Adaptive Chemistry Computations of Reacting Flow

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Background

- Hydrocarbon kinetics exhibit significant complexity and stiffness
  - Need simplified non-stiff chemical models with specified accuracy
- The requisite chemical kinetic model complexity varies in space and time
  - Need adaptive local chemical model reduction
- Computational Singular Perturbation (CSP) analysis provides
  - formal means of chemical model analysis
  - means for identification of low-dimensional manifolds
  - and chemical model reduction
- CSP analysis is expensive
  - Discretize chemical state space into hypercubes
  - Tabulate and reuse CSP analysis results in visited hypercubes
  - Piecewise Reusable Implementation of Solution Mapping (PRISM)

Key Elements of the Adaptive Chemistry Strategy

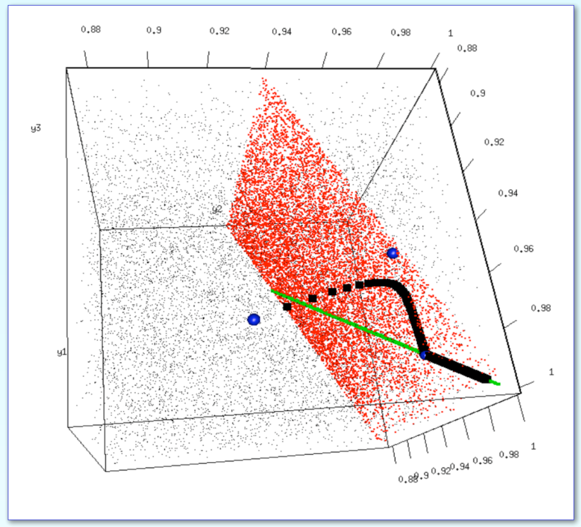
- Construct the state space tabulation a-priori and/or on the fly
  - Construct only those hypercubes visited by the solution state
  - Tabulate response surface fits for CSP quantities in each hypercube
  - Determine the size and dimensionality of each hypercube based on
    - the local manifold structure and quality of the response surface fit
- For a system with N species,
  - if, for a given chemical state, M modes are exhausted, then
  - the local hypercube dimensionality is only N-M.
  - Dimensionality reduction is key for efficient tabulation
- During time integration
  - Identify local hypercube
  - Use tabulated fits to evaluate CSP vectors and covectors
  - Use these to project the solution onto the manifold and
  - Integrate the resulting non-stiff source term efficiently

The CSP Homogeneous Correction

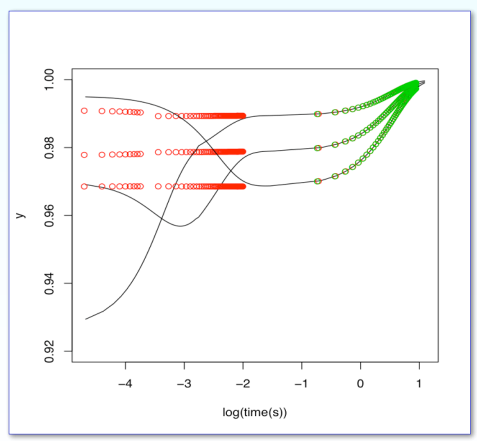
- Projects the solution along the fast directions towards the manifold
- Exhausts the fast processes with negligible effect on the slow processes
- Allows projection arbitrarily close to the manifold by repeated application
- Can be used to both
  - discover the manifold and
  - eliminate fast time scales and stiffness in time integration

Demonstration on a Model 3D Kinetic System

- Manifold identification and tabulation in a given hypercube
- Results highlight utility of tabulation with the CSP homogeneous correction
  - versus time integration of the original system
- Application to a H_2-O_2 system in progress



Model 3D kinetic system state space showing the 2D manifold for M=1 (red), and the 1D manifold for M=2 (green). Black squares denote the time integrated trajectory of the full system starting from the given initial condition.



Time integration starting from an arbitrary initial condition (black lines), after projection onto the 2D manifold (red), and onto the 1D manifold (green).

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