

Nouvelles de l'Europe

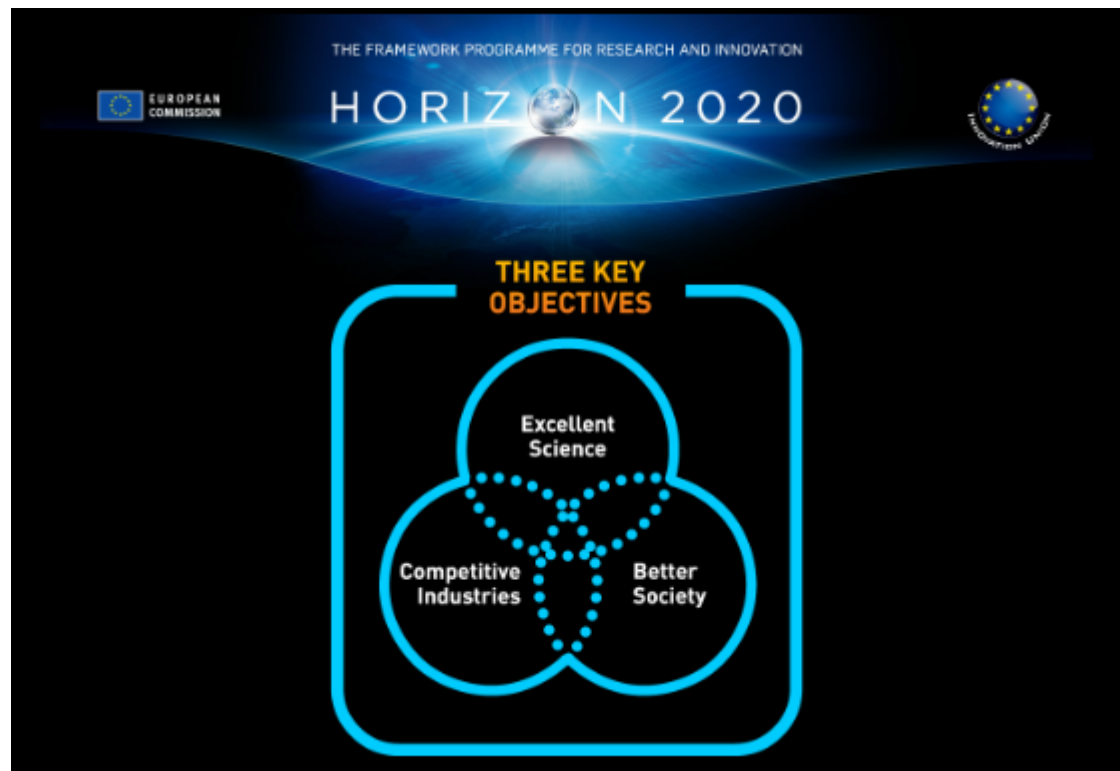
**Horizon 2020 et évolutions de la politique de la
Commission Européenne dans le domaine du HPC**

Jean-Philippe Nominé, CEA

Remerciements:
GENCI, S. Requena
J-Yves Berthou, ANR

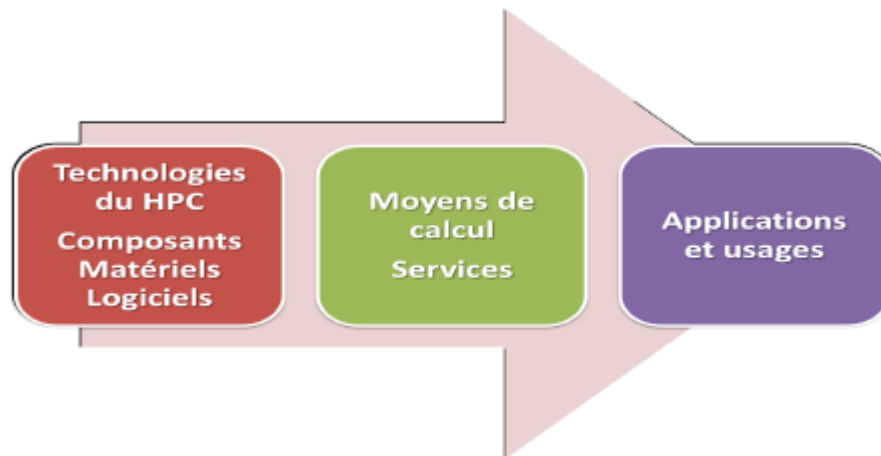
Contexte : H2020

- Horizon 2020 is the financial instrument implementing the [Innovation Union](#)², a [Europe 2020](#)³ flagship initiative aimed at securing Europe's global competitiveness. Running from 2014 to 2020 with an €80 billion budget, the EU's new programme for research and innovation is part of the drive to create new growth and jobs in Europe.



Fil directeur

- Politique EC
Vision « écosystème »
 - PRACE
 - Technologie: ETP
 - Applications & usages
 - EESI
 - CoE



Rappels communication EC

Les objectifs

- ❑ *Ensure independent access to HPC technologies, systems and services for the EU;*
- ❑ *Provide a world-class European HPC infrastructure, benefitting a broad range of academic and industry users, and especially SMEs,*
- ❑ *Ensure the EU's position as a global actor. The Commission shall raise inequalities in HPC market access, with the aim of ensuring that their national HPC procurement and R&D are open to EU-based industry*

Les budgets

The Union, Member States and Industry should increase their investments in HPC to some EUR 1.2 billion per year – equal in terms of GDP to other world regions.

La gouvernance

For industry, through

- ❑ *the industry-led technology platform for EU HPC suppliers,*
- ❑ *a network of competence centres providing expertise and services on HPC applications and software development;*



For science, through

- ❑ *PRACE, providing world class computing power to European research*
- ❑ *Centres of Excellence, addressing key societal and scientific challenges by deployment and application of HPC software and services;*



**Technologies
du HPC**

**Composants
Matériels
Logiciels**

**Moyens de
calcul
Services**

**Applications
et usages**



2012: PRACE is providing nearly 15 Pflop/s...

