SAND2011-5198C

Computational Singular Perturbation with Non-Parametric Tabulation of Slow Manifolds for Time Integration of Stiff Chemical Kinetics

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Supported by the US Department of Energy, Office of Basic Energy Sciences, SciDAC Computational Chemistry program

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Overview

- Introduction and motivation
- Computational Singular Perturbation
- Tabulation to improve computational efficiency
- Application to CH_4 ignition
  - Accuracy
  - Performance
- Conclusions and ongoing work

Reduction of chemical models needs to address both size and stiffness in an automated, efficient way

- Time integration of detailed kinetics is expensive
  - Large systems
  - Stiffness due to wide range of time scales
- Computational Singular Perturbation (CSP) analysis decouples fast and slow dynamics
  - Computation of fast dynamics is *expensive*; may be *irrelevant*
  - Fast dynamics constrain the system to lower-dimensional *slow manifolds*
  - Evolution along a CSP manifold is driven by slow dynamics
- How to do this **efficiently** and in **high-dimensional** state spaces?
  - CSP analysis is expensive; need to *re-use* relevant information
  - Goal: automated analysis of large kinetic models, typical of complex and realistic fuels

CSP projects the source term onto new basis vectors to decompose fast and slow components

- Decomposition of the source term:

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}) = \underbrace{\sum_{r=1}^{M} \mathbf{a}_r f^r}_{\text{fast}} + \underbrace{\sum_{s=M+1}^{N} \mathbf{a}_s f^s}_{\text{slow}}$$

  – New basis vectors **a** determined from eigenvalue analysis of the Jacobian

- Exhausted/Fast modes: largest *M* such that

$$\left| \tau_{M+1} \sum_{r=1}^{M} \mathbf{a}_r f^r \right| < \mathbf{y}_{error}$$

- $f^r \approx 0, r = 1..M$ describes slow manifold

Lam, Comb. Sci. Tech, 1993

The CSP integrator moves the system along the slow manifold

- After exhaustion of M fast modes: non-stiff reduced model:

$$\frac{d\mathbf{y}}{dt} \approx \underbrace{\sum_{s=M+1}^{N} \mathbf{a}_s f^s}_{\text{slow}} = \mathbf{Pg}$$

- Explicit *time-scale* splitting:

  – Slow dynamics along the manifold $\mathbf{y}(T+\Delta t) = \mathbf{y}(T) + \int_T^{T+\Delta t} \mathbf{Pg}\, dt$

  – Homogeneous correction (HC) to remain on manifold

$$\mathbf{y}(T+\Delta t) = \tilde{\mathbf{y}}(T+\Delta t) - \sum_{r,r'=1}^{M} \mathbf{a}_r \tau_{r'}^{r} f^{r'}$$

  (τ_m^n *are entries of* $\mathrm{T} = \Lambda^{-1}$)

  – This elimination of fast time scales allows the use of explicit time integrators

Valorani, Goussis, J. Comp. Phys, 2001

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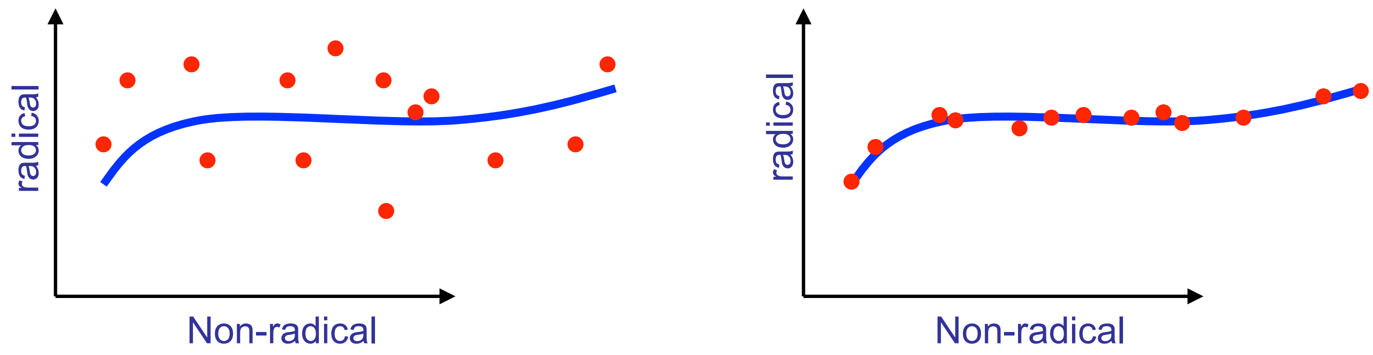
Tabulation allows re-use of CSP quantities to improve the efficiency of the CSP integrator

