Density matrix calculations of Doppler-broadened atomic systems implemented on GPUs

Teo Victor Resende da Silva and Marco P. M. de Souza
Departamento de Física, Universidade Federal de Rondônia, Ji-Paraná - RO, Brazil.

Important subjects in non-linear optics involving resonant interactions between lasers and atomic vapors has been very studied in recent years. We can mention the parametric four-wave mixing, the electromagnetically induced transparency, the photon echo and the slow light, for example. The Doppler broadening is usually the main contribution to the optical response of an atomic vapor. Thus, the numerical calculations of the density matrix elements must include the contribution of many group velocities, leading to time-consuming computations. On the other hand, graphical processing units (GPUs) has been extensively used in various fields of science, like molecular dynamics, magnetohydrodynamics simulations, Maxwell-Bloch equations, Monte Carlo simulations, and various others. In this work, we use GPUs to accelerate the calculations of the density matrix of the problem of a Doppler-broadened rubidium vapor in the presence of a resonant train of ultrashort pulses of 100 MHz repetition rate. We solve the Bloch equations in the time domain for the $5S_{1/2} \rightarrow 5P_{3/2}$ transition by using the standard fourth-order Runge-Kutta method. We use the Cuda cores of the GPUs to solve the Bloch equations for different atomic group velocities in parallel, while the CPU does it serially. We compare the performance of five GPUs and a Core i5 4460 CPU, where the results present a relative difference below $2.2 \times 10^{-5}$. For the Geforce GTX 760 Ti, it is necessary 55 group velocities to this GPU to be faster than the CPU. The maximum speedup is $960 \times$, reached for $10^6$ group velocities. This speedup should be useful in more realistic problems, like velocity-selective transitions in multilevel atomic systems, where the calculations on CPU for different group velocities and laser frequencies can lead several days.