PRACE: the European HPC Infrastructure and the Services for Industry

Stéphane Requena, member of the PRACE Board of Directors
435 scientific projects enabled

11.4 thousand million core hours awarded since 2010 with peer review, main criterion is scientific excellence. Open R&D access for industrial users with >50 companies supported

>7 350 people trained by 6 PRACE Advanced Training Centers and others events

21 Pflop/s of peak performance on 6 world-class systems

530 M€ of funding for 2010-2015, access free at the point of usage

25 members, including 4 Hosting Members (France, Germany, Italy, Spain)
Open R&D model since Jan. 2012
Access to leading-edge resources

- **Regular Calls open to industry twice a year**
  - Access is **free of charge**, based on scientific excellence only, but commitment to **publish results** in publicly available media
  - Already various companies benefited from PRACE allocations for > than 250M cpu hours!
    - **SMES**: HydrOcean on HERMIT, ARIA Tech on CURIE, SCC : JUQUEEN, …
    - **Large Companies**: Renault on CURIE, EDF R&D UK on HERMIT, MunichRé on Fermi, …
    - **Private-Public Research centers**: Cenaero on JUQUEEN, CERFACS on Marenostrum, …

  Next call will open on September 2016

- **Permanent Preparatory Access call**
  - Assess the scalability and port the codes preparation for future regular calls
  - Big companies: PSA, Renault, CS, Tetrapak, …
  - SMEs: ARIA, Thermofluids, Vratis, Dompé, …

Since 2012 more than 50 companies, > 250M cpu hours
More than half of them : SMEs
Open R&D model since Jan. 2012

Access to high-value services

- **Access to new knowledge enabled through PRACE**
  - Big science may be usable by industry in advance on leading edge HPC systems
  - PRACE as a **catalyzer of technological transfer**

- **Evangelization and Training**
  - Specific programme for SMEs HPC evangelisation (**SHAPE**)
  - Specific courses targeting industrial users are programmed in the 6 **PRACE Training Centers**
  - The online training portal is accessible by everyone

- **Code enabling**
  - The implementation projects work at developing **Open Source codes for industry**
    - Computational Fluid Dynamics: OpenFoam - Uncertainties analysis: **URANIE**, ...  
  - Real industrial test cases are used in the process
  - All the reports and white papers from PRACE are public!

- **Information, Promotion and Networking**
  - **PRACE Days Conferences**
    - Last edition in Prague (May’16) with more than 250 attendees
    - Good mix of large companies and SMEs, from various industrial domains
  - **PRACE Industrial Award**: in 2016 **Niels Aage from the Technical University of Denmark** awarded for “Ultra large scale structural optimisation-topology optimized wing structure”
Some PRACE breakthroughs for the EU industry

**IMPROVING CAR SAFETY**
A world premiere in the automotive industry

→ Performing more accurate crash optimization

- 42 million hours on Curie (France)
- Assess new large scale optimization methods: 200 parameters, 20 million finite elements
- Anticipate new security rules (EuroNCAP6)
- Impossible with internal Renault R&D HPC resources.

**DEVELOPING NEW DRUGS**
Molecular Dynamics Simulations for Computing Kinetic Constants for Drug Discovery

- Improve the process of drug discovery by taking into account for the first time kinetic properties of a drug and a candidate protein
- International collaboration K4DD (Kinetics for Drug Discovery) with NAMD and Gromacs
- 11 million core hours on Fermi (CINECA)

**IMPROVING SHIP SURVIVABILITY UNDER WAVE IMPACT AND AQUAPLANING FOR AUTOMOTIVE**

→ Major step: 32k cores simulations – Increased EU visibility and competitiveness for a SME

- 5 million core hours on Hermit (Germany)
- 8.2 million hours on CURIE (France)
Partnership for Advanced Computing in Europe
HPC for SME, a not so simple plan!

• Most of the SMEs are not aware of « what is HPC and what for » or think ”It’s not for me !”
  – Lack of trained resources/skills in HPC and simulation
  – Lack of knowledge of the ecosystem and tech transfer from academia
    • Who can help me and what tools/methodologies …
  – SME are not talking the HPC and the Cloud jargon
    • Access to rough cycles is NOT the solution

• HPC : **a strategic decision** for a SME
  – Need of training, new HR, new investments, …
  ✔ SME need to have a clear view and a ROI demonstration
A pan-European, PRACE-based, programme supporting HPC adoption by SME

- **Raise awareness** of SMEs of using HPC → increased competitiveness
  - Relying when existing on national HPC evangelisation prg. (UK, FR, DE, IT,...)

- **Support SMEs up to a proof-of-concept** with an integrated set of services
  - Training on PRACE PATC centers
  - Co-development of concrete industrial project with HPC and domain-specific experts
  - Demonstration using PRACE HPC resources (Open R&D model)

- **After the SHAPE demonstration, companies will have a clear view**
  - potential of HPC on their processes/business
  - investments to perform and skills to hire
  - software or methodologies to develop
  - next HPC Services to use: PRACE services for Open R&D, buying their own HPC facilities, remote access to HPC services on commercial Cloud platforms.
SHAPE : example of a recent result

A big German SME (450p) dedicated in the development and manufacture of filling and packaging machinery used in pharmaceutics

**Enhanced airflow simulations around filling machines in clean rooms**
- Assessment of various refinement levels of the mesh using snappyHexMesh
- Use and optimisation of the OpenFOAM software
- Scaling tests on turbulence model solvers (RANS, DDES, IDDES, …)
- Efficient post processing of the results

**Use of the CRAY Hermit system at HLRS (Germany)**
SHAPE: 29 SME supported in 2 years
• One call for proposals per year

Industrial domains:
• Naval engineering
• Renewable energies
• Genomics & health
• Micro electronics
• Cloud / HPC
• Automotive / crash
• Digital media
• Electromagnetism
• Agriculture, ...

www.prace-ri.eu/shape
Thank you very much for your attention!

SAVE the date

PRACEdays17
HPC for Innovation: when Science meets Industry

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