HPC PERSPECTIVES FOR EUROPE

Towards a European Exascale Ecosystem

Thomas Lippert – Director of Jülich Supercomputing Centre, Germany

Professor for Modular Supercomputing and Quantum Computing, Goethe University Frankfurt
PRACE | HBP | EuroHPC RIAG | DEEP-Projects | Groupe Mousquetaire

A SHORT HISTORY OF EUROPEAN HPC

THE PRACE ERA

THOMAS LIPPERT LED PRACE AS CHAIR FROM 2018 TO 2020

PRACE | Milestones

- Ancestor — 2002 – DEISA Project (Victor Alessandrini, F)
- First Steps — 2003 – HPC-Euro Interest Group (Hugh Pilcher Clayton, UK)
- Closing in — 2006 – HPC in Europe Task Force (HET) (Kimmo Koski, FL)
- ESFRI — 2006 – HPC on the Roadmap
- PRACE MoU — 2007 (Alain Lichnewsky, F, Achim Bachem, D)
- PRACE Signature — 2010 (Achim Bachem, D)
- PRACE II — 2016 (Anwar Osseyran, NL)
- PRACE meets EuroHPC — 2019 (Thomas Lippert, D)

PRACE | members

Hosting Members

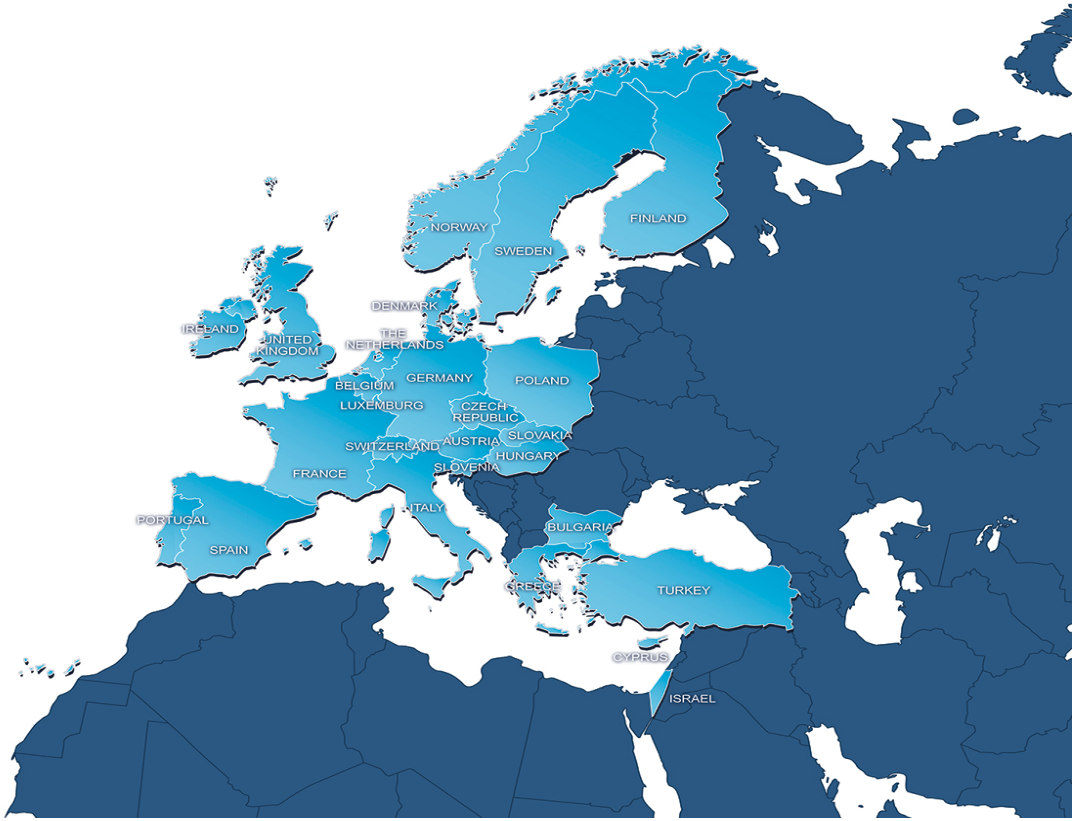
- France
- Germany
- Italy
- Spain
- Switzerland

General Partners (PRACE 2)

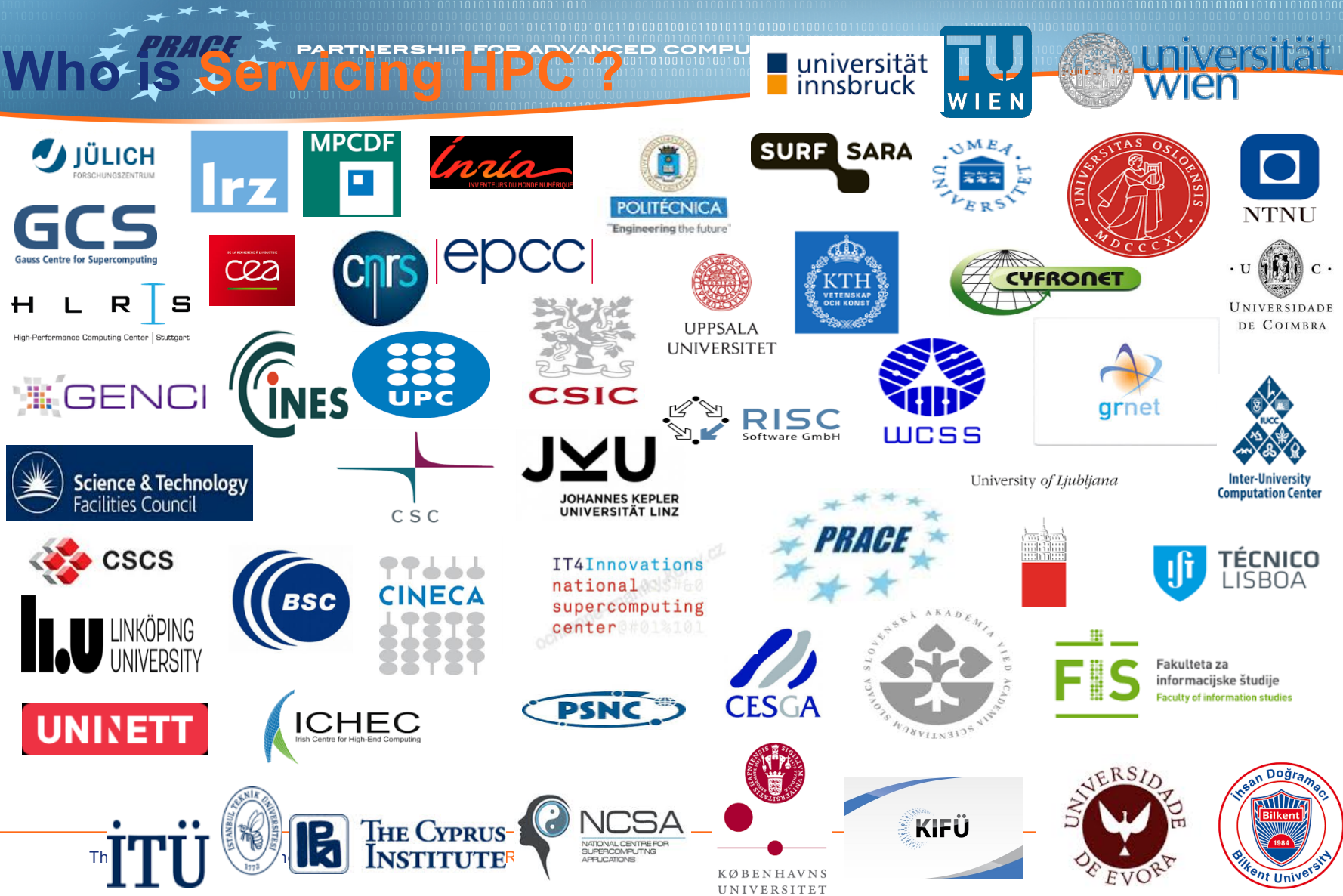
- Austria
- Belgium
- Bulgaria
- Cyprus
- Czech Republic
- Denmark
- Finland
- Greece
- Hungary
- Ireland
- Israel
- Luxembourg
- Netherlands
- Norway
- Poland
- Portugal
- Slovakia
- Slovenia
- Sweden
- Turkey
- United Kingdom

