Molecular dynamics simulations of electron-ion nonideal plasmas on GPU

R.G. Bystryi, Ya.S. Lavrinenko, I.V. Morozov

Joint Institute for High Temperatures of RAS, Moscow, Russia
Moscow Institute of Physics and Technology, Dolgoprundy, Moscow Region, Russia

Graphical procession units (GPUs) have shown their particular efficiency for classical molecular dynamics (MD) simulations [1,2,3]. In the case of long range interaction (Coulomb or gravitational) the so-called N-body problem is solved numerically which requires a relatively small amount of GPU memory and a large amount of computations. Such kind of algorithms fit the GPU architecture perfectly and allows one to achieve a significant performance gain (about 10 times comparing Intel Xeon X5670 CPU and Nvidia Tesla C2050 GPU).

In this work we applied GPU-accelerated MD simulations to study the electron-ion plasma generated by irradiation of nanosized metallic clusters by femtosecond laser pulses. Provided that the laser intensity is moderate (10^{13} – 10^{16} W/cm^2) the plasma becomes nonideal with the ratio of the mean potential to kinetic energy about unity. Electron plasma oscillations, electron-ion collisions, relaxation rates in such nonideal nanoplasma are of particular interest in view the size effects essential for the cluster plasma [3].

The use of GPUs allowed us to increase the number of particles by two orders of magnitude and to observe transitions of the electron oscillation spectra in the cluster plasma ranging from 55 to 10^5 ions. The dependence of frequency and damping of different collective plasma oscillation modes including Mie and Langmuir oscillations are presented. Influence of the choice of interaction potential is discussed.

GPU-accelerated program is also suitable for other problems of strongly coupled plasma. The example of convenient task is researching of equation of states of plasma. Computational aspects of this problem are discussed.

References

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