Partnership for Advanced Computing in Europe

PRACE for Science & Industry

Richard Kenway

Chairman, Scientific Steering Committee

CAPACITIES

e-infrastructure

PRACE past

- Mar 2004: Hugh Pilcher-Clayton and Richard Kenway attend German Science Council

ERA – NET
High Performance Computing Proposal

Aim: without prejudicing the national programmes for high performance computing, to create a European high performance computing service by 2009 with a capability that matches that of the current world leaders, the USA and Japan.

Partners: UK, Germany, France, and others

RESEARCH COUNCILS UK

German HSC 18.3.04

WR WISSENSCHAFTSRAT

- Apr 2006: Scientific Case for a European Supercomputing Infrastructure

The conviction that isolated European countries would not be able to provide their researchers and engineers with resources competitive on the world stage lies at the heart of the HPCEUR initiative.

- Jan 2007: HPC in Europe Task Force (HET)

HET recommends establishment of a small number of European HPC facilities to provide extreme computing power – exceeding petaflop capability – for the most demanding computational tasks. In addition, a funding model based on national investments with an additional European share and a possible new collaborative entity governing it is recommended.

PRACE Timeline

HPCEUR | HET | PRACE MoU | PRACE Preparatory

2004 | 2005 | 2006 | 2007 | 2008

EU-Grant: INFSO-RI-211528, 10 Mio. €

EC: 60 Mio. € + Member States: 60 Mio. € + 400 Mio. € cycles

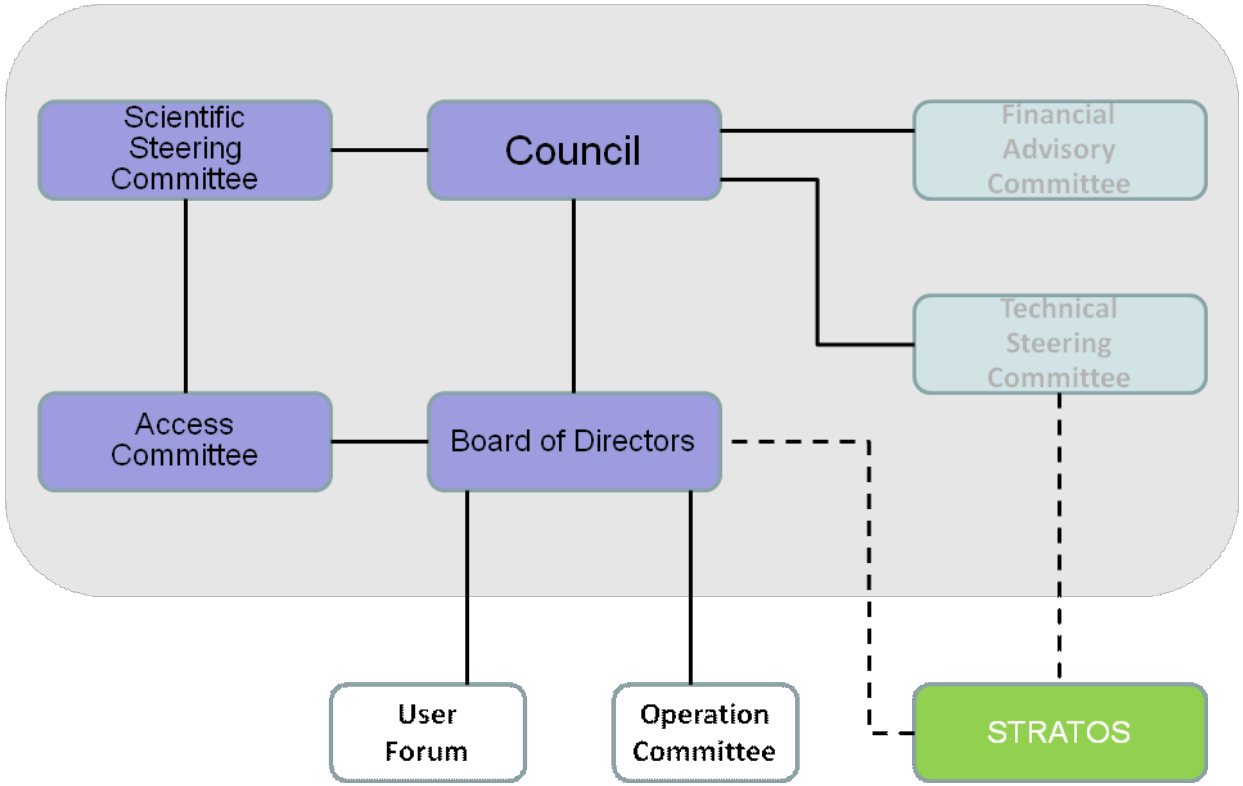
Phase | PRACE Operation

23.4. 2010 | PRACE Implementation Phase (1IP, 2IP, 3IP)

