

Hybrid Monte Carlo methods for simulation of complex systems

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Objective: working on development and implementation of the new class of hybrid simulation methods, GSHMCs, which are based on Hamiltonian dynamics and Monte Carlo and which provide effective sampling and exact temperature control during molecular simulation

Results:

GSHMC: generalized shadow Hamiltonian Monte Carlo: a thermodynamically consistent implementation of constant-temperature molecular dynamics

✓UK patent (2009), US patent (2009)

MTS-GSHMC: multiple-time-stepping GSHMC

✓2 US patent s (2011), 2 EU patents filed (2009)

meso-GSHMC: a Metropolis corrected dissipative particle dynamics method

✓ UK patent (2010), US patent (2010)

GSHmMC: generalized shadow Hamiltonian Monte Carlo: a reformulation of GSHMC for statistical simulation

✓UK patent (2009), US patent (2009)

In progress:

✓Performance optimization of GSHMCs

✓Efficient adaptation of GSHMCs to new applications