WPMD-DFT CALCULATIONS OF THE DEUTERIUM HUGONIOT

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A new quantum method for non-ideal plasmas simulations is proposed based on the wave packet molecular dynamics (WPMD) and density functional theory (DFT). The method is called WPMD-DFT. It allows to study simultaneous dynamics of electrons and ions, obtain thermodynamic properties of non-ideal plasmas, electron-ion relaxation rates, plasma conductivity and interaction of plasma with the laser irradiation.

In the WPMD-DFT approach the electrons are represented as Gaussian wave packets whereas the Hartree approximation for the many-body wave function is used. The exchange and correlation effects are treated using an additional energy term taken from DFT (LSDA approximation). This term is determined by an exchange-correlation functional and a correction to the kinetic energy. It is calculated via integration over the mesh values of the function that depends on the electron density. The local electron density distribution is determined by the positions and widths of the wave packets. The proposed approach is meant as a replacement for the antisymmetrized WPMD (AWPMD) method which is more time consuming.

Evaluation of exchange-correlation energy is a time-consuming operation due to the integration over a simulation cell space. Different optimization techniques like an adaptive mesh refinement and GPU-accelerated computing are applied to speed up the computations. Moreover, the algorithm is parallelized to be used for multi-CPU/multi-GPU computational clusters. The computational efficiency of the method is considered.

The WPMD-DFT method is applied for direct simulation of deuterium shock compression. As a contrast to other QMD studies of the Hugoniot [], the simulation is performed by a direct method, i.e. as a series of compression and relaxation stages. This technique is more efficient computationally, because it requires equilibrium calculations along the Hugoniot curve only. The convergence of simulation results as a function of compression speed, which is critical to the direct method, is studied. The results are compared with experimental data and other QMD simulations.