

Langevin Thermostat for Rigid Body Dynamics

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We present a new method for isothermal rigid body simulations using the quaternion representation and Langevin dynamics. It can be combined with the traditional Langevin or gradient (Brownian) dynamics for the translational degrees of freedom to correctly sample the NVT distribution in a simulation of rigid molecules. We propose simple, quasi-symplectic second-order numerical integrators and test their performance on the TIP4P model of water. We also investigate the optimal choice of thermostat parameters. The talk is based on a joint work with Ruslan Davidchack and Richard Handel (Leicester).