2009 | 2010 | 2011 | 2012 | 2013

PRACE (AISBL), a legal entity
with seat location in Brussels

PRACE present … 2010 - 14



6 PRACE Advanced Training Centres

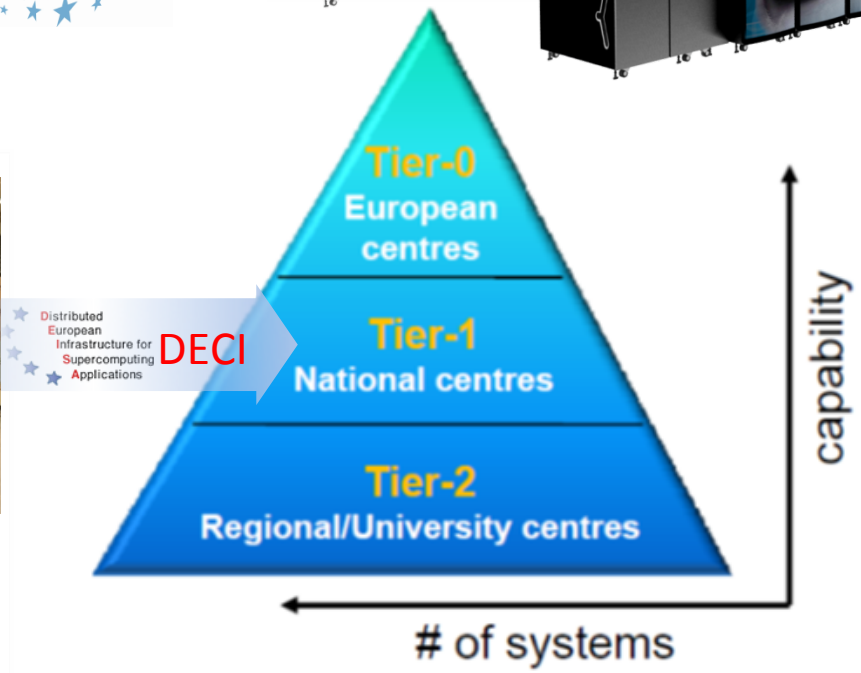
- BSC
- CINECA
- CSC
- EPCC
- GAUSS
- Maison de la Simulation

24 Member States

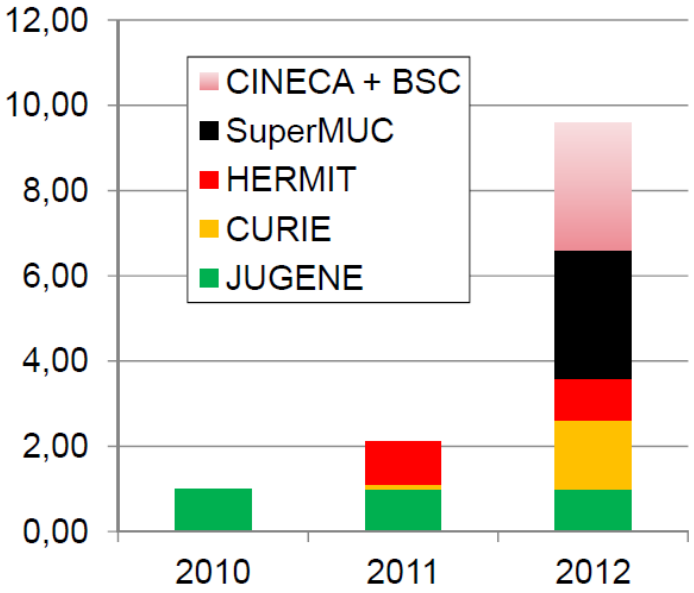
- Hosting members: France, Germany, Italy, Spain
- 100M€ each in kind