Mare Nostrum: IBM
at BSC



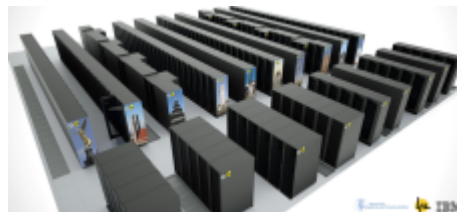
JUQUEEN: IBM BlueGene/Q
at GCS partner FZJ
(Forschungszentrum Jülich)



FERMI: IBM BlueGene/Q
at CINECA



CURIE: Bull Bullx at
GENCI partner CEA.



SuperMUC: IBM
at GCS partner LRZ
(Leibniz-Rechenzentrum)



HERMIT: Cray
at GCS partner HLRS
(High Performance Computing Center Stuttgart).

.../...

The PRACE 7th Project Access Call for Proposals is now open from February 13 to March 26.

The entire PRACE Tier-0 Research Infrastructure is available:

- CURIE (GENCI@CEA, France)
- FERMI (CINECA, Italy)
- HERMIT (GCS@HLRS, Germany)
- JUQUEEN (GCS@Jülich, Germany)
- MareNostrum (BSC, Spain)
- SuperMUC (GCS@LRZ, Germany)

Allocations will be for 1 year starting from early September, 2013 intended to individual researchers as well as multi-national research groups, asking for resources on a single or multiple machines.

The 7th Call is open to academia and industry under specific mandatory conditions including that access is devoted solely for open R&D research purposes. Please carefully check the full eligibility criteria listed in the text of the call for proposals.

All applications whether submitted by academia or by commercial companies will be evaluated against the highest peer-review standards. Applications must demonstrate scientific excellence, include elements of novelty, transformative aspects and have a recognised scientific impact.

The PRACE 7th Call for Proposals can be found on the PRACE website:

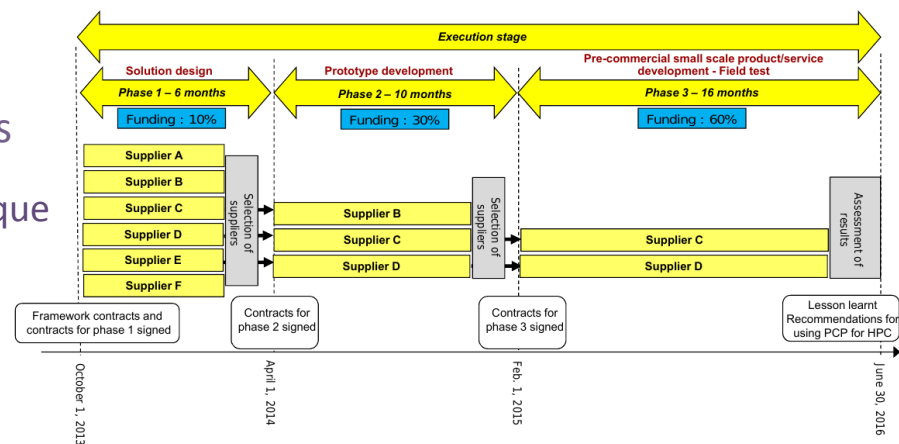
<http://www.prace-ri.eu/Call-Announcements>.



Point d'activité de PRACE (1/2)

Lancement d'un appel d'offre PCP

- ❑ Travaux menés dans le cadre du projet PRACE 3IP financés par la Commission Européenne
- ❑ Objectifs
 - **Evaluer pour la 1^{ère} fois en Europe le mécanisme de PCP (Pre-Commercial Procurement) pour le HPC**
 - PCP = financement en avance de phase de R&D, utilisé notamment aux US par DoE
 - Thème retenu : **Efficacité énergétique globale**
 - Nœud de calcul, réseau, stockage, alim, cooling, ...
 - Gestionnaire de ressources, runtime, filesystem, checkpoint/restart,
- ❑ Partenaires du groupe d'acheteurs
 - CINECA : pouvoir adjudicateur
 - GENCI, Juelich (Allemagne), CSC (Finlande) et EPCC (UK)
 - PRACE aisbl : sans contribution, pour appropriation méthodologique
- ❑ Budget : autour de 9M€
- ❑ Démarrage en juillet 2012 pour une durée de 4 ans
 - Information aux vendeurs
 - En cours : définition du cadre légal, juridique et technique
- ❑ Lancement de la procédure en avril 2013
 - Première phase ouverte de pré sélection
 - Trois phases d'exécution, typiques d'un PCP
 - Solution Design
 - Prototype development
 - Pre-commercial small scale product/service development





Point d'activité de PRACE (2/2)

Définition de la stratégie de PRACE 2.0

Quelques rappels

- Infrastructure de recherche créée en avril 2010, siège à Bruxelles, 25 partenaires
- Budget de la période initiale (2010-2015) : **530 M€**
 - 400 M€ apportés par 4 pays (Allemagne, Espagne, France et Italie) → 6 systèmes Tier0
 - 70 M€ par des projets d'implémentations cofinancés par EC (PRACE-PP et PRACE (1,2,3)-IP)
 - 60 M€ apportés par les partenaires de PRACE

