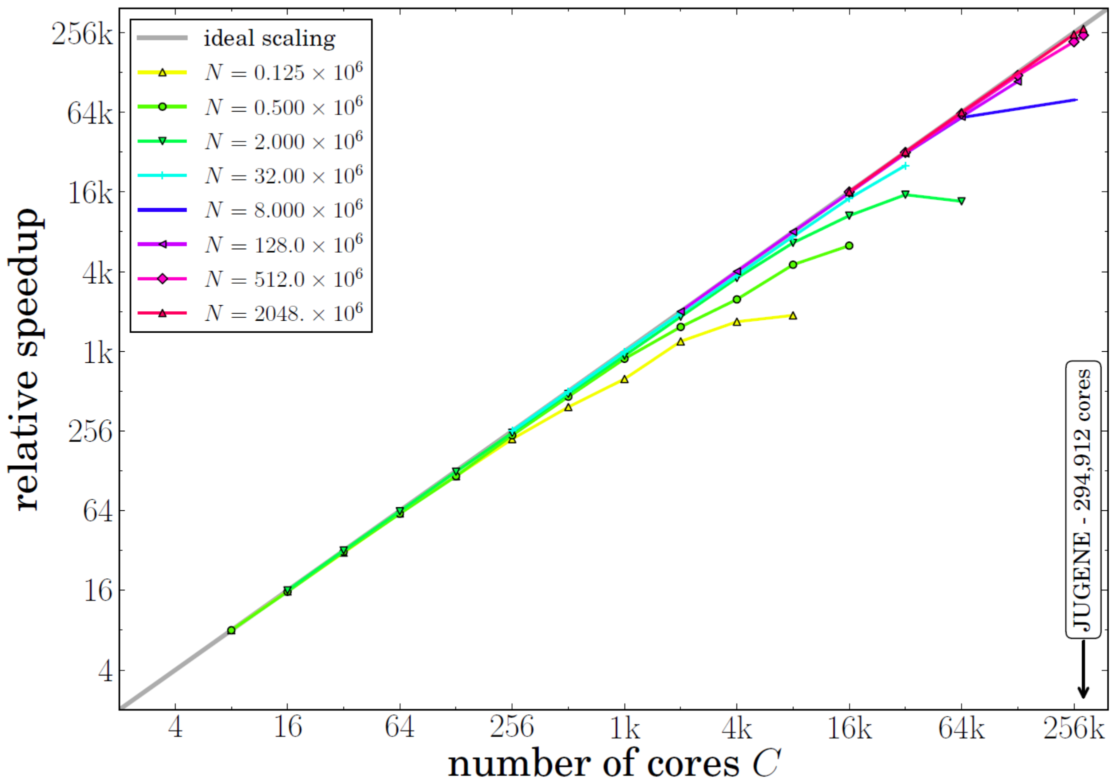
# SUPERCOMPUTER STRATEGY 2010-2015-2020

# The Jülich Dual Scalability Concept



# JUGENE

# Scalability unltd.? MD code PEPC for modelling strongly coupled plasmas



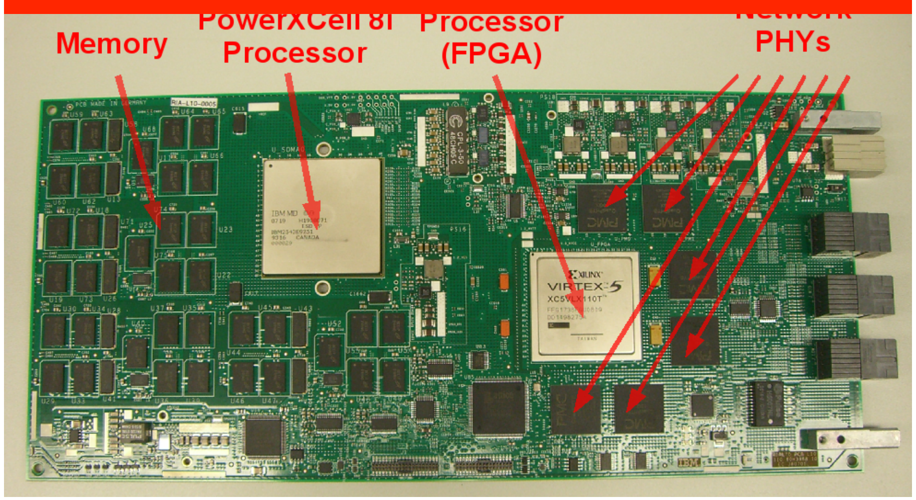

- Hybrid O(N log N) tree algorithm to compute forces (MPI + pthreads)
- Parallel scaling to 288k cores of BlueGene/P
- Multi-billion *ab-initio* simulation with charged particles

*Winkel, Speck, Hübner, Arnold, Krause, Gibbon, Comp. Phys. Commun. (accepted, 2011)*

# JUROPA + HPCFF (5/2009 – 308 TF)


# QPACE (made in Europe, 2009)

**No 1 in Green TOP 500 from 2009 to 2010**




## Massively parallel architecture for LQCD

- 4+4 racks installed in 2009
  = 400 SP TFlops (peak)

## Developed by an academic-industrial team (SFB/TR 55)

- U Regensburg
  U Wuppertal
  U Ferrara/Milano
  FZJ, DESY
