SAND2007-1817C

Paper # C31 **Topic: Kinetics**

5th US Combustion Meeting
Organized by the Western States Section of the Combustion Institute
and Hosted by the University of California at San Diego
March 25-28, 2007.

Efficient slow manifold identification for tabulation based adaptive chemistry

José M. Ortega[1], Habib Najm[1], Mauro Valorani[2], Dimitris Goussis[3] and Michael Frenklach[4]

[1]Sandia National Laboratories, Livermore, CA, USA
[2]Università di Roma “La Sapienza”, Rome, Italy,
[3]National Technical University of Athens, Greece,
[4]Univ. of California at Berkeley & LBNL, Berkeley CA, USA

OUTLINE OF PRESENTATION

① **Background**

- ➜ Computational Singular Perturbation (CSP) for Automatic Simplification/Reduction of Chemical Kinetics Systems
- ➜ Reusing CSP Information Through Tabulation

② **CSP Homogeneous Correction**

- ➜ Slow Invariant Manifold Dimension
- ➜ Identification of Active Species and CSP Radicals

③ **Homogeneous Correction for Adaptive tabulation**

- ➜ Partition of Chemical Composition Space
- ➜ Response Surfaces of CSP Quantities
- ➜ Construction of Local Slow Manifold Models

④ **Example: A 3-species kinetics Problem**

CSP ANALYSIS FOR MODEL REDUCTION/SIMPLIFICATION

① Addresses **wide range of time scales** in the dynamics of chemical kinetics systems

② **Automatic decomposition** of fast and slow dynamics

- ➜ Fast dynamics constrain the system evolution to a lower dimensional manifold. Irrelevant, Expensive, Difficult
- ➜ Slow dynamics drive the system along the manifold

③ Building a **reduced model** focusing on the subprocesses of the slow scales let us

- ➜ describe the system as a function of **fewer (active) species**
- ➜ integrate the **non-stiff system** with efficient **explicit** one-step algorithms

