What Can We Learn from the Numerical Simulation of Far from Equilibrium Steady States?

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Linear constitutive relations such as Newton's law of viscosity, Fourier's law of heat conduction and Fick's law of diffusion relate thermodynamic forces to fluxes and hence provide the means for closing the partial differential equations describing the conservation of mass, momentum and energy in continuum mechanics. Numerical simulation, using non-equilibrium molecular dynamics (NEMD), provides a powerful means to study the realm of applicability of these constitutive relations, test new relations and formulating new ones. In the last few decades, NEMD has shown that Newton's law of viscosity requires generalizing to account for the non-local dependence of the stress on the strain rate for flowing fluids in highly confined geometries, while Fourier's law of heat conduction must be modified when describing heat flows through the centre of a stationary shockwave, to account for a time lag between the temperature gradient and the heat flux. Central to the success of these numerical discoveries has been the use of well-designed NEMD algorithms able to generate far from equilibrium states with simple boundary conditions. A new simulation algorithm has recently been introduced which enables the generation of Joule-Thomson states of a throttled fluid. The significance of this new method is that it uses simple equilibrium boundary conditions and does not require the use of artificial thermostats. In the main part of this presentation, we describe the algorithm for creating Joule-Thomson states, in both 2 and 3 physical dimensions for fluids using a number of different force laws. We examine the non-equilibrium steady states that are formed, explore the validity of the linear constitutive relations, demonstrate tensor temperature and examine the usefulness of configurational temperature. Simple extensions of the NEMD algorithm include the use of multiple 'porous plugs' to generate multiple Joule-Thomson states from a single simulation. These extensions will be discussed together with an analysis of the throttling process in which non-zero flow velocity can be properly accounted for, thus explaining the counterintuitive result of cooling in a gas governed by a purely repulsive force law.