



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

Campus School HPC 2014

Introduction to HPC and PRACE, Leon Kos, UL





25 members of PRACE

- Germany: [GCS - GAUSS Centre for Supercomputing e.V](#)
- Austria: [JKU - Johannes Kepler University of Linz](#)
- Belgium: [DGO6-SPW – Service Public de Wallonie](#)
- Bulgaria: [NCSA - Executive agency](#)
- Cyprus: [CaSToRC –The Cyprus Institute](#)
- Czech Republic: [VŠB - Technical University of Ostrava](#)
- Denmark: [DCSC - Danish Center for Scientific Computing](#)
- Finland: [CSC - IT Center for Science Ltd.](#)
- France: [GENCI - Grand Equipement National de Calcul Intensif](#)
- Greece: [GRNET - Greek Research and Technology Network S.A.](#)
- Hungary: [NIIFI - National Information Infrastructure Development Institute](#)
- Ireland: [ICHEC - Irish Centre for High-End Computing](#)
- Israel: [IUCC - Inter-University Computation Center](#)
- Italy: [CINECA - Consorzio Interuniversitario](#)
- Norway: [SIGMA – UNINETT Sigma AS –](#)
- The Netherlands: [SURFSARA: SARA Computing and Networking Services](#)
- Poland: [PSNC – Instytut Chemii Bioorganicznej Pan](#)
- Portugal: [FCTUC – Faculdade Ciencias e Tecnologia da Universidade de Coimbra](#)
- Serbia: [IPB - Institute of Physics Belgrade](#)
- **Slovenia:** [ULFME - University of Ljubljana, Faculty of Mechanical Engineering](#)
- Spain: [BSC – Barcelona Supercomputing Center – Centro Nacional de Supercomputación](#)
- Sweden: [SNIC – Vetenskapsrådet – Swedish Research Council](#)
- Switzerland: [ETH – Eidgenössische Technische Hochschule Zürich](#)
- Turkey: [UYBHM – Ulusal Yuksek Basarimli Hesaplama Merkezi.](#)
- UK: [EPSRC – The Engineering and Physical Sciences Research Council](#)



PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE



PRACE HAS A MEMORANDUM OF UNDERSTANDING (MOU) WITH:

	<p>The European Middleware Initiative provided Middleware services to PRACE. This also includes the provision of robust, well-designed, user-centric services to scientific user communities and the development of specific open standards.</p>
	<p>The Initiative for Globus in Europe (IGE) provides Middleware services to PRACE. This allows PRACE to leverage Globus training and support from IGE.</p>
	<p>The European Data Infrastructure and PRACE are working towards seamless access to HPC and data services, including the use of the dedicated PRACE network by EUDAT and a close collaboration in the use of iRODS.</p>
	<p>The LinkSCEEM-2 project which aims at the establishment of a high performance computing (HPC) eco-system in the Eastern Mediterranean and PRACE are collaborating in dissemination, outreach and training activities.</p>
	<p>The Scalable Software Service for Life Science and PRACE organised joint training and dissemination events. ScalaLife provided support to its target community in applying for and using PRACE resources efficiently.</p>

PRACE IS A CONSORTIUM MEMBER AND PARTNER OF THE FOLLOWING PROJECT:



The European Exascale Software Initiative and PRACE collaborate on dissemination and exchange of experience and information including the alignment on application scalability and participation in the definition of a European policy and Roadmap.

PRACE IS A CONSORTIUM MEMBER OF:

EEF -
European E-infrastructure Forum

PRACE is a member in the European E-Infrastructure Forum which coordinates the European e-Infrastructures.

PRACE HAS COLLABORATED IN OTHER WAYS WITH:



PRACE and XSEDE jointly organise the EU-US HPC Summer School and work on the enhancement of interoperable services between PRACE and XSEDE through a joint call for request for support.



RIKEN Advanced Institute for Computational Science (AICS) joined up with PRACE and XSEDE to organise the 4th "International Summer School on HPC Challenges on Computational Sciences"



Within the e-Infrastructure Reflection group PRACE is a stakeholder in the provision of an ICT based Research Infrastructure.



PRACE participated in the Exchange of Experience group in the project for ESFRI: Communication and Policy development for Research Infrastructures in Europe.

sCi (security for Collaborating infrastructures)

PRACE Security Forum is represented in the Security for Collaborating Infrastructures, a collaborative activity of security staff from several large-scale distributed computing infrastructures, including EGI, OSG, PRACE, wLCG, and XSEDE.

PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

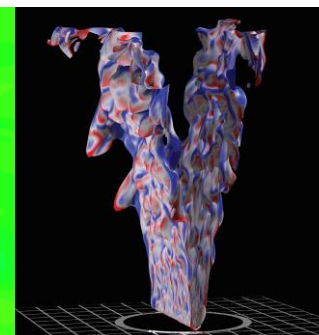
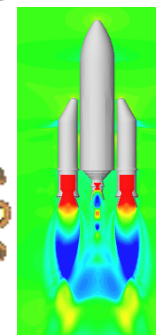
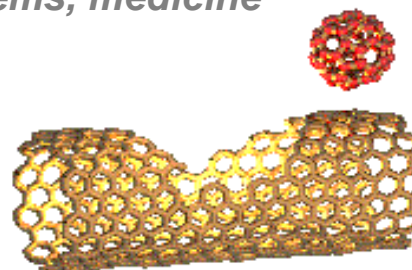
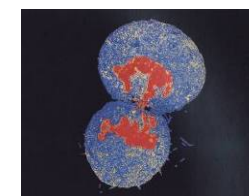
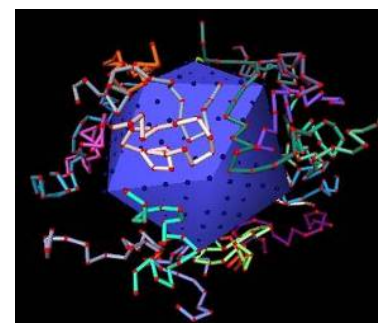
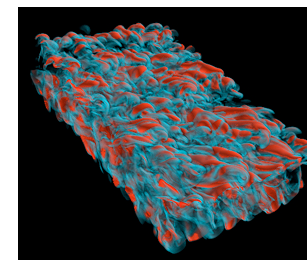
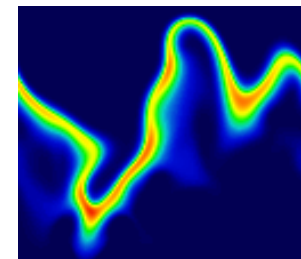
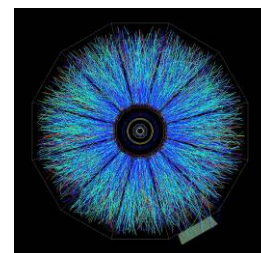
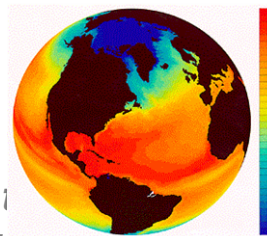


