Session E-infrastructures and Their Services for Research Infrastructures

The Partnership for Advanced Computing in Europe

Thomas Lippert
Chair of the PRACE Council

Ostrava, 6 November 2018

PRACE Helps Creating Leadership Science

- **Ground-breaking results of European science are**
  - achieved by supercomputing in various areas of science and industry
  - medicine, biology, geology, physics, engineering, social sciences etc
- **Leadership-class supercomputers in Europe currently are**
  - provided by 5 hosting countries
  - to be boosted by (pre)exascale and petascale systems through EuroHPC
  - Today provisioned by the PRACE in strict scientific peer review
  - mandatory for the success of European science and industry

Support by the European Commission

- **European Commission:** has supported the development of the PRACE infrastructure through a series of 1+6 pan-European implementation projects (PRACE IP-Projects)
- **26 Member States of PRACE:** PRACE IP-projects create and unite competence and efforts of experts on a pan-European scale

IT4Innovations & PRACE since 2010

- **Helps to access EU HPC resources for researchers in Czech Republic**
- **Contributes to EU HPC roadmap**
- **Commits 5-10% of IT4I resources for EU researchers (>DECI-9)**

June 2010
VSB Tech.
Univ. Ostrava
becomes PRACE
member

PRACE-4IP Kick Off Meeting April 2015

Int. HPC Summer School 2018

PRACE SUMMER SCHOOL 2013
17-21 June
Ostrava, Czech Republic

PRACE WINTER SCHOOL 2015
12 - 15 January
Ostrava, Czech Republic

PRACEdays16

WP6 – Co Lead

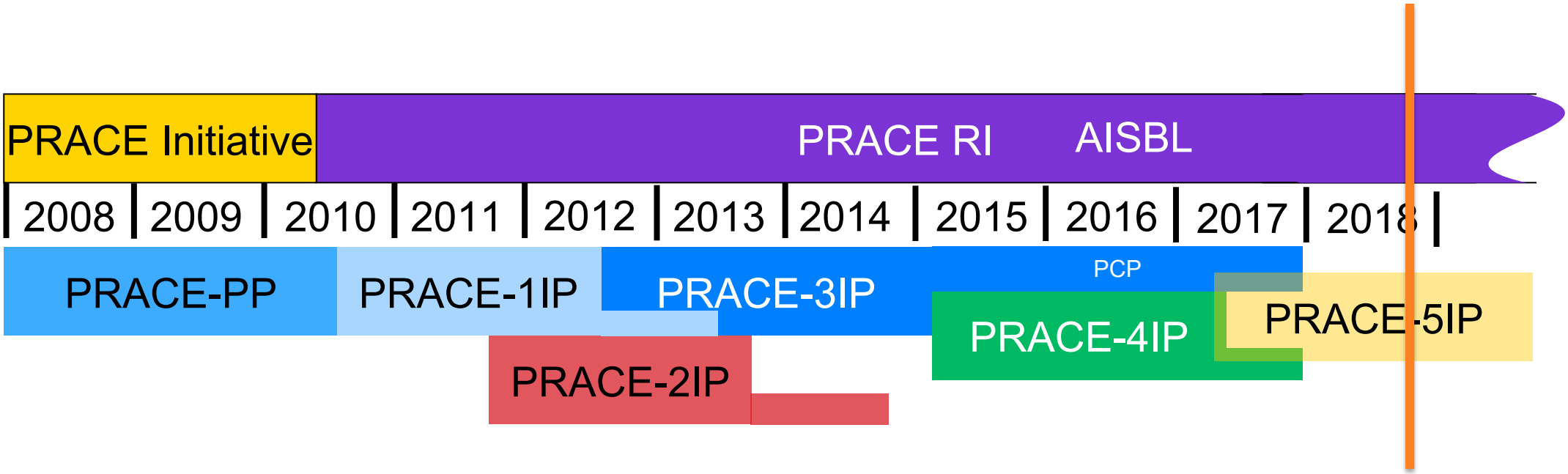
THE PRACE History

- **Precursor** The DEISA Project (Victor Alessandrini, F)
- **First Ideas** 2003 – HPC-Euro Interest Group (Hugh Pilcher Clayton, UK)
- **Closing in** 2006 – HPC in Europe Task Force (HET) (Kimmo Koski, FL)
- **ESFRI** 2006 – HPC is on the Roadmap
- **PRACE MoU** 2007 (Alain Lichnewsky, F, Achim Bachem, D)
- **PRACE Signing** 2010 (Achim Bachem, D)
- **PRACE II** 2016 (Anwar Osseyran, NL)
- **PRACE Future** 2018 …, TL, D

PRACE Mission

1. **Enable high-impact scientific discovery** and **engineering research** and development across all disciplines to enhance **European competitiveness** for the benefit of society.
2. Offering world-class computing and data management resources and services through a **peer review process**.
3. Strengthen the European users of HPC in **industry**