  Industrial partner: IBM

## Concept

- Fast commodity processor
  = IBM PowerXCell 8i
- Custom network
  → custom network processor
- Custom system design

# JUQUEEN (2012)

## Jülich's Novel Scalable Petaflop System (PoF funded)

### IBM Blue Gene/Q

- IBM PowerPC® A2
- 1.6 GHz
- 16 cores per node
- 8 racks, 131072 cores
- 1,7 PF peak, 1.4 PF Linpack
- 128 TByte main memory
- Global Parallel File System
  - *8 PByte online disk*
  - *up to 80 PB tape*
  - *full end-to-end data integrity*
  - *fast rebuilt-technology*
- 5D network
- Production start: May 16, 2012

**Extension to 20 (28) racks in September 2012 (December 2012)**

# Dynamical Exascale Entry Platform

## FP7-ICT-2011-7 Integrated Project No. 287530

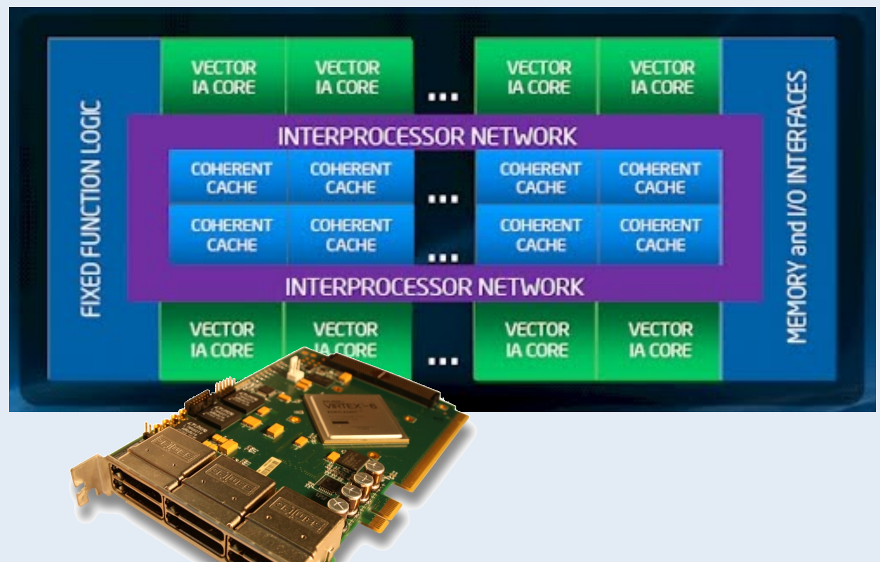
- **16 partners from 8 countries:**
- **3 PRACE Hosting Members**
- **5 industry partners**