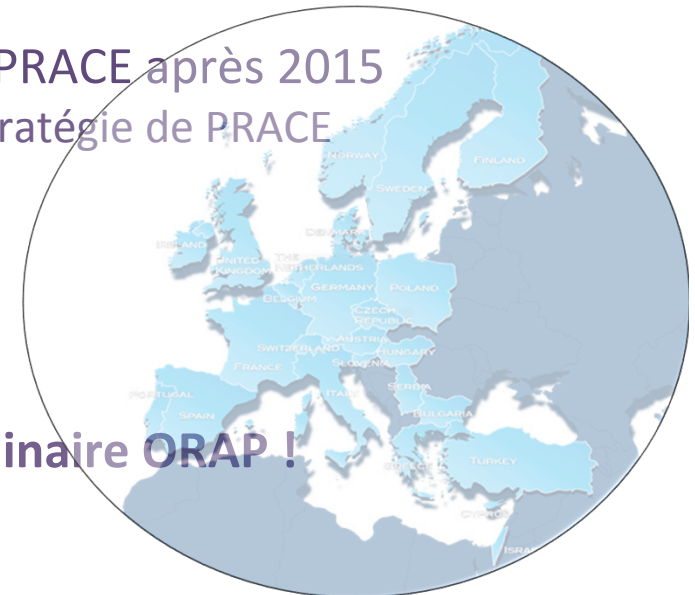
Et des résultats

- 6 systèmes Tier0 déployés pour un total de **15 PFlops**
- Accès ouvert aux chercheurs académiques et industriels (par l'Open R&D)
- Plus de **5.5 milliards d'heures** allouées depuis mi 2010
- Des services à haute valeur ajoutée :
 - information, formation, optimisation, co développement, support utilisateurs, ...

☐ PRACE 2.0 : Pérenniser l'infrastructure de recherche PRACE après 2015

- Discussions en cours entre les partenaires autour de la stratégie de PRACE
- Fenêtre politique **majeure** en mai 2013 :
 - Conseil Européen de compétitivité à Dublin
 - HPC à l'agenda

✓ **Un beau sujet de présentation pour le prochain séminaire ORAP !**



PRACE

**THE SCIENTIFIC
CASE FOR HIGH
PERFORMANCE
COMPUTING
IN EUROPE
2012 - 2020**

**FROM PETASCALE
TO EXASCALE**

PRACE

PARTNERSHIP FOR ADVANCED
COMPUTING IN EUROPE

PRACE

PRACE | DIGEST **2012**

**PRACE – SPECIAL ISSUE ON THE DISTRIBUTED
EUROPEAN COMPUTING INITIATIVE**

**Technologies
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Logiciels**

**Moyens de
calcul
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**Applications
et usages**

Technologie: ETP

- Cf exposé de J. Gonnord, Forum 30, octobre 2012

DE LA RECHERCHE À L'INDUSTRIE

cea

Jean GONNORD
Chef de projet
Simulation numérique
CEA/DAM

www.cea.fr

ETP4HPC

*Une Plateforme technologique
Européenne*

Pour le calcul haute performance

HORIZON 2020: Une politique nouvelle pour le HPC en Europe

La plateforme ETP4HPC

30^{ème} Forum de l'ORAF
PARIS
4 octobre 2012

allinea

ARM

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

BULL

CAPS

cea

CINECA

EUROTECH Imagine. Build. Succeed.

Fraunhofer

IBM

intel

JÜLICH FORSCHUNGSZENTRUM

Lrz

PARTEC CLUSTER COMPETENCE CENTER

ST life.augmented

xyratex

MAXELER Technologies MAXIMUM PERFORMANCE COMPUTING

INFN Istituto Nazionale di Fisica Nucleare

epcc

gnodal

numascale

Inria

Ter@tec

ROGUE WAVE SOFTWARE

KALRAY

HLRIS

NVIDIA

TF

FINMECCANICA

THE EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

HPC

DOCUMENTS

NEWS AND EVENTS

High Performance Computing

The European Technology Platform (ETP) for High Performance Computing (HPC) was created to improve HPC technologies and to foster collaboration among all players in the HPC

European suppliers of High Performance Computing (HPC) technologies in research centres.

The ETP for HPC is a unique initiative that recognizes the importance of HPC and sees a European Technology Platform (ETP) playing a leading forum open to any organization performing research in the area of HPC



ETP4HPC



Thank you for your plan for the development of HPC in Europe. As I already said during our meeting on 27 September, your efforts are fully aligned with the implementation of the Commission strategy for HPC. I am therefore positive about your suggestion to prepare the grounds for a Public-Private Partnership in this area in Horizon 2020. Such an initiative should include the three elements of the strategy: development of exascale technologies, access to world-class HPC facilities and services for both industry and academia; and excellence in HPC applications. I encourage you to continue working with all stakeholders, to encompass these three components.