THE PRACE Timeline



IP Projects supported by EC with >110 Million €

Hosting Members

General Partners

IP Projects funded by EC

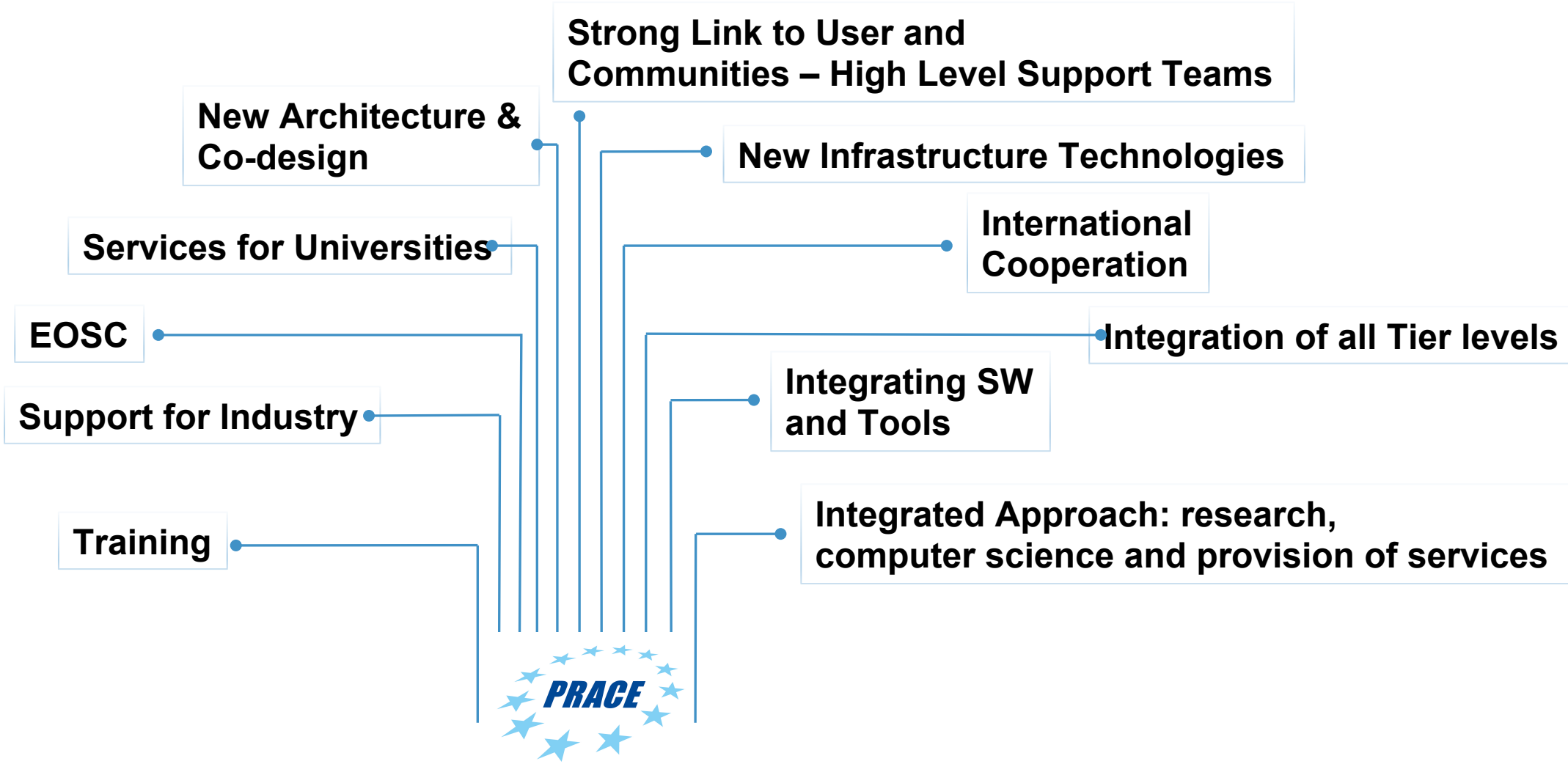
PRACE
AISBL

Scientific Steering
& Access Committees

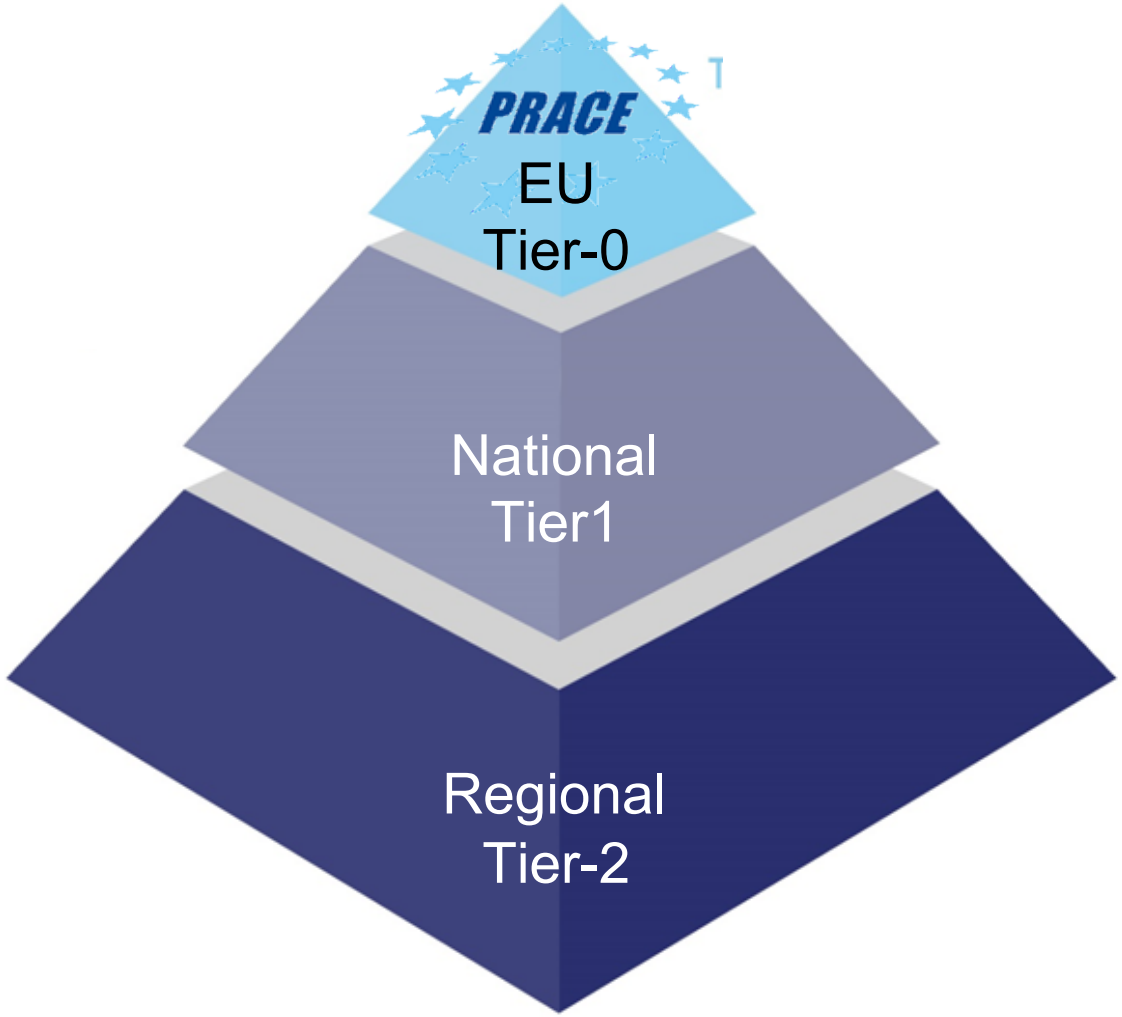
High Level Support Teams

European Application
Teams

PRACE Tree of Competences



Europe's HPC Provisioning Pyramid



PRACE Tier-0 Systems in 2018

NEW ENTRY 2018

JUWELS: Bull Sequana
GAUSS @ FZJ, Jülich, Germany

In the future: EuroHPC will provide Pre-Exascale and Exascale Machines

MareNostru
BSC, Barcel
#16 Top 500

enovo
Germany

TRY 2018

Piz Daint: Cray XC50
CSCS, Lugano, Switzerland
#3 Top 500

NEW ENTRY 2018

JOLIOT CURIE : Bull Sequana
GENCI/CEA, Bruyères-le-Châtel, France

Hazel Hen: Cray
GAUSS/HLRS,
Stuttgart, Germany
#19 Top 500

MARCONI: Lenovo
CINECA, Bologna, Italy
#14 Top 500

Close to 110 PFlops cumulated peak performance

http://82.116.198.186:8080/

The European HPC Systems Map


PRACE
universität innsbruck
TU WIEN
universität wien
JÜLICH FORSCHUNGSZENTRUM
lrz
MPCDF
Inria INVENTEURS DU MONDE NUMÉRIQUE
POLITÉCNICA "Engineering the future"
SURF SARA
UMEÅ UNIVERSITET
UNIVERSITAS OSLOENSIS MDCCCXI
NTNU
GCS Gauss Centre for Supercomputing
cea
cnrs
epcc
KTH VETENSKAP OCH KONST
CYFRONET
UNIVERSIDADE DE COIMBRA