PRACE IS REPRESENTED IN AN ExTERNAL BOARD OF:

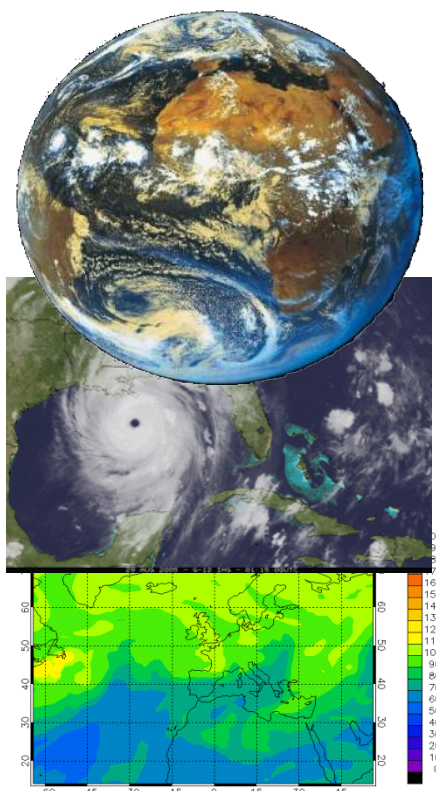
	<p>PRACE is represented in the European Grid Infrastructure (EGI)-InSPIRE External Advisory Committee.</p>
	<p>PRACE is represented in the Advisory Board of e*inventory, an FP7 project dealing with impact assessment of eInfrastructures.</p>
	<p>The European Policy Management Authority for Grid Authentication in e-Science is a body to establish requirements and best practices for grid identity providers. PRACE is represented as relying party.</p>
	<p>PRACE is using the GÉANT network services, the pan-European research and education network interconnecting Europe's National Research and Education Networks. It is represented in the International User Advisory Committee</p>
	<p>PRACE is an observer in the European Technology Platform for High Performance Computing.</p>
	<p>PRACE is represented in the advisory board of e-Fiscal, an FP7 project dealing with the assessment of costs of Research Infrastructures.</p>

Why supercomputing?

- **Weather, Climatology, Earth Science**
 - degree of warming, scenarios for our future climate
 - understand and predict ocean properties and variations
 - weather and flood events
- **Astrophysics, Elementary particle physics, Plasma physics**
 - systems, structures which span a large range of different length and time scales
 - quantum field theories like QCD, ITER
- **Material Science, Chemistry, Nanoscience**
 - understanding complex materials, complex chemistry, nanoscience
 - the determination of electronic and transport properties
- **Life Science**
 - system biology, chromatin dynamics, large scale protein dynamics, protein association and aggregation, supramolecular systems, medicine
- **Engineering**
 - complex helicopter simulation, biomedical flows, gas turbines and internal combustion engines, forest fires, green aircraft,
 - virtual power plant



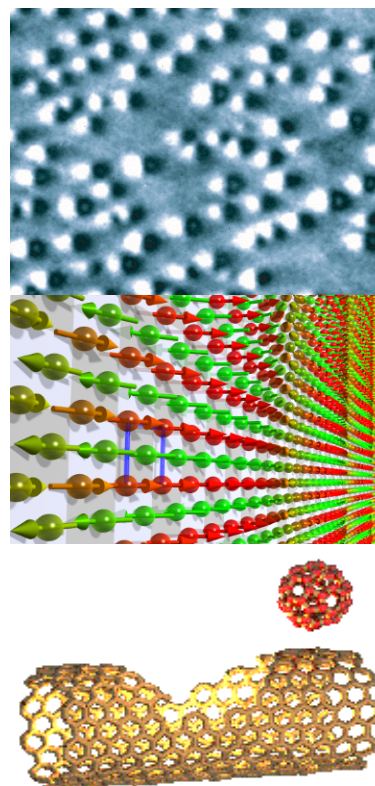
Supercomputing drives science with simulations



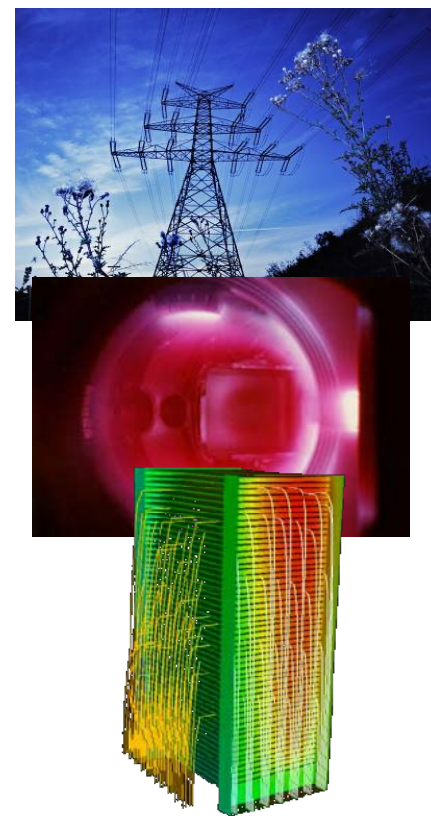
Environment
Weather/ Climatology
Pollution / Ozone Hole