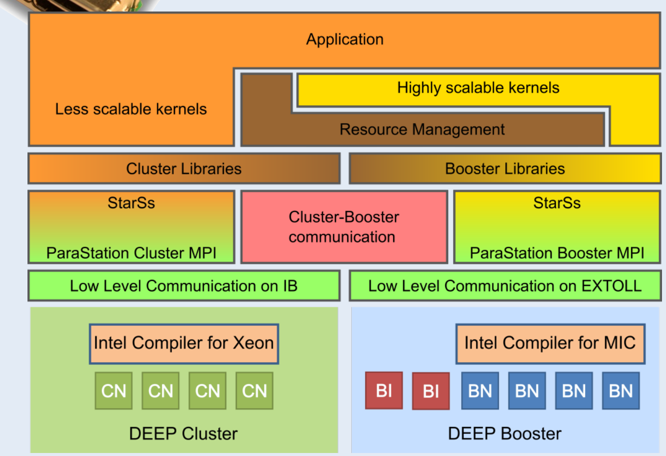
**Knights Corner Processor**
**EXTOLL network**
**ParaStation cluster operation**
**StarSS programming env.**

- **Start: 1st Dec 2011**
- **Duration: 3 years**
- **Budget: 18.5 M€ (8.03 M€ funded by EU)**

