Inria Project Lab C2S@Exa
Computer and computational sciences at exascale

Radioactive waste management application
Kickoff meeting at ANDRA
April 24, 2013

Location: ANDRA headquarters, 1/7, rue Jean Monnet, Parc de la Croix-Blanche, 92298 Châtenay-Malabry cedex

This one day technical meeting aims at discussing numerical modeling and high performance computing issues related to ANDRA's use case on radioactive waste management.

ANDRA's participants
Marc Leconte
Laurent Loth
Guillaume Pépin
Jean Roger
Bernard Vialay

Inria' s participants
Nabil Birgle, POMDAPI project-team
Edouard Canot, SAGE project-team
Jérôme Jaffré, POMDAPI project-team
Cédric Lachat, BACCHUS project-team
Rachid El Khaoulani, NACHOS project-team
Luc Giraud, HIEPACS project-team
Michel Kern, POMDAPI project-team
Stéphane Lanteri, NACHOS project-team
Christian Perez, AVALON project-team
Souhila Sabit, SAGE project-team

Participants and talks

Guillaume Pépin, ANDRA
ANDRA's use case for the C2S@Exa IPL
This talk will aim at presenting the use case selected by ANDRA for the activities undertaken in the C2S@Exa IPL. The application context will be described together with the objectives and expected achievements, as well as the positioning of this action in the strategic plan of the Agency for what concern the use of large-scale numerical simulation in its studies.

Laurent Loth, ANDRA
The TRACES software
In this talk we will present the history of the development of the TRACES simulation software for reactive transport in porous media. The physical functionalities and numerical characteristics of the software will be described.

Marc Leconte, ANDRA
Ongoing high performance computing initiatives at ANDRA
This talk will be dedicated to a presentation of ongoing high performance computing initiatives at ANDRA in connection with the PORFLOW simulation software.

Stéphane Lanteri, NACHOS project-team
C2S@Exa – An INRIA Project Lab on high performance computing for computational sciences
In this talk we will present the objectives and associated activities of the recently launched C2S@Exa Project Lab. The C2S@Exa IPL is concerned with the development of numerical modeling methodologies that fully exploit the processing capabilities of modern massively parallel architectures in the context of a number of selected applications related to important scientific and technological challenges for the quality and the security of life in our society. At the current state of the art in technologies and methodologies, a multidisciplinary approach is required to overcome the challenges raised by the development of highly scalable numerical simulation software that can exploit computing platforms offering several hundreds of thousands of cores. Hence, the main objective of the C2S@Exa IPL is the establishment of a continuum of expertise in the computer science and numerical mathematics domains, by gathering researchers from INRIA project-teams whose research and development activities are tightly linked to high performance computing issues in these domains.

Luc Giraud, HiePACS project-team
On hierarchical parallel sparse linear systems
In this talk we will review the parallel numerical techniques and implementations of sparse linear solvers currently designed in the HiePACS project. Starting from dense linear algebra kernels up to hybrid techniques through sparse direct solvers, we will describe the complete solution stack and the underlying methodologies. Numerical and parallel performances for the solution of large 3D problems on distributed manycore, possibly heterogeneous, platforms will be discussed.

Cédric Lachat, BACCHUS project-team
The PaMPA tool for parallel mesh partitioning and adaptation
This talk will present the structure and operations of PaMPA (Parallel Mesh Partitioning and Adaptation), a middleware library dedicated to the management of unstructured meshes distributed across the processors of a parallel machine. Its purpose is to relieve solver writers from the tedious and error prone task of writing again and again service routines for mesh handling, data communication and exchange, remeshing, and data redistribution.

Souhila Sabit, SAGE project-team
Numerical models of reactive transport in porous media
Modeling of reactive transport in porous media is a complex problem combination the difficulties of transport modeling with those of chemistry. After spatial discretization, the semi-discrete model is a coupled algebro-differential system. The objective of this work is to compare in this framework the explicit Euler scheme (SNIA method) with an implicit BDF scheme (GDAE method). SNIA decouples transport from chemistry but has stability constraints. GDAE, combined with a specific software, does not have these constraints and provides a dynamic time-step adaptation, but each time-step is computationally expensive.

Christian Perez, AVALON project-team
Programming HPC applications with software components
This talk will deal with the programming of parallel applications with software components. It will discuss about the benefits of software component models (in general and for HPC). It will present models (L2C and HLCM) that are developed within the AVALON team.