it's not size that counts … yet

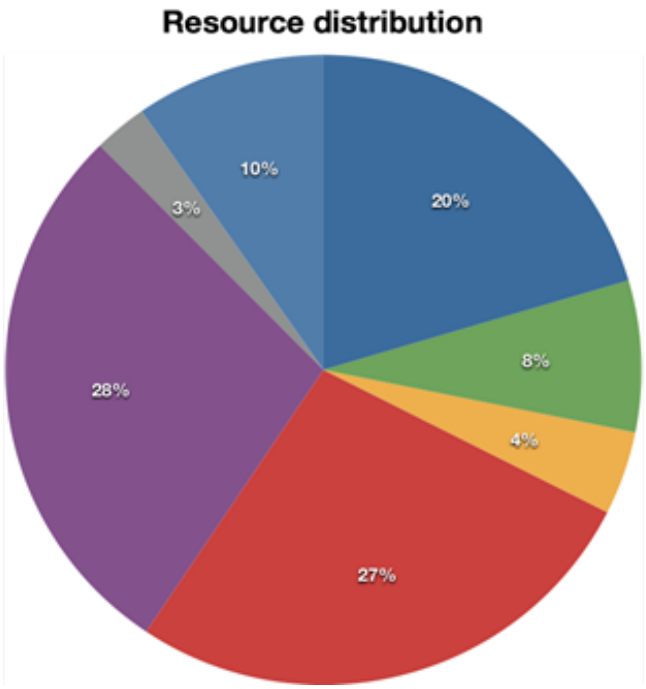
- Phase 1: differentiated by time allocation
- Phase 2: size/cost?



Tier-0 Capability



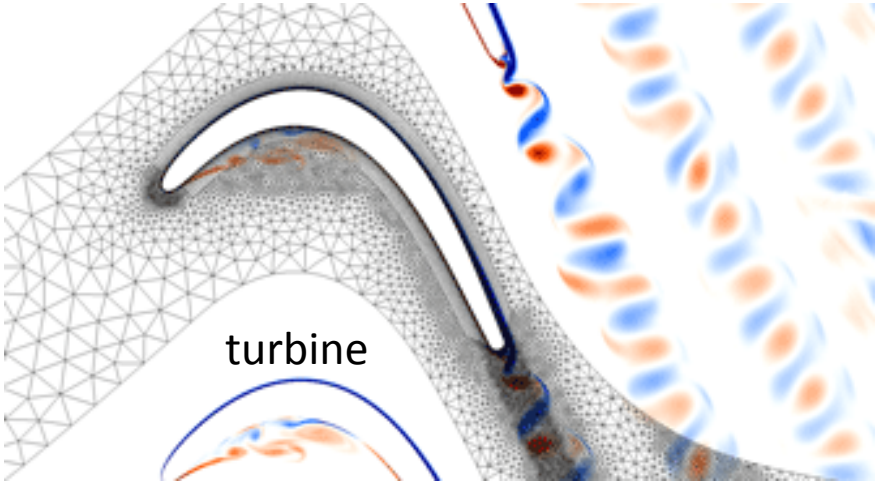
Tier-0 Project Allocations



- Competitive peer review for
  - academic research worldwide
  - open industry research in Europe
- projects with the greatest potential for new knowledge that are only possible at tier-0
  - up to 3 year allocations

Call	Requested Hours (million core hours)	Requested Projects	Awarded Hours (million core hours)	Awarded projects
Early Access	1870	68	324	10
1st	2900	59	362	9
2nd	1250	47	398	17
3rd	1700	53	721	24
total	**7720**	**227**	**1805**	**60**
			inc. 4th Call 2941	103

