Autumn School 2013 INTRODUCTION
Industry oriented HPC simulations

Introduction to HPC and PRACE, Jožef Duhovnik, UL

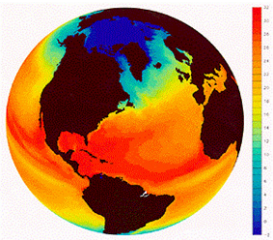
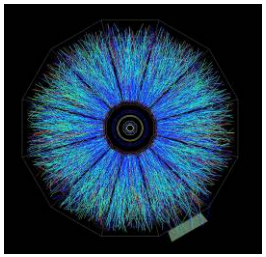
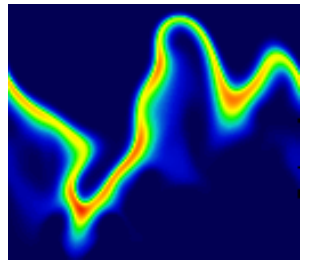
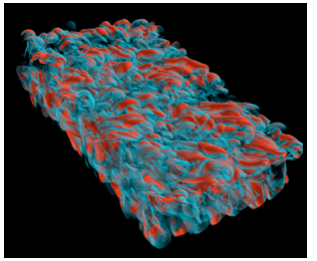
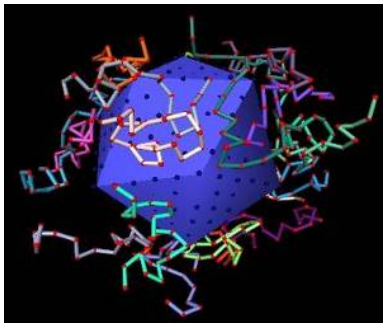
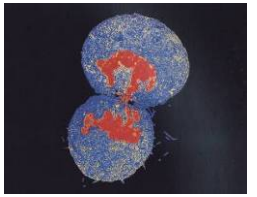
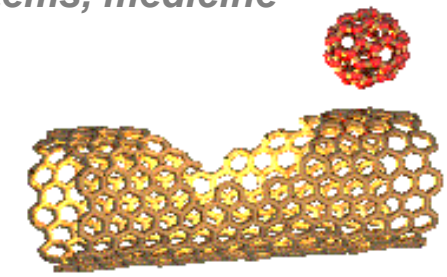
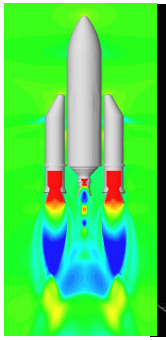
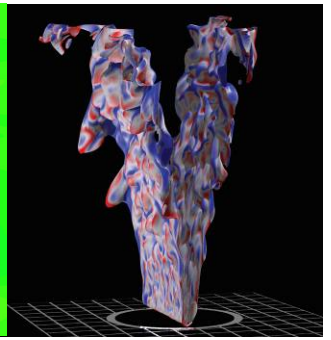
CAPACITIES

e-infrastructure

25 members of PRACE

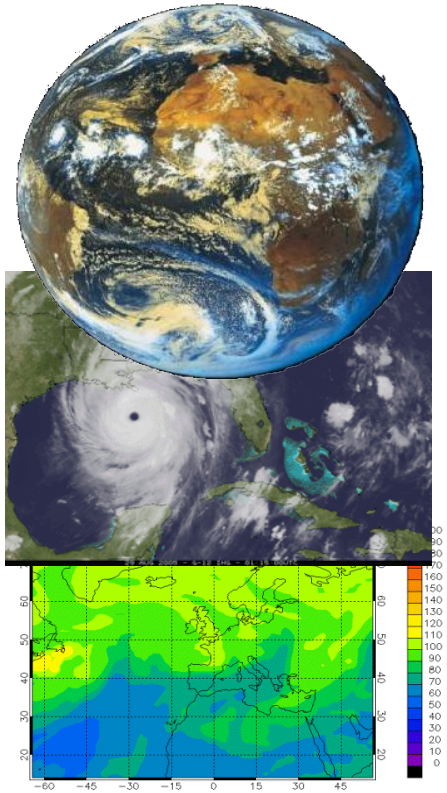
- Germany: GCS - GAUSS Centre for Supercomputing e.V
- Austria: JKU - Johannes Kepler University of Linz
- Belgium: DGO6-SPW – Service Public de Wallonie
- Bulgaria: NCSA - Executive agency
- Cyprus: CaSToRC –The Cyprus Institute
- Czech Republic: VŠB - Technical University of Ostrava
- Denmark: DCSC - 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

Why supercomputing?

