BSC / MSC ASSIGNMENT

Accelerating Computational Quantum Chemistry software package ADF using GPU's

Background

Computational Chemistry is used to predict and understand chemical processes, including reactions, on the computer. The software package ADF (Amsterdam Density Functional) focuses on the quantummechanical description of molecules. The computations on large molecules are very time-consuming and are typically performed on Linux clusters or supercomputers at computing centers and may take days even then. There is increasing interest in our field for usage of GPU's to accelerate the calculations to enable users to simulate on their desktop what used to require a supercomputer. SCM closely follows these developments and wishes to investigate to what extent GPU's can be meaningfully used in ADF. ADF video op YouTube: http://www.scm.com/Videos/Welcome.html

Description of assignment

Feasibility study into acceleration of modules in ADF using GPU's. ADF contains various modules each with their own computational bottlenecks, which can usually be reduced to a linear algebra task. The most compute intensive tasks in the ocde, such as numerical integration, have been isolated into a stand-alone code that can be easily used for various tests without prior ADF knowledge. ADF is a Fortran90 program that has been vectorized and parallelized, it uses performance libraries such as BLAS and LAPACK, and is well structured. The student's task is to adapt the algorithms of the most time-consuming parts such that they will run efficiently on GPU's. Initially this will be compared to serial CPU usage, later possibly also in combination with multiple CPU cores.

Company

Scientific Computing & Modelling NV (SCM, www.scm.com) is a spin-off company of the VU University, located inside the VU building and conveniently located near train station Amsterdam-Zuid. SCM employs six experienced PhD chemists and physicists. Four of them do software development and one is specialized in speeding up code. He will act as supervisor for the student. SCM's software is used worldwide to predict material properties. Only part of the assignment work needs to be performed in Amsterdam.

More information

Further information can be obtained from Dr. Stan van Gisbergen, managing director of SCM (vangisbergen@scm.com, 020-5987626). Various forms and durations of the assignment can be discussed.