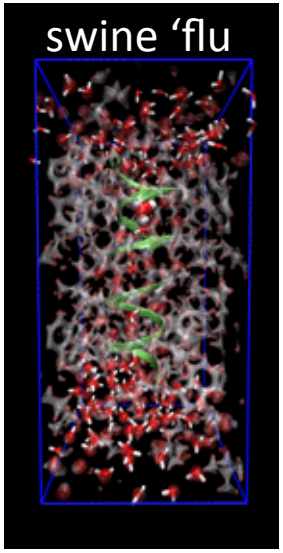
First Results

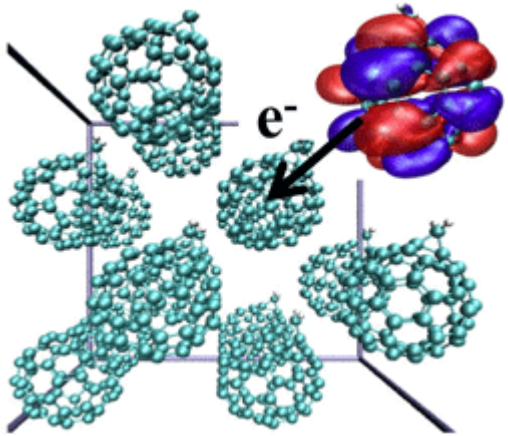


fusion

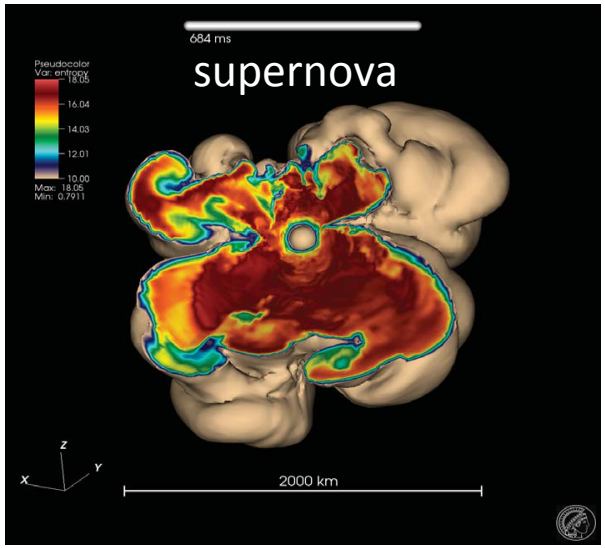
gene.rzg.mpg.de

GENE

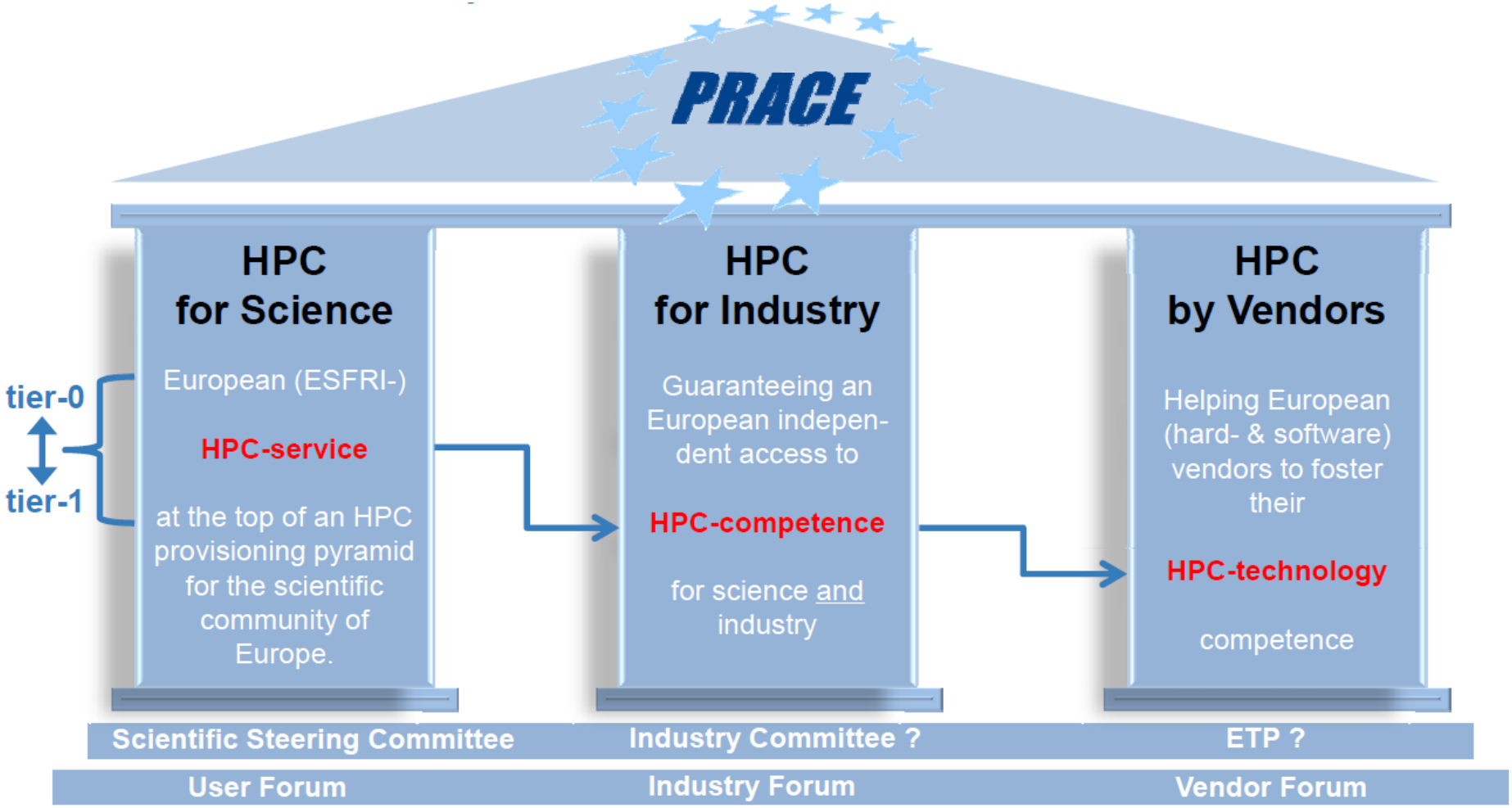




organic solar cell material



3 Pillar Mission



PRACE future … 2015-19

EUROPEAN COMMISSION

Brussels, 15.2.2012
COM(2012) 45 final

COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS

High-Performance Computing: Europe's place in a Global Race

The 2009 investment level of EUR 630 million per year[5] for acquiring high-end HPC resources across Europe is not sufficient to sustain HPC systems and services at a globally competitive level. It would need to double to some EUR 1.2 billion per year to bring Europe back as a major actor in the field of HPC[5]. Consultations with stakeholders have confirmed such an increased investment.

