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Numerical master equation approach for complex transport processes[1] JANNE KAUTTONEN, JUHA MERIKOSKI, University of Jyvaskyla — Applicability of the numerical master equation analysis in studies of complex non-equilibrium systems is discussed. For small systems (up to $\sim 10^6$ states), solving of master equations directly is found very useful especially when studying parameter sensitive and elusive properties, such as drifts caused by the ratchet effect. Also various types of optimization methods can be applied. Efficient numerical methods for solving large master equation systems are discussed. Properties that can be readily computed include mean values and fluctuations of trajectory and state dependent observables, such as velocity, diffusion coefficient and shape deformations of the object. To further study the microscopic mechanisms of complex transport processes, we apply a graph optimization method to master equation sets. This allows one to identify the dominating processes that are responsible for the transport. We present detailed case studies for reptating polymers and metal-on-metal atomic islands in non-homogeneous potentials. These models represent complex many-particle systems with rich nonlinear behavior, such as inversions and increasing of velocity and large shape deformations in external potentials.

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