Nonequilibrium Molecular Dynamics Integrators Using Maple

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Abstract

The Conjugate Pairing Rule states that for Hamiltonian systems to which a Gaussian or Nosé-Hoover thermostat is applied, the spectrum of Lyapunov exponents should exhibit a simple symmetry: that the sum of conjugate pairs of exponents should be a constant independent of the pair index. This symmetry is important for it enables one to calculate the entropy production and thereby the nonequilibrium transport coefficient, by summing just two exponents, say the maximal exponents. However, the Conjugate Pairing Rule has never been proved for the standard computer simulation algorithm for shear flow namely the Sllod algorithm.

We use the symbolic algebra program, Maple, to examine the validity of the Conjugate Pairing Rule for the Sllod algorithm. We do this by using the multiple precision facility of Maple to carry out computer simulations for Sllod to very high accuracy. We also use the symbolic algebra capability of Maple to prove the Conjugate Pairing Rule for ideal gases subject to thermostatted shear flow and also for unthermostatted shear flow of fluids at arbitrary density.

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