PRACE ensures the wide availability of HPC resources on equal access terms. It has to be further strengthened to acquire the competence to (i) pool national and EU funds, (ii) set the specifications and carry out joint (pre-commercial) procurement for leadership-class systems, (iii) support Member States in their preparation of procurement exercises, (iv) provide research and innovation services to industry, and (v) provide a platform for the exchange of resources and contributions necessary for the operation of high-performance computing infrastructure.

Update of Scientific Case 2012-20: petascale to exascale

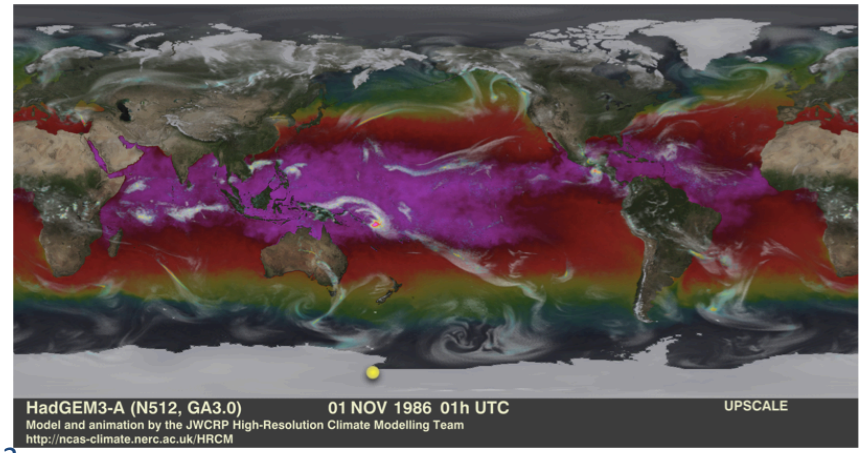
- Expert panels
  - Weather, Climatology, Solid Earth Sciences
  - Astrophysics, HEP, Plasma Physics
  - Materials Science, Chemistry, Nanoscience
  - Life Sciences, Medicine
  - Engineering Science, Industry Applications
- Update original case, incorporate EESI reports
- Deadline Jun 2012

Weather, Climatology, Solid Earth Sciences

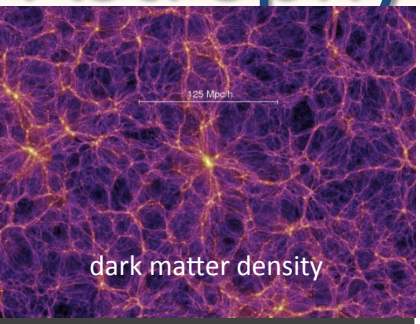
- Climate & Weather
  - whole Earth system models (bio/chem, cloud-aerosol) → coupled, multiscale
  - improved resolution: global 100km → 20km, regional 10km → 1km
  - better extreme event, regional climate, weather and air quality forecasts
- Ocean
  - critical for climate change, food, transport, natural hazards
  - include better observational surface data (ARGO), biogeochemistry
  - improved resolution: global 10km → 1km
- Solid Earth
  - earthquake protection of buildings, hydrocarbon exploration, waste sequestration
  - > 4Hz resolved frequency for ground shaking + geological timescales
  - 10x better spatial resolution, better soil models, 3D seismic imaging of Earth's interior

enes European Network for Earth System Modelling

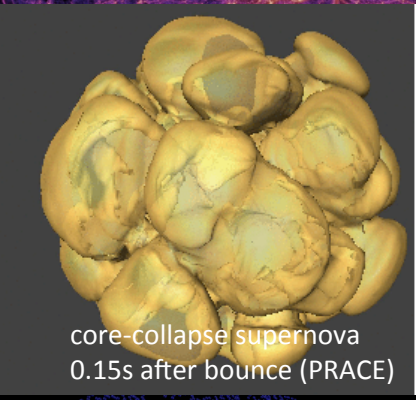
- Requirements
  - quantify uncertainties (ensemble + multimodel)
  - large spatial, long time scales → most powerful HPC available
  - 2x resolution → 10x, bio/chem → 10x, ensembles → 10-100x compute
  - full spectrum of HPC systems = tiers 0, 1 and 2
    - 10-100 x 100 Pflop/s sustained + 10 PB on-line + 100 PB off-line
    - supporting both capacity and capability jobs
    - end-to-end data infrastructure for analysis + visualisation
  - multiyear access to stable tier-0 platforms for bit-level reproducibility
    - possibly dedicated with high volume data storage and fast I/O
    - co-design and competence centres supporting software development (strong scaling challenge)
  - community coordination of codes, simulations (different models) and data, training