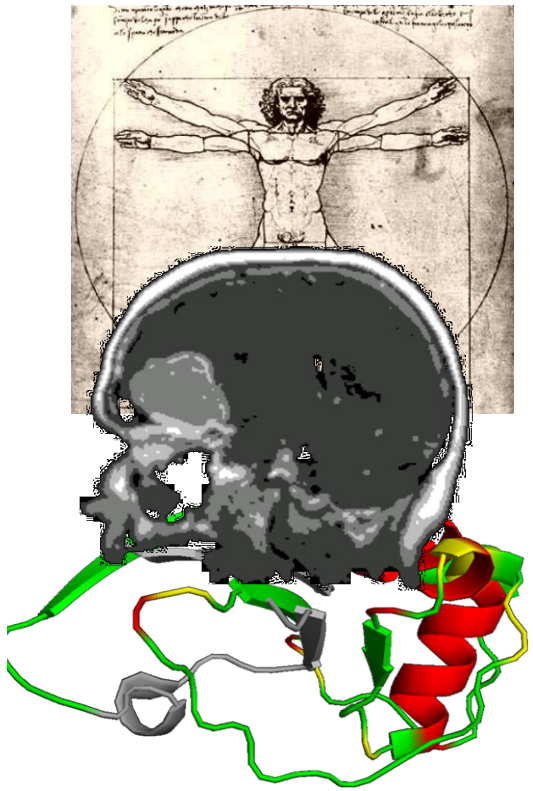










- ***Weather, Climatology, Earth Science***
  - *degree of warming, scenarios for our future climat*
  - *understand and predict ocean properties and variations*
  - *weather and flood events*
- ***Astrophysics, Elementary particle physics, Plasma physics***
  - *systems, structures which span a large 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*

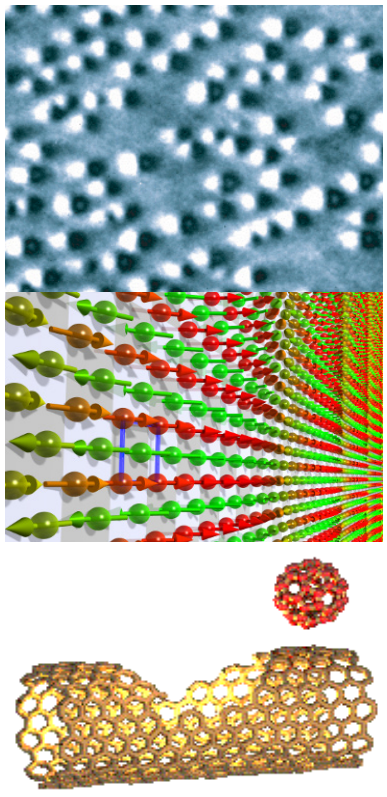
Supercomputing drives science with simulations



