WARWICK
THE UNIVERSITY OF WARWICK

Novel stochastic thermostats for rigid body dynamics

Michael Tretyakov

School of Mathematical Sciences.
University of Nottingham

Tuesday, 8th Dec, 4 p.m.
B2.04/5, Science Concourse, 2nd Floor

Abstract: We introduce two new thermostats, one of Langevin type and one of gradient (Brownian) type, for rigid body dynamics. We formulate rotation using the quaternion representation of angular coordinates; both thermostats preserve the unit length of quaternions. The Langevin thermostat also ensures that the conjugate angular momenta stay within the tangent space of the quaternion coordinates, as required by the Hamiltonian dynamics of rigid bodies. Geometric integrators play an important role in simulating dynamical systems, in particular in molecular dynamics, on long time intervals with high accuracy. We have constructed three geometric numerical integrators for the Langevin thermostat and one for the gradient thermostat. The numerical integrators reflect key properties of the thermostats themselves. Namely, they all preserve the unit length of quaternions, automatically, without the need of a projection onto the unit sphere. The Langevin integrators also ensure that the angular momenta remain within the tangent space of the quaternion coordinates. The Langevin integrators are quasi-symplectic and of weak order two. The first-order numerical method for the gradient thermostat was constructed using ideas of Lie-group type integrators for differential equations on manifolds. We numerically compare the discretization errors of the Langevin integrators, as well as the efficiency of the gradient integrator compared to the Langevin ones when used in the simulation of rigid TIP4P water model with smoothly truncated electrostatic interactions. The talk is mainly based on joint recent work with Rusland Davidchak and Tom Ouldridge.

More info: http://www2.warwick.ac.uk/fac/sci/wcpm/seminars

WCPM

Warwick Centre for Predictive Modelling