Observers

- Croatia
- Romania



Who is Servicing HPC ?



PRACE | Tier-0 Systems in 2020

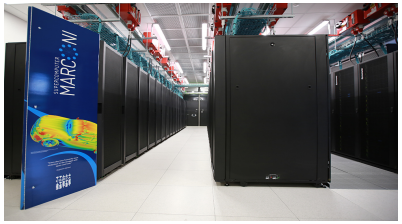
MareNostrum: IBM
BSC, Barcelona, Spain
#38 Top 500

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

NEW ENTRY 2018/2019
SuperMUC NG: Lenovo cluster GAUSS @ LRZ, Garching, Germany #13 Top 500

NEW ENTRY 2018
JUWELS (Module 1):
Atos/Bull Sequana
GAUSS @ FZJ, Jülich, Germany #39 Top 500

NEW ENTRY 2018
JOLIOT CURIE : Atos/Bull Sequana X1000;
GENCI @ CEA, Bruyères-le-Châtel, France
#34 Top 500

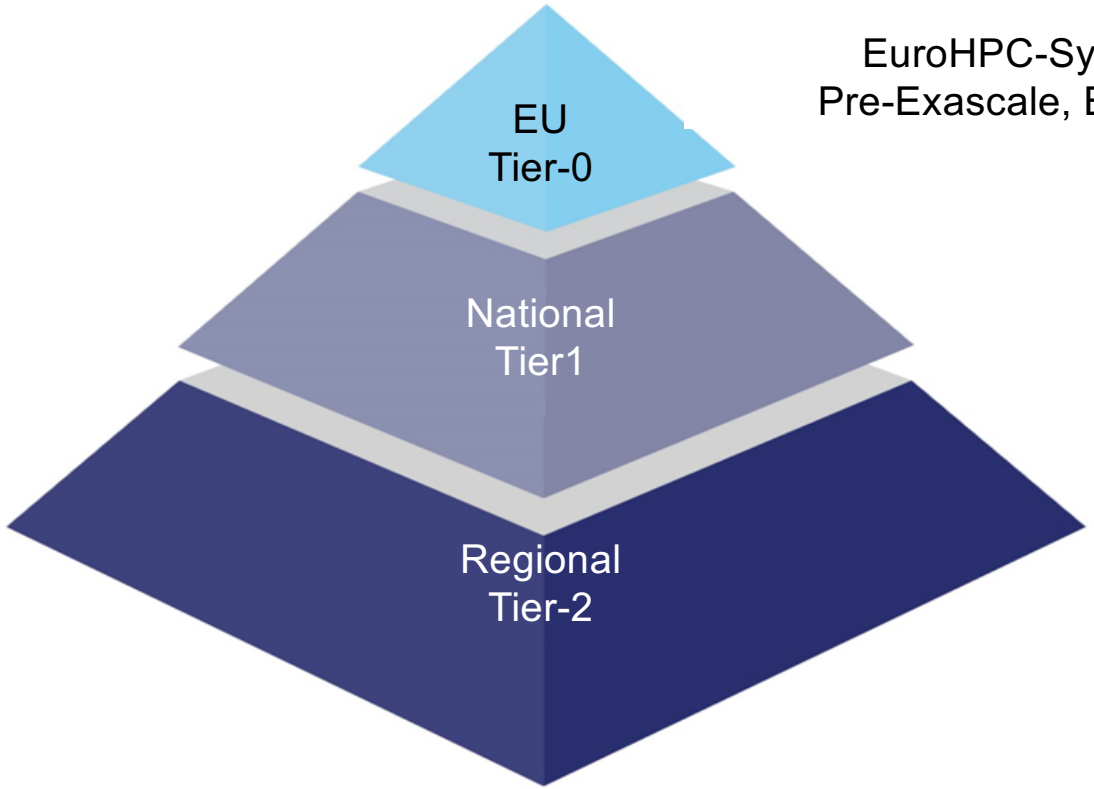


MARCONI-100: IBM
CINECA, Bologna, Italy
#9 Top 500

NEW ENTRY 2020
HAWK: HPE Apollo
GAUSS @ HLRS, Stuttgart, Germany

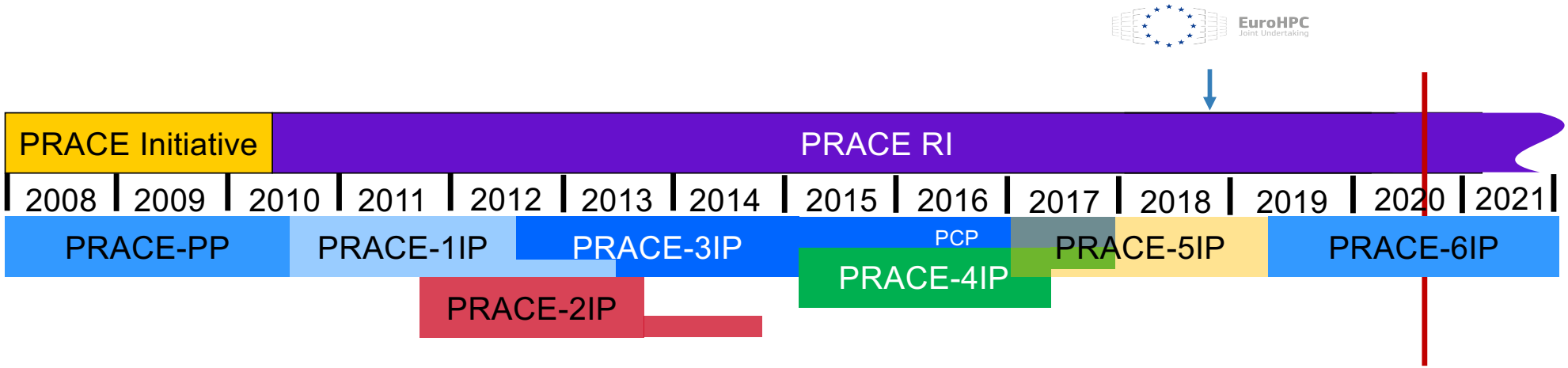
Close to 110 Petaflops total peak performance

European Provisioning Pyramid in the Future



EuroHPC-Systems
Pre-Exascale, Exascale

PRACE | Implementation Projects



- PRACE-IP projects accelerate the implementation of the PRACE RI
- IP Projects supported by EC with >100 Million €

PRACE | Achievements

- 688 scientific projects enabled
- 110 Petaflops of peak performance on 7 Tier-0 systems
- >21 billion since 2010 – 63% led by PI not from HM
- >50 companies supported
- >12 000 people trained through PRACE Training

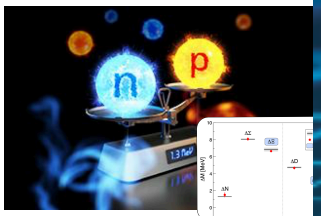
PRACE | Scientific Case 2018–2026

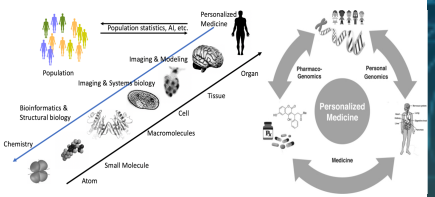
"Future Infrastructures and operations will need to be much more diverse to support HPC, Data Science and different types of accelerators - but we also need to avoid fragmentation."

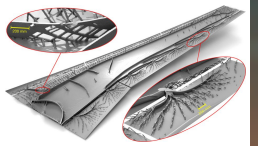
PRACE Scientific Case
by PRACE SSC

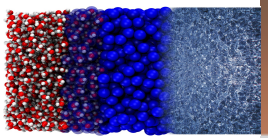
THE EUROPEAN SCIENTIFIC CASE

- **Fundamental Sciences**
  - Astrophysics, Cosmology, Particle Physics
- **Climate, Weather, and Earth Sciences**
  - Climate Change, Meteorology, Oceanography, Solid Earth Sciences
- **Life Sciences**
  - **Bioinformatics, Systems & Structural Biology, Neuroscience**
- **Energy**
  - **Renewable Energy, Fusion Energy, Sustainable Energy**
- **Infrastructure & Manufacturing**
  - Engineering, Integrative Design, Manufacturing
- **Future Materials**
  - Atomic and Electronic Structure, Data-driven Materials Design
- **Complexity & Data**
  - AI, Deep Learning, GANs, Convergence with Simulation









Access Mode	Extreme Scale	Regular	Benchmark	Development	Academic Fast Track	Industry Fast Track
Duration	1y renewable	1y renewable	2 to 3 months	1y renewable	< 6 months	1y renewable
Periodicity	1x / y	3x / y	Continuous call, weekly cut-offs	Continuous call, weekly cut-offs	Continuous call, cut-offs ev. 2w/1m	Continuous call, cut-offs ev. 2w/1m
