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Efficient interacting many body similations using GPUs TOBIAS KRAMER, Universität Regensburg — Graphics Processing Units (GPUs) provide an ideal tool to study interacting systems using classical machanics 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.

[1] Time dependent approach to transport and scattering in atomic and mesoscopic systems, T. Kramer AIP Conf. Proc., 1334, 142 (2011)

[2] Self-consistent calculation of electric potentials in Hall devices, T. Kramer, V. Krueckl, E. Heller, and R. Parrott Phys. Rev. B, 81, 205306 (2010)

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