Ageing Society
Medicine
Biology



Materials/ Inf. Tech
Spintronics
Nano-science

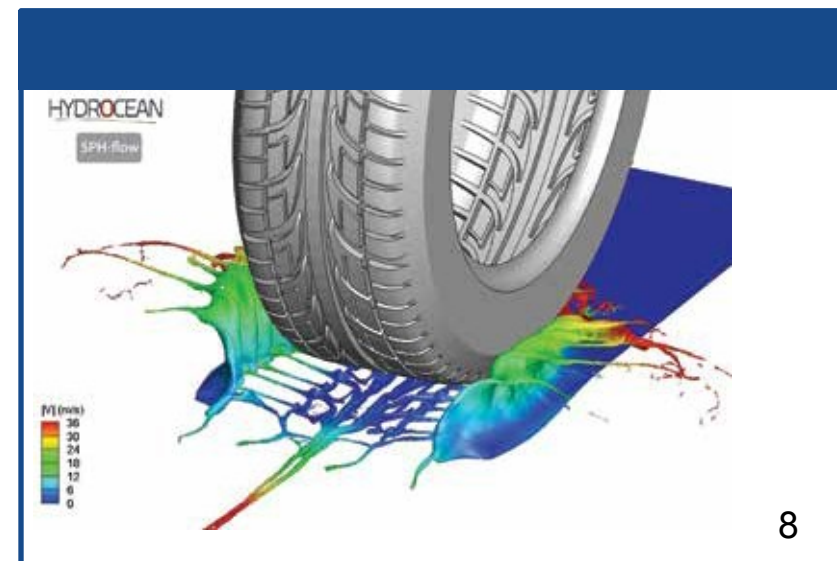
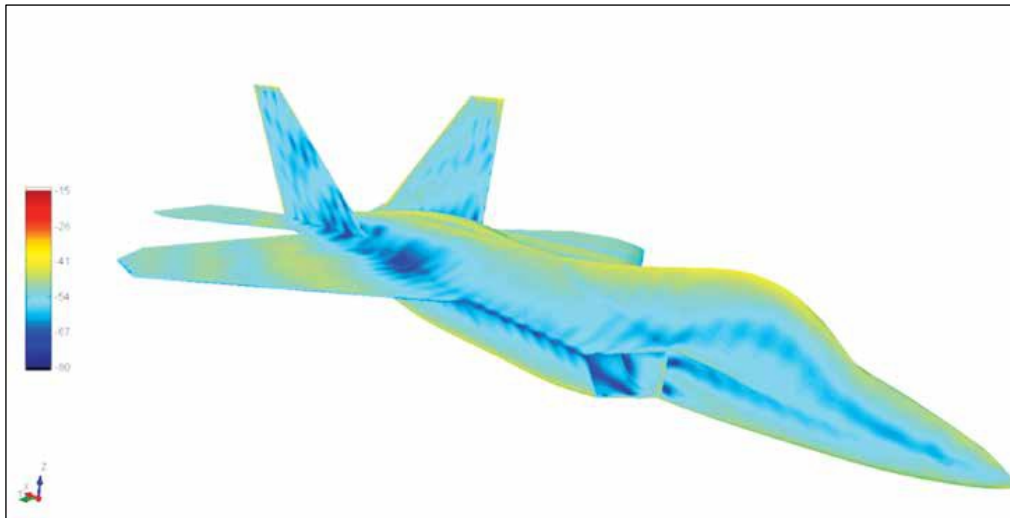


Energy
Plasma Physics
Fuel Cells

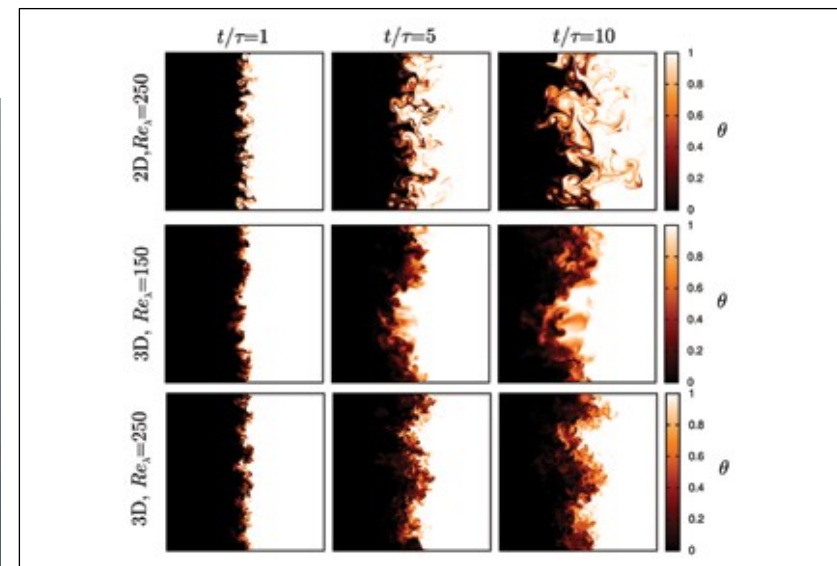
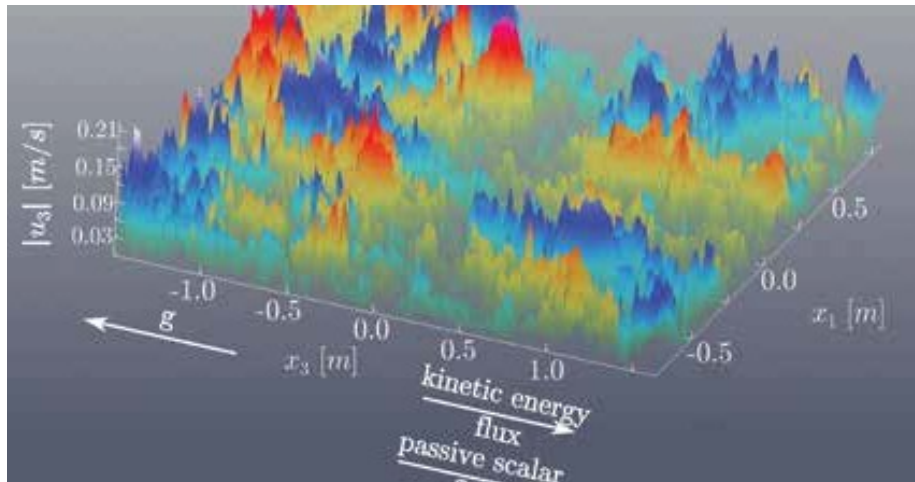
SHAPE

- HPC to accelerate growth and innovation for European SMEs through open R&D

HydrOcéan was again awarded under the PRACE 6th Call for Proposals for Project Access with 8.2 million core hours on CURIE @ GENCI@CEA, France



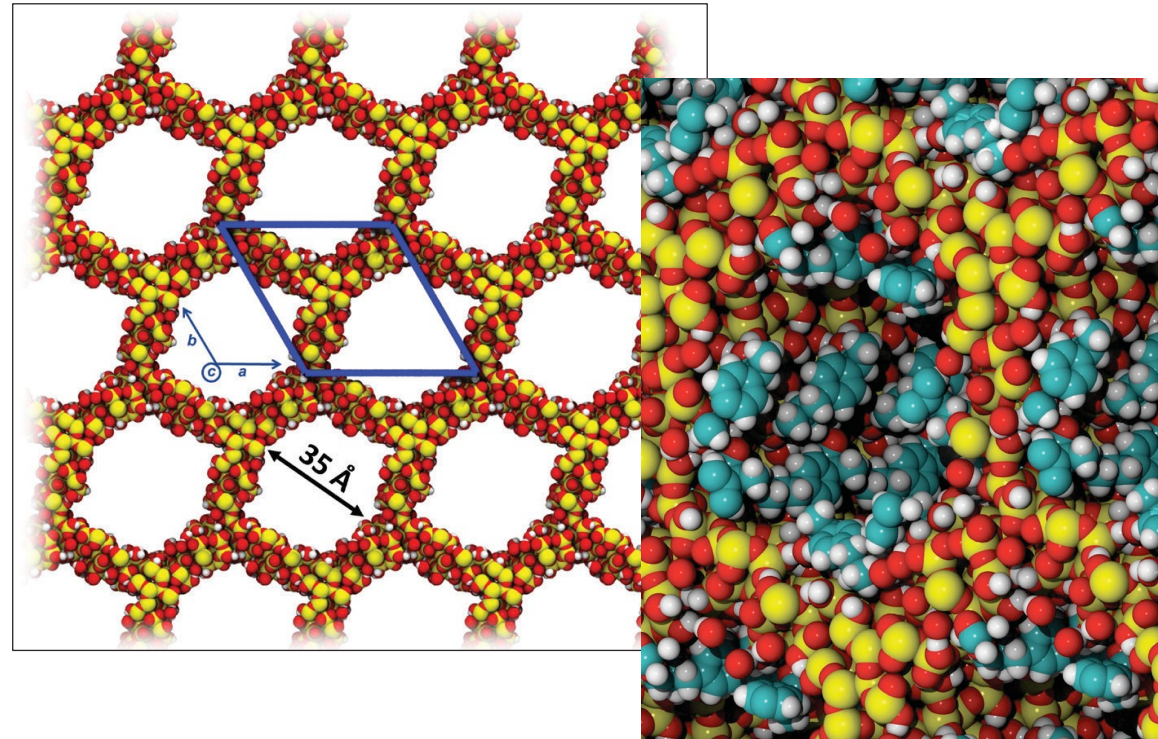
Analysing cloud behaviours through HPC modelling