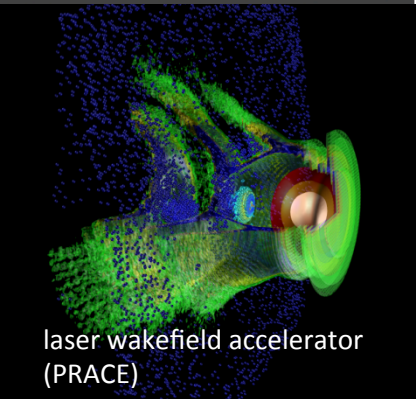


Astrophysics, HEP, Plasma Physics

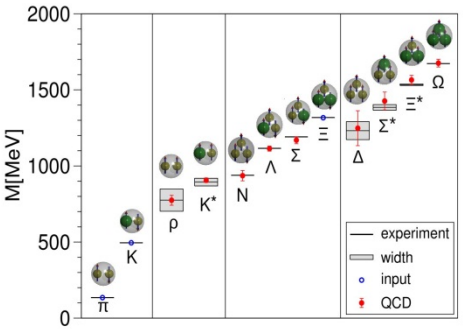


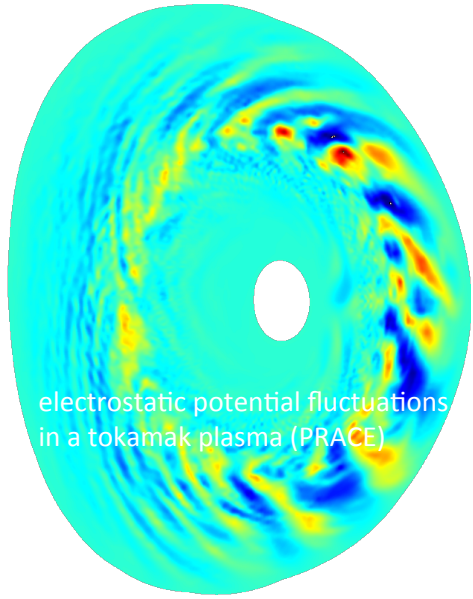
dark matter density


core-collapse supernova 0.15s after bounce (PRACE)


laser wakefield accelerator (PRACE)

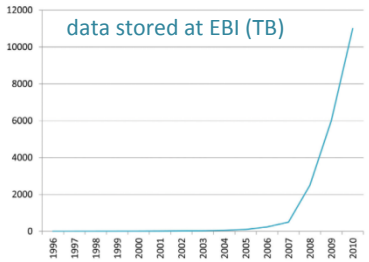
- Tied to long-term big-science projects
  - essential for interpreting experiments & observations
  - LHC, FAIR, SKA, Euclid, LIGO, ITER, …
- Precision theory
  - discrepancy from standard model = signal of new physics
- Model exploration
  - which virtual world matches observation?
  - fills a methodological gap in astrophysics (can't do controlled experiments)
- Today
  - codes scale to 100,000+ cores
  - successful track record of co-design
  - efficient use of accelerators
- Requirements
  - large range of scales in space and time → weak scaling
  - huge simulations (precision)
    - 2015: 10 x 10 Pflop/s year sustained
    - 2020: 10 x 100 Pflop/s year sustained (1 Eflop/s peak)
  - many smaller simulations (model exploration)
    - integrated large-memory clusters
  - observational, experimental and simulation data storage and integration
  - 10-20 year commitment to HPC infrastructure
  - algorithm and software development

