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Optimal closure for nonequilibrium statistical models

This talk outlines an unconventional approach to nonequilibrium statistical mechanics that relies on statistical modeling and information theory. Given a deterministic microscopic dynamics, taken to be a Hamiltonian system with many degrees of freedom, and a macroscopic description, defined by a vector of relevant observables, the goal is to derive reduced equations for the mean macrostate from the microdynamics. To do so, this approach avoids the usual projection operator technique, or Mori-Zwanzig method. Instead, one constructs a parametric statistical model (or nonequilibrium ensemble) whose parameter vector is in one-to-one correspondence with the macrostate, and one chooses that path in the model's parameter space along which the rate of information loss is minimized. This optimal path is the best fit to the underlying dynamics within the imposed statistical model, as quantified by relative entropy (Kullback-Leibler divergence). The equations governing the optimal path are deduced by applying Hamilton-Jacobi theory to this classical optimization problem. These reduced equations have a nonequilibrium thermodynamic structure – they are "GENERIC"(=General Equations of NonEquilibrium Reversible Irreversible Coupling) in the sense of Grmela and Öttinger, or "metriplectic" in the terminology of Morrison.

This optimal closure has been applied to several test problems motivated by coarse-graining questions in hydrodynamics. Specifically, it has been implemented in a shell model, the spectrally-truncated Burgers equation, and two-dimensional inviscid flow. These tests show that it is capable of predicting relaxation rates toward statistical equilibrium without introducing tuned constants, and approximating linear response kernels without recourse to full auto-correlation data.