- Tabulate the information sufficient to assemble the slow-manifold projectors P and the homogeneous correction
  - Local M
  - CSP radicals
  - *Fast* CSP vectors/covectors; and timescales $\tau_{1:M+1}$
- Tabulation in a reduced dimension state space
  - These quantities depend on the *N - M* ***non-radical species***
  - No need to tabulate or search in the full *N*-dimensional space
- Other desirable features
  - Adaptivity…
  - Scalability…
  - Support “online” learning…

Table design points are obtained by sampling the configuration space

- Generate a set of initial conditions by sampling key parameters of the reacting system
  - T
  - φ
  - Dilution (extra mol N_2 per mol air)
- Run the detailed simulation for each initial condition
- Collect relevant snapshots in time as samples of the configuration space
  - Discard runs that do not ignite
  - Only collect configurations that are sufficiently different from previously saved conditions

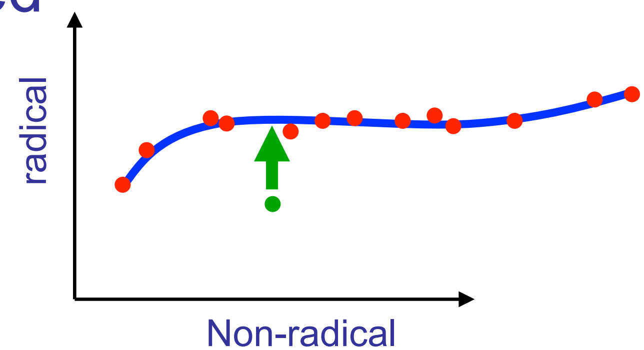
Successive homogeneous corrections from sampled conditions discover points on slow manifolds



- For each sampled state space condition
  - Get number of exhausted modes M from CSP analysis
  - Perform homogeneous corrections onto manifold
  - Repeat until norm of fast modes sufficiently small
- Gather points that are on same manifold

In forward integration, manifold CSP information approximated with local regression

- Storage in kd-trees for efficient storage and queries
  - Very flexible. No assumed spatial partitioning
  - Efficient nearest-neighbor (NN) or *k*-nearest-neighbor (*k*-NN) queries in ***N - M*** dimensions
- Coordinates scaled to range from 0 to 1 in all dimensions
  - Gives equal relative weight to deviations in all state space coordinates
- Use local interpolation between tabulated points near current condition
  - Currently *nearest-neighbor* interpolation
    - Over all manifolds
    - Subject to limit d_{Max} on distance
  - Easily extended to smoother interpolants via k-NN queries
- Use full CSP when table has no appropriate entry