state vector Y

↓ Analytical Jacobian
Finite Differences, AD

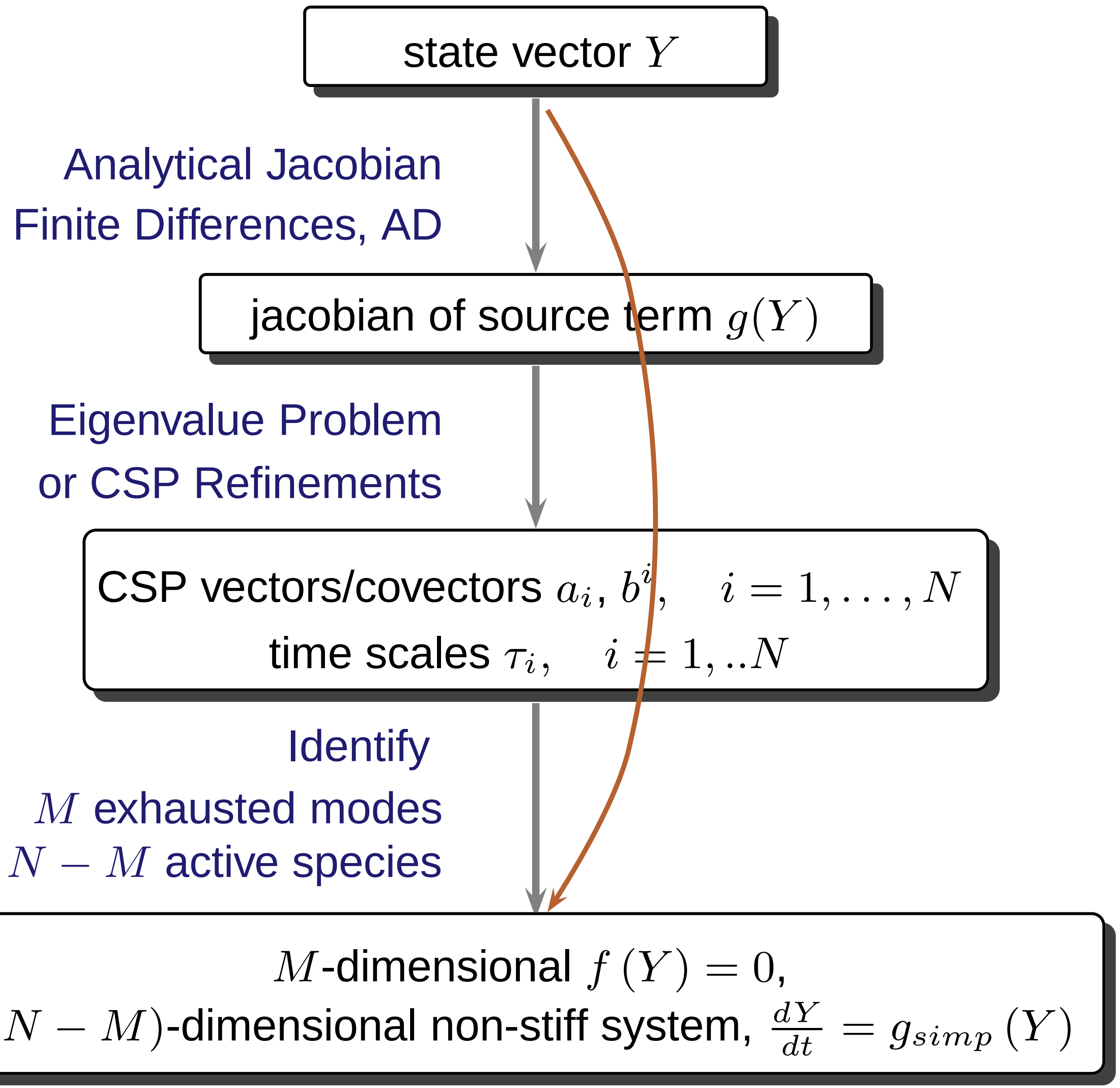
jacobian of source term $g(Y)$

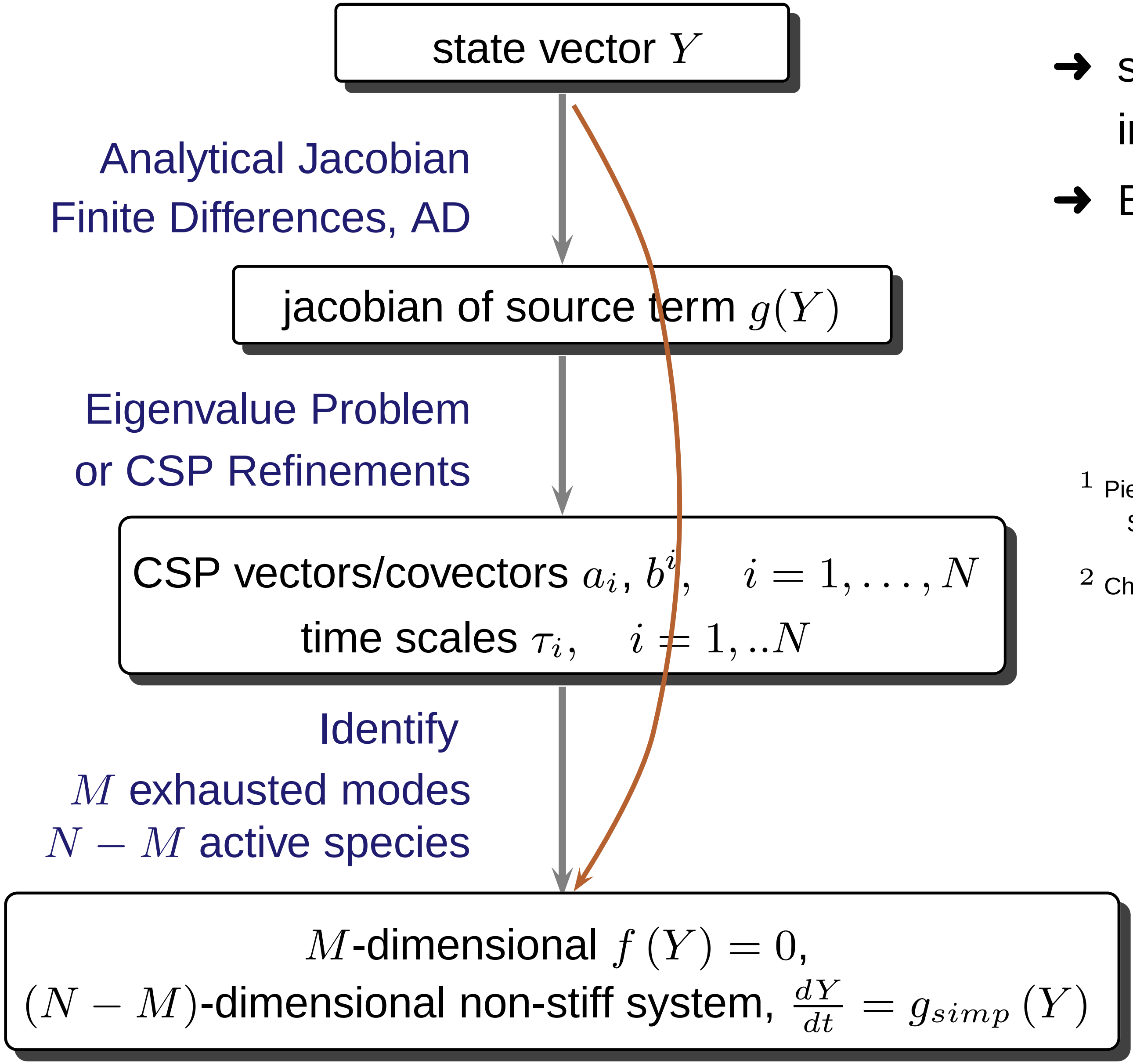
↓ Eigenvalue Problem
or CSP Refinements

CSP vectors/covectors a_i, b^i, $\quad i = 1, \ldots, N$
time scales τ_i, $\quad i = 1, ..N$