Project size (core hours)	> 75 M	< 75 M	200 k to 500 k	1 M to 5 M	Up to 75 M	Up to 75 M
Share of resources	50 to 70% Mostly pre-exascale	20 to 30% Mostly multi-petascale	Few % All systems	Few % All systems	~5% All systems	~5% All systems
Data storage needs	Large storage for medium to long term	Large storage for medium to long term	Limited	Data processing environment and platform		
Accessible to industry	Yes – Open R&D With specific track	Yes – Open R&D With specific track	Yes – Open R&D	Yes – Open R&D	Yes – Open R&D	Exclusively Open R&D
External sc. review	Yes	Yes	No	No	No / Pre-identified	No / Pre-identified
Tech. review	Yes	Yes	Yes	Yes	Yes	Yes
DMP required	Yes	Yes	No	No	Yes	Yes
Proposal type	Full proposal	Full proposal	Technical proposal	Technical proposal	Light request + support documents	Full proposal
Prerequisite	Benchmark	Benchmark	None	None	Previous allocation or Benchmark	Benchmark
Submission period	> 2 months	> 2 months	N/A	N/A	N/A	N/A
Duration of evaluation process	5 months	2 months	≥1 week <2 weeks	≥1 week <2 weeks	≥2 weeks <1 month	≥2 weeks <1 month

PRACE fighting COVID-19

- PRACE runs a **Fast Track Call for Proposals** for projects that will use supercomputers to contribute to fight against **COVID-19**
- Access to the **Europe's most powerful supercomputers**
- More than 25 proposals have been awarded since end of March 2020 with research topics such as:
  - Bio-simulations to develop therapeutics and/or vaccines
  - Epidemiologic analysis to understand and forecast the spread of the disease
  - Biomolecular research to understand the mechanisms of the virus infection

EuroHPC
Joint Undertaking

EUROHPC ERA – 2018 ---

JÜLICH
Forschungszentrum

EUROHPC MEMBERS

- Commission (represents the Union)
- Austria, Belgium, Bulgaria, Croatia, Cyprus, Czech Republic, Denmark, Estonia, Finland, France, Germany, Greece, Hungary, Iceland, Ireland, Italy, Latvia, Lithuania, Luxembourg, Montenegro, the Netherlands, North Macedonia, Norway, Poland, Portugal, Romania, Slovakia, Slovenia, Spain, Sweden, Switzerland, and Turkey
- European Technology Platform for High Performance Computing (ETP4HPC)
- Big Data Value Association (BDVA)

EuroHPC Activities 2019-2020

Infrastructure & Operations

R&I, Applications & Skills

JU Admin/Running costs

HPC Ecosystem

- **Infrastructure + Operations**

  Procurement of 2 pre-exascale machines and at least 2 petascale machines

- **Applications & Skills + R&I**

  R&I, exascale technologies and systems (incl. low-power processor); applications

- **JU Admin/running costs**

JU Operation: 2019 to 2026

Indicative only!