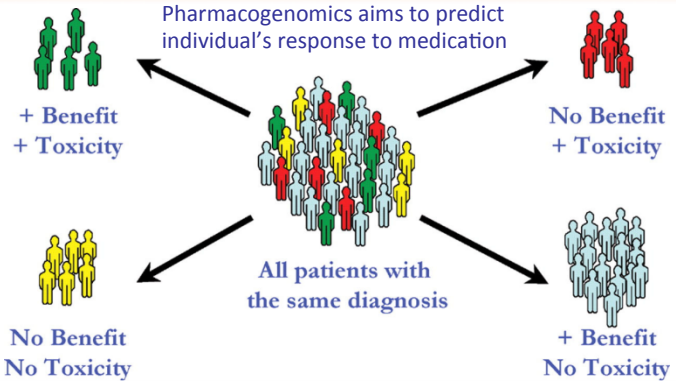


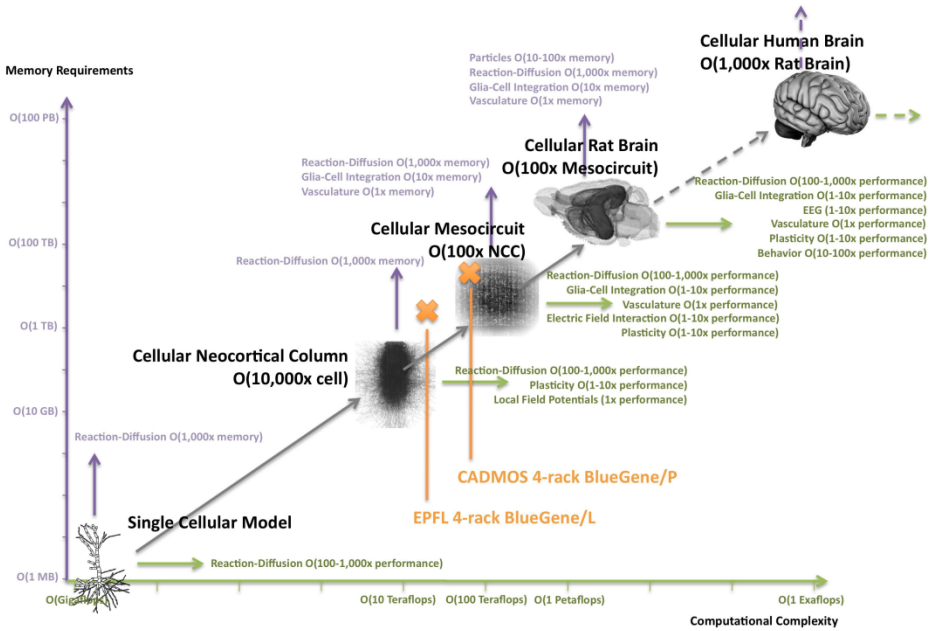

electrostatic potential fluctuations in a tokamak plasma (PRACE)

Life Sciences, Medicine

- Human genome sequencing
  - 2000: scientific milestone (100 Gflop/s, 1TB)
  - 2012: 100 per week (100 Tflop/s, 1PB)
  - soon: $1000 per genome, sequences integrated into clinical trials
- Drug discovery
  - virtual screening of molecular compounds for therapeutic target
- Multiscale simulation
  - DNA → proteins → cells → organs → whole body
  - hierarchical parallelisation
- Requirements
  - few huge simulations (eg brain)
    - 2020: 1 Eflop/s (peak)
    - (strong) scaling difficult on flat architectures
    - academic + industrial co-design centre for exascale
  - flexible access to a range of computational resources
    - high data rates, up to 100PB/y
    - real-time access for patient treatment
    - visualisation and computational steering
  - security for private data
  - exascale software and data management tools