↓ Identify
M exhausted modes
$N - M$ active species

M-dimensional $f(Y) = 0$,
$(N - M)$-dimensional non-stiff system, $\frac{dY}{dt} = g_{simp}(Y)$


state vector Y
Analytical Jacobian
Finite Differences, AD
jacobian of source term $g(Y)$
Eigenvalue Problem
or CSP Refinements
CSP vectors/covectors a_i, b^i, $\quad i = 1, \ldots, N$
time scales τ_i, $\quad i = 1, ..N$
Identify
M exhausted modes
$N - M$ active species
M-dimensional $f(Y) = 0$,
$(N - M)$-dimensional non-stiff system, $\frac{dY}{dt} = g_{simp}(Y)$



- ➜ store and reuse CSP information
- ➜ Based on PRISM[1]
  - local response surfaces
  - hypercubes in CCS[2]

[1] Piecewise Reusable Implementation of Solution Mapping

[2] Chemical Composition Space

REUSE STRATEGY

based on the ability to store basic information from CSP analysis and retrieve it when needed without expensive computations :

tabulate the CSP basis vectors/covectors using local –low-order– polynomial response surfaces of the first M

① vectors $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_M$ and

② covectors $\mathbf{b}^1, \mathbf{b}^2, \ldots, \mathbf{b}^M$

as a function of the $N - M$ active species

Equations of State $Y_M = f\left(Y_{N-M}\right)$

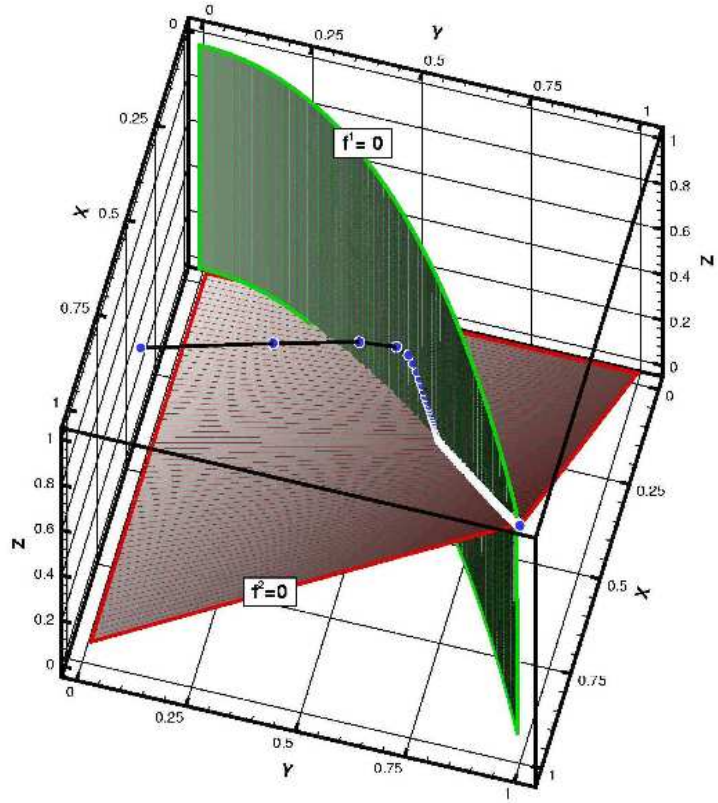
Non Stiff Model $\frac{dY}{dt} = \left(\mathbf{I}_N - \sum_{r=1}^{r=M} a_r b^r\right) \times g(Y)$

Main Challenges during table construction

① identification of the $N - M$ active species and M CSP radicals

② identification of $(N - M)$ dimensional manifold surfaces in a N-dimensional space

③ optimal size of hypercubes for accurate local response surfaces of the CSP quantities



Computing trajectories to identify the manifolds is very expensive

THE CSP "HOMOGENEOUS CORRECTION"