Environment
Weather/ Climatology
Pollution / Ozone Hole



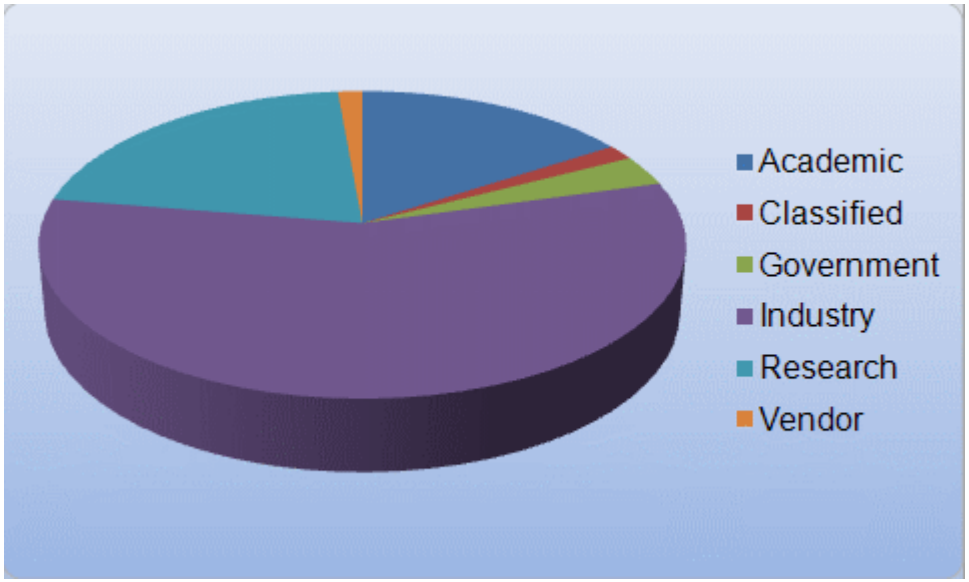
Ageing Society
Medicine
Biology

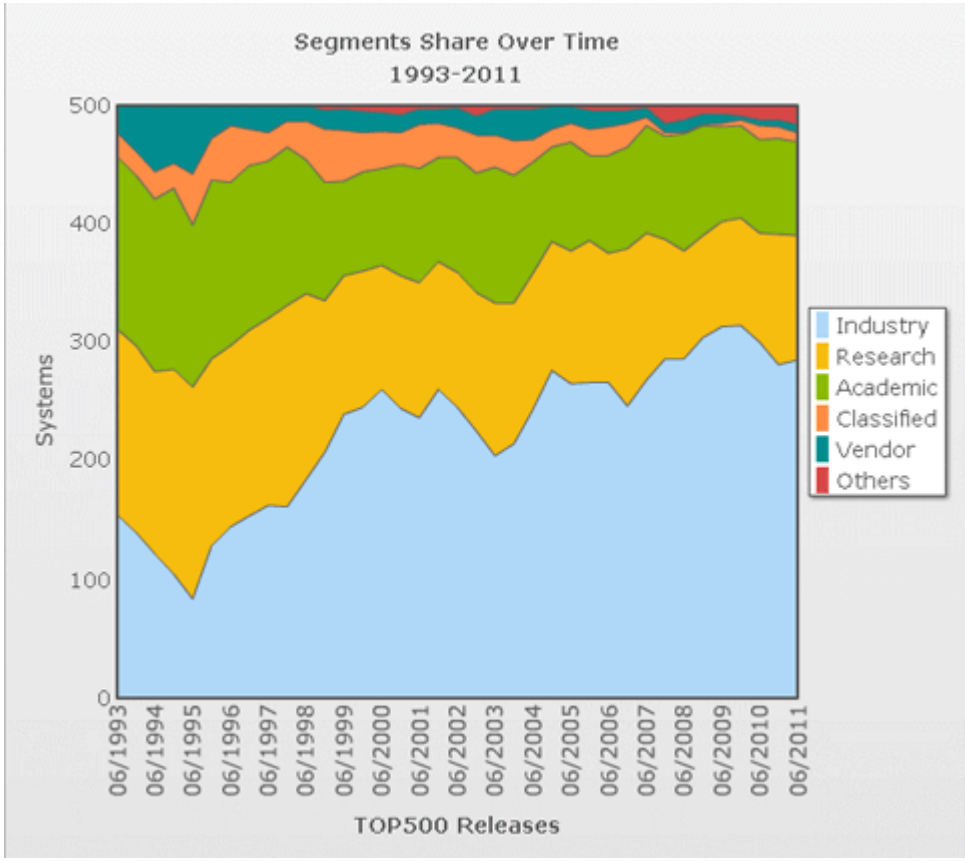


Materials/ Inf. Tech
Spintronics
Nano-science

Energy
Plasma Physics
Fuel Cells

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

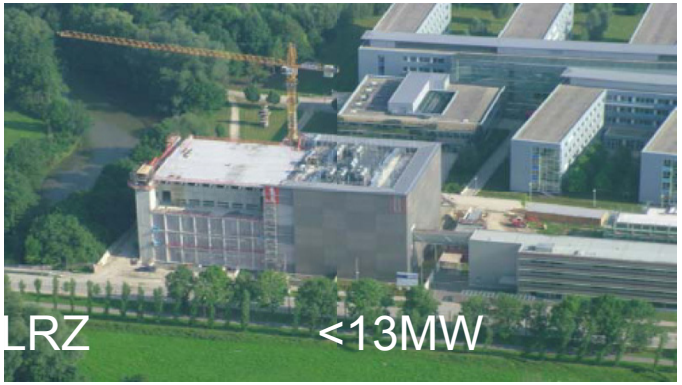
- ***Cray XE6 (Multi-year contract for $60+M)***
  - ***Phase 0 – 2010***
    10TF, 84 dual socket 8-core
    AMD Magny-Cours CPUs,