~270	min 180	10	In M€
~290	~186	10	486
560	392	20	486
0	~420 (in kind)	2	972
			422

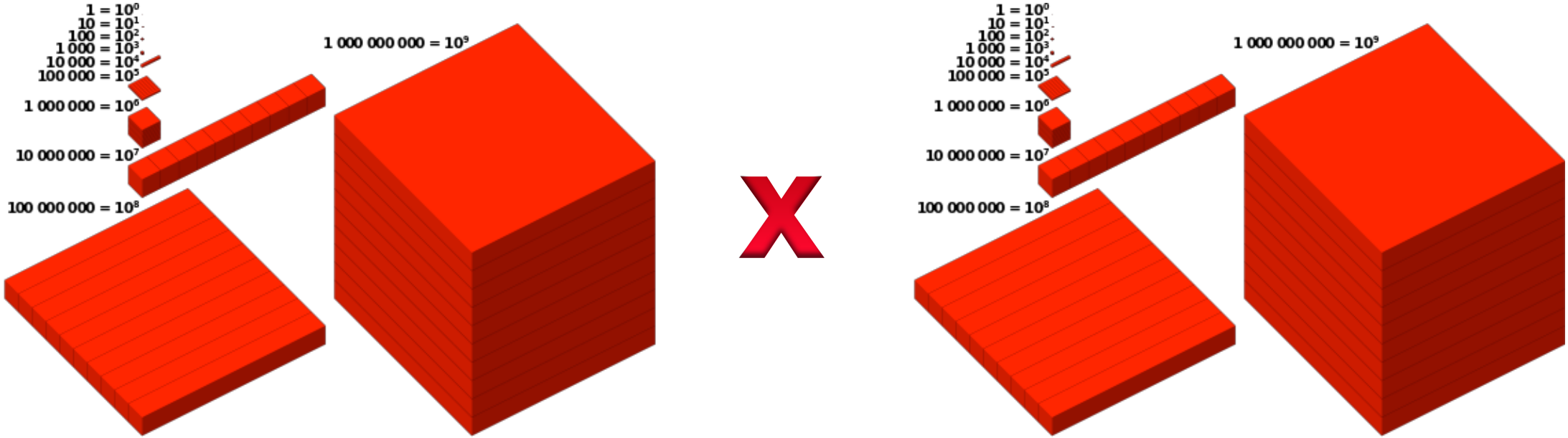
EC
Participating States
Total
Private Members

EUROHPC PETASCALE SYSTEMS

Country	System Name
Bulgaria	PetaSC
Czech Republic	EURO_IT4I
Luxembourg	MeluXina
Portugal	Deucalion
Slovenia	VEGA

EUROHPC PRE-EXASCALE SYSTEMS

Country	System Name
Finland	Lumi
Italy	Leonardo
Spain	Mare Nostrum 5



TOWARDS THE EXASCALE ERA IN EUROPE

THE JÜLICH APPROACH

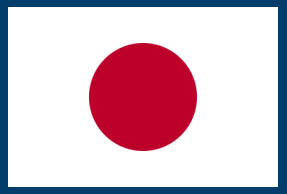
EXASCALE PLANS WORLDWIDE

2020+ (3)

Integrator: China
Processors: China

2021+ (3)

Integrator: US
Processors: US



2021 (1)