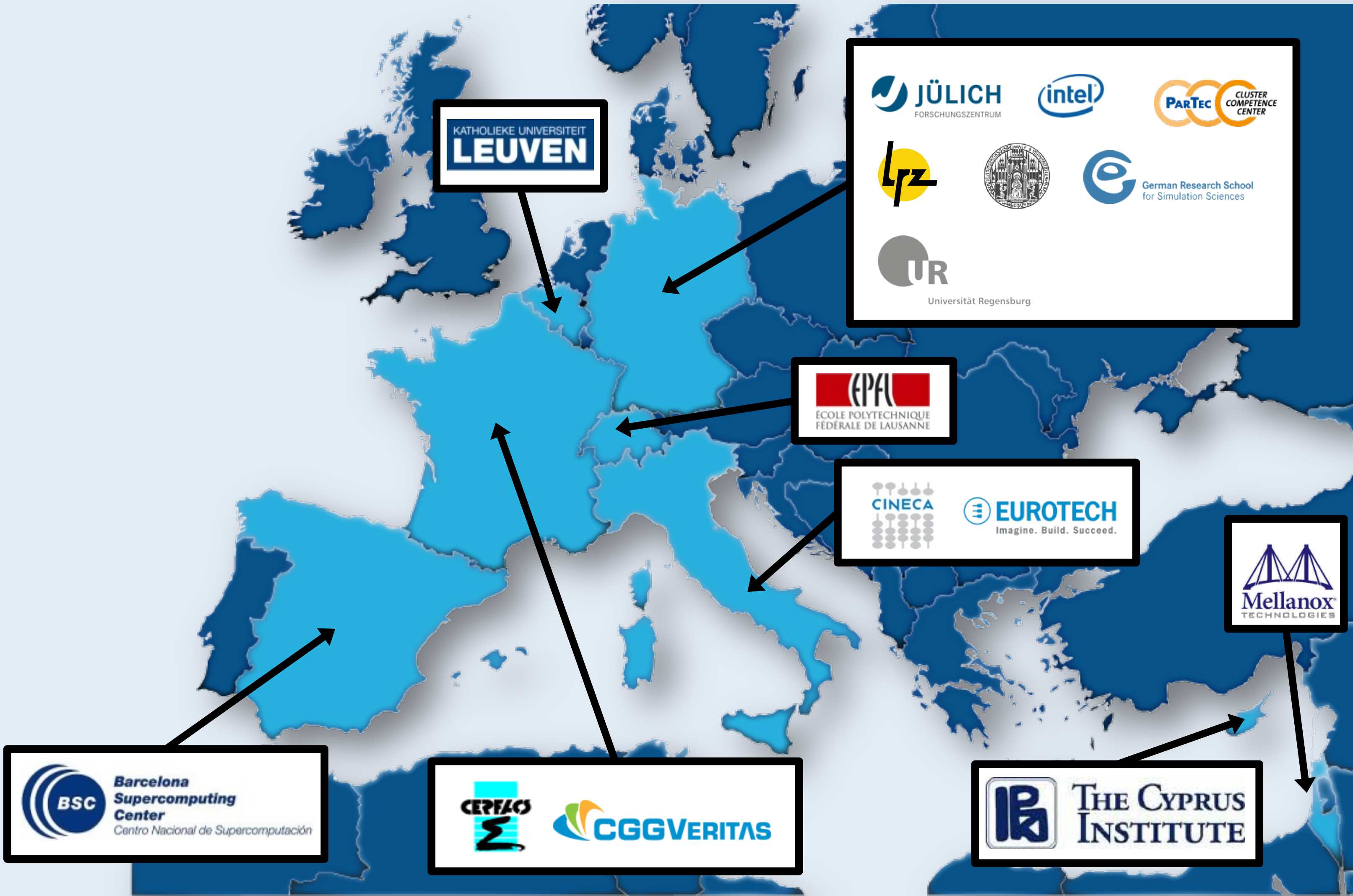
# DEEP Cornerstones

- Knights Corner Processor
  - > 50 Cores
  - 22 nm process
- EXTOLL network
  - Ultra low latency
  - Cut-through routing
- ParaStation
  - Cluster operation
- StarSS
  - Programming environment



# DEEP Partners



# Exascale Computer (ExaCom)

## Timeline

| | |
|---|---|
| Construction: | 2016–2020 (continuously) |
| Operation: | 3 to 5 years after last upgrade |

## Estimated Costs

| | |
|---|---|
| Preparation: | 2 Mio. € |
| Implementation: | 150 Mio. € (GCS funding expected) |
| Operation: | 6 Mio. € p.a. |