Nabil Birgle, POMDAPI project-team
A mixed finite element method for deformed cubic meshes
We present a mixed finite element method in 3 dimensions for second order elliptic equations in a domain discretized with a mesh of deformed cubes. The goal is to define a numerical method with one pressure per cell and one flux per face, even for the case of the deformed cubes with non-planar faces. The deformed cube is approximated by a submesh of 24 tetrahedrons by introducing a new mesh point at the barycenter of the cube and one mesh point at the barycenter of each cube face. Now each face of this approximate deformed cube is actually the union of four triangles. Then the standard RTN mixed finite element method is used on this underlying tetrahedral mesh. From this point, we show how to use static condensation to obtain a method with only one pressure per approximate deformed cube (instead of 24) and one flux per face of the approximate deformed cube (instead of 4). This work is a preliminary study for introducing the new mixed finite element method in the TRACES simulation software before undertaking HPC studies with this code.

Edouard Canot, SAGE project-team
Activities of the SAGE project-team in relation to the C2S@Exa IPL
In this talk we will present the activities of the SAGE project-team on numerical modeling and high performance computing in relation with the C2S@Exa IPL.

Michel Kern, POMDAPI project-team
Activities of the POMDAPI project-team in relation to the C2S@Exa IPL
In this talk we will present the activities of the POMDAPI project-team on numerical modeling and high performance computing in relation with the C2S@Exa IPL. In particular, we will discuss about space-time domain decomposition methods, a posteriori error estimation for iterative methods and parallel computing with Ocaml and skeletons.

Michel Kern, POMDAPI project-team
Maison de la Simulation
The *Maison de la Simulation* is a joint project of five partners (CEA, CNRS, INRIA, University of Orsay and University of Versailles-StQuentin) with the status of a "Unité de Service et de Recherche" (Service and Research Unit), whose aim is to support and stimulate the scientific community in order to get the best out of supercomputers, in particular those managed by the French GENCI and the European PRACE programs. The *Maison de la Simulation* promotes among others the emergence in France of a HPC community, and develops the strong synergies between researchers and engineers from various fields, necessary for the important scientific breakthroughs expected from HPC to materialize. These initiatives are targeted to the current HPC users, as well as to the research of new application fields for the HPC.

Preliminary program

9h30-10h00 Welcome of the participants

10h00 - 10h20
Stéphane Lanteri, NACHOS project-team
C2S@Exa – An INRIA Project Lab on high performance computing for computational sciences

10h20 – 10h40
Guillaume Pépin, ANDRA
ANDRA's use case for the C2S@Exa IPL

10h40 – 10h55
Laurent Loth, ANDRA
The TRACES software

10h55 – 11h10
Marc Leconte, ANDRA
Ongoing high performance computing initiatives at ANDRA

11h10 – 11h30
Luc Giraud, HiePACS project-team
On hierarchical parallel sparse linear systems

11h30 – 11h50
Michel Kern, POMDAPI project-team
Activities of the POMDAPI project-team in relation to the C2S@Exa IPL

11h50 – 12h00
Michel Kern, POMDAPI project-team
Maison de la Simulation

12h00 - 12h20
Nabil Birgle, POMDAPI project-team
A mixed finite element method for deformed cubic meshes

12h20 – 14h00 Lunch

14h00 – 14h20
Edouard Canot, SAGE project-team
Activities of the SAGE project-team in relation to the C2S@Exa IPL

14h20 - 14h40
Souhila Sabit, SAGE project-team
Numerical models of reactive transport in porous media