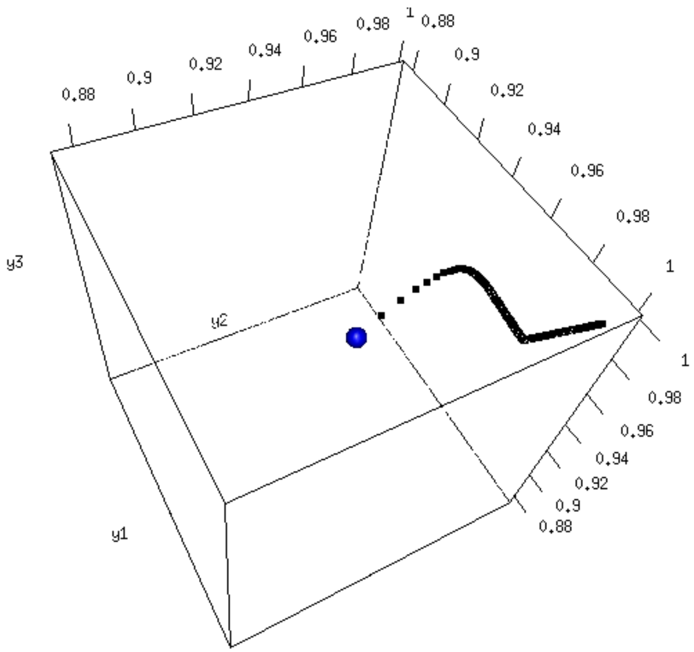
brings the state vector $\mathbf{y}$ arbitrarily close to an $(N-M)$-dimensional manifold where M fast scales exist

$$\delta\mathbf{y} = -\sum_{m,n=1}^{M} \mathbf{a}_m \tau_n^m f^n$$

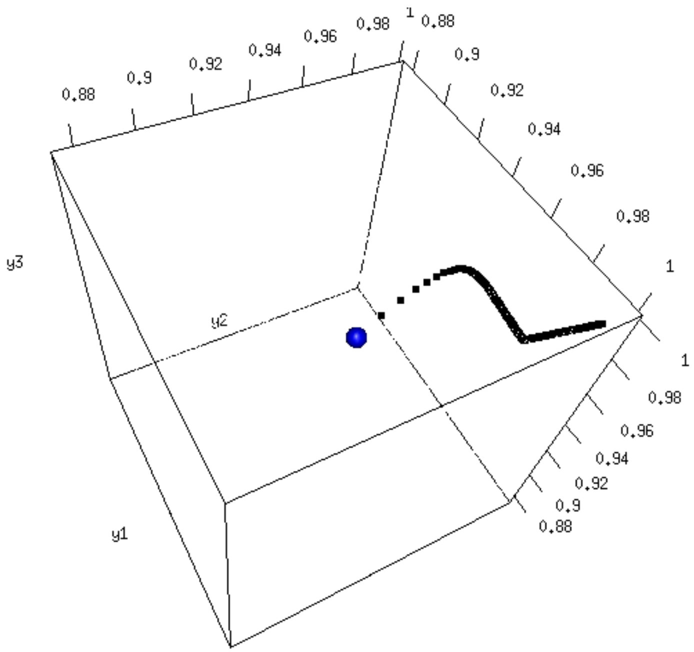
where

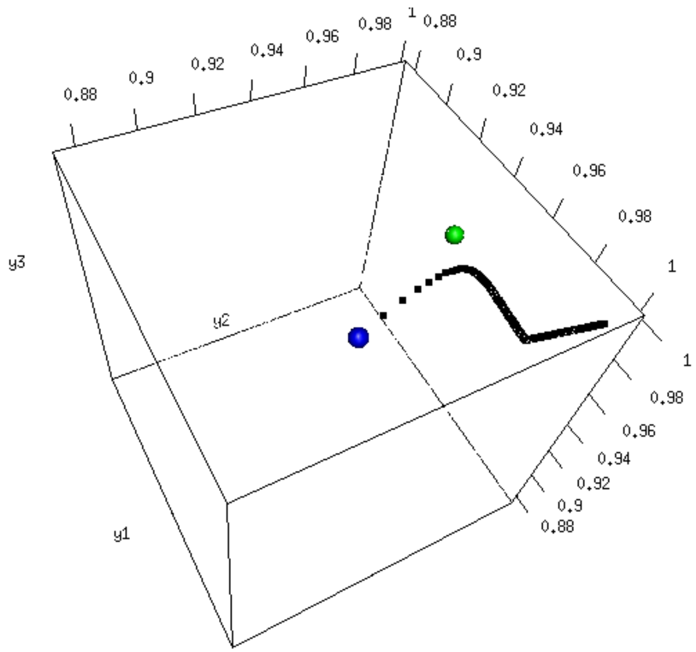
- ➜ $\{f^n = \mathbf{b}^n \cdot \mathbf{g}\}_{n=1}^{M}$, non-vanished fast mode amplitudes
- ➜ $\mathbf{g}$, right hand side (RHS) of ODE
- ➜ $\mathbf{J}$, jacobian of RHS
- ➜ τ_n^m, inverse of λ_n^m

$$\lambda_j^i = \left(\frac{d\mathbf{b}^i}{dt} + \mathbf{b^i J}\right)\mathbf{a}_j$$