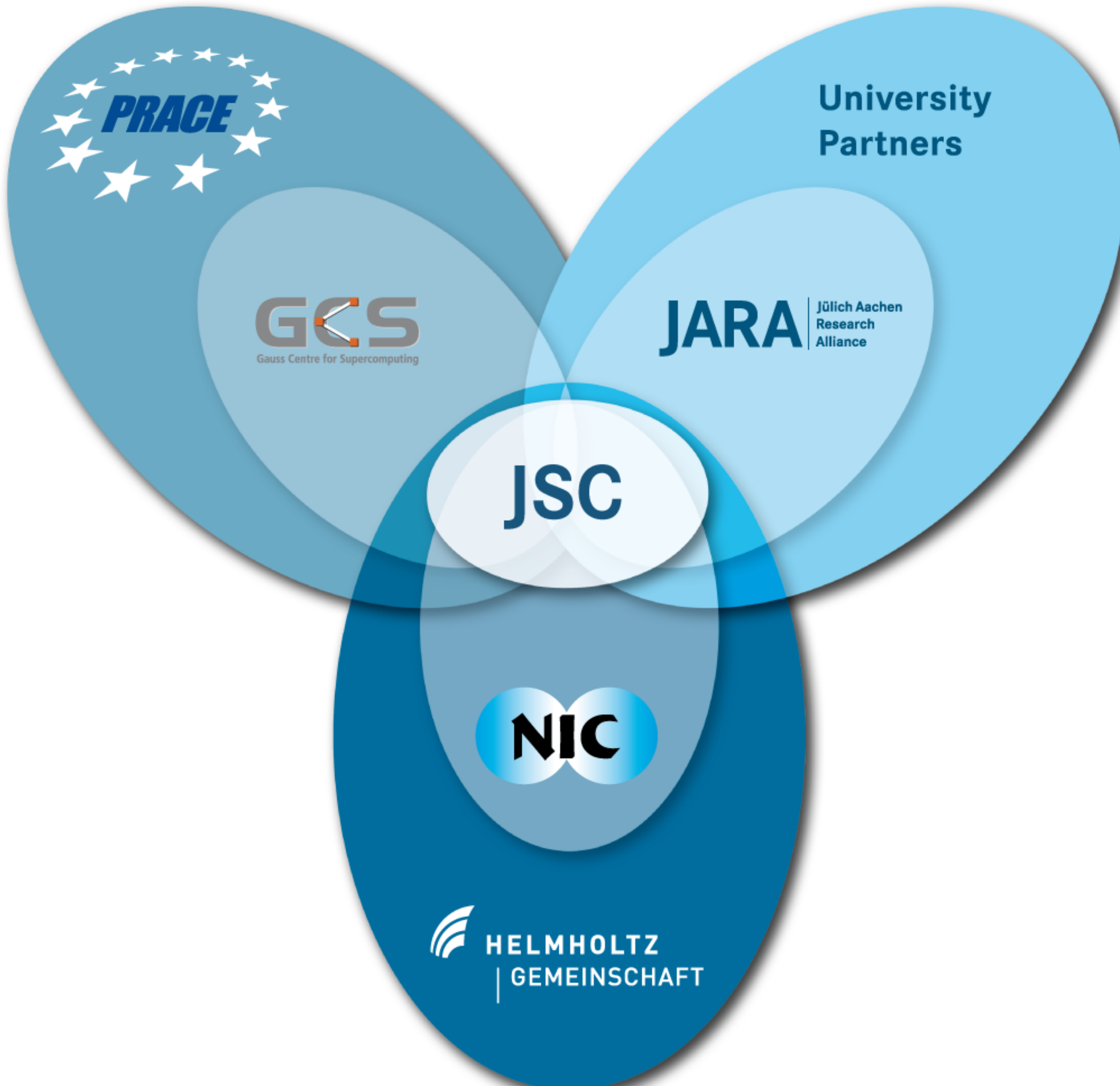
## International Dimension

The planned Exascale Computer for Jülich will be the leadership-system of the EuropeanTier-0 centres. It will give researchers in the HGF a substantial competitive advantage

## Role of the Centre

With 25 years experience and excellence in development, implementation and operation of national and European Supercomputers FZJ is an ideal location and architect of the infrastructure

# STRATEGIC ACTIVITIES AND PERSPECTIVES


PRACE
University
Partners
GCS
Gauss Centre for Supercomputing
JARA
Jülich Aachen
Research
Alliance
JSC
NIC
HELMHOLTZ
GEMEINSCHAFT

# Local: Institute for Advanced Simulation

JÜLICH
FORSCHUNGSZENTRUM

**Institute for Advanced Simulation (IAS)**
Structure, Topics and Integration

**IAS-1**
**Quantum Theory of Materials**
Investigation of the complex structural, electronic and magnetic qualities of solids and molecules
Prof. Stefan. Blügel

**IAS-2**
**Theoretical Soft Matter and Biophysics**
Exploration of the structure and dynamics of complex fluids, soft matter and biological systems
Prof. Gerhard Gompper

**IAS-3**
**Theoretical Nanoelectronics**
Information processing based on the quantum mechanical nature of matter
Prof. David DiVincenzo

**IAS-4**
**Theory of the Strong Interactions**
Analysis of the structure and dynamics of hadrons and atomic nuclei
Prof. Ulf Meissner

**IAS-5**
**Computational Biomedicine**
Integrating the *in silico* approach with *in vitro* and *in vivo* experiments
Prof. Paolo Carloni

**IAS-6 (planned)**
**Computational and Systems Neuroscience**
Development of multi-scale models of the brain
Prof. Markus Diesmann