    1344 cores in total, 2 GHz,
    2GB/core,
    Gemini interconnect
  - ***Phase 1 Step 1 – Q3 2011***
    AMD Interlagos, 16 cores,1 PF
    2 – 4 GB/core
    2.7 PB file 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.***

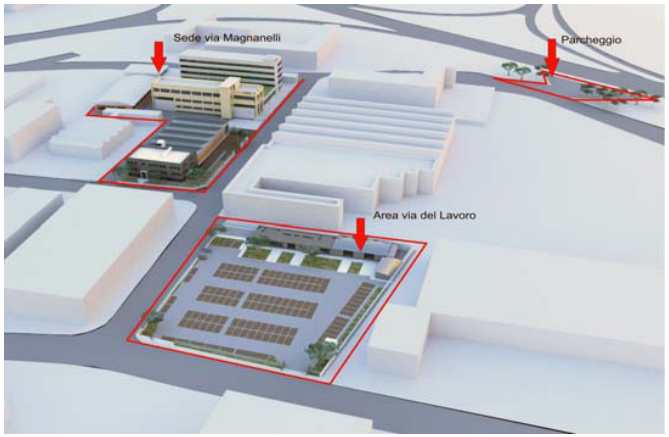
Prof. Arndt Bode, LRZ, and Martin Jetter, IBM, with a SuperMUC component prototype. (C) LRZ

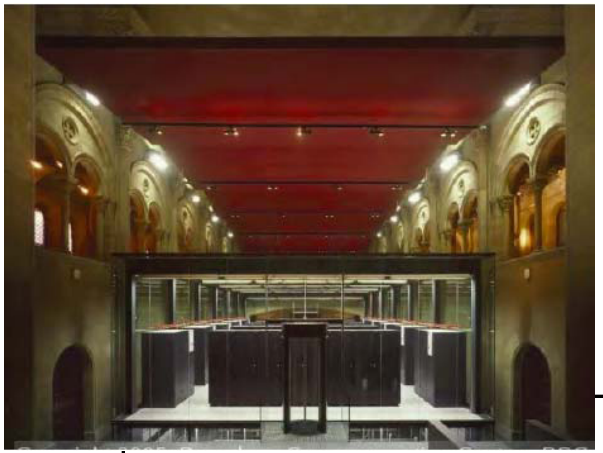


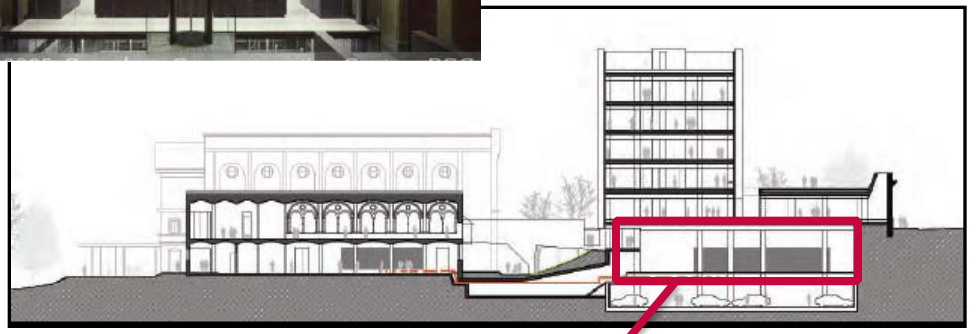
BSC and CINECA - Bologna (Italy)