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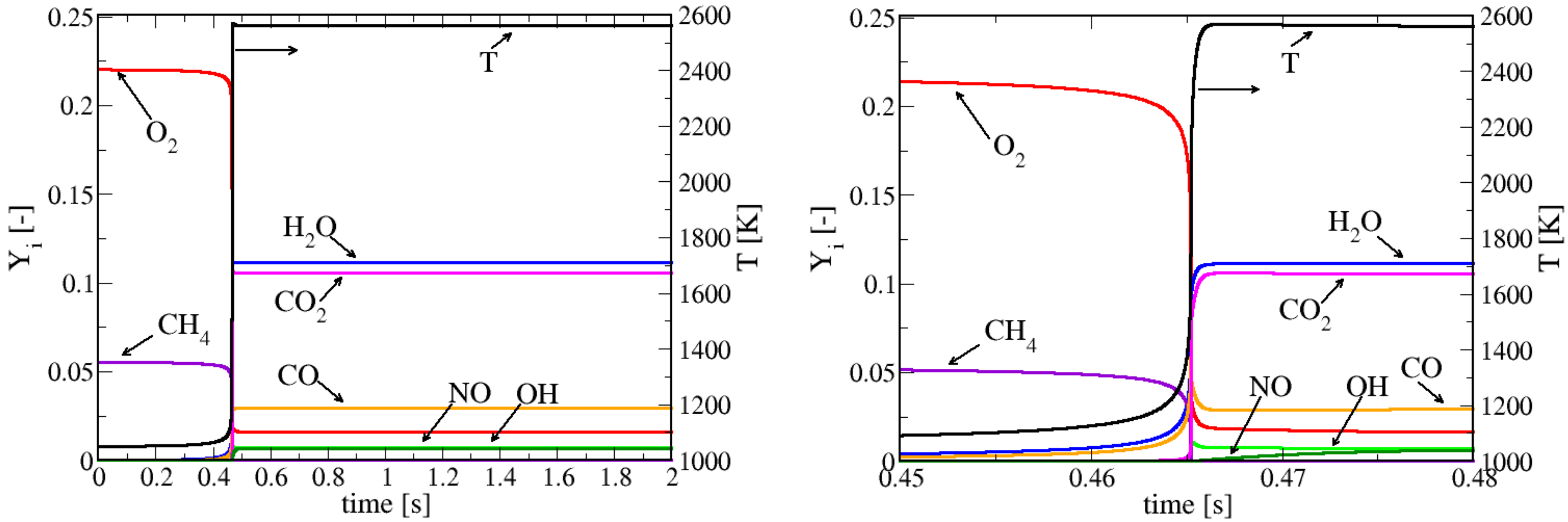
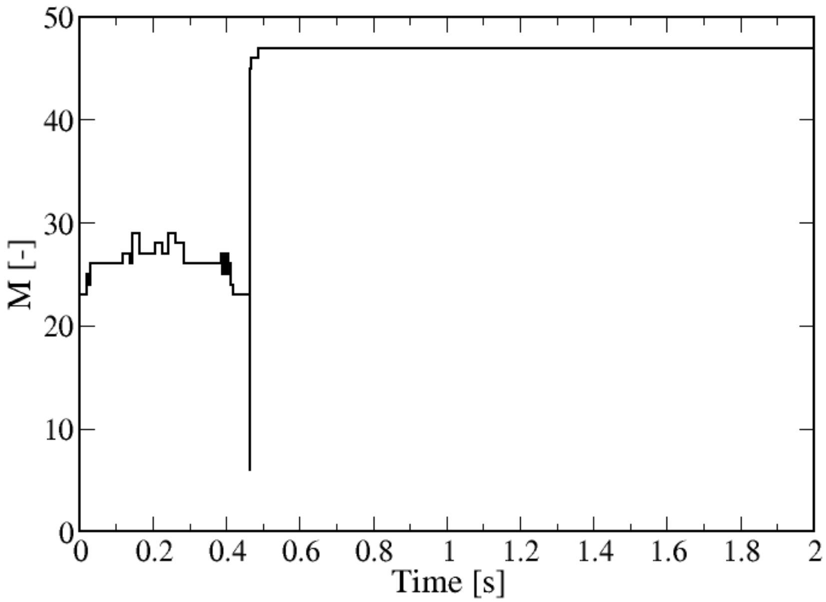
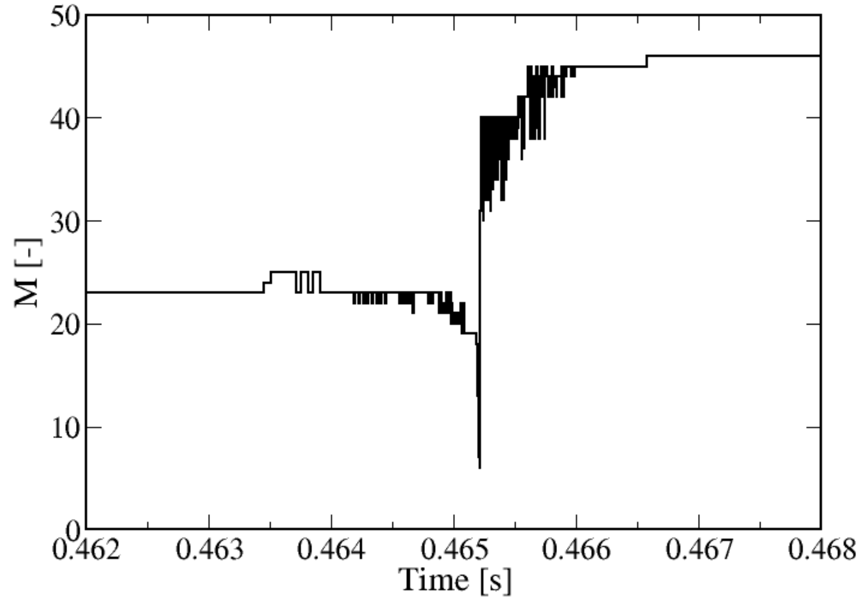
Application to CH_4-air ignition