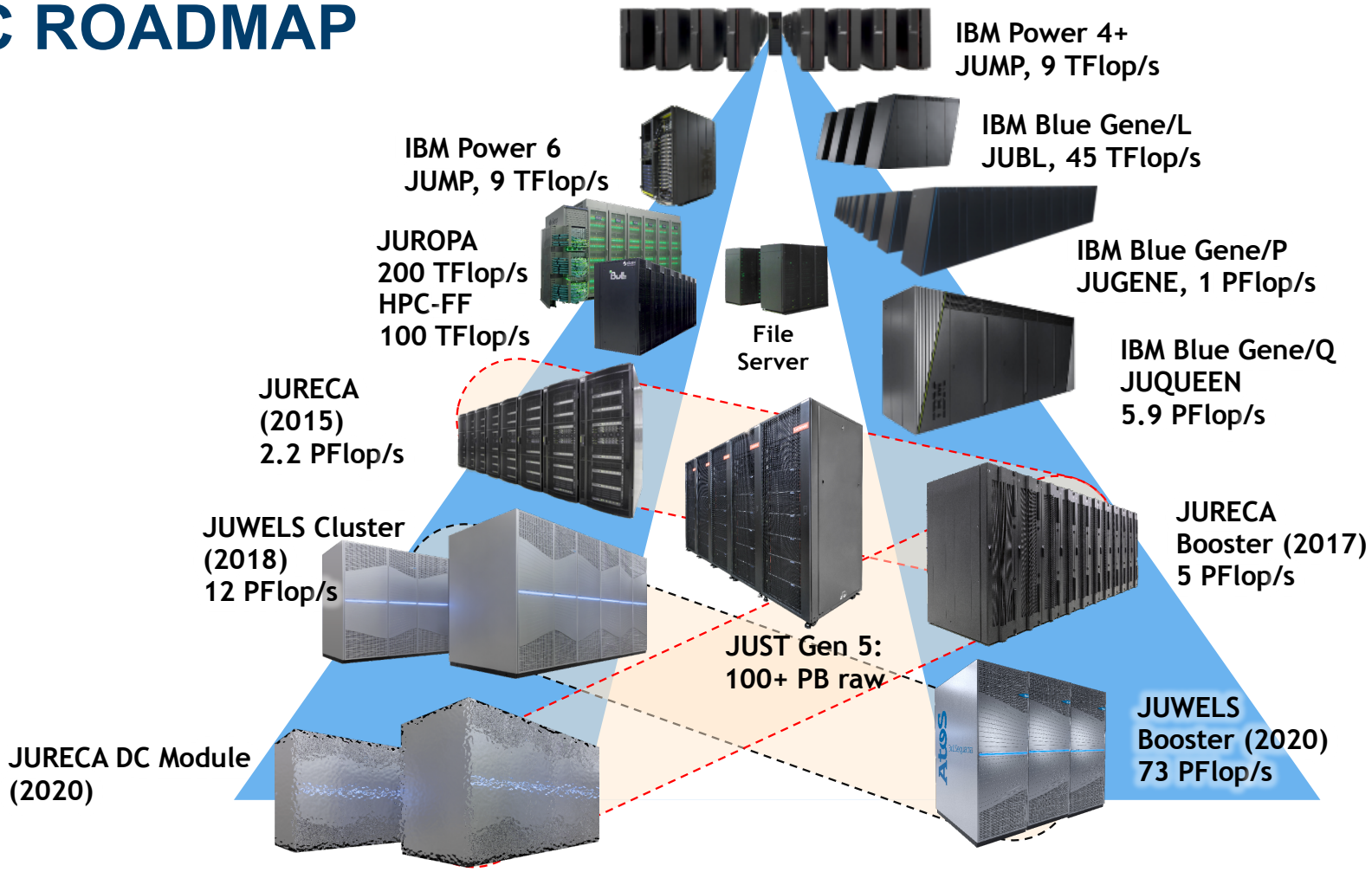
Integrator: Japan
Processors: Japan

2023+ (2)

Integrator: EU-US
Processors: EU-US

Data Source: hpcwire / hyperion

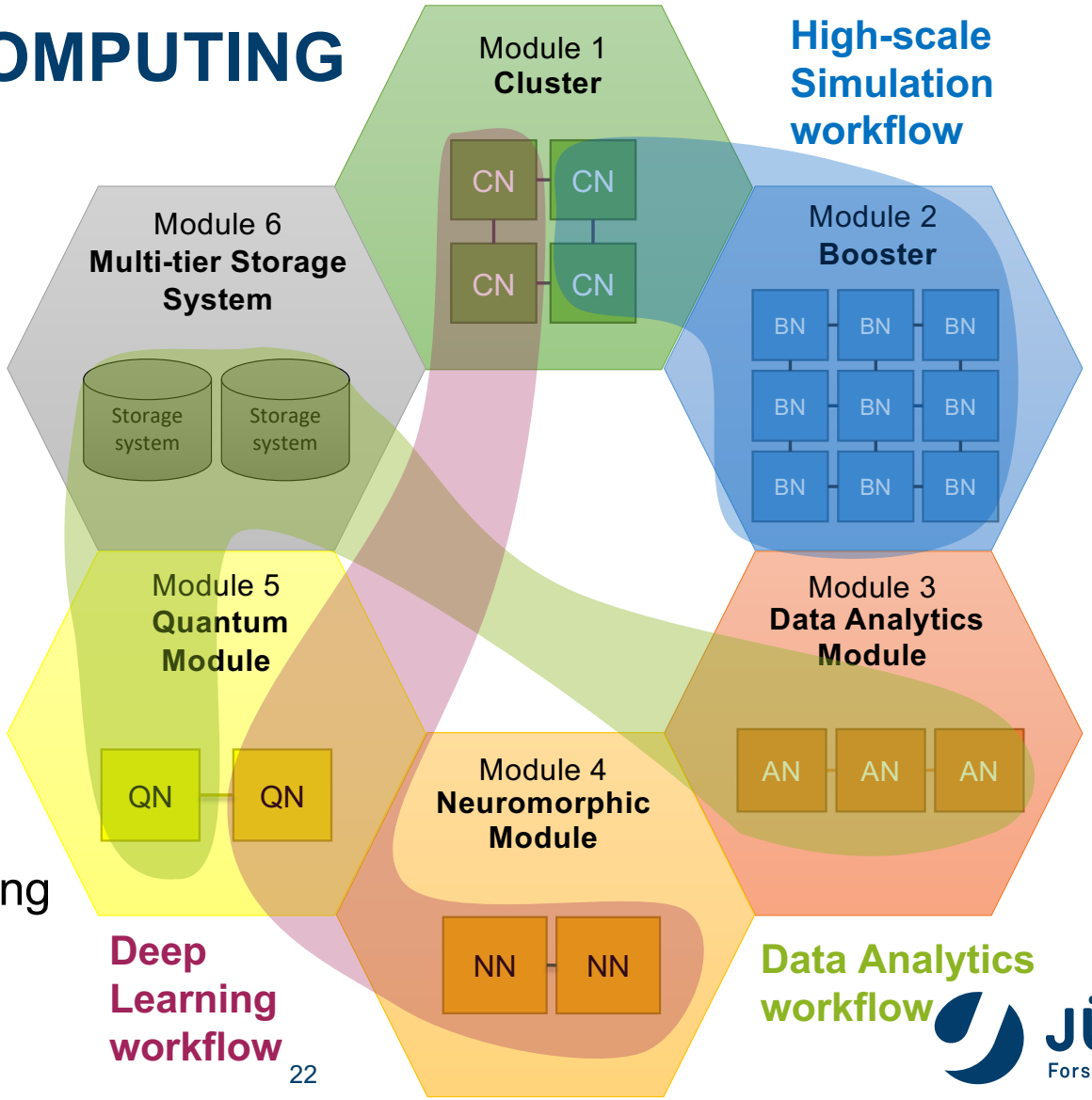
JSC ROADMAP


IBM Power 4+
JUMP, 9 TFlop/s
IBM Power 6
JUMP, 9 TFlop/s
IBM Blue Gene/L
JUBL, 45 TFlop/s
JUROPA
200 TFlop/s
HPC-FF
100 TFlop/s
IBM Blue Gene/P
JUGENE, 1 PFlop/s
File
Server
IBM Blue Gene/Q
JUQUEEN
5.9 PFlop/s
JURECA
(2015)
2.2 PFlop/s
JUWELS Cluster
(2018)
12 PFlop/s
JURECA
Booster (2017)
5 PFlop/s
JUST Gen 5:
100+ PB raw
JUWELS
Booster (2020)
73 PFlop/s
JURECA DC Module
(2020)