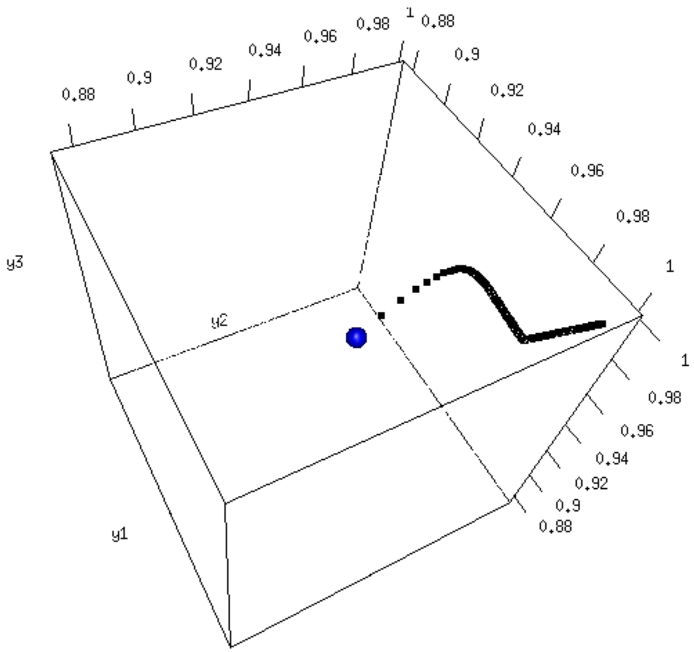

0.88
0.9
0.92
0.94
0.96
0.98
1
0.88
0.9
0.92
0.94
0.96
0.98
1
1
0.98
0.96
0.94
0.92
0.9
0.88
y3
y2
y1

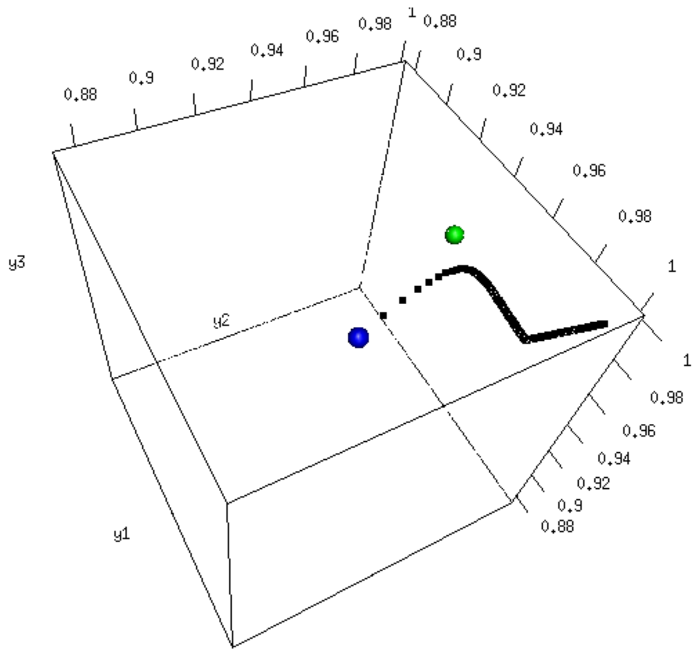
Homogeneous Correction Computed with $M = 1$