- GRI 3.0
- N = 54 (53 species + T), 325 reactions
- Nominal initial conditions:
  - T_0 = 1050K, stoichiometric
  - No N_2 dilution, 1 atm

Large number of exhausted modes offers large potential for stiffness reduction





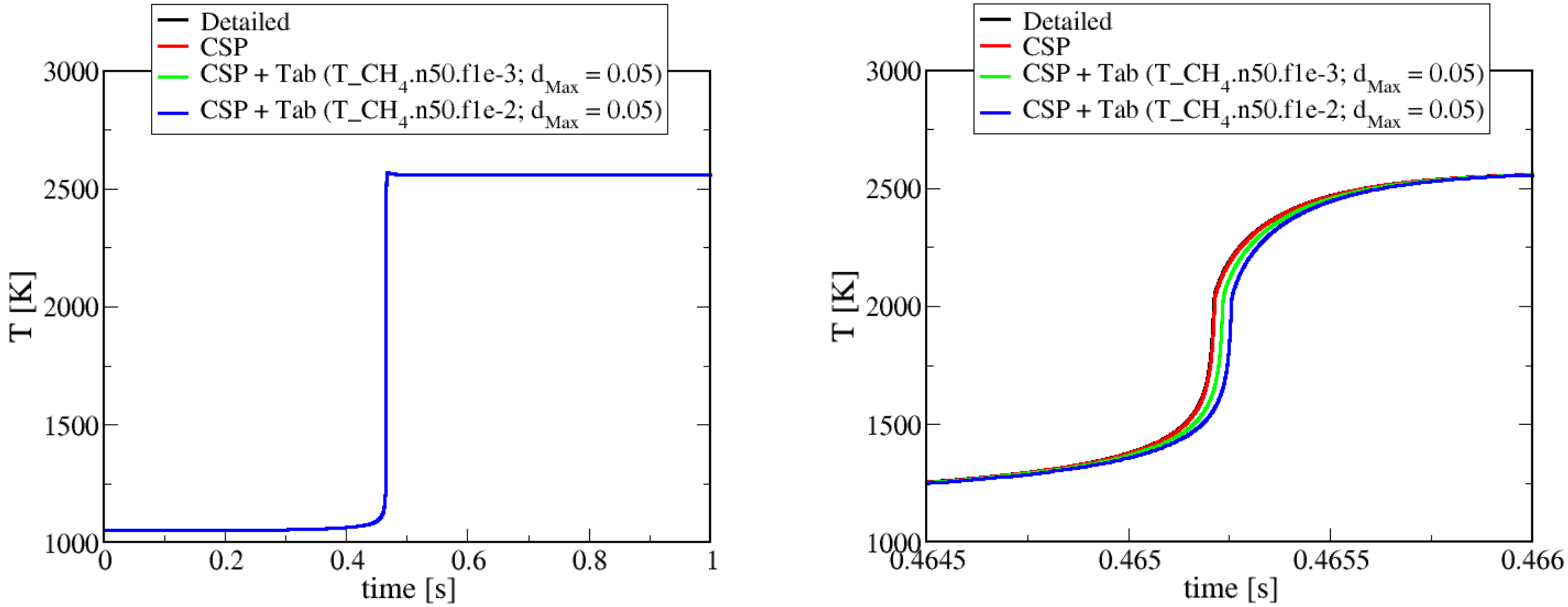
- Minimum number of exhausted modes about 4
- As many as 47 exhausted modes
  - only 7 dimensional table needed in those areas
  - Significant stiffness reduction enables explicit integration with time step on the order of slowest active time scale