**JSC**
**Jülich Supercomputing Centre**
Prof. Thomas Lippert

**Management:**
Managing Director, elected for one year from Board of Directors; permanent Deputy Director

**Organisation:**
Most IAS divisions are as well divisions in disciplinary departments

JARA Jülich Aachen Research Alliance

## Regional: Cooperation with Excellence University RWTH Aachen

**JARA-BRAIN**

**JARA-ENERGY**

**JARA-F-IT**

**JARA-HPC**

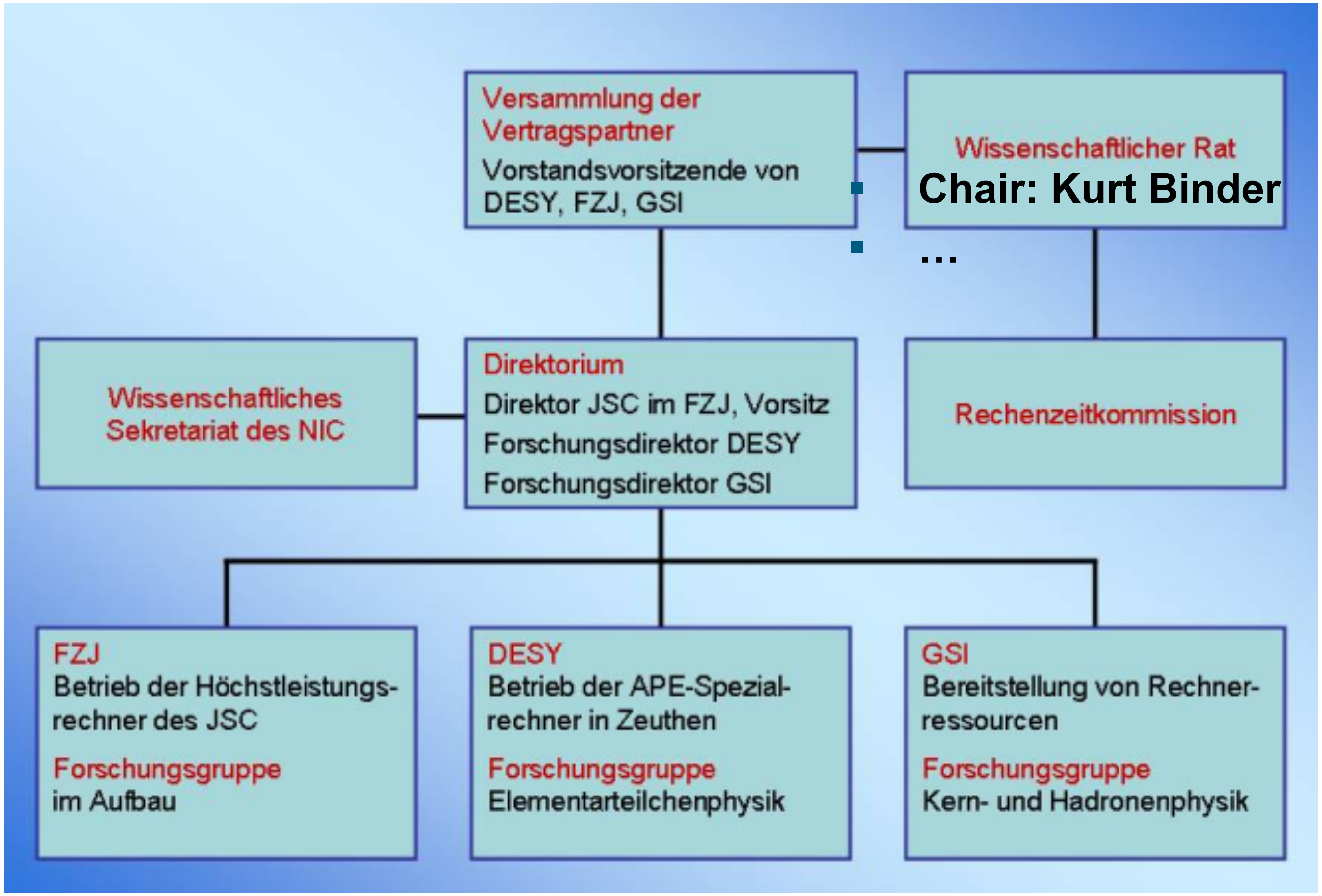
# JARA

- is unique in Germany
- joins University and Research Centre
- cooperates in
    - Research
    - Education
    - Infrastructure
    - Knowledge transfer
    - Services