Homogeneous Correction Computed with $M = 1$

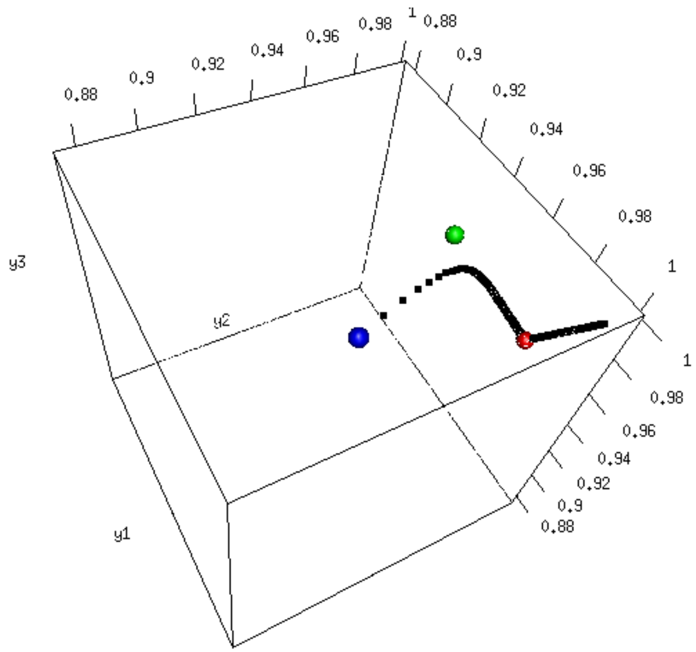




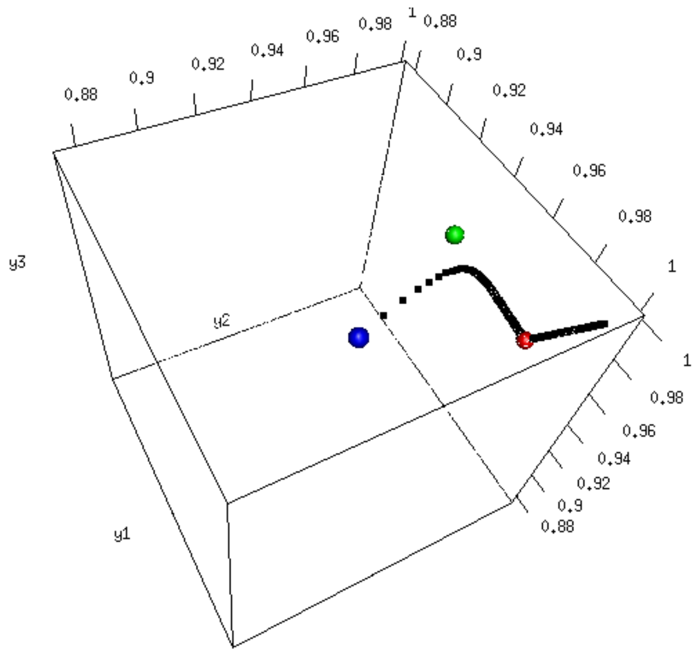
$M = 1$	y_1	y_2	y_3	dy_1/y_1	dy_2/y_2	dy_3/y_3	f^1
Initial	0.97003	0.92696	0.99514				-128.35270
1 HC	0.94726	0.97593	0.99401	0.02346	-0.05283	0.00113	2.41797
2 HC	0.94768	0.97504	0.99403	-0.00044	0.00091	-0.00002	0.00454

$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_1 f^1 + \mathbf{a}_2 f^2 + \mathbf{a}_3 f^3$$

Homogeneous Correction Computed with $M = 2$



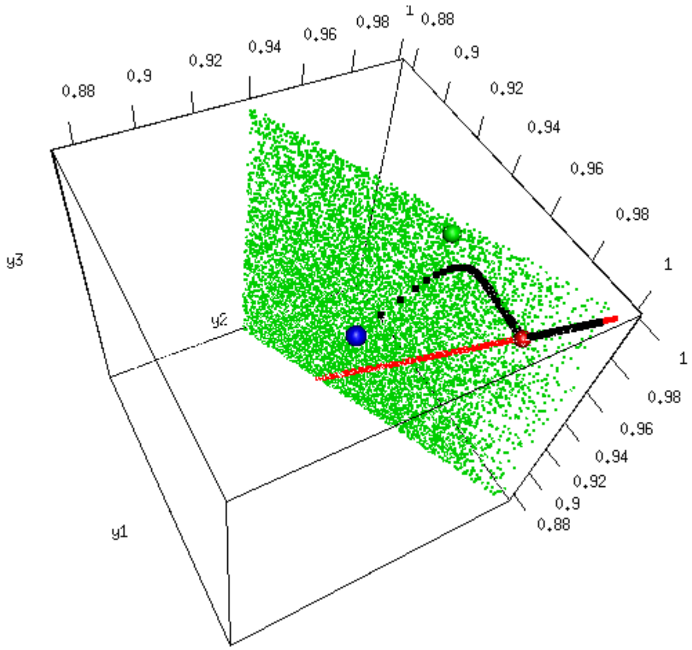
Homogeneous Correction Computed with $M = 2$



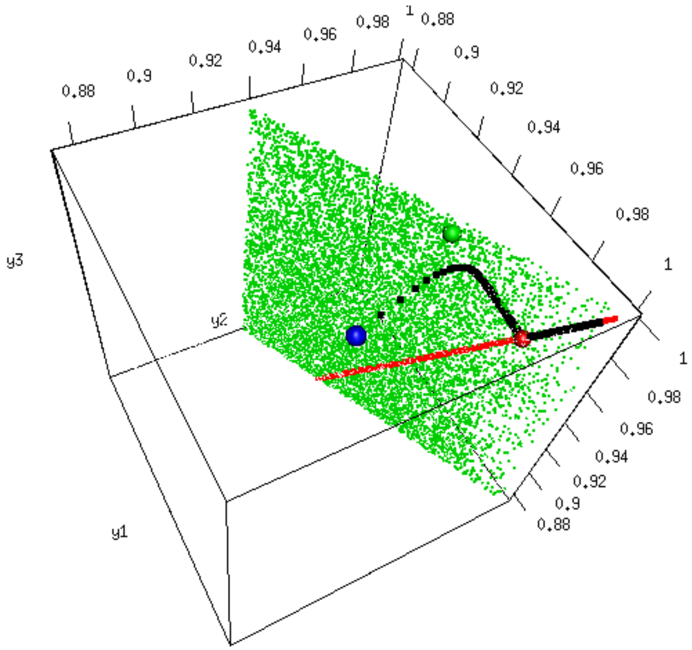
$M = 2$	y_1	y_2	y_3	dy_1/y_1	dy_2/y_2	dy_3/y_3	f^1	f^2
Initial	0.97003	0.92696	0.99514				-128.35269	-11.47343
1 HC	0.97782	0.99093	0.96854	-0.00804	-0.06901	0.02673	4.59536	-0.06144
2 HC	0.97876	0.98934	0.96844	-0.00096	0.00160	0.00010	0.00275	-0.00033

