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High Performance Computing / Le Calcul Intensif

Foreword

On June 28, 2010 the French Academy of Sciences held a seminar on high performance computing (HPC). Consequently, conscious of the importance of this field, it was then decided to put together this special issue of *the Comptes Rendus de Mecanique*. The contributions are not those of the seminar, and being in a journal of mechanical and computational engineering, algorithms and methods are discussed rather than applications, which for some of them are in geophysics, chemistry and mathematics.

HPC deals with algorithms and simulations on supercomputers. Few fields in science have seen their means of investigation doubling every 12 to 18 months for the past 50 years. It seems that this rate of growth will be sustained for another 10 years at least, and most likely we will see ExaFlop machines around 2018.

Extreme simulations seem to advance all fields of science. Mathias Steinmetz[1] in astrophysics can reproduce the evolution of the universe from an initial state near the Big Bang, subject to the far reaching hypothesis that 99% of the energy of the universe is dark matter. In fundamental physics Lattice Quantum Chromo Dynamics may yield a much better understanding of elementary particles.[2] In engineering, the simulation of a complete jet engine has contributed greatly to the understanding of certain combustion instabilities.[3] In geology the detection of fossil energy is systematically assisted by numerical seismology (see the *rapport annuel de l'IFP 2009*). In chemistry everyone agrees that new materials, in particularly for the walls of commercial fusion reactors – ITER's successors – will be found with the help of ab-initio chemistry.[4] In molecular biology the progress made by Molecular Dynamics and ab-initio chemistry is immense: a real revolution.[5]

ExaFlop machines will probably have millions of computing units, possibly hybrid (x86 type + GPU type), each having its local memory yet accessible by others through an intricate high speed network, with the result that the locality of data is of prime importance for optimal performance. In short, the architecture of the supercomputer is now an integral part of the numerical method, algorithm and programs of any simulation.

Concurrently at the high end of personal computers, general-purpose graphic processing units have appeared. Although their prime objective is to accelerate graphics for realistic rendering, they can also be programmed with dedicated languages such as CUDA and OpenCL. The difficulties are similar: localization and communication of data. Despite these difficulties a surprising number of numerical analysts have turned to CUDA. It is a good thing, because in the end it will enlarge the scientific community of HPC developers, which is too small as lamented in all government reports.[6]

So in this issue we have solicited HPC and GPU users. Most will tell us of their experience and how to achieve performance.

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[1] Films can be seen at http://www.aip.de/People/msteinmetz/Movies.html.
[2] See for example http://en.wikipedia.org/wiki/Lattice_QCD.
[3] Films can be seen at http://www.cerfacs.fr/cfd/Gallery/movies/Ignition_high.mov.
[4] Slides of a conference at http://fire.pppl.gov/sofe09_zinkle.pdf.
[5] See for examples the pictures and films at http://www.ks.uiuc.edu/Gallery/.
[6] See for example the annual report of the CSCI, downloadable from http://www.genci.fr.

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