**JARA HPC Partition: 500 TF (JSC), 100 TF (Aachen)**

AN INITIATIVE OF RWTH AACHEN UNIVERSITY JÜLICH FORSCHUNGSZENTRUM

# Supporting German University Groups: John von Neumann-Institute for Computing




- **Chair: Kurt Binder**
- …

The NIC is a guarantee for highest quality of scientific proposals for CPU time.
The NIC was blueprint for the PRACE scientific steering committee

# Germany: Gauss Centre for Supercomputing


- **Alliance of the three German SC centres**

  **HLRS, JSC, LRZ**
- **Creating joint scientific governance**
- **German representative in PRACE**
- **More information: http://www.gauss-centre.de**

# Europe: PRACE

HPC part of the ESFRI Roadmap; creation of a vision involving 15 European countries



Creation of the Scientific Case

Signature of the MoU

Creation of the PRACE Research Infrastructure

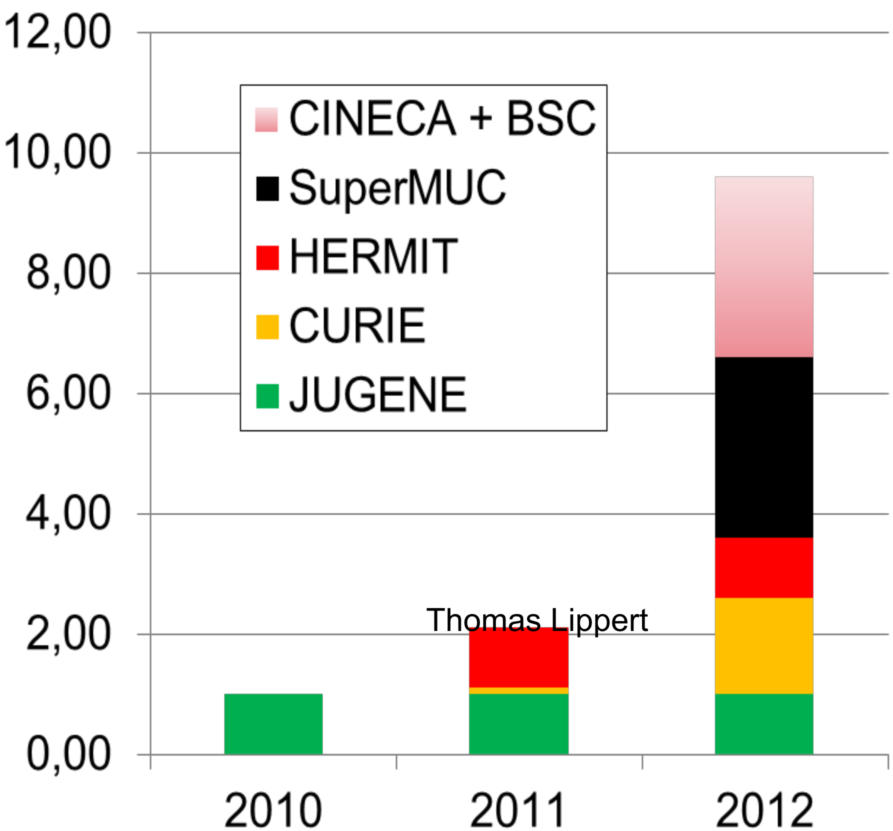
HPCEUR | HET | PRACE Initiative | PRACE RI