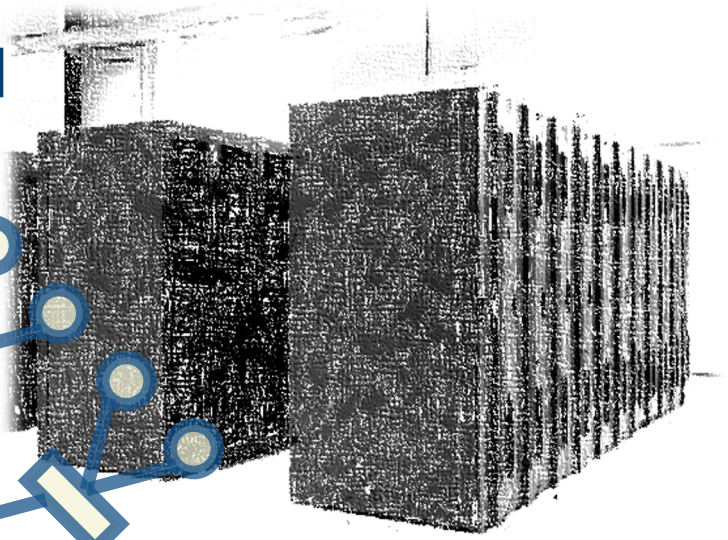
MODULAR SUPERCOMPUTING

Composability of heterogeneous resources

- Cost-efficient scaling
- Effective resource-sharing
- Fit application diversity
  - Large-scale simulations
  - Data analytics
  - Machine- and Deep Learning
  - Artificial Intelligence



THE JUWELS MODULAR SYSTEM



JUWELS Cluster (2018)

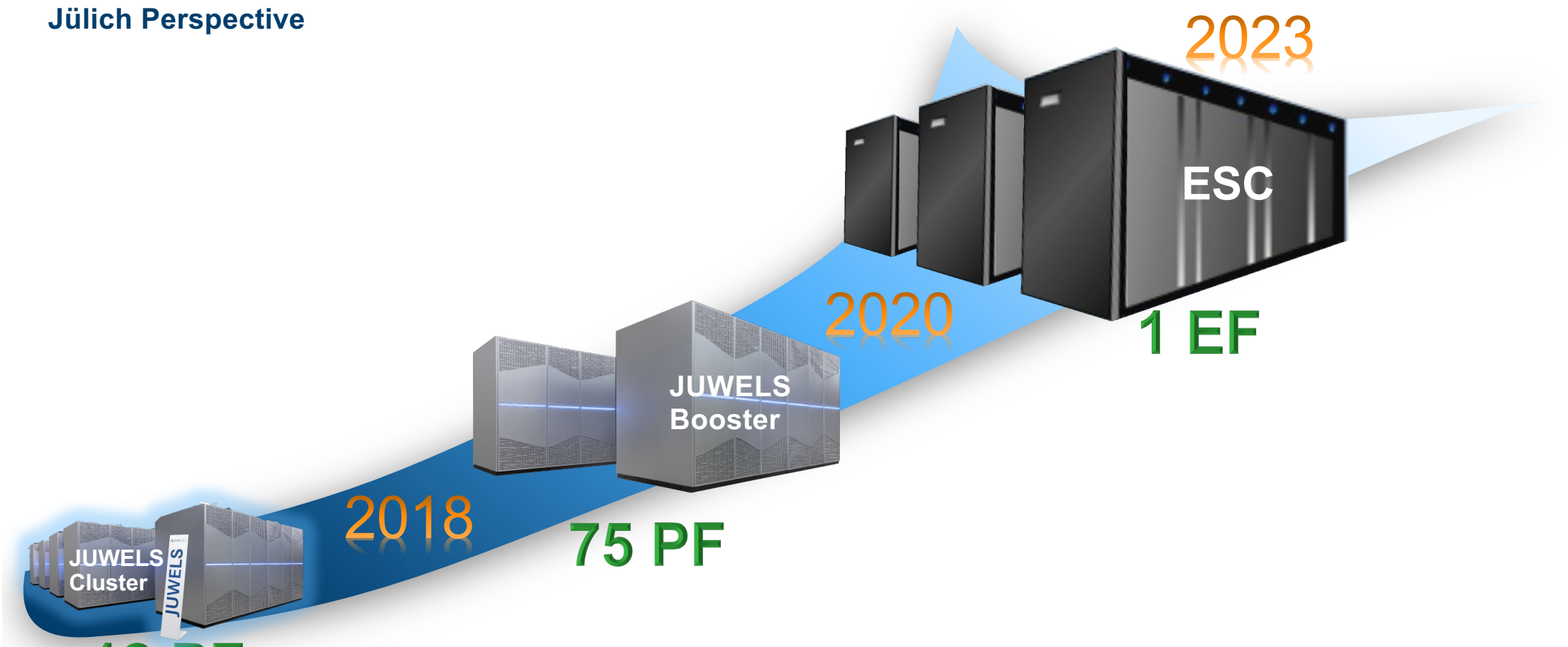
- 2511 compute nodes based on dual-Socket Intel Xeon Skylake
- 48 GPU nodes (4× V100 w/ NVLink2)
- Mellanox InfiniBand EDR 100 Gb/s network:
  Fat-tree topology (1:2@L1)
- 12 PF/s

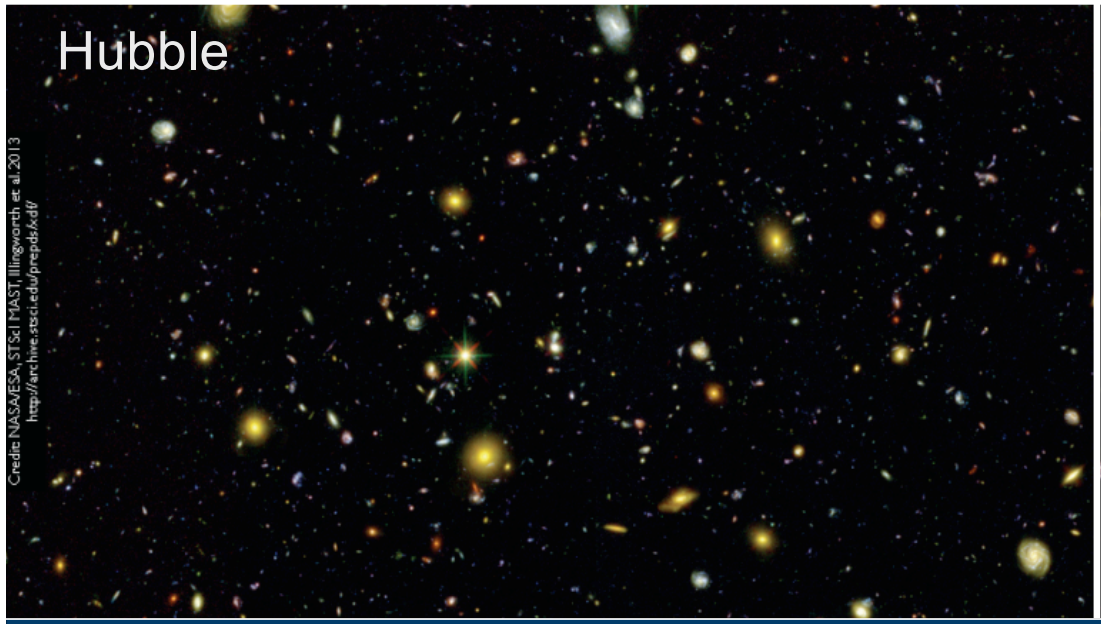
JUWELS Booster (2020)

