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An invariant manifold of molecular dynamics and its relation to continuum mechanics

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Inhaltsangabe
We describe an invariant manifold of the equations of molecular dynamics associated with a given discrete group of isometries. It is a time-dependent manifold, but its dependence on time is explicit. In the case of the translation group, it has dimension 6N, where N is an assignable positive integer. The manifold is independent of the description of the atomic forces within a general framework. Most of continuum mechanics inherits some version of this manifold, as do theories in-between molecular dynamics and continuum mechanics, even though they do not inherit the time reversibility of molecular dynamics on this manifold.

The manifold implies a natural statistics of molecular motion, which suggests a simplifying ansatz for the Boltzmann equation which, in turn, leads to new explicit far-from-equilibrium solutions of this equation. In some way the manifold underlies experimental science, i.e., the viscometric flows of fluids and the bending and twisting of beams in solids and the procedures commonly used to measure constitutive relations, this being related to the fact that the form of the manifold can be prescribed independent of the atomic forces.