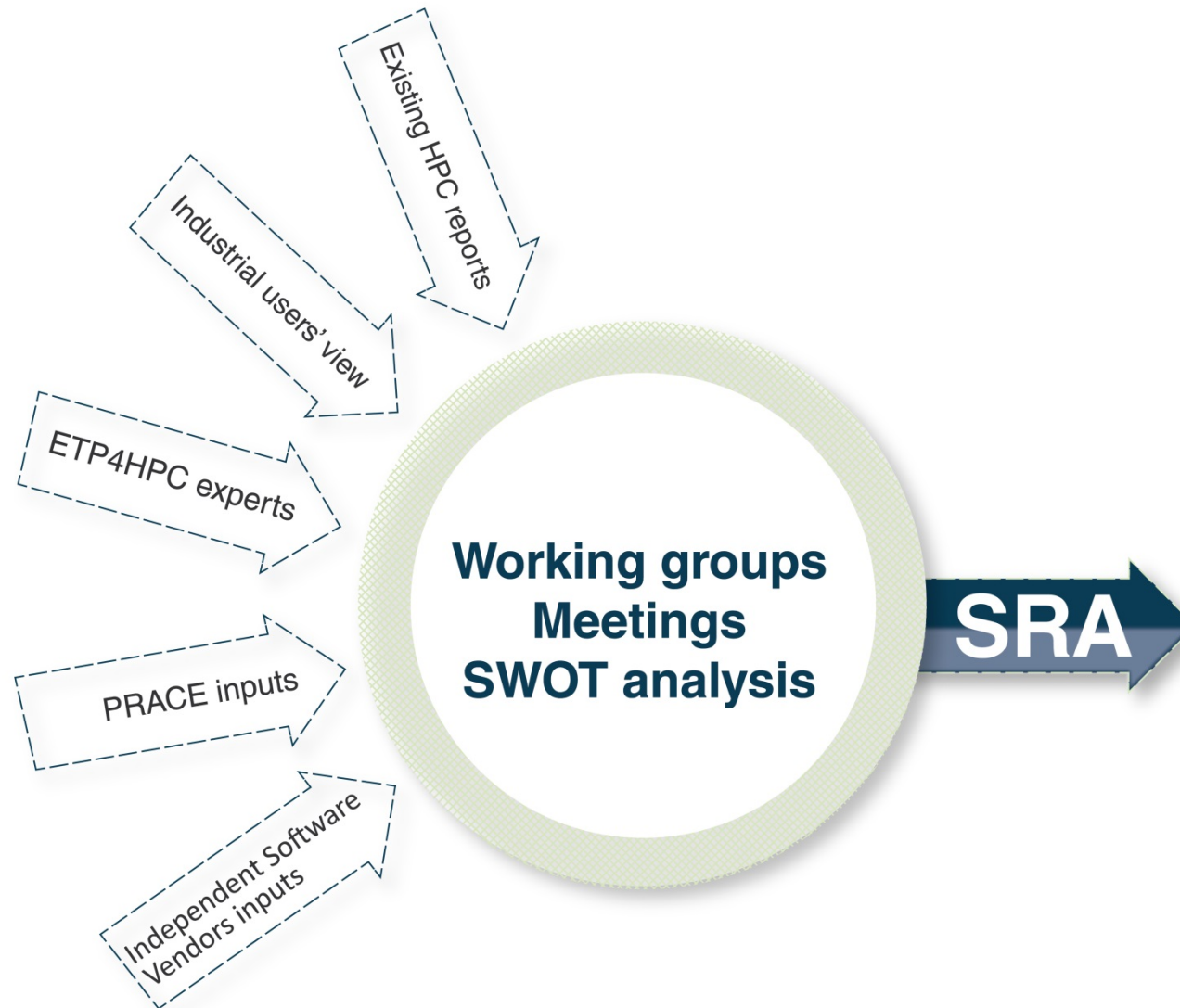
These plans are, of course, subject to availability of resources in Horizon 2020. The ambitious goals of the HPC strategy will need substantial means, and in this sense I also count on a strong mobilisation of your constituency to support the Commission's ambitious budget proposal for research and innovation 2014-2020, and to actively champion HPC in Council and Parliament.

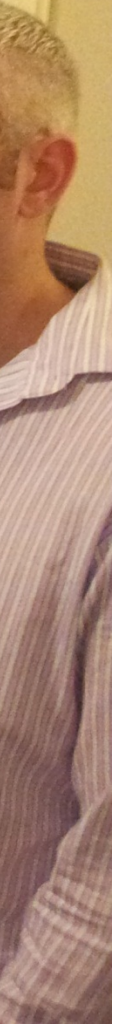
Yours sincerely,

A handwritten signature in black ink, consisting of a large, stylized 'N' followed by a horizontal line and a small flourish at the end.

Neellie KROES
Vice Présidente de la Commission Européenne
Commissaire à la société numérique

Creation of the SRA







European Technology Platform for High Performance Computing

ETP4HPC Strategic Research Agenda Achieving HPC leadership in Europe

February 2013

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Jean-François Lavignon

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Arndt Bode
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Ian Phillips
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Tim Courtney
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Marc Dollfus
Marc Duranton
Ton Engbersen
Thomas Fieseler
Hartmut Fischer
Uwe Fischer
Tony Ford
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Brent Gorda
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Horst Schwichtenberg
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Burkhard Steinmacher-Burow
John Taylor
Ralph Thesen
Thomas Weigold
Michele Weiland
Robert W. Wisniewski

Independent Software Vendor

Representatives

Laurent Anné
Philippe Barabinot
Jean-Pierre Delsemme
Matt Dunbar
Rolf Fischer
Claude Gomez
Charles Hirsch
Koutalba Kassem-Manthey
Dominique Lefebvre
Mark Loriot
Gino Perna
Antoine Petitot
Struan Robertson
Christian Saguez

ISV companies interviewed

Accelrys, DISTENE, EnginSoft, ESI Group, GNS-
mbH, INTES, LMS Samtech, NUMECA, Scilab,
SIMULIA