HLRS High-Performance Computing Center | Stuttgart
UPPSALA UNIVERSITET
GENCI
INES
UPC
CSIC
RISC Software GmbH
WCSS
grnet
IUCC Inter-University Computation Center
Science & Technology Facilities Council
CSC
JKU JOHANNES KEPLER UNIVERSITÄT LINZ
University of Ljubljana
PRACE
CSCS
BSC
CINECA
IT4Innovations national supercomputing center
TÉCNICO LISBOA
LINKÖPING UNIVERSITY
CESGA
FIS Fakulteta za informacijske študije Faculty of information studies
UNINETT
ICHEC Irish Centre for High-End Computing
PSNC
İTÜ
THE CYPRUS INSTITUTE
NCSA NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS
KØBENHAVNS UNIVERSITET
KIFÜ
UNIVERSIDADE DE EVORA
İhsan Doğramacı Bilkent University

Top Infrastructure → Top Science

EuroHPC

- Infrastructure: huge investment
- Infrastructure: managed top-down
- EuroHPC
  - **EU** coordination and funding
  - Joint undertaking (JU)
  - 25 member states
  - Focus on **acquisition** & **operation**
  - Focus on **research** & **innovation**
- Declaration, Rome, 23-3-2017

- **Science** is community effort
- Science: develops **bottom-up**
- **PRACE**
  - Engagement of **many scientists**
  - Pan-European association (AISBL)
  - 26 members states
  - Established record in **provision**
  - Europe-wide **training**, **user support**
- **Foundation, Brussels, 17-4-2010**