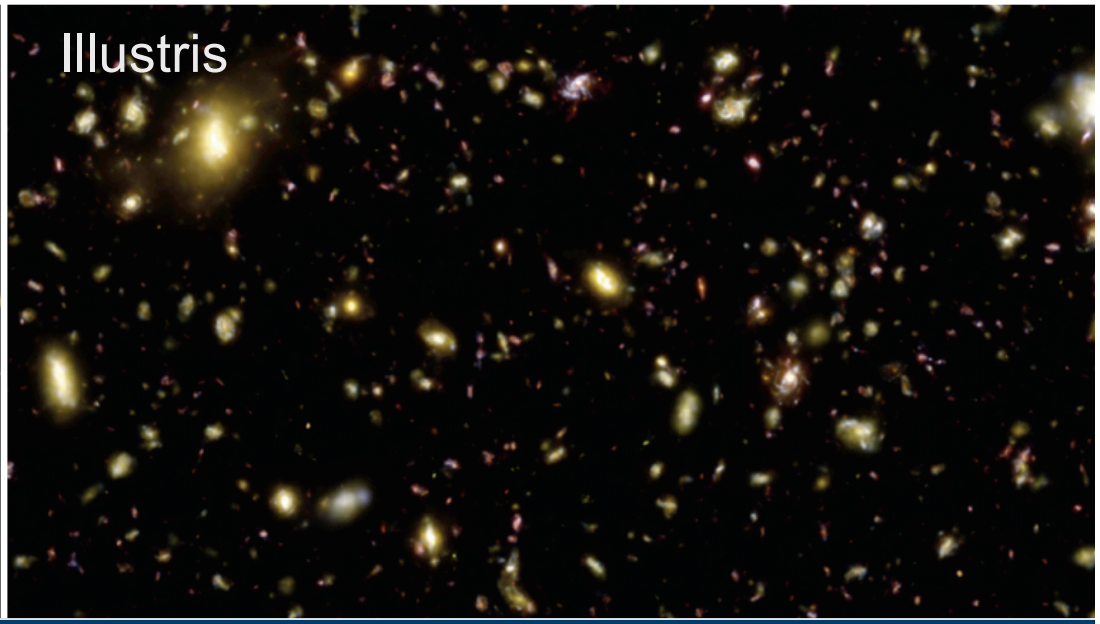
- 936 nodes (4× A100 w/ NVLink3)
- Mellanox InfiniBand HDR200: DragonFly+ network
- Focus on massively-parallel and learning applications
  - GPUs
  - Balanced network
- 73 PF/s peak

EXASCALE ROADMAP

Jülich Perspective







SELECTED HIGHLIGHTS FROM THE PRACE PETASCALE ERA

AND WHAT WE MIGHT EXPECT FOR EXASCALE

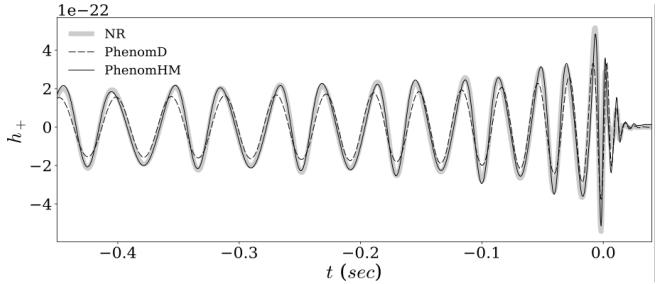
Lead Institution: UIB (Spain) - collaborators from UK, Germany, India; 33 Mio Core hrs

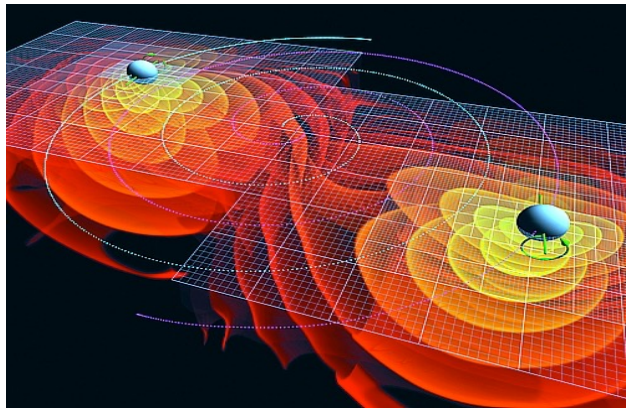
Modelling Gravitational Wave Signals

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

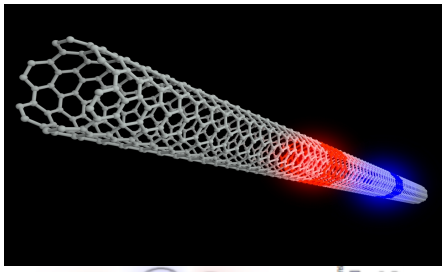


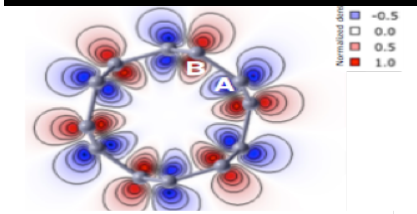


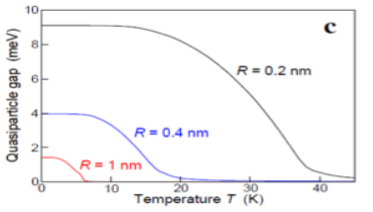
Carbon Nanotubes as Excitonic Insulators