14h40 – 15h00
Cédric Lachat, BACCHUS project-team
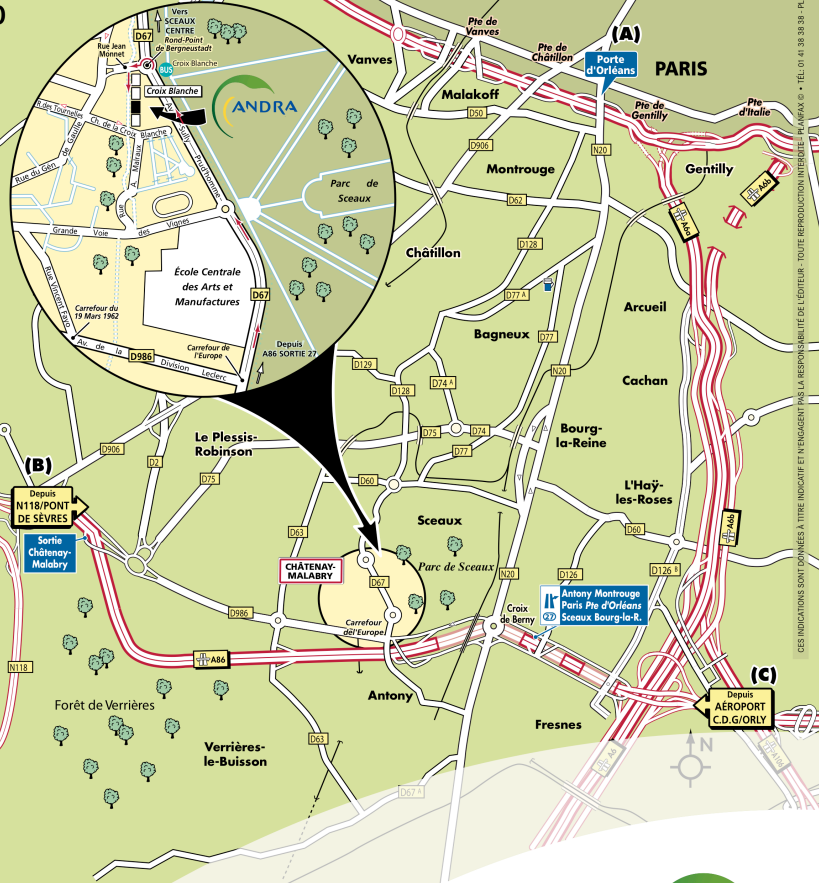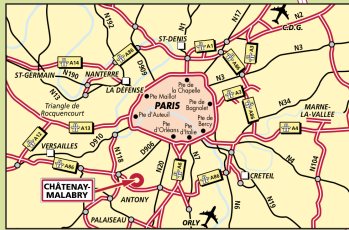The PaMPA tool for parallel mesh partitioning and adaptation

15h00 – 15h20
Christian Perez, AVALON project-team
Programming HPC applications with software components

15h20 – 17h00 Discussion

17h00 End of the meeting

Siège social de l'Andra
1/7 rue Jean-Monnet
92298 CHATENAY-MALABRY CEDEX
Tél. : 01 46 11 80 00

■ **Depuis PARIS/PORTE D'ORLÉANS : (A)**
Rejoindre la PORTE D'ORLÉANS puis emprunter la N20 direction ANTONY. À la CROIX DE BERNY, prendre à droite direction CHÂTENAY-MALABRY puis au CARREFOUR DE L'EUROPE emprunter la D67 direction SCEAUX CENTRE (puis voir loupe).

■ **Depuis PARIS/PONT DE SÈVRES : (B)**
Rejoindre la N118 direction MEUDON/BIÈVRES. Prendre la sortie 4 VERSAILLES/ROUEN/VÉLIZY puis continuer direction A86/CRÉTEIL. Prendre la sortie CHÂTENAY-MALABRY. Emprunter la D986 vers CHÂTENAY-MALABRY puis la D67 vers SCEAUX CENTRE (puis voir loupe).

■ **Depuis AÉROPORT CHARLES-DE-GAULLE : (C)**
Rejoindre l'A1 direction PARIS puis l'A3 direction PARIS/PTE DE BAGNOLET. Prendre l'A86 direction FONTENAY-S-BOIS/CRÉTEIL puis l'A4 direction PARIS/PTE DE BERCY. Continuer sur l'A86 direction CRÉTEIL/VERSAILLES puis emprunter la sortie 27 ANTONY/MONTROUGE/PARIS/PORTE D'ORLÉANS/SCEAUX/BOURG-LA-REINE. À la CROIX DE BERNY, prendre la direction de CHÂTENAY-MALABRY puis au CARREFOUR DE L'EUROPE emprunter la D67 en direction SCEAUX CENTRE (puis voir loupe).

■ **Depuis AÉROPORT D'ORLY : (C)**
Rejoindre la N7 direction VILLEJUIF/CRÉTEIL. Prendre l'A86 direction VERSAILLES. Emprunter la sortie 27 ANTONY/MONTROUGE/PARIS/PORTE D'ORLÉANS/SCEAUX/BOURG-LA-REINE puis à la CROIX DE BERNY, prendre en face en direction de CHÂTENAY-MALABRY. Au CARREFOUR DE L'EUROPE emprunter la D67 en direction SCEAUX CENTRE (puis voir loupe).

■ **Transports en Commun :**
Prendre le RER B direction ST-RÉMY-LÈS-CHEVREUSE. Arrêt ANTONY Prendre ensuite le bus n° 395 direction CLAMART. Arrêt CROIX BLANCHE.

ANDRA
La maîtrise des déchets radioactifs