This project was awarded 2,440,500 core hours on CURIE Fat Nodes (FN) and 536,850 on CURIE Thin Nodes (TN), CURIE @ GENCI@CEA, France

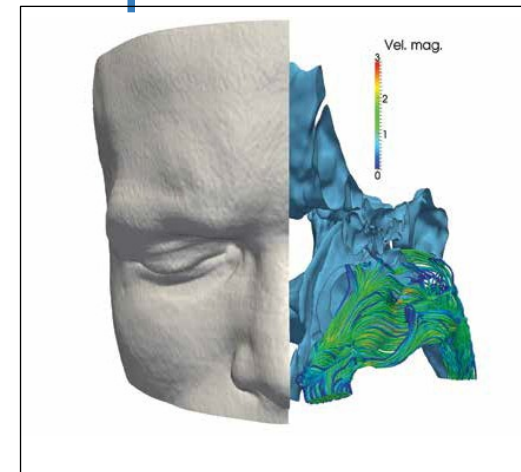
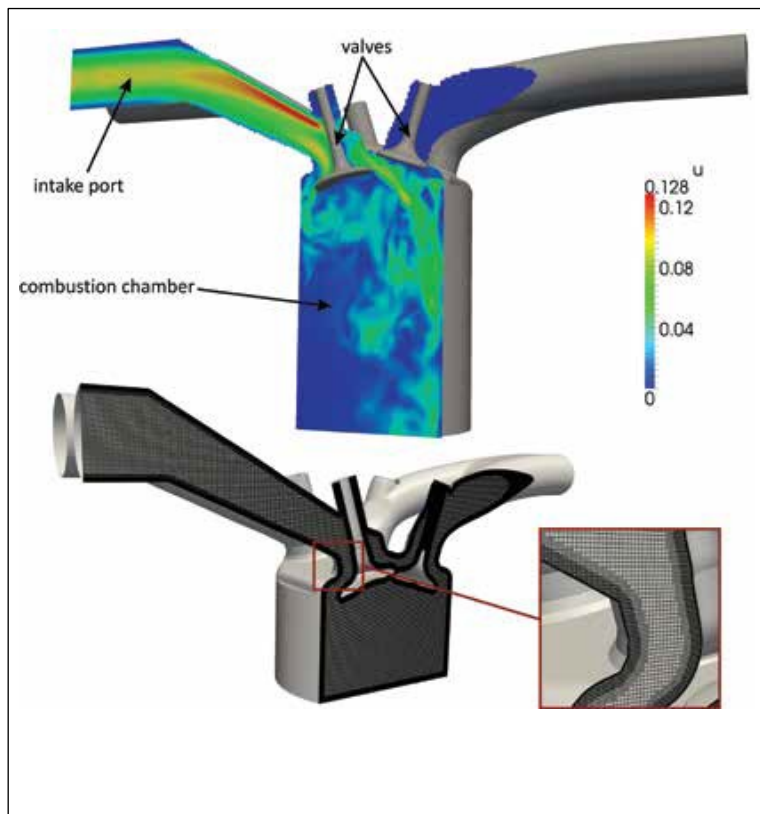
Harnessing European HPC to improve nanomedicines

Drugs can be delivered to specific areas of the body and benignly dispensed, using nanomedicines, and mesoporous silica is a material which possesses the properties to fulfil this role.



This project was awarded
20,000,000 core hours on SuperMUC @
GCS@LRZ

Simulating turbulent airflows to inform energy-saving engine designs and pioneer surgical technologies



Direct Numerical Simulation of the Flow in an Internal Combustion Engine
Project leader: Prof. Dr.-Ing. Wolfgang Schröder at RWTH Aachen University
Project details: This project was awarded 72,700,000 core hours on Hermit @ GCS@HLRS, Germany

Creating end-user systems to calculate real world physical phenomena

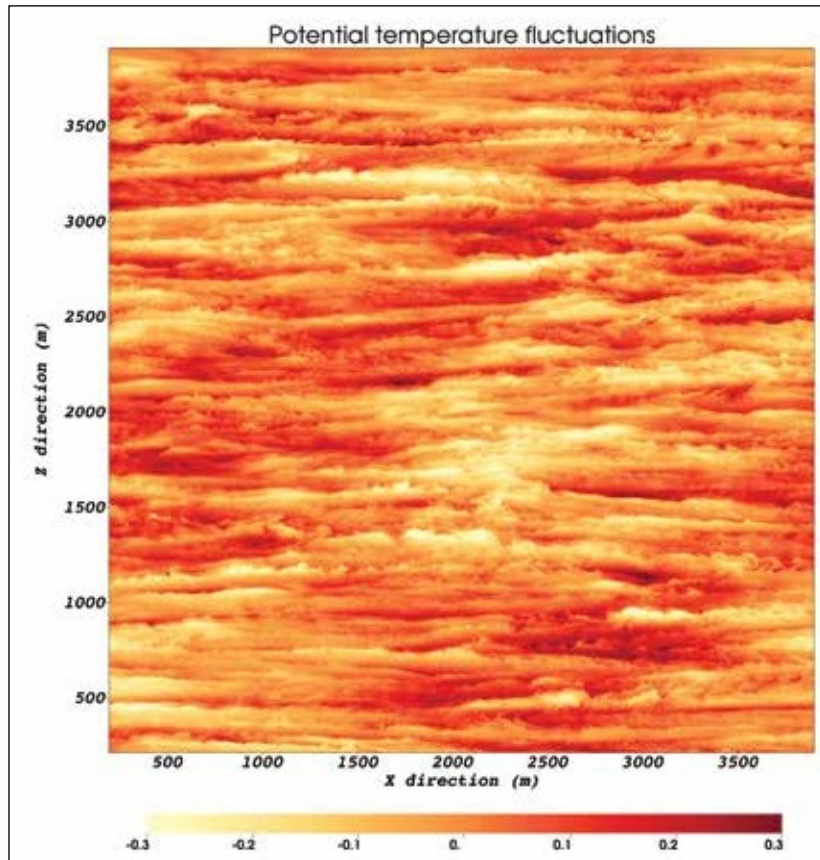


Example of a geometry used for performing large- scale physical simulations

High Performance Computing with Generic Solvers for Partial Differential Equations (HPC-PDE) Project leader: Dr. Frederic Nataf, Senior scientist at CNRS