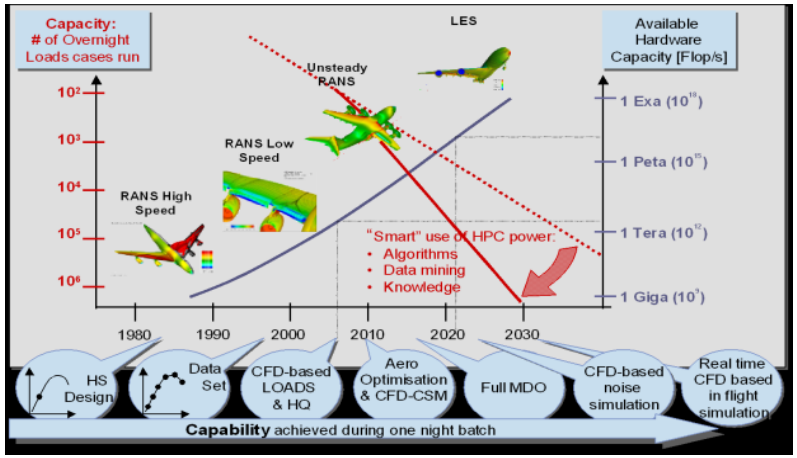


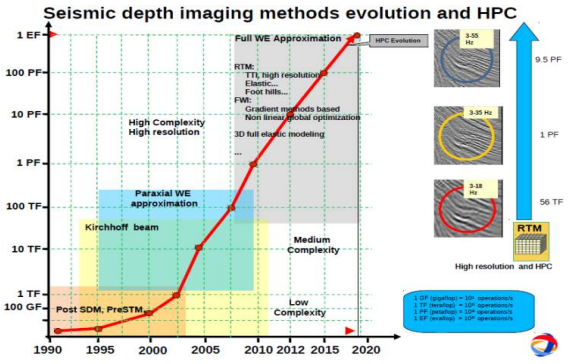




Engineering Science, Industry Applications

- Replace experiment to achieve faster/cheaper/better design
  - horizontal coupling: structures, fluids, acoustics, heat transfer, passengers → multiphysics
  - vertical coupling: continuum, mesoscale, molecular dynamics, quantum chemistry → multiscale
  - digital prototyping: engine performance, fuel efficiency, crash tests, noise reduction (whole aircraft > 1 Zflop/s)
- When experiment is not possible
  - nuclear power plant safety (> 1 Eflop/s), biomedical flows
- Codes are not well organised: in-house + commercial packages
- Turbulence
  - critical: combustion (good), drag (bad)
  - need 5x Reynolds no → 1000x compute, 100x storage
  - replace models by DNS
- Combustion
  - fast chemical reactions over a large range of spatial scales
  - burners, turbines, forest fires, explosions
- Oil & Gas
  - seismic imaging, reservoir modelling, multiphase fluids (> 1 Eflop/s)





- Requirements
  - pre-processing: parallel mesh generation tools
  - post-processing: visualisation of massive data
  - multi 1 Eflop/s + 10-100 PB
  - dedicated HPC + large data store + fast I/O
  - centres of competence, co-design
  - security of codes and data

Scientific Requirements for PRACE 2.0

- **tier-0 exascale capabilities (compute + data)**
  - multi 100 Pflop/s sustained, some > 1 Eflop/s
  - fast I/O to multi PB on-line storage
  - some dedicated facilities (climate, industry, medicine)
- **integrated, diverse, flexible, responsive tier-1 infrastructure**
  - real-time interactive access (medicine, industry)
  - end-to-end data management (including tier-2)
  - co-scheduling, computational steering and visualisation
- **software and algorithm development support and training**
  - strong scaling challenges
  - skills shortages
  - long-term investment
- **centres of competence**
  - thematic: expertise, programme management, support
  - co-design: algorithms, application software, architectures
  - software/tools: development, expertise, support
  - skills retention, career development
- **long-term funding horizon: 10-20 years**
  - match lifetimes of experimental programmes
  - hardware stability: 3-5 years

Industry Issues

- Pre-Commercial Procurement (PCP)
  - co-design doesn't fit
  - distinct from PRACE objectives
  - PRACE 3IP trial (10M€, energy-efficient HPC)
  - ETP4HPC industry forum
- ISV licencing
  - must change to "pay per use"
  - need support to rewrite codes
- Tier-0 access
  - support for software development + demonstrators
  - large companies buy their own production facilities
  - business model/access for SME's?

- Member States are invited to carry out joint procurement activities and to use PCP to stimulate the development of advanced HPC systems and services. Each Member State should actively encourage the use of PCP and devote in the order of 10 % of its annual HPC procurement budget to it.
- The Commission should contribute to the funding provided collectively by Member States for PCP of R&D on HPC systems services with an EU-level mission and with EU-wide availability.
- HPC e-Infrastructure projects receiving funding from the Commission should be encouraged to use PCP where relevant.
- EU Industry is encouraged to actively engage in advanced HPC and application development efforts in response to PCP.

ETP 4 HPC

"develop HPC technology link in HPC value chain"

- public-private partnership (ETP/ PRACE/EC)
- increase European vendors' share of global HPC supply chain

Hicham Lahlou, Xcelerit, receives the Award for the Most Innovative Industrial HPC Application in Europe

Governance and Funding Issues

- Strategy Workshop (14 May) & Council (6 Jun)
  - Restate PRACE strategy
  - Elect new Chair and Vice-Chair

- Questions
  - What are the unique characteristics and added value of PRACE?
  - What will be the relationship between tier-0 and tier-1 access?
  - Is representation by providers on Council appropriate and how will national funding agencies be involved in policy making?
  - Should members contribute money or cycles and how will juste retour work?
  - What will the relationship be with industry users and vendors?

PRACE for Science and Industry

- **Strategy**

  to support world-leading open research by academia and industry through the provision of a level of computing infrastructure and access which is beyond the capabilities of any one European nation
  - world-wide competition + best-practice peer review
  - multi-national facility procurement and operation (tier-0)
  - shared access to national infrastructure (tier-1)
  - larger-scale resource allocation than is possible nationally
- **Governance**

  European organisation owning and operating
  - tier-0 facilities
  - centres of competence
- **Funding**

  Long-term national commitments
  - EC leverage where/when strategies align
- **Direction**

  Jointly by researchers and providers
  - to meet the needs of the most demanding computational research
  - to provide industry with expertise and development opportunities