- 2012/2013 5th and 6th PRACE Systems

CINECA
Target ~2.5 PF



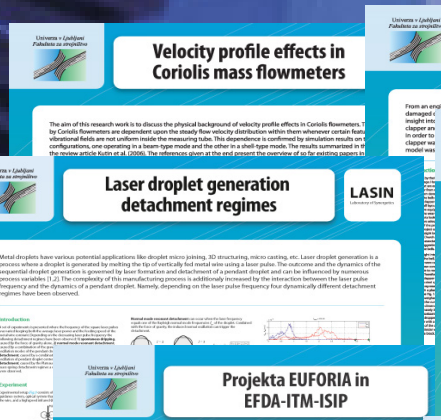


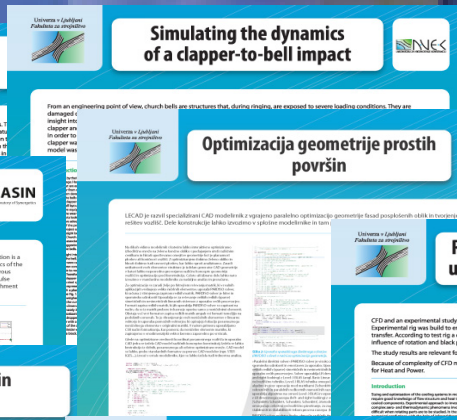


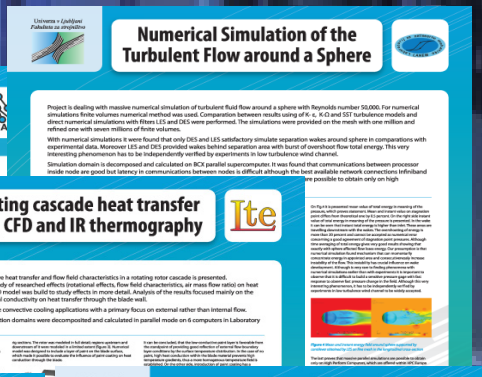
Computing Facility
10 MW 2013

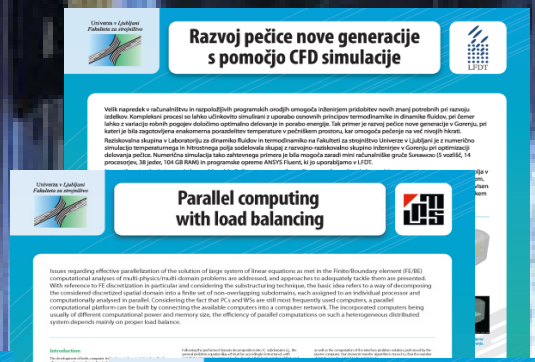
Supercomputing at UL FME --HPCFS for ?

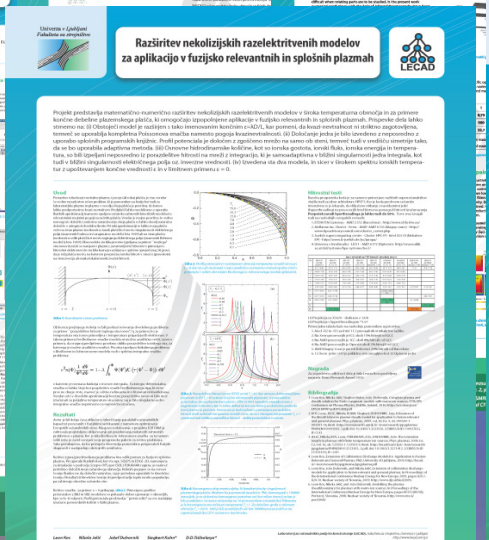
- ***Some examples of previous projects***