Project details: This project was awarded 1,000,000 hours on CURIE @ GENCI@CEA, France

Investigating the structure of atmospheric turbulent flows



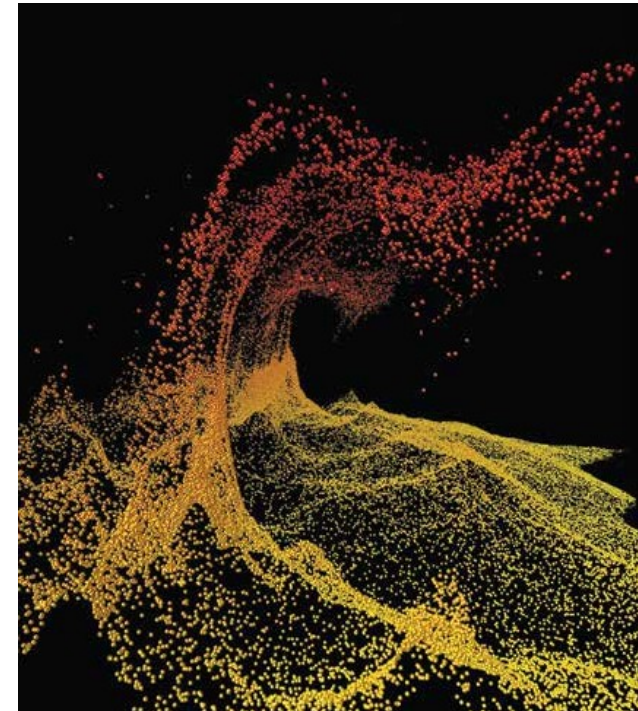
Large-eddy simulations of stratified atmospheric turbulent flows with Meso-NH: application to safety in meteorology and environmental impact of aviation

Project leader: Dr. Roberto Paoli, Research scientist CERFACS

Project details: This project was awarded 21.5 million core hours on CURIE @ GENCI@CEA, France

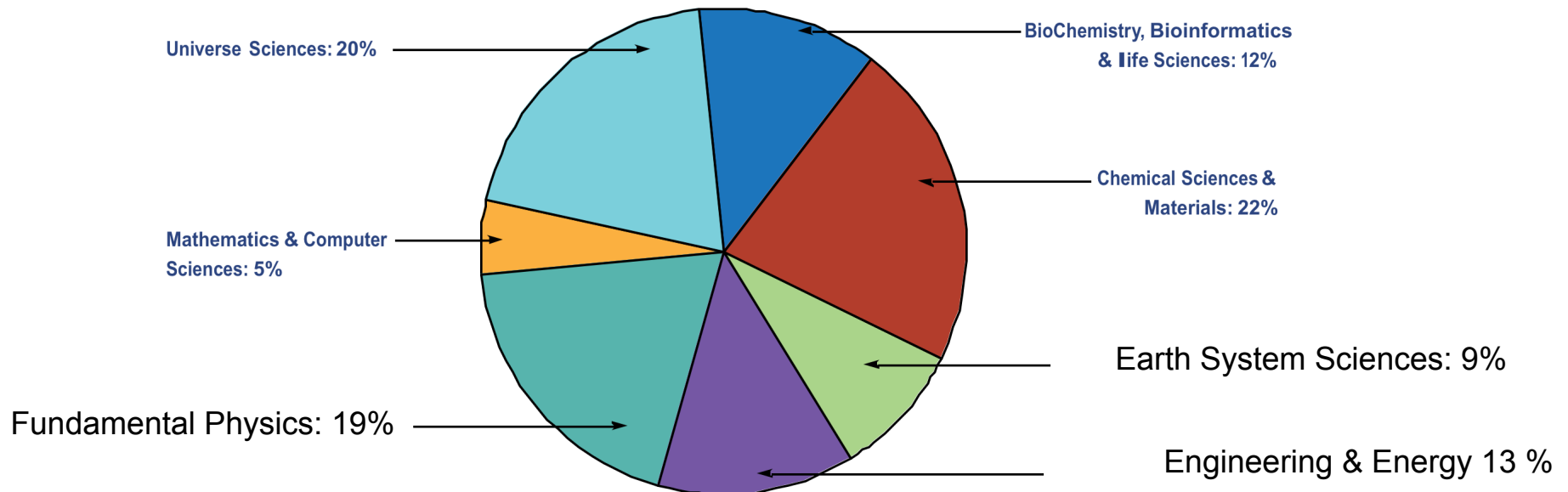
Evaluating the physical properties of plasma

Understanding how collisionless shocks behave within plasma is a fundamental scientific question. Exploiting the power of HPC to examine these phenomena has enabled scientists to create detailed models of them, revealing new facets of their behaviour



