Efficient interacting many body simulations using GPUs

TOBIAS KRAMER, Universität Regensburg — Graphics Processing Units (GPUs) provide an ideal tool to study interacting systems using classical mechanics with huge speedups for example in molecular dynamics. The quantum-mechanical calculations of many-body systems require additional work, but are feasible using additional degrees of freedom to incorporate quantum-mechanical effects [1]. As an example of the method I show the self-consistent solution to the current transport in a magnetic field can be obtained from a microscopic model with thousands of Coulomb interacting electrons. This yields a microscopic model of the Hall effect [2]. For few electron systems I compare the electronic density evolution based on the GPU classical-quantum model to TD-DFT calculations and discuss prospects of GPUs for solving the Schrodinger equation for many-particles.