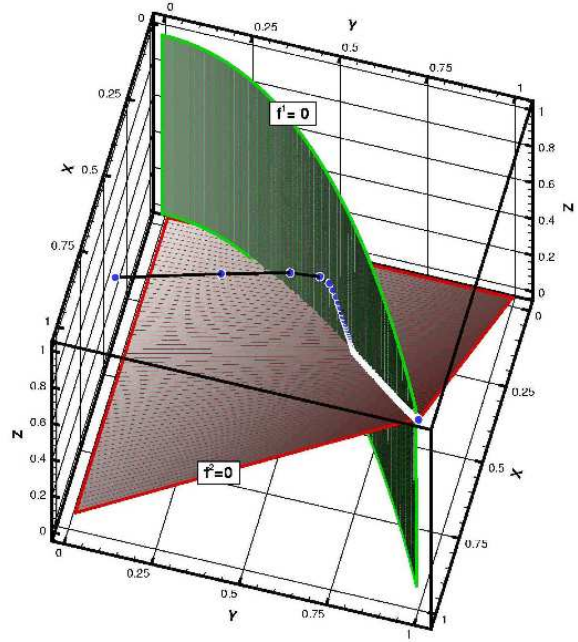
$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_1 f^1 + \mathbf{a}_2 f^2 + \mathbf{a}_3 f^3$$

Manifold surfaces for $M = 1$ and $M = 2$

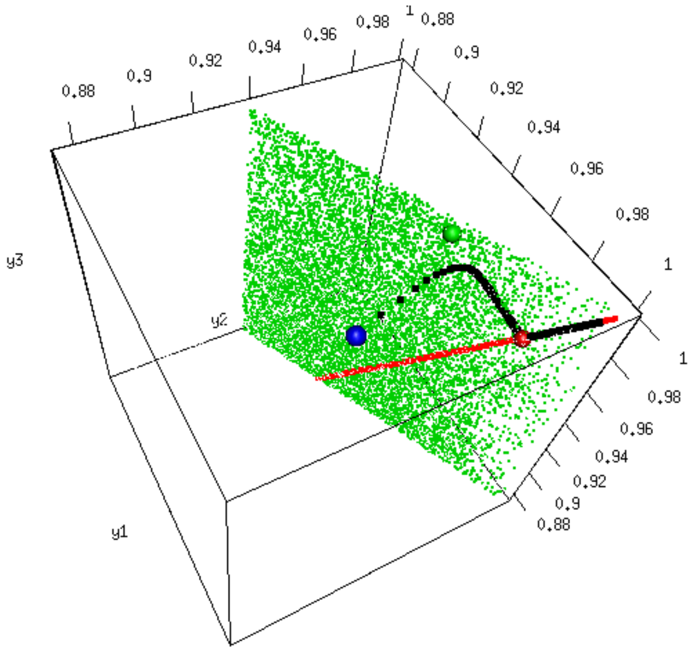


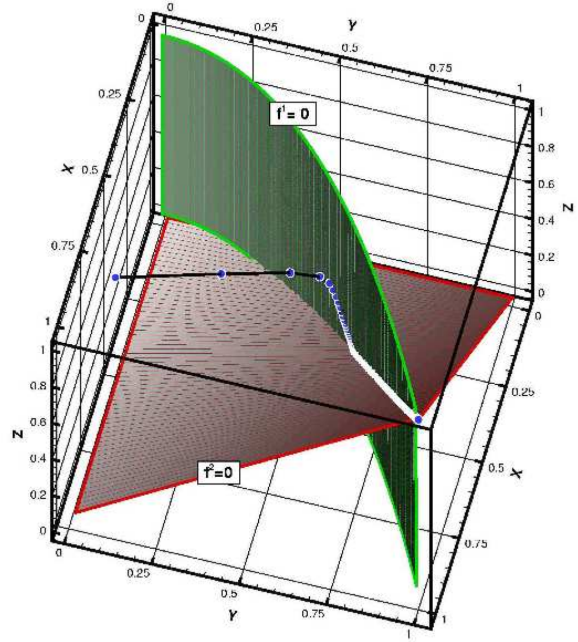
Manifold surfaces for $M = 1$ and $M = 2$