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)







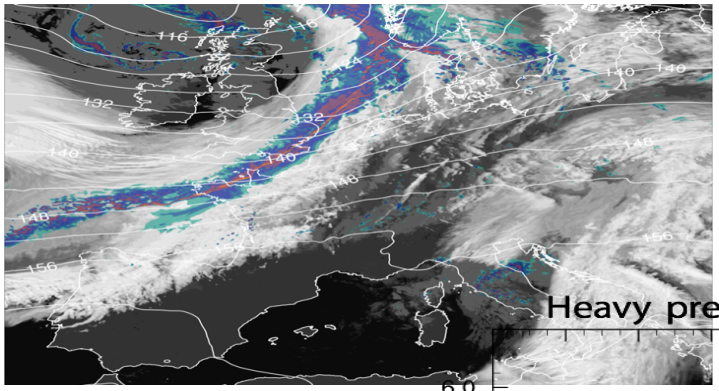
PI: Christoph Schaer, ETH, Convection-resolving Climate on GPUs (gpuCLIMA
170 Million core-hours

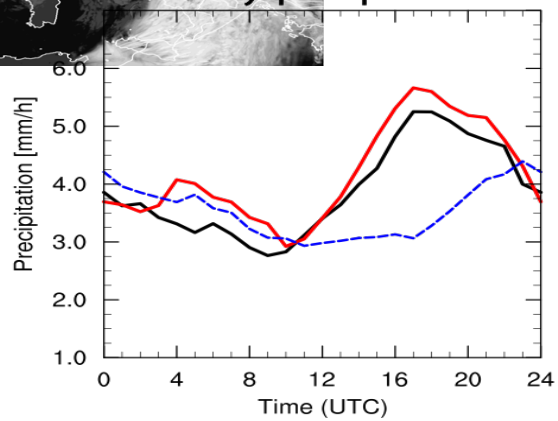
Convection Resolving Climate Simulations

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)



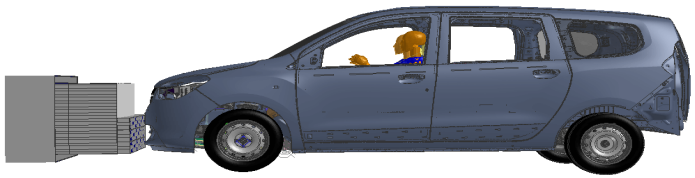


Biggest Crash Optimization Ever

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

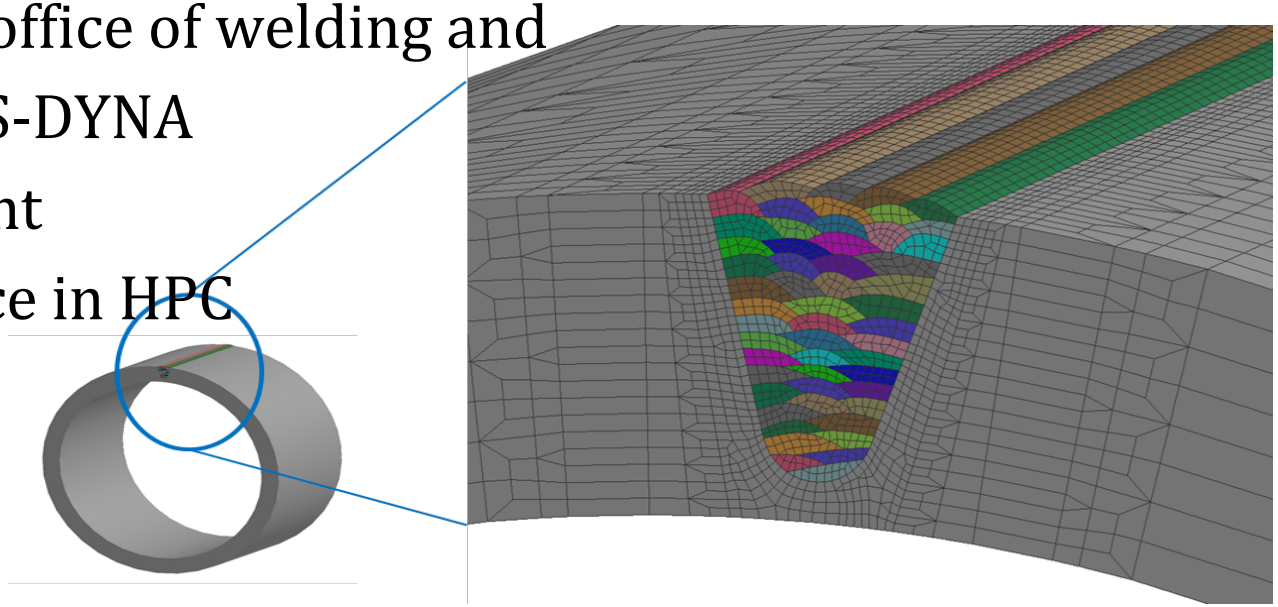
cea

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

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



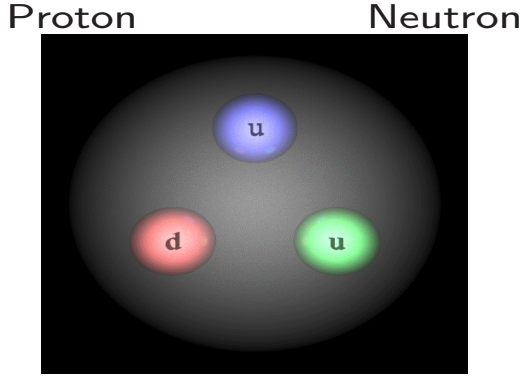
PI: Zoltán Fodor, Thomas Lippert et al., Ab inition calculation of the neutron-proton mass difference, Science 347 (2015) 1452-1455, 150 Mio core hours.

Daß ich erkenne, was die Welt, im Innersten zusammenhält

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

Universität Regensburg

Science

AAAS

Luciao Rezzolla et al.

Black Hole Simulations

- How to evaluate the black hole EHT data?
- Simulate about 60 k magneto-hydro-dynamical models of the space around the event horizon
- Highly efficient, well parallelized numerical implementation on SuperMUC
- Essential to understand physics separated from background

Enabling Breakthrough Observations

lrz GCS Gauss Centre for Supercomputing