GPU ACCELERATED SHAKE AND RATTLE ALGORITHMS FOR SYSTEMS WITH HOLONOMIC CONSTRAINTS

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Introduction. The dynamic of complex fluid can be described by including viscoelastic stress tensor into the equation of Non-Newtonian fluid. Different models are used to evaluate the stress tensor at various levels, with the multi-scale model being the most effective.

Methodology. In our work we will present the new approach to the macro-kinetic-micro model, and show the use of GPU technologies to accelerate the kinetic and molecular scales. Because it is impossible to track all relevant microscopic variables for each polymer in a polymer-laden solution due to the huge number of degrees of freedom, we use the statistical representation of polymer conformations at kinetic level.

Results. We developed a GPU algorithm for systems satisfying holonomic constraints. In our work we implemented an analog of the original SHAKE algorithm and its velocity version RATTLE using NVIDIA CUDA computer language. Several numerical experiments were performed to examine an acceleration and validity of the algorithms, including a simulation of a stochastic dynamics of lambda DNA. In our simulations, performed using NVIDIA Tesla C2075, the algorithm demonstrates significant acceleration (ten and more times for large systems) in comparison to serial CPU code.