Curvature-based criteria for model reduction in chemical kinetics via optimization of trajectories

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The need for reduced chemical kinetics is motivated by the fact that the computational effort for a full simulation of reactive flows, e.g. of fluid transport involving combustion processes, is computationally extremely expensive. For a simulation in reasonable time reduced models of chemical kinetics are needed. In dissipative systems different time scales cause an anisotropic phase volume contraction behavior. Most common model reduction approaches in chemcial kinetics are explicitly based on multiple time scales and often assume and directly exploit a clear time scale separation into fast and slow reaction processes. In previous work we proposed an approach for the approximation of slow invariant manifolds by computing trajectories as solutions of an optimization problem with respect to their initial values. The slow invariant manifold is spanned by these solution trajectories. The objective functional for the identification of suitable trajectories in the optimization problem is supposed to represent the extent of relaxation of chemical forces along these trajectories. Various geometrically motivated ideas for the formulation of possible optimization criteria are discussed. They are compared to each other through three sample mechanisms: the Davis-Skodje problem, a simple hydrogen combustion mechanism, and a temperature-dependent ozone decomposition mechanism.