This project was awarded 37,000,000 core hours on JUQUEEN @ GCS@Jülich, Germany

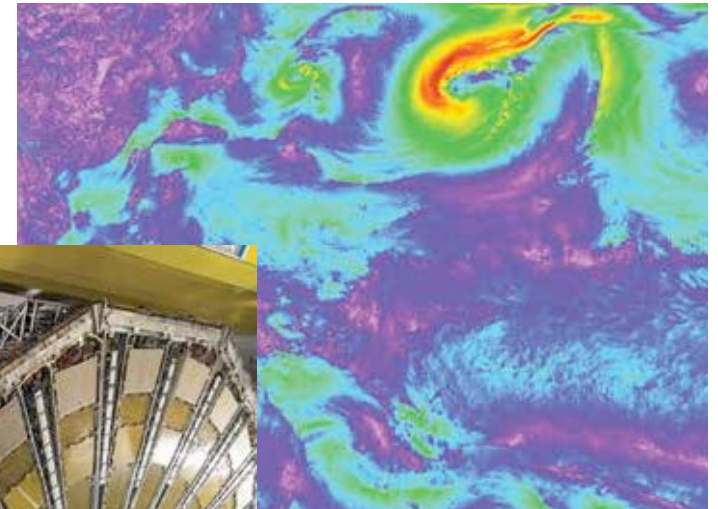
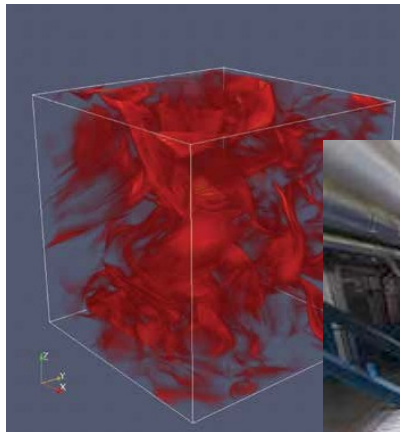
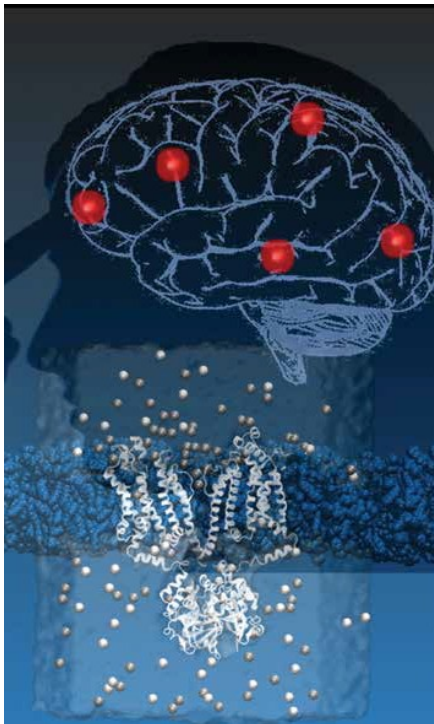
Total core hours dedicated in calls 1-7



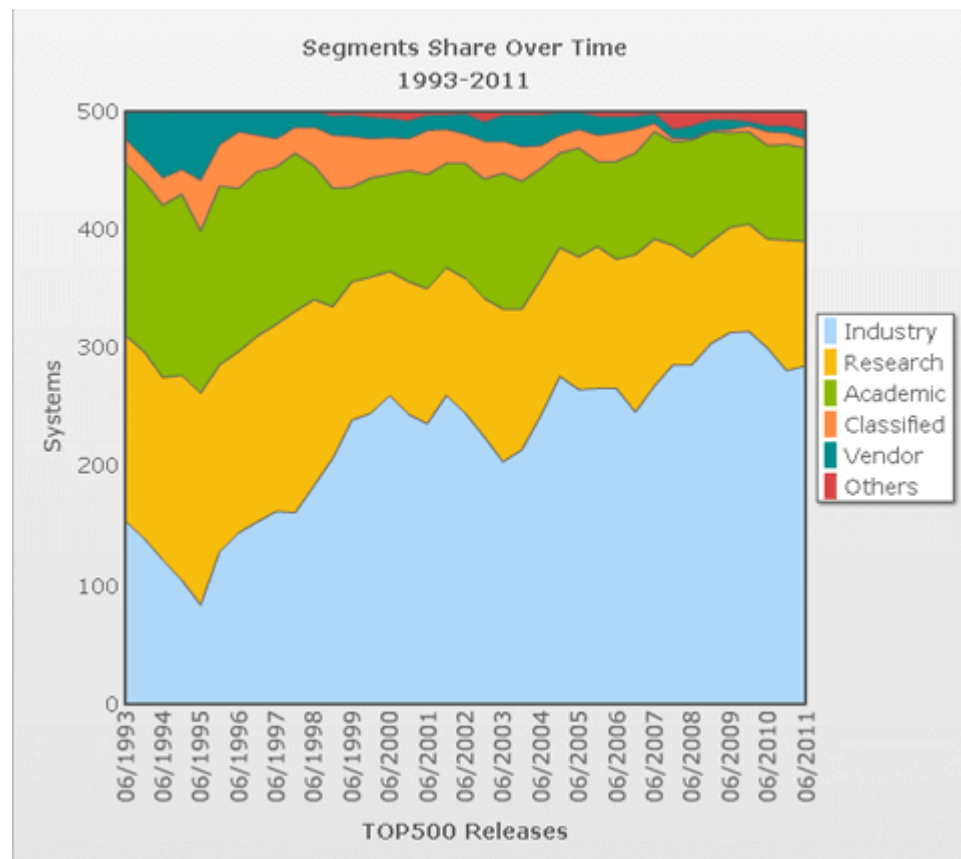
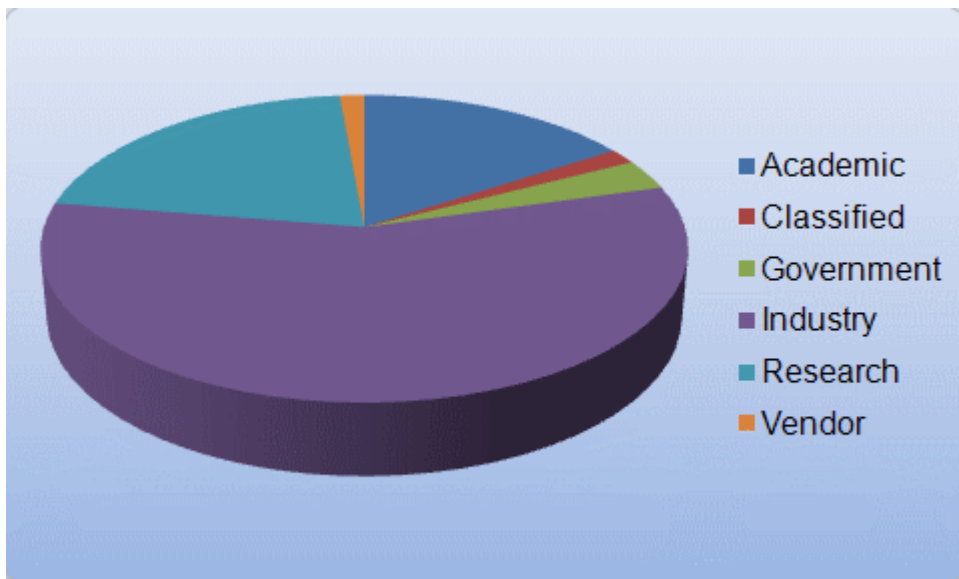
“Starting mid-2014, PRACE 2.0 will come into life, continuing and increasing the access to Europe’s largest and most capable systems through a single peer-review process”

Thinking ahead

PRACE wraps up the evaluation of a multi-year allocation pilot to encourage and support long-term execution of vital research



Systems share in TOP500 list



Large HPC systems around the world



FZJ - at Juelich (Germany)

2010 1st PRACE System - JUGENE

- BG/P by Gauss Center
for Supercomputing

294,912 CPU cores, 144 TB memory
1 PFlop/s peak performance
825.5 TFlop/s Linpack
600 I/O nodes (10GigE) > 60 GB/s I/O
2.2 MW power consumption
35% for PRACE