Manifold surfaces for $M = 1$ and $M = 2$





	Q_{m11}	Q_{m22}	Q_{m33}
$M = 1$	0.18	0.82	7.4E-04
$M = 2$	0.36	0.46	0.17

$\Rightarrow$ CSP Radicals $\{y_2\}$

$\Rightarrow$ CSP Radicals $\{y_2, y_1\}$

Using the Homogeneous correction for adaptive tabulation

Optimization Problem

Maximize model reduction $M = argmax\ M^*$

Maximize size of hypercube $S = argmax\ S^*$

subject to

- ➜ $S^* \in \{S_1, S_2, S_3, \ldots, S_n\}$, where $S_1 > S_2 > \ldots S_{n-1} > S_n$
- ➜ $0 < M^* < N$
- ➜ Identical M^* CSP radical pointers and $N - M^*$ active species.
- ➜ Corrections computed with M^* do NOT take the state vector outside the hypercube
- ➜ After $n \leq 2$ corrections amplitudes vanish $f \approx 0$, and CSP tolerance errors are met
- ➜ goodness-of-fit statistics $\chi^2 < \chi^2_{max}$ for low order polynomial model of $\mathbf{a_i}$ and $\mathbf{b^i}$, $i = 1, \ldots, M^*$ w.r.t. $N - M^*$ active species.

Initialization

- Initial Hypercube $\{0, 0, 0\}$, $S = 1$
- Hypercube Sizes: $S = [1, \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}]$
- Goodness-of-fit statistics threshold $\chi^2 < 0.01$

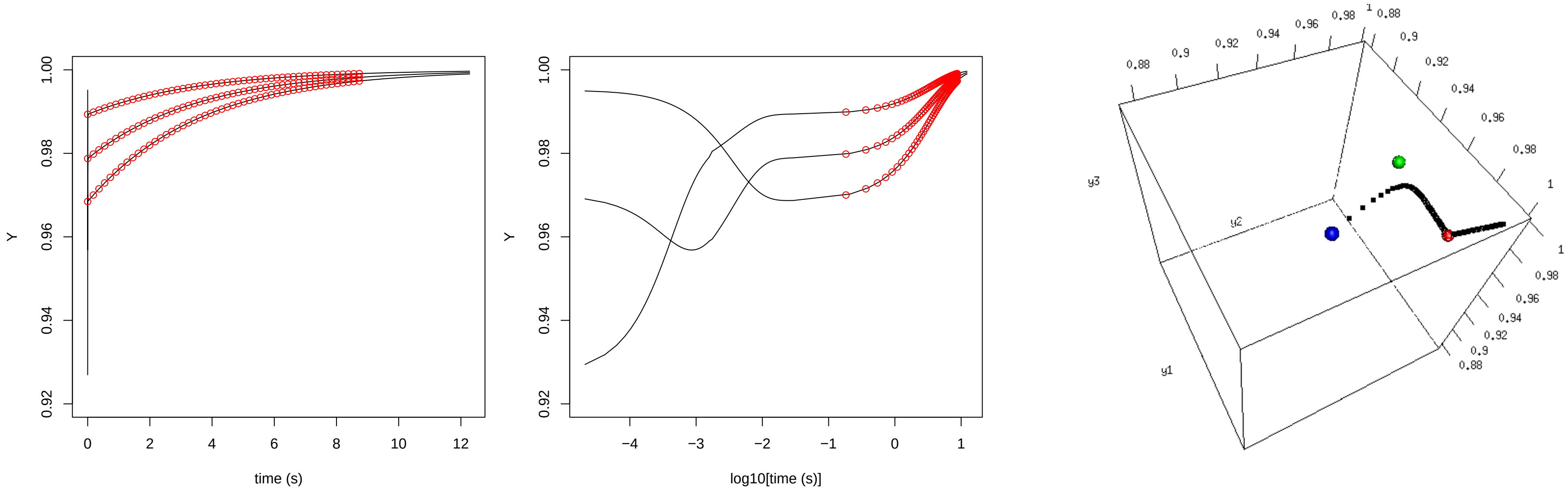
Generated Table Entry

- Hypercube: $\{0.875, 0.875, 0.875\}$, $S = 1/8$
- Number of fast and exhausted time scales $M = 2$
- Active species $Y_{N-M} = \{y_3\}$
- CSP radicals $Y_M = \{y_1, y_2\}$
- Response surface polynomial

$$\left[\ \mathbf{a_1}^T \, \mathbf{a_2}^T \, \mathbf{b}^1 \, \mathbf{b}^2 \ \right]^T = \Theta \mathbf{X}$$

$$\mathbf{X} = [1 \ \log(y_3) \ (\log(y_3))^2]^T$$

After 2 homogeneous corrections:



- ➜ maximum error < 0.2 %
- ➜ time integration step $O(3.8)$ seconds
- ➜ Computational cost comparison:
  0.550 ms (full CSP) vs 40 ms (Tabulated CSP)

CONCLUSIONS

- ➜ The CSP homogeneous correction provides an efficient way to identify an SIM
- ➜ No need to resort to expensive trajectory calculations
- ➜ An effective dimensionality reduction is obtained ($N - M$ major species)
- ➜ Significant CPU savings can be achieved by skipping the fast dynamics and tabulating the CSP information