Nonequilibrium Steady States: Theory and Simulation

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The world around us in a nonequilibrium state, and although nonequilibrium statistical mechanics has seen some advances over recent decades, there are many problems that are still intractable. Problems become particularly difficult when a system is inhomogeneous and evolving in time, but even for nonequilibrium steady state systems predictive theories are not always available. Using deterministic dynamics, the evolution of a phase space distribution from an initial equilibrium distribution can be rigorously obtained, but it is path dependent. This leads to complications in determining properties of steady state systems that are far from equilibrium.

An example of a nonequilibrium property of importance is the viscosity of complex non-Newtonian fluids undergoing shear flow. Nonequilibrium molecular dynamics simulations give us a way of predicting properties and understanding what happens at the molecular level in cases where theories currently do not exist – and in some cases this can lead to new theories. They might also provide equilibrium properties when the equilibrium state is not readily accessible or numerical errors are too high at equilibrium. In this talk I will discuss how we can proceed if a time-independent distribution function is unknown and also highlight the importance of nonequilibrium molecular dynamics simulations which can be used to model a range of systems . We also highlight some of the technical issues that need to be considered in carrying out this type of simulation.

References

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