GENCI - Paris (France)

2011 2nd PRACE system – CURIE

- ***Bull, 1.6PF, 92160 cores, 4GB/core***
- ***Phase 1, December 2010, 105 TF***
 - ***360 four Intel Nehalem-EX 8-core nodes, 2.26 GHz CPUs (11,520 cores), QDR Infiniband fat-tree***
 - ***800 TB, >30GB/sec, local Lustre file system***
- ***Phase 1.5 Q2 2011***
 - ***Conversion to 90 16-socket, 128 core, 512 GB nodes***
- ***Phase 2, Q4 2011, 1.5 TF***
 - ***Intel Sandy-Bridge***
 - ***10PB, 230GB/sec file system***



HLRS - Stuttgart (Germany)

2011 3rd PRACE System – HERMIT

- ***Cray XE6 (Multi-year contract for \$60+M)***

- ***Phase 0 – 2010***

- 10TF, 84 dual socket 8-core
AMD Magny-Cours CPUs,
1344 cores in total, 2 GHz,
2GB/core,
Gemini interconnect***

- ***Phase 1 Step 1 – Q3 2011***

- AMD Interlagos, 16 cores, 1 PF
2 – 4 GB/core
2.7 PB file system, 150 GB/s I/O***

- ***Phase 2 – 2013***

- Cascade, first order for Cray, 4- 5 PF***



LRZ - Munich (Germany)

2011/12 4th PRACE system

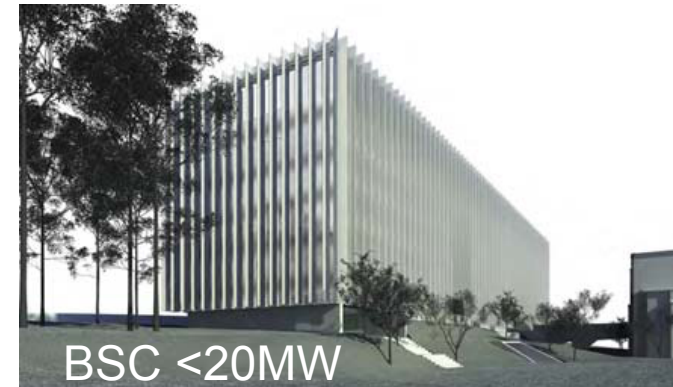
- **IBM iDataPlex**
- **(€83M including operational costs)**
 - **>14,000 Intel Sandy-Bridge CPUs, 3 PF (~110,000 cores), 384 TB of memory**
 - **10PB GPFS file system with 200GB/sec I/O, 2PB 10GB/sec NAS**
 - **LRZ <13MW**
 - **Innovative hot water cooling (60C inlet, 65C outlet) leading to 40 percent less energy consumption compared to air-cooled machine.**



BSC and CINECA - Bologna (Italy)

- 2012/2013 5th and 6th PRACE Systems

CINECA
Target ~2.5 PF



Computing Facility
10 MW 2013

PRACE continues to train the next generation of HPC experts

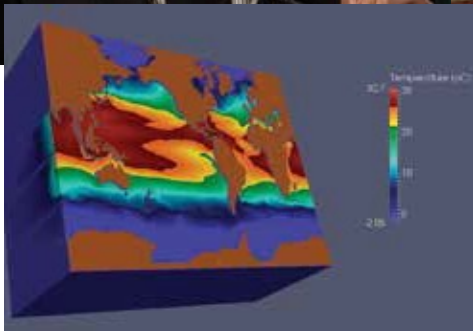
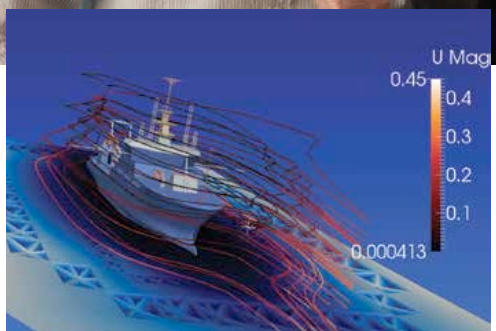
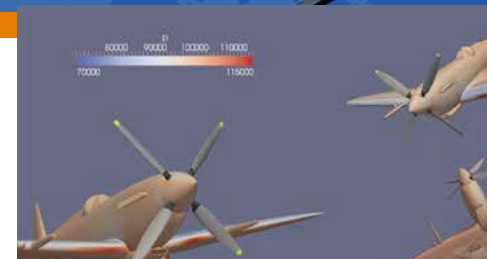
Six Advanced Training centers across Europe with regular curricula



International Summer School on HPC Challenges in Computational Sciences

PRACE Summer of HPC

Vito Simonka and Niki Loppi, SoHPC Awards Ceremony, BSC 2013



PRACE Projects support the Research Infrastructure

- Prototypes
- The PRACE-3IP project is running a joint Pre-Commercial Procurement (PCP) pilot targeting “Whole System Design for Energy Efficient HPC”.



Supercomputing at UL FME --HPCFS for ?

• Some examples of previous projects

The image displays a collection of scientific posters from various research projects at UL FME. The posters are arranged in a collage, overlapping each other. Each poster typically features a title, a brief description of the project, and some graphical elements like charts or diagrams. The projects include:

- Velocity profile effects in Coriolis mass flowmeters**: Discusses the physical background of velocity profile effects in Coriolis flowmeters.
- Simulating the dynamics of a clapper-to-bell impact**: Focuses on the dynamics of a clapper on a bell structure.
- Numerical Simulation of the Turbulent Flow around a Sphere**: Describes a project dealing with massive numerical simulation of turbulent flow around a sphere.
- Razvoj pečične nove generacije s pomočjo CFD simulacije**: Discusses the development of a new generation of furnaces using CFD simulation.
- Laser droplet generation detachment regimes**: Investigates metal droplet generation in a process where a droplet is generated by melting the tip of a wire.
- Optimizacija geometrije prostih površin**: Focuses on the optimization of the geometry of free surfaces.
- Rotating cascade heat transfer using CFD and IR thermography**: Presents an experimental study of convective heat transfer and flow field characteristics in a rotating rotor cascade.
- Parallel computing with load balancing**: Discusses issues regarding effective parallelization of the solution of large systems of linear equations.
- Projekta EUFORIA in EFDA-ITM-ISIP**: Focuses on the development of a new generation of furnaces using CFD simulation.
- Razširitev nekolijskih razelektivnih modelov za aplikacijo v fuzijsko relevantnih in splošnih plazmah**: Discusses the extension of non-linear models for application in fusion-relevant and general plasmas.
- Numerične simulacije na področju varnosti cestnih in terenskih vozil**: Focuses on numerical simulations in the field of road and off-road vehicle safety.
- Strateški raziskovalno-razvojni projekt INTELLIGENT FIT**: A strategic research and development project.
- Modeling of breathing process influence personal exposure effectiveness**: Focuses on the influence of breathing process on personal exposure effectiveness.