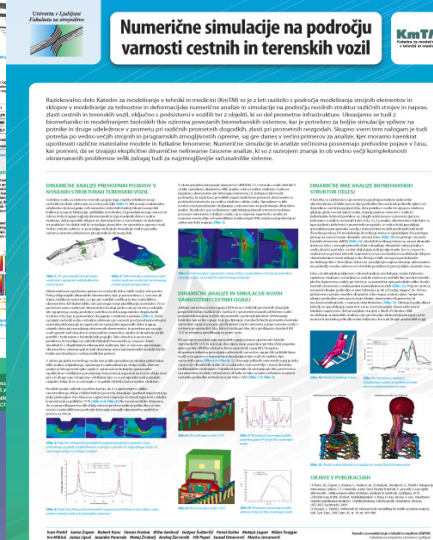






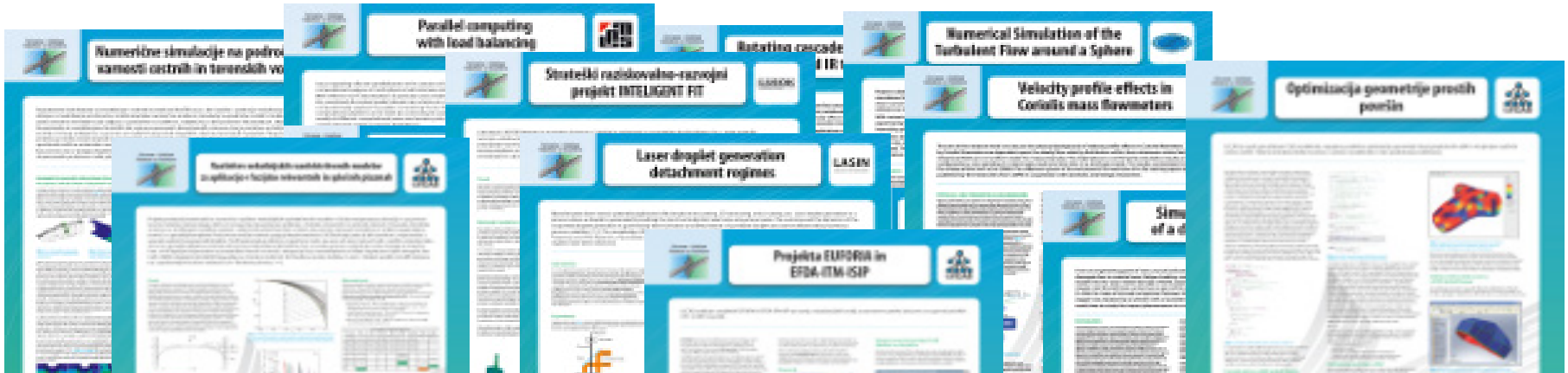






What HPCFS is used for?

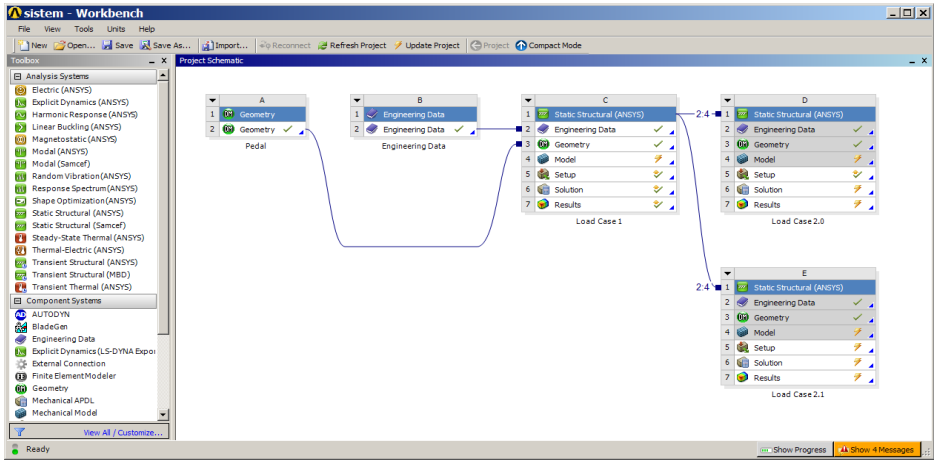
- ***Complex enginering research problems demands parallel processing***
- ***Education of new generation of students on II cycle ob Bologna process***
- ***Cooperation with other GRID and HPC centres***



