Integrated Project (IP)

Code analysis and profiling

Tasks

Develop the following tasks for each proposed theme (list below):

1. Read and characterize the supplied code, converting it into C code if necessary; analyse qualitative and quantitatively the performance of this version (using profilers, including PAPI); identify those parts of the algorithm/code that are better suited for optimization and/or parallel computing.
2. Design and implement a shared-memory parallel version of the critical parts of the code with OpenMP (no need to struggle for optimum code); test and evaluate the resulting performance on one node in the SeARCH cluster.
3. Design and implement a hybrid code that combines a CPU core (the host portion of the code) with a CUDA-enabled GPU device (the kernel with the critical parts; no need to struggle for highly efficient code); test and evaluate performance on one node in the SeARCH cluster.

Methodologies, reports and presentations

1. Theme allocation:
   a. 6 teams, 2 MEI students each, competitive allocation;
   b. Themes allocated to teams on Tuesday Dec 11, with reading assignments before end 2012;
   c. Themes source code with min 3 input/output data sets at 1st Tuesday in January.
2. Deliverables: extended abstracts, presentations and reports in English; when and what:
   a. An extended abstract (max. 2 A4 pages) before Thursday 31st January;
   b. An individual oral presentation and discussion (20 min) on Tuesday 5th February;
   c. A final report (produced by the team, no longer than 8 pages plus plots and/or annexes) by Tuesday 12th February.

List of themes (provisional titles)

1. **Heat transfer in solids**
   (*CPD Advisor & co-Advisor: AProença & Miguel Nóbrega*)
   (*Team: Cristiano Sousa & David Pereira*)
   Description:
   Current work by the project team includes a port of some CFD numerical computations from "home-designed" code to library functions from the OpenFoam project. The project in this course will be mainly based on a set of functions to solve a particular problem that uses OpenFoam functions that have not been yet fully ported to a parallel environment nr in a a CUDA-based platform. More details soon...
   Preliminary readings:
   Some work on the issue of porting the application (without OpenFoam) to a CUDA environment has already been performed under an MSc dissertation (Simão's) and some work has already been developed to port OpenFoam to parallel and heterogeneous environments. A compilation of these documents can be found in http://gec.di.uminho.pt/minf/cpd1213/PI/OpenFoam.zip.

2. **Quantum modelling of carbon nanomaterials with millions of atoms with HPC**
(*CPD Advisor & co-Advisor: APina & Manuel Melle Franco*)
(*Team: Diogo Barbosa & Luís Gomes*)
Description:
The aim of this project is to informally explore different strategies to test the efficiency of current Quantum Mechanics models with different parallelization strategies. More details in in http://gec.di.uminho.pt/minf/cpd1213/PI/QMsimulationsCPD2013.pdf.
Preliminary readings:
These are in the document mentioned above.

3. **Solving the Poisson-Boltzmann equation for 3D problems**
(*CPD Advisor & co-Advisor: AProença & Nuno Micaêlo*)
(*Team: Daniel Gomes & Rui Silva*)
Description:
This project aims to get efficient parallel solutions (mainly in CUDA/GPU) to solve the Poisson-Boltzmann equation for 3D problems.
More details in http://gec.di.uminho.pt/minf/cpd1213/PI/Project_SOR.pdf
Preliminary readings:
The slides of the presentation and the project description mentioned above. The software can be directly downloaded from the author website in http://stjuderesearch.org/site/lab/bashford/.

4. **Finite volume method for steady-state convection-diffusion**
(*CPD Advisor & co-Advisors: RRalha, JSobral & Stéphane Clain*)
(*Team: José Alves & Rui Brito*)
Description:
A classical finite volume method for the 2D or 3D steady-state convection-diffusion problem based on the Patankar formulation has been developed using a matrix-free implementation. It provides an afine operator: for any vector $\phi \to \G(\phi)$ such that the solution is given by $G(\phi)=0$.
We compute the approximation using an iterative method where no matrix is needed (GMRES method for instance). The core of the problem is (i) to improve the efficiency of the routine which compute $G(\phi)$ for any vector ϕ since it is easy to parallelize and (ii) to improve the iterative solver.
Preliminary readings:
Read these 3 documents in http://gec.di.uminho.pt/minf/cpd1213/PI/FinVolMethods.zip

5. **Hydrodynamic modelling**
(*CPD Advisor & co-Advisor: APina, JSobral & José Luís Pinho*)
(*Team: Nuno Fernandes & Ricardo Costeira*)
Description:
Work related to the open package Delft3D. More details and context in the document below.
Preliminary readings:
Context in http://gec.di.uminho.pt/minf/cpd1213/PI/HydrodynModelling.pdf; follow the Webinar in http://content.oss.deltares.nl/delft3d/Webinar/Baart_LinuxCodeCompiling/WebinarBaart_11012012_v3.html before attempting to install the software.
Please try to run the 1st example (./examples/01_standard/)

6. **Code optimization in High Energy Physics: challenges at the LHC**
(*CPD Advisor & co-Advisors: APina & António Onofre and Nuno Castro*)
(*Team: Diogo Lopes & Fábio Correia*)
Description:
More details soon...
Preliminary readings:
Read these 2 documents in http://gec.di.uminho.pt/minf/cpd1213/PI/LIPstuff.zip