What HPCFS is used for?

- ***Complex engineering research problems demands parallel processing***
- ***Education of new generation of students on II cycle ob Bologna process***
- ***Cooperation with other GRID and HPC centres***

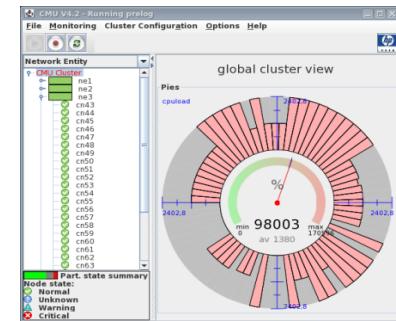
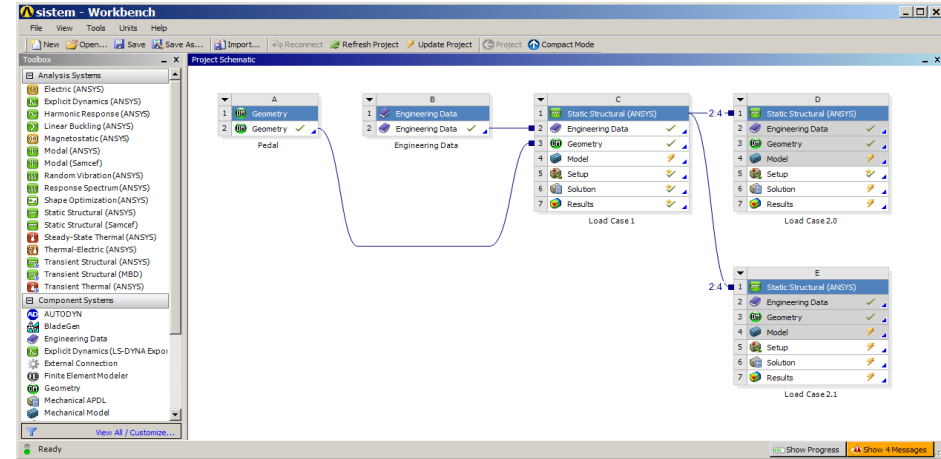


Long term goals

- Extension of computing capabilities
- In-house development of custom codes
- ***Installation of commercial and open-source codes***
- ***ANSYS multiphysics, OpenFOAM,..***
- ***Cooperation in EU projects***
- ***Advantage is if having HPC and knowledge about it***
- ***Introducing (young) researchers***
 - ***Center for modelling, simulations and optimization in cooperation on severale levels at university and intra universities***
- ***Promotion of FS/UL, science, research and increased awareness***
- ***Nacional HPC centre?***

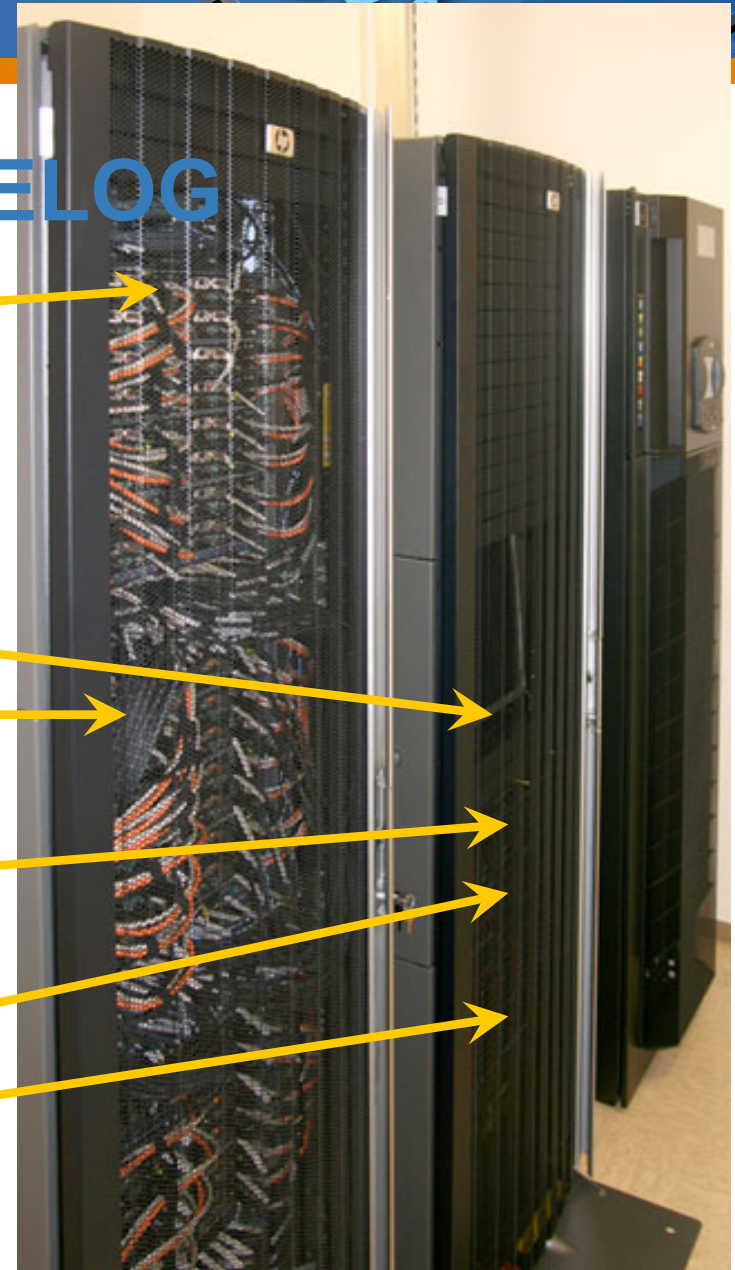
Software at HPCFS

- Linux (CentOS 6.4)
- Remote desktop NX
- Development environment and LSF batch scheduler
- Compilers C++, Fortran (Python, R, ...)
- Parallel programming libraries with MPI, OpenMP
- Open-source and commercial packages for simulations (ANSYS)
- Servers for support of the research and development



Hardware of the cluster PRELOG

- 64 computing nodes
 - 768 cores X5670
 - 1536 threads
- 3 TB RAM
- Login node
- **Infiniband network**
- QDR x4 „fat tree“
- **File servers**
 - NFS 25TB
- LUSTRE 12TB+22TB
- Virtualization servers
- 1Gbit Connection to ARNES



I wish you fulfillment
of your expectations about this week
and nice memories from
the University of Ljubljana

And in the future,
new ways for research & collaboration
between all participants of the school,
lecturers and trainers.

Backup slides for Lustre and ZFS



LLNL Sequoia installation



LLNL Sequoia Lustre Architecture