PRACE

- Achievements

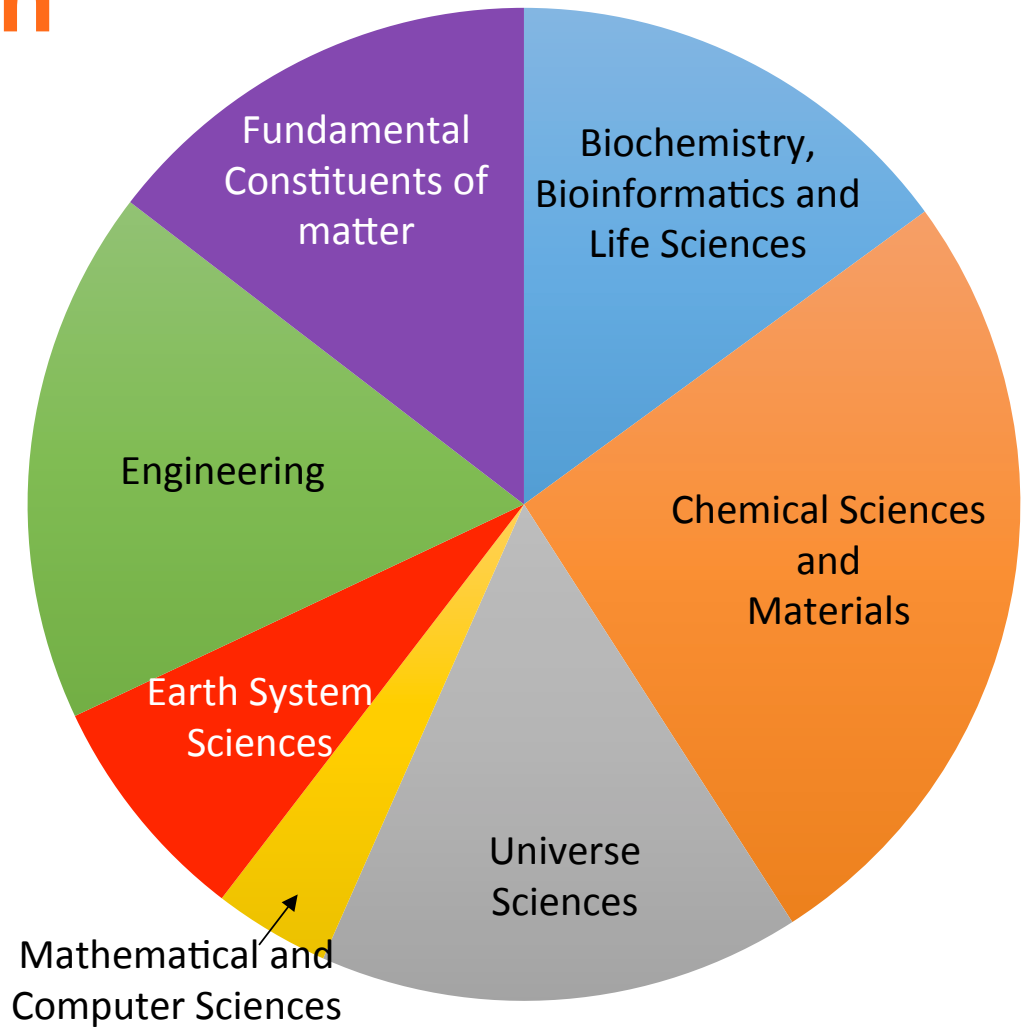
PRACE Main Achievements to-date

- >650 scientific projects enabled
- >17 billion core hours since 2010, 63% led by another PI than HM
- R&D access to industrial users with >50 companies supported
- >11 000 people trained through PRACE Training
- Close to 110 Petaflops of peak performance on 7 systems
- PRACE is only e-infrastructure landmark on ESFRI Roadmap 2016

PRACE Peer Review

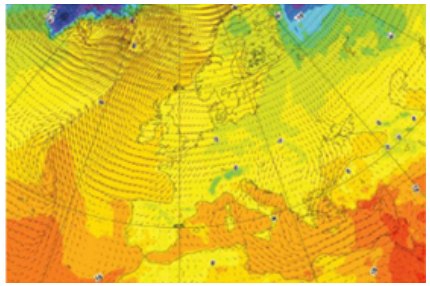
- Know-how over 8+ years
- ERC standard peer review process
- Peer Review Office (PRO)
  - check of proposals
  - coordination of the process
- Technical Review of proposals
- Access Committee – Domain and HPC specific criteria
- Resource Allocation Panel (RAS)

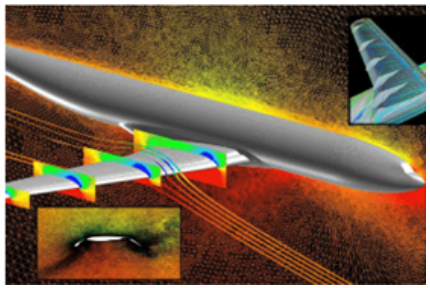
Application Spectrum

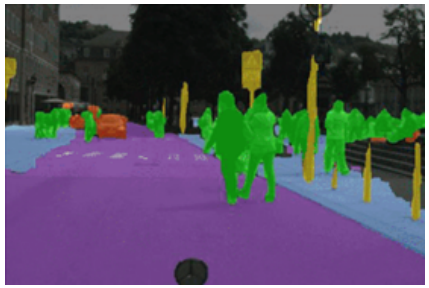


PRACE – Scientific Case

- **Scientific applications**
  - urgent need for more compute cycles, AND
  - huge demands memory bandwidth & I/O
- **Need new approaches**
  - Ensemble parallelism, deep learning, and statistical models
  - systems able to handle tens of thousands of active jobs and large I/O requests
- **Software & algorithms** take longer to change than hardware
  - PRACE & Europe need a much more ambitious strategy to develop the SW part of next-generation computing





PRACE Schools

Excellence in Education and Training for HPC in Europe

PRACE WINTER SCHOOL 2017
6-9 February 2017
Tel Aviv, Israel

PRACE MOOC

Supercomputing Online Course

PRACE Spring School
School for Developers of Petascale Applications

#CODE VAULT

PRACE Advanced Training Centres

&

PRACE Training Centres

SHAPE

SME HPC Adoption Programme in Europe

- PRACE-based programme supporting HPC adoption by SMEs
- PRACE Council endorsed SHAPE as a permanent PRACE service
- Calls for applications

"The decision of the PRACE Council to make SHAPE (SME HPC Adoption Programme in Europe) a permanent service was keenly welcomed by the PRACE Industrial Advisory Committee (IAC)"

Jürgen Kohler, Chair of the IAC

OUR PRACE DAYS

Where Science meets Industry

PRACE IP All-Hands Meeting

Athens, 31 January - 2 February 2017

EDI

The European Data Initiative

The European Data Initiative (EDI)

- Combination of world-class supercomputing (HPC) capability, high-speed connectivity, data storage and interfaces for cloud-based service delivery.
- Only with High-performance ICT infrastructures the current and expected scale of future data flows can be managed.
- European science, industry and public services need world-class infrastructures to compete in the digital economy.

Towards EDI | challenges

- Target Exascale building up on PRACE's momentum
- Move towards a data-centric approach
- Extend services towards industry and to public sector
- Enhance integration of the Tiers and connects to EOSC

The Role of PRACE in EDI

- **Support EuroHPC → establishment of EDI**

  PRACE and GÉANT should interact as core providers of EDI.