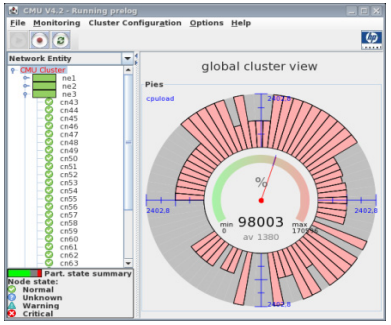
Long term goals

- 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

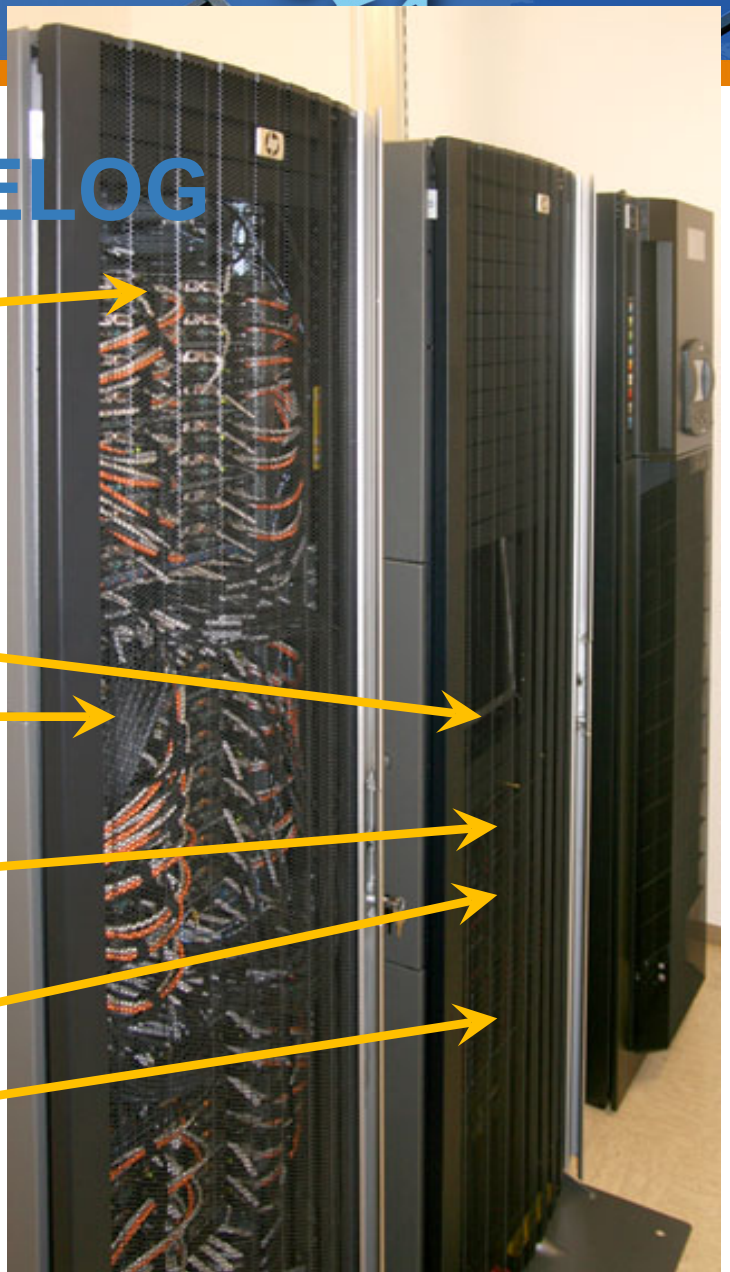


- Linux (CentOS 6.4)
- Remote desktop NX
- Development environment and LSF batch scheduler
- Compilers C++, Fortran (Python, R, ...)
- Parallel programming libraries with MPI, OpenMP
- Open-source anc commercial packages for simulations (ANSYS)
- Servers for support of the researsch and development



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.