Document Editing

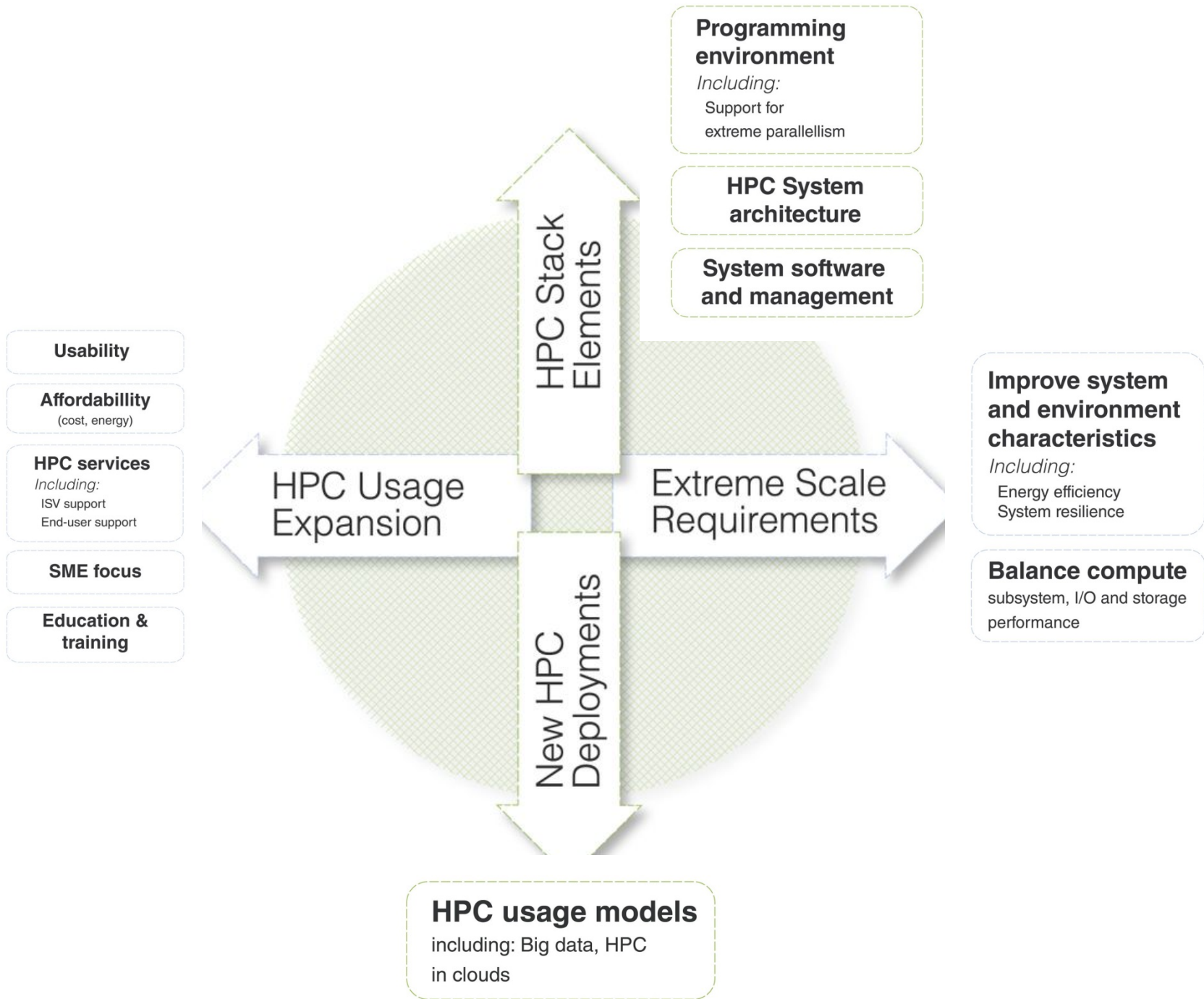
Charlotte Bolliger
Laura Bermúdez
Sonia Piou

End-User Representatives

Nicola Bienati
Serge Bogaerts
Ricard Borell
Norbert Boumeix
Ange Caruso
Thierry Chevalier
Alfred Geiger
Andy Jenkinson
Oscar Laborda Sanchez
Oriol Lehmkühl
Felix Manchado Perdiguero
Gael Mathis
Alessandro Prandi
Hugues Prisker
Bernard Querleux
Michel Ravachol
Philippe Ricoux
Francisco Santistevé Puyuelo
Francesco Spada
Yves Tourbler
Mauro Varasi

End-user organisations and companies interviewed

Airbus, Arcelor Mittal, CENAERO, Dassault
Aviation, EBI, EDF, ENI, Epsilon Meteo,
Finmeccanica, L'OREAL, Renault, SAFRAN,
Termofluids, TOTAL, T-Systems



2013 directions

- Making it happen
 - Working with stakeholders and EC to make the HPC development plan a reality
- Strengthening our ecosystem
 - Recruit new members
 - Creation of 2 workgroups : SMEs, Education and training
- Coordination
 - PRACE
 - Centres of Excellence
 - Future common JU Artemis+Eniac+EPoSS
 - Prospect, Teratec, EESI2



Technologie: rappel FP7

- In FP7 (~49 m€):
 - 3 exascale IPs (Mont-Blanc, DEEP and CRESTA)
 - 2 support actions (EESI and EESI2)
 - (expected) 2 more IPs and 2/3 STREPs



ICT – Information
and communication
technologies

Work programme 2013



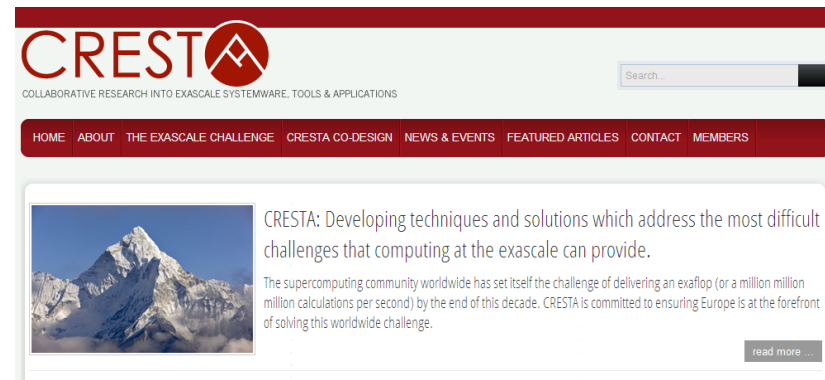
DEEP - Dynamical Exascale Entry Platform

DEEP is an Exascale project funded by the EU 7th framework programme. The main goal is to develop a novel, Exascale-enabling supercomputing platform.



Europe on Exascale

The project DEEP will develop a novel, Exascale-enabling supercomputing platform along with the optimisation of a set of grand-challenge applications highly relevant for Europe's science, industry and society. The DEEP System will realise a Cluster Booster Architecture that will serve as proof-of-concept for a next-generation 100 PFlop/s production system.
→ More



7.12 Special Action

Objective ICT-2013.12.1 Exascale computing platforms, software and applications

ANR en France

- Les call INFRA et MN mettent comme priorité le HPC et en cible l'Exascale pour ce qui concerne MN.

1.2. OBJECTIFS DU PROGRAMME

Les objectifs du programme MN sont de faire progresser les connaissances scientifiques en mathématiques appliquées et en informatique dans les domaines du calcul intensif, du traitement des grandes masses de données, de l'optimisation et de la conception de systèmes, du traitement des incertitudes afin de résoudre de grands défis applicatifs scientifiques dans tous les domaines scientifiques tel que le climat, les sciences de l'univers, la biologie, la santé, l'ingénierie ... ou industriels (gestion du cycle de vie de produits (PLM), logiciels...). Cette édition 2013 s'attache en priorité à relever les défis scientifiques et technologiques de calcul scientifique intensif dont *l'exascale computing et le big data*.

