State-to-state reactive scattering dynamics implemented on graphics processing unit

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Abstract

Graphics processing unit (GPU) computing has been successfully applied in some scientific simulations. In this work we developed an efficient GPU version of a time-dependent wave-packet code for atom-diatom state-to-state reactive scattering processes. Both the reactant Jacobi coordinates and product Jacobi coordinates approach are implemented, and the efficiency and convergence are compared. Since we use the split operator method to propagate the wave-packet, most of the runtime on each time step in the program is consumed in two parts: (1) the transformation of wave-packet between discrete variable representation (DVR) and finite basis representation (FBR) and (2) the actions of the several parts of Hamiltonian on the wave-packet. Both of these parts are actual matrix multiplication and are therefore very viable to realize paralleling in GPU with careful structuring of the matrices and manipulation of multiplication.

In our tests GPU and CPU are Tesla C2050 GPU and CPU E5620 @ 2.40GHz, respectively. The propagation of wave-packet is entirely on a single GPU. Thus after preparation of the initial wave-packet, the CPUs of the computing node can still be used to do other calculations. The result shows a global speedup of more than 15 comparing the parallel computation of GPU and serial computation of CPU.

Paralleling in a single GPU rather than between computing nodes, the code allows us to study the adiabatic/nonadiabatic reactive dynamics to obtain the state-to-state information. It is hoped that the approach of accelerating reactive dynamics by GPU can be used in polyatomic reaction systems involving more than three atoms.