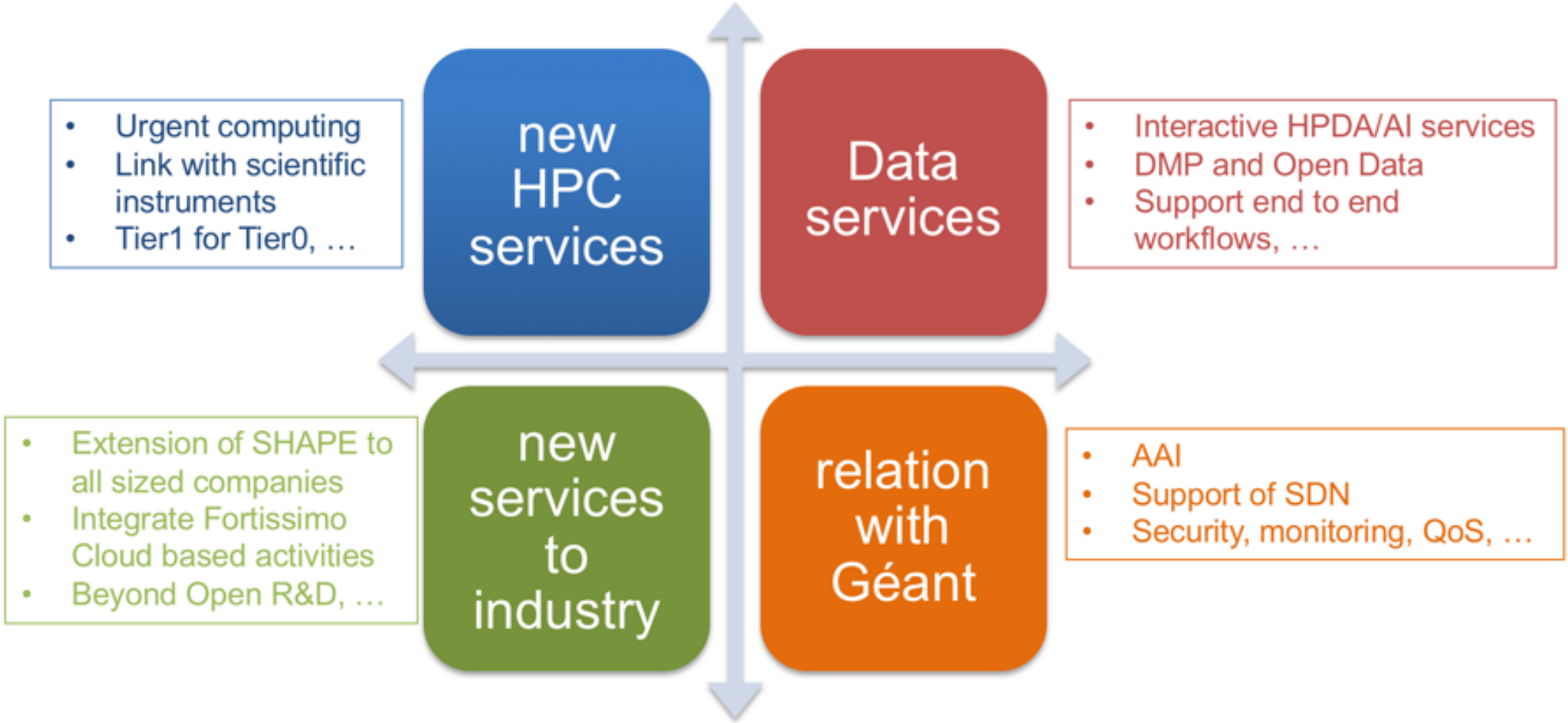
- **New HPC / HPDA / AI services**

  Urgent computing, link with scientific instruments

- Scale up SME Adoption Programme (SHAPE)

- **Pan-European federated data infrastructure**

  PRACE will feature a data management and access layer based on infrastructures like **ICEI / Fenix** (HBP) and EUDAT


new HPC services
Data services
new services to industry
relation with Géant
• Urgent computing
• Link with scientific instruments
• Tier1 for Tier0, …
• Interactive HPDA/AI services
• DMP and Open Data
• Support end to end workflows, …
• Extension of SHAPE to all sized companies
• Integrate Fortissimo Cloud based activities
• Beyond Open R&D, …
• AAI
• Support of SDN
• Security, monitoring, QoS, …

THANK YOU FOR YOUR ATTENTION

www.prace-ri.eu

PRACE

Enabling Leading Edge Simulations for European Science

- Selected Results from PRACE Systems

Mare Nostrum @ BSC – 2017

3456 nodes
394 TB RAM, 830 TB SSD
14 PB disk
tape storage n/a

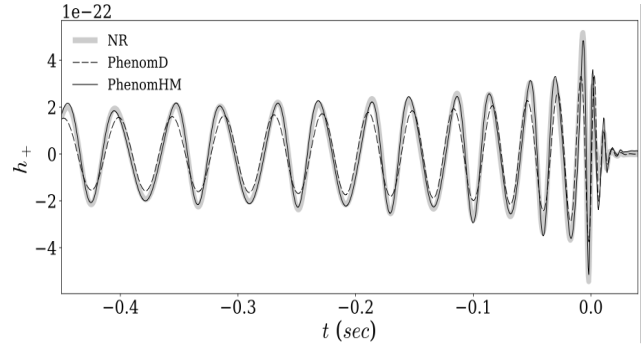
OPA	
Mare Nostrum 6480 Skylake	Mare Nostrum 2016 p9+Volta