Le programme INFRA recouvre tous les travaux de recherche visant à produire les architectures et infrastructures matérielles et logicielles qui vont permettre de mettre en œuvre un accès ubiquitaire aux diverses infrastructures de communication, de stockage et de calcul. Ces infrastructures sont réparties, à des échelles très diverses (multi-échelle) et impliquent des équipements de nature très différentes et hétérogènes, allant de réseaux d'objets (capteurs, micro et nano contrôleurs, etc.) jusqu'à des architectures massivement parallèles (dont le parallélisme multi-cœurs) et des grilles de machines à l'échelle d'internet.

**Technologies
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Applications et usages

EESI

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SKIP INTRO

e-infrastructure CAPRIELES

More than 35 partners and 100 contributors working together on the future of exascale technology

EESI PARTNERS

Project information

- ★ **Start dates:**
EESI2: 01/09/2012 – 30 months
EESI1: 01/06/2010 – 18 months
- ★ **Coordinator EESI2:**
Philippe Ricoux
TOTAL SA Direction Scientifique
philippe.ricoux@total.com
tel.: +33 1 47 44 75 35
- ★ **EESI2 Partners:**
TOTAL & PRACE and 29 organisations.
- ★ **Coordinator EESI1:**
Jean-Yves Berthou EDF R&D

Homepage

More on the European Exascale Software Initiative:

The objective of this Support Action, co-funded by the European Commission is to build a european vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020**.

- More information on the project and its structure and objectives are available in the section [Project](#).
- Details on Work Groups and experts involved can be found in the section ["Working Groups"](#)

*The speed of a supercomputer is measured in "FLOPS", FLoating Point Operations Per Second "Petascale" supercomputers can process 10¹⁵ FLOPS Exascale

News 02-16-2012

EESI invited to participate in eChallenges e2012

Supported by the EC, the 22nd annual eChallenges e-2012 Conference & Exhibition takes place in Lisbon, Portugal, 17 - 19 October.

Events 2013

March

Mon Tue Wed Thu Fri Sat Sun

<http://www.eesi-project.eu/>

Objectives

One of the EESI2 main objectives is to provide recommendations on strategic European actions with a particular focus on software key issues improvement, cross cutting issues advances, and gap analysis.

The objective of EESI2 is to build on the work done within EESI1 and to extend this role of external and independent representative of the European Exascale community. EESI2 aims to:

1. Contribute to the coordination and the monitoring of the European Exascale Open Source software production, toward an implementation.
2. Produce a dynamic updated roadmap of Exascale industrial applications, Exascale applications for Climate, earth sciences, fundamental physics, life science with a particular emphasis on the breakthroughs and gap analysis.
3. Produce a roadmap of Numerical Libraries, Software eco-system, scientific software engineering and programmability. Once again, emergence of breakthroughs in linear or non linear algebra or in particle simulation for example, will be monitored ex: eigenvalues of tensors?
4. Follow up of research program in massively parallel stochastic programming, Uncertainties, Power, Performance, Data management, Resilience, with a particular emphasis on the breakthroughs and gap analysis.
5. Exchange and dissemination
6. Act as a pro-active European voice in the international community and propose an International Exascale Software Initiative
7. Prepare periodic synthesis by key issues – Recommendations for EC, Funding agencies and R&D stakeholders



Applications et usages: CoE?

There are two main dimensions to such governance. They are linked to each other via the HPC/PRACE centres driving development and innovation.

- (a) For industry, through the industry-led technology platform for EU HPC suppliers, and a network of competence centres providing expertise and services on HPC applications and software development;
- (b) For science, through PRACE and centres of excellence addressing key societal and scientific challenges by deployment and application of HPC software and services;

- The EU Industry engaged in supply of HPC systems and services should coordinate research agendas through the technology platform and thereby create critical mass of industrial R&D in HPC.

- Centres of excellence should be established for the application of HPC in scientific or industrial domains that are most important for Europe (e.g. in the area of energy, life-sciences and climate).