2004 | 2005 | 2006 | 2007 | 2008 | 2009 | 2010 | 2011 | 2012

PRACE Preparatory Phase Project | PRACE-1IP | PRACE-3IP

PRACE-2IP

# PRACE Tier-0 Capability and Support

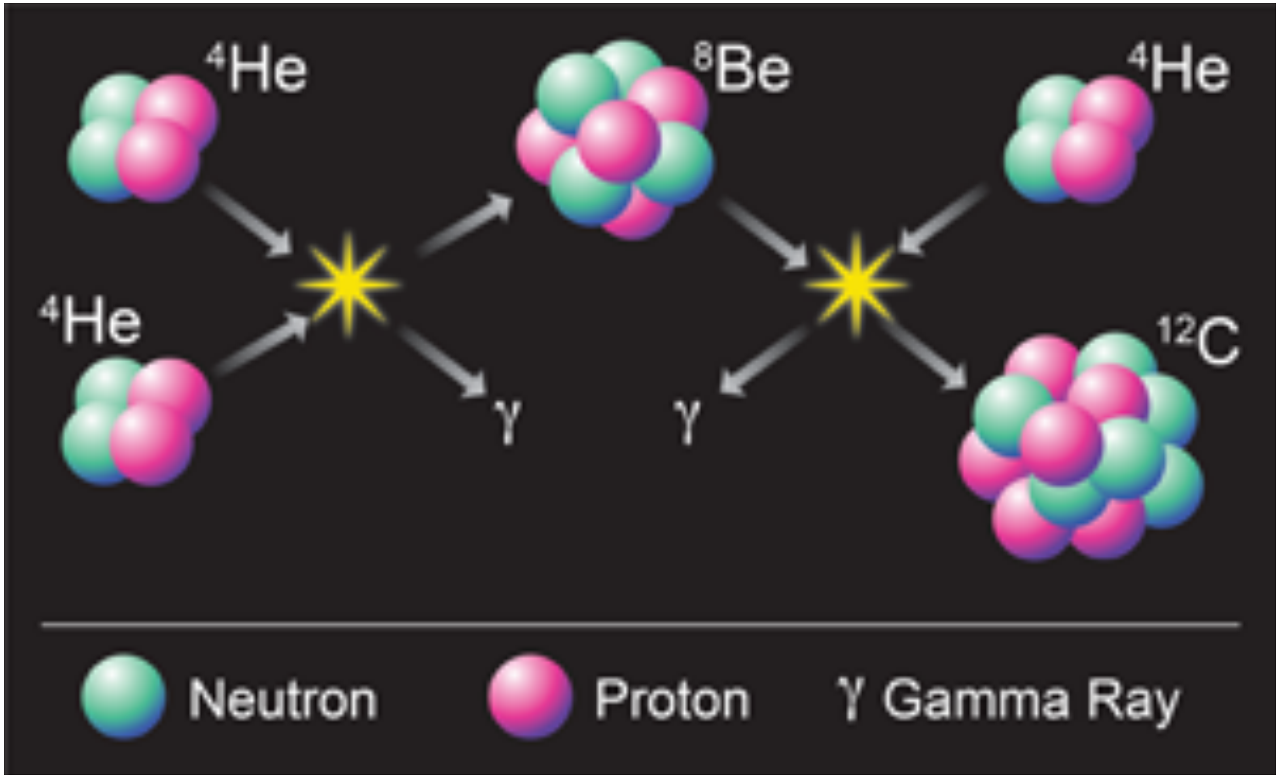



Thomas Lippert

- Accumulated Tier-0 performance > 15 Pflop/s in 2013/14
- PRACE includes 18 Tier-1 systems with accumulated capability of > 2 PF (building on DEISA / DECI)
- PRACE provides capability support competence centres over several sites

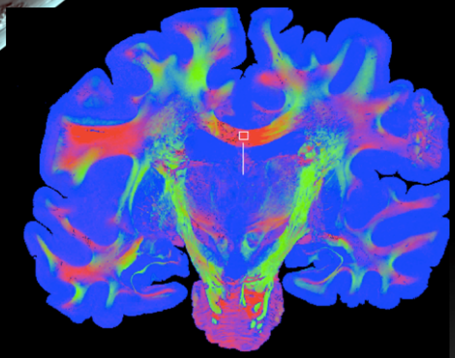
# OUR MOTIVATION

# Ab Initio Calculation of the Hoyle State

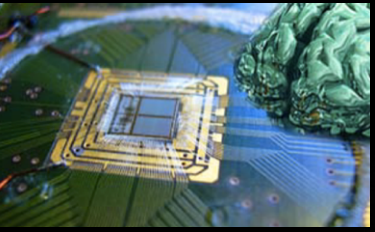



**Epelbaum, Meissner et al. (2011)** (JUGENE)

# Simulating the human brain



Needs Exascale Compute Power and Data Management



# Jülich Supercomputing Centre