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GPU-based Integration with Application in Sensitivity Analysis

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The presented work is an important part of the grid application MCSAES (Monte Carlo Sensitivity Analysis for Environmental Studies) which aim is to develop an efficient Grid implementation of a Monte Carlo based approach for sensitivity studies in the domains of Environmental modelling and Environmental security. The goal is to study the damaging effects that can be caused by high pollution levels (especially effects on human health), when the main modeling tool is the Danish Eulerian Model (DEM).

Generally speaking, sensitivity analysis (SA) is the study of how the variation in the output of a mathematical model can be apportioned to, qualitatively or quantitatively, different sources of variation in the input of a model. One of the important classes of methods for Sensitivity Analysis are Monte Carlo based, first proposed by Sobol, and then developed by Saltelli and his group. In MCSAES the general Saltelli procedure has been adapted for SA of the Danish Eulerian model. In our case we consider as factors the constants determining the speeds of the chemical reactions in the DEM and as output a certain aggregated measure of the pollution.

Sensitivity simulations lead to huge computational tasks (systems with up to 4×10^9 equations at every time-step, and the number of time-steps can be more than a million) which motivates its grid implementation. MCSAES grid implementation scheme includes two main tasks: (i) Grid implementation of the DEM, (ii) Grid implementation of the Monte Carlo integration.

In this work we present our new developments in the integration part of the application. We have developed an algorithm for GPU-based generation of scrambled quasirandom sequences which can be combined with the CPU-based computations related to the SA. Owen first proposed scrambling of Sobol sequence through permutation in a manner that improves the convergence rates. Scrambling is necessary not only for error analysis but for parallel implementations. Good scrambling is especially important for GRID applications. However, scrambling is often difficult to implement and time consuming. Here we propose and study effective generation of the most popular quasirandom sequence, Sobol sequence, with Owen scrambling using GPU computing and interacting with the CPU-based computational tasks using MPI. The model for GPU computing is to use a CPU and GPU together in a balanced heterogeneous computing model. Our implementation works in a Grid environment on a combination of worker nodes from a Grid cluster with a high number of CPUs and special GPU nodes with powerful graphical cards supporting CUDA.

From the user's perspective, the application just runs faster because it is using the high-performance of the GPU to boost performance. Numerical and timing results for integration of multiple integrals (dimension 100) using scrambled Sobol sequence, using the combined power of hundreds of CPU cores and thousands of GPU cores demonstrating the advantages of our approach are presented and discussed.