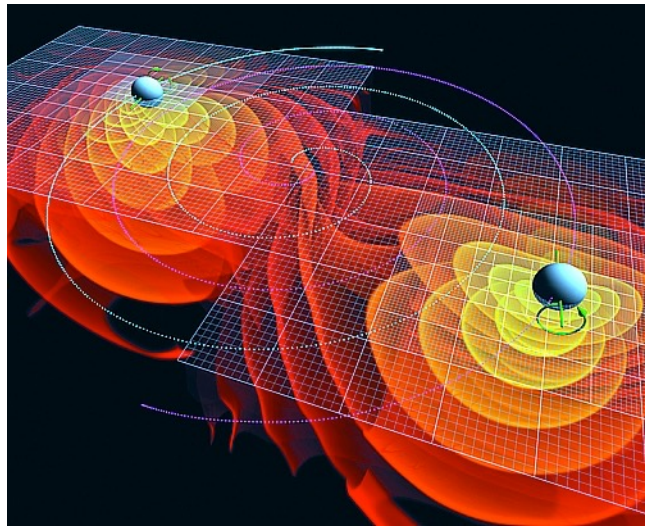
Modelling Gravitational Wave Signals

Models For Nobles

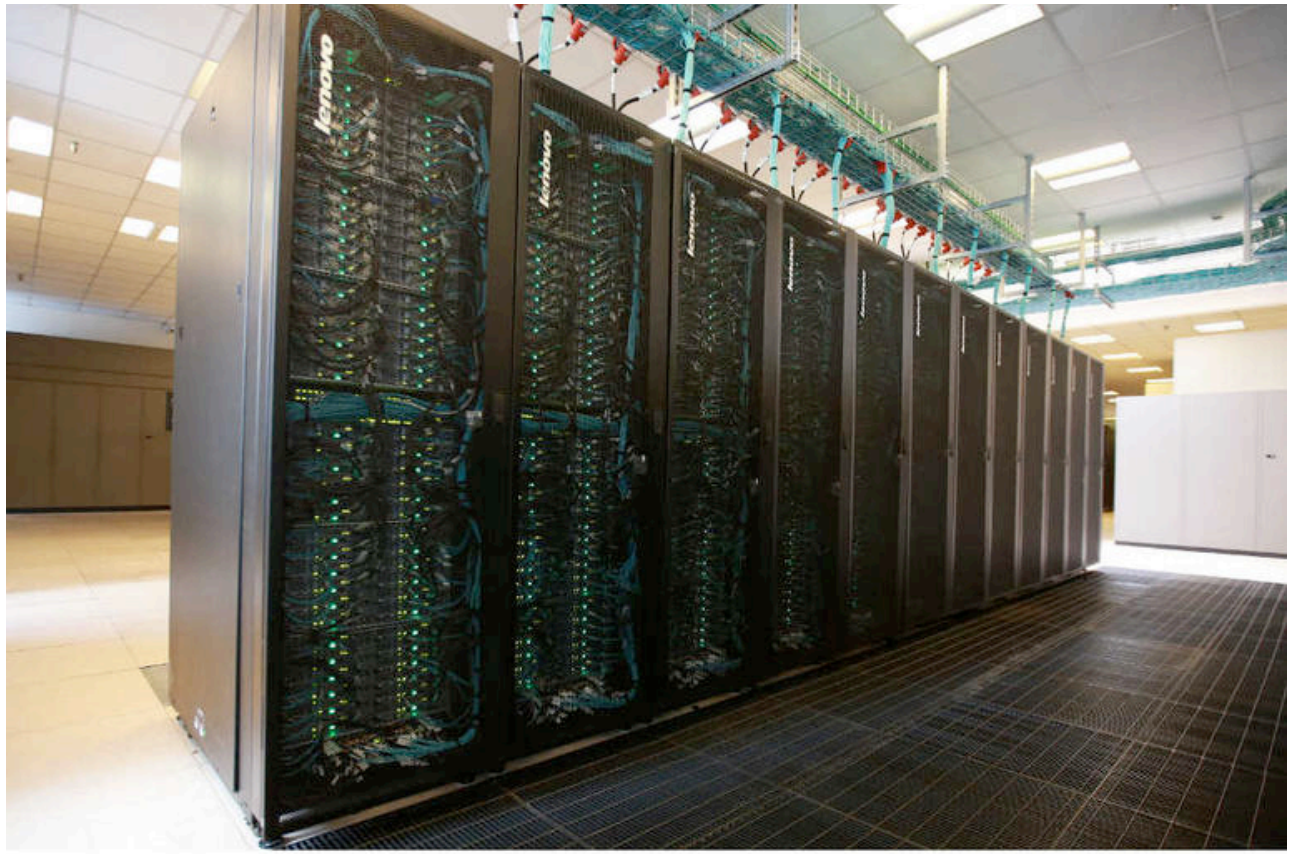
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

- Identification of gravitational wave signals from merging black holes
- Model signals across the parameter space of plausible binary mergers ≧ 7 dimensions!
- Model Input: solutions of Einstein's Equations
- 1 point in parameter space ~ O(10^5) CPU hours
- Templates for analysis: LIGO/Virgo detectors





Marconi @ CINECA – 2017



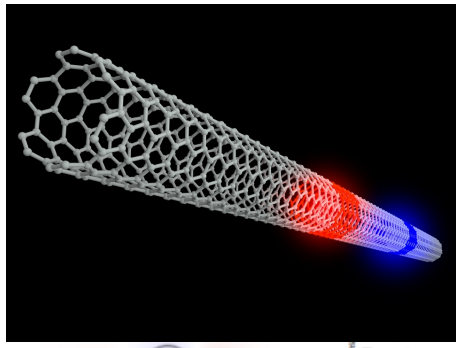
6600 server nodes
560 TB memory
15 PB disk
60 PB tape storage

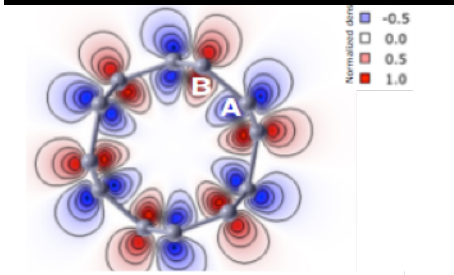
OPA		
Marconi 1440 Broadwell	Marconi 3600 KNL	Marconi 4608 Shkylake