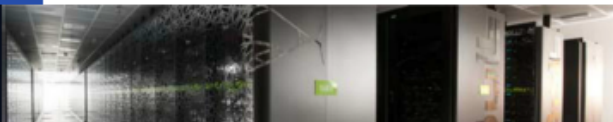
Rappel

Ecoles d'Eté
CEA/EDF/INRIA
2013

Analyse numérique
&
HPC

<http://www-hpc.cea.fr/SummerSchools2013.htm>

  	
SUMMER SCHOOLS 2013 Scientific Committee: B. BIGOT (CEA), B. SALHA (EDF), M. COSNARD (INRIA)	
NUMERICAL ANALYSIS June 10 to June 21, 2013 <i>MOLECULAR DYNAMICS: AB INITIO AND CLASSICAL METHODS</i>	COMPUTER SCIENCE June 24 to July 5, 2013 <i>PROGRAMMING HETEROGENEOUS PARALLEL ARCHITECTURES</i>
Introduction to Molecular Dynamics and Monte Carlo for classical models Michel MARESCHAL (ZCAM, Zaragoza)	Directive-based Programming Michael WOLFE (Portland Group)
Numerical Methods in Computational Statistical Physics Gabriel STOLTZ (CERMICS, Ecole des Ponts ParisTech & MICMAC, Inria Rocquencourt)	Programming Massively Parallel Processors Using CUDA and C++AMP Wen-Mei HWU (University of Illinois at Urbana-Champaign)
Density functional theory: formalism, implementation, dynamical properties Xavier GONZE (UC Louvain)	Implicit and Task-based Approaches to Heterogeneous Parallel Programming Josef WEIDENDORFER (Technical University Munich)
Ab initio Molecular Dynamics Gilles ZERAH (CEA)	
– Hands on session – – Seminars: various conferences by international specialists –	
Coordinator of the Numerical Analysis Summer School Johann BOUCHET, CEA e-mail: johann.bouchet@cea.fr	Coordinator of the Computer Science Summer School Brice GOGLIN, Inria e-mail: brice.goglin@inria.fr
Website: www-hpc.cea.fr/SummerSchools2013.htm Information: Jean CONNARD Phone: 01 69 26 75 35 Fax: 01 69 26 70 03 Secretary of the summer schools: Régis VIZET Phone: 01 69 26 47 45 - Fax: 01 69 26 70 80 - regis.vizet@cea.fr Mail address: Ecoles d'Eté CEA-EDF-INRIA - CEA DAM Ile de France - DAMISENDe - Bruyeres-Le-Châtel - 91297 ARPAJON CEDEX	
Registration Deadline: May 10, 2013 Summer schools are intended for researchers, engineers and PhD students. They allow them to review the state of progress of the proposed subjects and to confront their experience. The teaching is done in English. It is complemented by practical works, in small groups, hosted by assistants. Both schools will take place in the castle of Cadarache - 13115 Saint Paul Lez Durance - FRANCE Cost of the registration (accommodation and all expenses included), Computer Science school (10 days) or Numerical Analysis school (10 days): Full rate: € 5000 - Universities and public research institutes: € 2800 - PhD students: € 1400	



Numerical analysis Summer school 2013

Molecular dynamics: ab initio and classical methods

Cadarache, from June 10 to June 21, 2013.



Abstract

The aim of the summer school is to give thorough knowledge of ab initio and classical methods for molecular simulation. The first week will be dedicated to classical molecular simulation. The basic principles will be tackled both for the physical (Michel Mareschal's lectures) and the numerical (Gabriel Stoltz's lectures) point of view: various ensembles, numerical schemes, stochastic methods, ... For each theme various applied exercises will be proposed. The second week will be dedicated to ab-initio molecular dynamics with an introduction to the density functional theory (DFT). Implementation of ab initio molecular dynamics within the framework of plane wave pseudopotential density functional theory will be given in detail. Specific topics include : Car-Parinello molecular dynamics (CPMD), Path Integral molecular dynamics (PIMD), Tight-Binding methods, Lean on the fly (LOTF)... Emphasis will be given to problems that can only be tackled using ab-initio molecular dynamics as matter in extreme conditions, or properties related to electronic excitations. The participants will use the Abinit program to perform molecular dynamics : parallelism, calculations of melting temperature, phonons density of state, transport properties, PIMD...

Place, Dates, Public

Accommodation and courses take place in a castle depending of the CEA (French Alternative Energies and Atomic Energy Commission) at Cadarache, South of France, from June 10 to June 21, 2013.

These courses can interest a public of industrial engineers as well as academics (in particular researchers from CEA, EDF and INRIA), confirmed or not, in particular the PhD and the post-doctorate students.

Contents

* Lecture 1:

Introduction to Molecular Dynamics and Monte Carlo for classical models

Michel MARESCHAL (ZCAM, Zaragoza)

The lectures will introduce the basics of the Molecular Dynamics and Monte Carlo methods for systems which can be modeled by classical mechanics. The techniques allowing to compute static and transport properties will be introduced, based on equilibrium statistical mechanics. Applications in various ensembles will be presented, with an emphasis on thermostating the dynamics. The last part of the course will be dedicated to direct non-equilibrium modeling.

* Lecture 2:

Numerical Methods in Computational Statistical Physics

Gabriel STOLTZ (CERMICS, Ecole des Ponts & MICMAC, INRIA Rocquencourt)

The aim of this set of lectures is to present the mathematical underpinnings of the most common numerical approaches to integrate dynamics in molecular simulation. The first part will be devoted to the numerical integration of

Reminder:

Summer schools are intended for researchers, engineers and PhD students.

They allow them to review the state of progress of the proposed subjects and to confront their experience.

The teaching is done in English. It is complemented by practical works, in small groups, hosted by assistants.

Schedule

Registration:

If you wish to join, thank you for filling this [registration form](#) and sending it to Régis VIZET before May 10, 2013

Contacts:

Summer Schools secretary

Régis VIZET - CEA
tel: 01 69 26 47 45
fax: 01 69 26 70 80

Coordinator of the numerical analysis summer school:

Johann ROUCHET - CEA

Location

Registration fees:

Full rate: 5000 euros
Academia/ University & Public Research rate: 2800 euros
PhD student rate: 1400 euros (accommodation and meals included)

Hamiltonian dynamics, with an emphasis on symplectic algorithms (such as the celebrated Verlet method). The second part will focus on stochastic methods, namely stochastic differential equations such as the Langevin dynamics, and Markov chain approaches such as the Metropolis algorithm. We will give rigorous results on the convergence of time averages along trajectories of the system, and present numerical schemes to approximately integrate the corresponding dynamics. An important point will be the estimation of numerical errors.

* Lecture 3:

Density functional theory: formalism, implementation, dynamical properties.

Xavier Gonze (UC Louvain)

<http://www.uclouvain.be/xavier.gonze>

Density functional theory (DFT) is nowadays the workhorse for the first-principle prediction of properties of condensed matter, i.e. without parameterization relying on experimental data. Any type of system can be examined, provided the computing resources are available.

In this lecture, I will first present the basic theorems of density functional formalism, and the approximations leading to realistic calculations. I will then detail how DFT equations can be implemented, using plane wave and pseudopotentials.

I will present the computation of forces acting on the nuclei, when these are treated using classical mechanics.

This opens the way to the use of Born-Oppenheimer molecular dynamics.

Finally, I will also focus on the computation of vibrational properties of solids (and related thermodynamical properties), based on density functional perturbation theory.

