Model reduction in chemcical kinetics based on the optimization of trajectories

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Pursuing the ideas of Lebiedz [1], we present a general framework for the application of modern optimization techniques in model reduction. The underlying idea is a minimization of chemical forces along state trajectories subject to given constraints including the system dynamics and especially the choice of progress variables (by the fixation of initial values). Using this approach some remedies for common problems of other model reduction approaches can be found without having to use complicated extensions.
For instance for the formulation of the model reduction task as a variational boundary value problem highly sophisticated mathematical solution strategies exist, assuring high accuracy and fast convergence. Although the convergence properties can even be improved by the utilization of continuation strategies, good initial values as supplied by a continuation method are not mandatory for the successful solution of the underlying variational boundary value problem. On the contrary trajectory-based optimization approaches for model reduction can be applied for local species reconstruction due to their little dependence on initial values.
A drawback of model reduction techniques directly exploiting time-scale properties of the underlying ODE system is the requirement of clear time-scale separation. In domains where most processes are slow, e.g. the low temperature domain, this requirement demands an increase of the desired dimension. The optimization foundation of our approach avoids this problem, as the computation of an optimal solution to the underlying variatonal boundary value problem is always feasible, independent of the desired reduced dimension.
Underlining the applicability of trajectory-based optimization approaches in model reduction we present promising results for the construction of low-dimensional attracting manifolds of higher order in chemical kinetics.

References

[1] D. Lebiedz. Computing minimal entropy production trajectories: An approach to model reduction in chemical kinetics. *J. Chem. Phys.*, 120:6890 – 6897, 2004.