GPU implementation of molecular quantum scattering codes: MOLSCAT code for astrophysical applications

1 Introduction

In order to solve the quantum dynamics of scattering, several codes have been devised and are presently running on an OpenMP implementation. While this implementation used to be efficient enough for all applications, the advent of new instruments and new physical questions make the OpenMP implementation prohibitively slow. Indeed, we are now interested in molecule-molecule scattering at higher temperatures, involving the physical conditions of our atmosphere or the exo-atmospheres, in the Solar System (like Venus or Titan) or else in exo-planets [1, 2, 3]. Computing these collisions entails solving the Schrödinger equation with representative matrices too large to fit in the usual CPU programs in reasonable times. The quantum codes have been running and evolving for several decades (fortran code MOLSCAT [4]), but need to be ported towards newer, faster environments, with GPU computations.

2 Techniques

The MOLCAT code comprises three conceptual parts :

1. Setting up the problem : bases, potentials, preparation of angular momentum algebra. This part is fast and, in principle, need not to be touched upon. However, some size effects may occur, that will have to be addressed and possible MPI-type of implementation of this part of the code is not ruled out.
2. Propagation of the representative quantum matrix. This part takes about 95% of the time. Each step involves several matrix multiplication and a matrix inversion ; this is the stage that has to be completely implemented anew.

3. Final stage, summing up the work, outputs. Very fast.

Representative matrices are real, symmetric and their size varies from 100 up to more than 30,000, with extensions forecast to 50,000 or more. With those sizes of matrices, simple MPI extension are not expected to represent a breakthrough speed up of the code, and using the full capabilities of GPU's is looked for.

The new implementation of the propagation scheme should be on one or several GPU's, backed with the relevant fast MAGMA [6] and/or OpenACC environments and routines [5]. Several side problems of memory sizes and of sparse vector dense matrix multiplications will be treated too. A full rewriting of the code is not necessary, only the parts dealing with linear algebra should be handled, even if some understanding of the overall machinery is necessary.

The aim of this internship will be to implement the GPU capabilities in the propagation scheme of the existing quantum scattering code MOLSCAT, thanks to MAGMA subroutines and OPEN-ACC environments.

During this internship, the student will work at the Laboratoire Aimé-Cotton (LAC)[8], a world class atomic and molecular physics laboratory (Theomol team), and the Idris [7] which is one of the most important HPC institution in France. The student will be free to work on the multi-GPU optimization of the matrix algebra and/or the GPU implementation of the MOLSCAT. An access to the Jean Zay supercomputer located at Idris [9] will be also granted during the internship, together with front-ends at LAC, in order to get acquainted with the MOLSCAT code.

Keywords : Molecules, astrophysics, quantum scattering, HPC, Linear Algebra, Fortran, MAGMA, OpenACC

Training places : Laboratoire Aimé-Cotton, CNRS-U. Paris Saclay, Bât 505, Campus Universitaire d'Orsay
and
IDRIS (Institut du Développement et des Ressources en Informatique Scientifique), Campus Universitaire d'Orsay.

Training period : Tentatively from middle of March till beginning of September

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[5] https://www.openacc.org/

[6] http://icl.cs.utk.edu/magma/

[7] http://www.idris.fr/

[8] http://www.lac.u-psud.fr/

[9] http://www.idris.fr/eng/jean-zay/jean-zay-presentation-eng.html