DFT

1.A. Formal DFT (1h30) (Theorems, XC functionals, the band gap problem)
1.B. DFT mapped into a computer (1h) (Planewave, pseudopotentials, k point sampling)
1. C. Algorithms (1h) (Computation of forces, conjugate gradient, self-consistency, optimization of geometry)

DFPT

2. A. Formal DFPT (1h30) (Perturbations, Sternheimer equation, 2n+1 theorem)
2. B. Phonon and dielectric properties (1h) (incl. phonon band structure, DOS, thermodynamical properties)

* Lecture 4:

Ab initio Molecular Dynamics

Gilles ZERAH (CEA)

Coupling molecular dynamics and ab initio calculation has made possible a qualitative investigation of the properties of many states of matter, from quantum solids to high temperature plasmas.

This set of lectures will present some of the methodological developments and applications which occurred in this respect during the past twenty years.

A special emphasis will be given to the interplay between these theoretical developments and experimental results.

Don't forget the possibility of using your company's training budget.

Computer Science Summer school 2013

Programming Heterogeneous Parallel Architectures

Cadarache, from June 24 to July 5, 2013.



Accommodation and courses take place in a castle depending of the CEA (French Alternative Energies and Atomic Energy Commission) at Cadarache, South of France, from June 24 to July 5, 2013.

Aim:

The aim of the summer school is to give a thorough introduction of tools, languages and execution models for efficient programming of heterogeneous multicore architectures with accelerators. Three lectures will describe the existing programming levels for accelerators as well as techniques for simultaneously using multicores and accelerators within a single application, while trying to maintain performance portability. All courses consist of lectures and hands-on sessions where everyone can try out the tools on several exercises using different parallel computing hardware. No preliminary knowledge of accelerator programming is required, but basic knowledge of parallel programming is recommended.

Lectures:

* Lecture 1:

Directive-based programming
Michael WOLFE (Portland Group)

The lecture will introduce high-level directive-based programming for heterogeneous architectures, such as CPUs connected to GPUs or Intel Xeon Phi coprocessors. We will discuss what kinds of programs are amenable to acceleration with these architectures, and the advantages and penalties of high-level programming. We will go into details of OpenACC, and compare to OpenMP and Intel Languages Extensions for Offload, and will use the PGI compilers for demonstration.

Michael WOLFE has over 35 years of experience developing languages and compilers for high performance and parallel computers in industry and academia. He joined The Portland Group in 1996, where his responsibilities and interests include deep compiler analysis and optimizations ranging from improving the efficiency of programs on parallel clusters to designing and implementing features for high level GPU programming. He was an associate professor at the Oregon Graduate Institute from 1988 until 1996, and was a cofounder and lead compiler engineer at Kuck and Associates, Inc., prior to that. He has published one textbook, "High Performance Compilers for Parallel Computing", a monograph, "Optimizing Supercompilers for Supercomputers," and a number of technical papers, and holds one patent.

References:

Easy GPU Parallelism with OpenACC, June 11, 2012
<http://www.drjdoobs.com/parallel/easy-gpu-parallelism-with->

Reminder:

Summer schools are intended for researchers, engineers and PhD students.

They allow them to review the state of progress of the proposed subjects and to confront their experience.

The teaching is done in English. It is complemented by practical works, in small groups, hosted by assistants.

Schedule

Registration:

If you wish to join, thank you for filling this [registration form](#) and sending it to Régis VIZET before May 10, 2013

Contacts:

Summer Schools secretary
Régis VIZET - CEA
tel: 01 69 26 47 45
Fax: 01 69 26 70 80

Coordinator of the computer science summer school:
Brice GOGLIN - INRIA

Location

Registration fees:

Full rate: 5000 euros
Academia/ University & Public
Research rate: 2800 euros
Phd student rate: 1400 euros

openacc/240001776

(accommodation and meals included)

The OpenACC Execution Model, August 27, 2012
<http://www.drjdoobs.com/parallel/the-openacc-execution-model/240006334>

Creating and Using Libraries with OpenACC, October 29, 2012
<http://www.drjdoobs.com/parallel/creating-and-using-libraries-with-openacc/240012502>

The PGI OpenACC Getting Started Guide
http://www.pgroup.com/docs/openacc_gs.pdf

Tips for Maximizing Performance with OpenACC in Fortran
http://www.pgroup.com/resources/openacc_tips_fortran.htm

* Lecture 2:

Programming Massively Parallel Processors Using CUDA and C++AMP
Wen-Mei Hwu (University of Illinois at Urbana-Champaign)
<http://parallel.illinois.edu/people/wen-mei-hwu>

Description: This course introduces the principles and basic techniques for programming a CPU+GPU heterogeneous parallel computing system. We will start with CUDA, a low-level programming interface where the programmers must explicitly specify the details in data movement, thread index to data index mapping, and use of scratchpad memory. Once the students are familiar with the details, we will also cover C++AMP, a higher-level programming interface where the compiler takes care of a good portion of the details, improving code maintainability. However, the programmer still needs to go through the same thought process in order to achieve performance goals. We will cover some important parallel computation patterns with both CUDA and C++AMP.

References:

"Programming Massively Parallel Processors - A Hands-on Approach", Kirk and Hwu, Morgan-Kaufmann Publisher, 2012.

* Lecture 3:

Implicit and task-based approaches to heterogeneous parallel programming
Josef WEIDENDORFER (Technical University Munich)
<http://www.lrr.in.tum.de/~weidendo/>

After introducing general-purpose processors and their issues, the lecture will detail the design space for accelerators and why some codes are good or bad candidates for these architectures. We describe ways to manage heterogeneity, such as work partitioning, granularity, load balancing, scheduling and data transfers. We also explain how memory namespaces between devices and/or nodes can be managed before presenting some existing programming models and runtime systems that address these issues using task-based models.

References:

Barcelona Supercomputing Center: Programming with StarSS
https://pm.bsc.es/sites/default/files/tutorial_omps_PATC_single.pdf

StarPU handbook:
http://runtime.bordeaux.inria.fr/StarPU/starp_u.html

Don't forget the possibility of using your company's training budget.