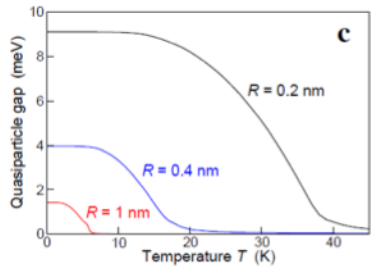
Carbon Nanotubes as Excitonic Insulators

Forefront Simulation

- Excitonic Insulator Phase: instability of a zero gap semiconductor against tendency of mutually attracting electrons and holes to form bound pairs
- Idea: W. Kohn in 1968, but observation of EIP still elusive
- Finally Proved on CINECA systems by ab initio simulations (QMC): below a critical temperature the exciton phase is present theoretically, EIP is realized in zero gap carbon nanotubes (CNT)







Piz Daint @ CSCS – 2016

6751 server nodes
600 TB memory
10 PB disk
tape storage

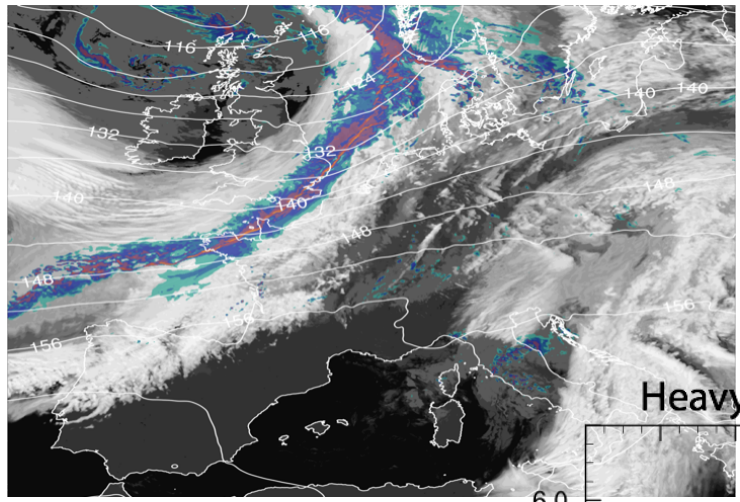
Cray Aries	
Piz Daint 5320 Haswell + Tesla	Piz Daint 2862 Broadwell

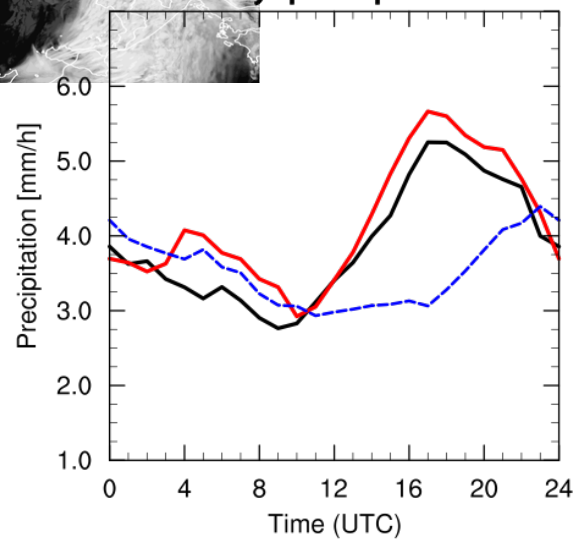
Convection Resolving Climate Simulations

World Record in Code Acceleration

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

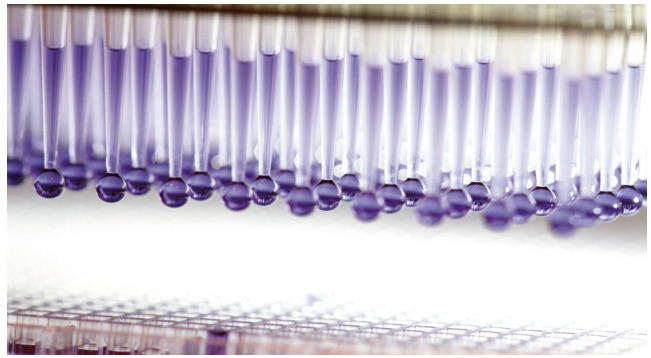
- Convection needs km-scale resolution
- Significant improvements in representation of diurnal cycle, heavy precipitation and clouds
- COSMO model scales to 5300 GPU accelerated nodes, runs 2-3x faster than on TaihuLight (present #1 on Top500)





The Grand Challenge of Drug Design

- Office of Health Economics study of 2011
- Cost of developing new drugs
  - $ 200 million in the 1970s
  - $ 2 billion in 2010 (scaled to 2011 currency values)
- Development time
  - 6 years in the 1970s
  - 13.5 years in 2010
- Classical search technology for new drugs not scalable (costs and time)
  - For new drugs: > 1 million candidates to test
  - For each candidate: $ 20 to $ 130



Boost Prototyping and Reduce Costs by Supercomputers

- Industry
  - Novartis – Swiss Pharmaceutical
  - Schrödinger – German life and materials science software
- The Task
  - 21 million drug candidate molecules tested by Novartis
  - New HPC algorithm by Schrödinger
- The Costs
  - Production run costs: EUR 10,000 on Piz Daint
  - Gain Factor: O(1000) in costs and person hours

Curie @ GENCI – 2013

5588 server nodes
360 TB memory
6 PB disk
10 PB tape storage

Mellanox IB QDR

Curie 10080 Sandy Bridge	Curie 1440 Nehalem	Curie 188 Westmere + Tesla

Biggest Crash Optimization Ever

Push Competitiveness of European Industry

- Renault: New optimization methods based on 20 million d.o.f. finite elements meshes with 200 different parameters
- Anticipate new security rules (EuroNCAP6)
- Impossible with existing Renault R&D facilities
- World premiere:

  5 years lead for

RENAULT NISSAN

Ter@tec

cea

Best use of HPC in Automotive
HPC wire
Readers' Choice Awards 2014

Hazel Hen @ HLRS – 2015

7712 server nodes
964 TB memory
10 PB disk
tape storage

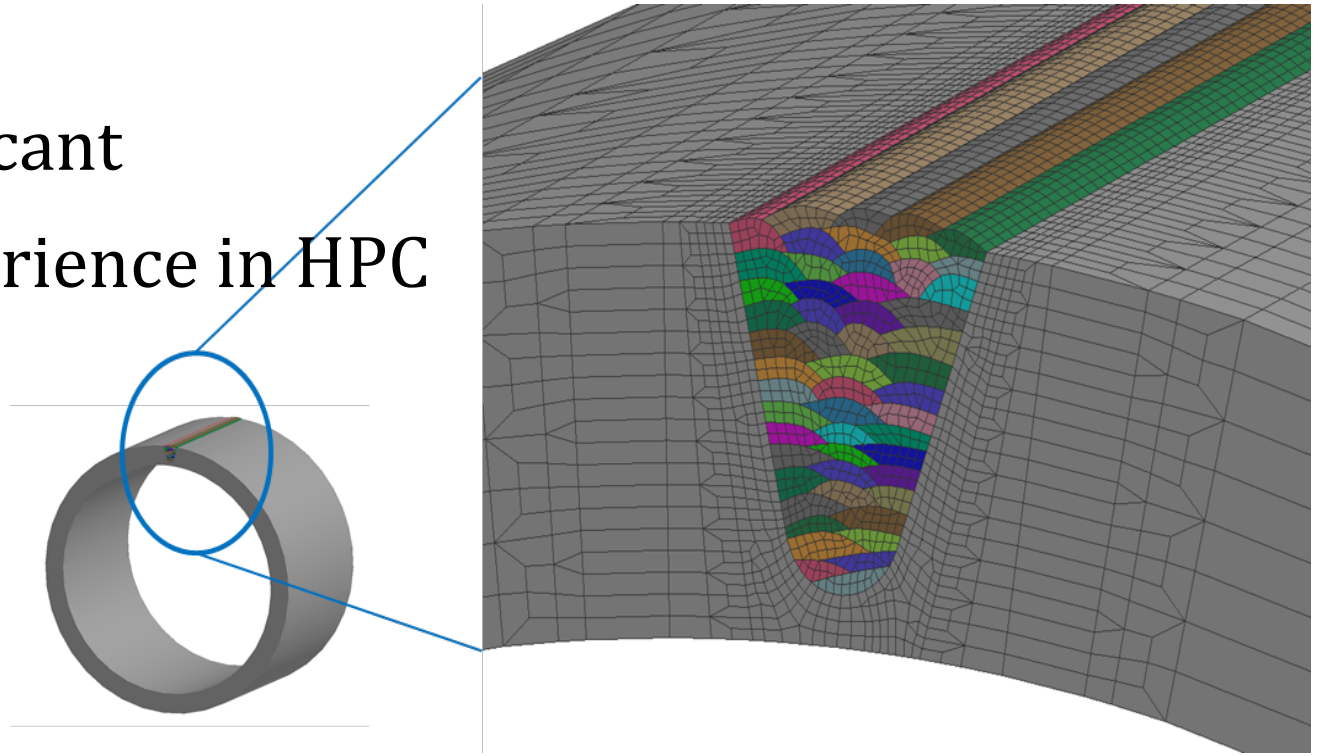
Cray Aries

Hazel Hen
15424
Haswell

HPC Welding - A SHAPE Project

PRACE Brings SMEs to HPC

- Simulation of multi-layered welding lines
- Close collaboration with office of welding and DYNAmore supporting LS-DYNA
- The SME gained significant knowledge and experience in HPC
- The SME sees high commercial benefit as to better cost estimates



JUQUEEN @ JSC – 2012

28672 nodes
448 TB memory
18 PB disk
75 PB tape storage

BGQ 5D Torus

JUQUEEN
28672
Power BQC

PI: Zoltán Fodor, Ab inition calculation of the neutron-proton mass difference, Science 347 (2015) 1452-1455, 150 Mio core hours.

JÜLICH FORSCHUNGSZENTRUM

GCS Gauss Centre for Supercomputing

Daß ich erkenne, was die Welt im

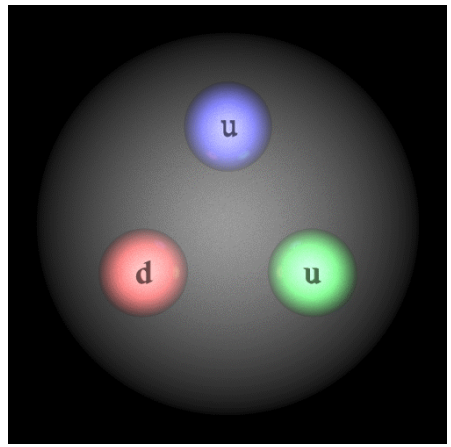
That I may understand whatever,
Binds world's inner core together

Faust, J. W. Goethe

Results for Textbooks

- Solving an 80 year old riddle
- Understanding the mass difference of proton and neutron by simulation of the fundamental theory, QCD
- 80 years after the experimental detection: simulation on JUQUEEN

Proton Neutron



SFB TRR55

Universität Wuppertal

Universität Regensburg

Science

AAAS

SuperMUC @ LRZ – 2015

15062 server nodes
537 TB memory
15 PB disk
30 PB tape storage

Mellanox IB QDR	Mellanox IB FDR	Mellanox IB FDR
SuperMUC 19252 Sandy Bridge	SzperMUC2 10752 Haswell	SuperMuc3 60 KNL

Supernova Simulations

Breakthrough Predictions

- How do neutron stars form?
- We know by the most advanced 3D simulation of supernovae
- Highly efficient, well parallelized numerical implementation on SuperMUC
- A New Neutrino-Emission Asymmetry in Forming Neutron Stars is predicted