Multiple tables with varying density were constructed from sampled detailed chemistry ignition simulations

Table	n_ϕ	# Manifolds	M_{min}	M_{max}	# points
T_CH_4.n50.f1e-2	50	60	4	47	14895
T_CH_4.n50.f5e-3	50	61	4	47	299228
T_CH_4.n50.f1e-3	50	69	4	47	125948
T_CH_4.n100.f1e-2	100	60	4	47	29791
T_CH_4.n100.f5e-3	100	65	4	47	58451

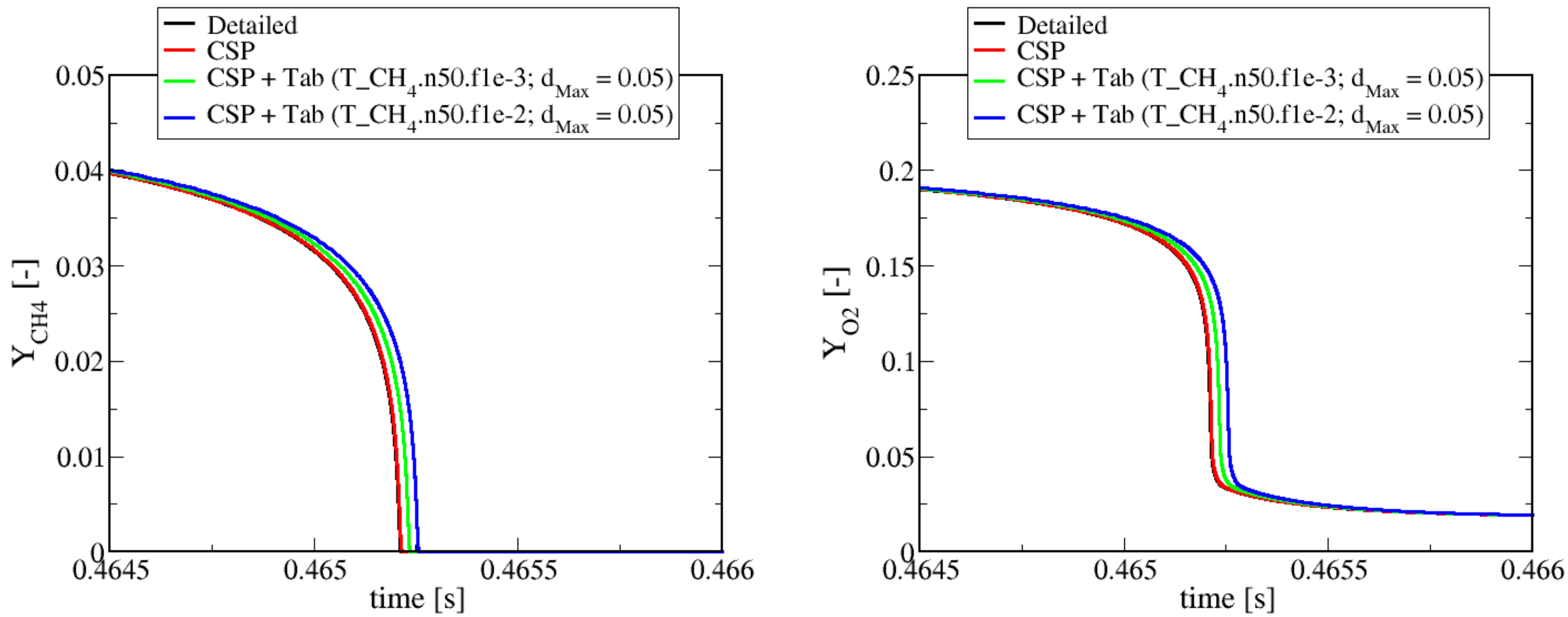
- Initial conditions sampled on uniform grid:
  - Φ ranging from 0.95 to 1.05
- Two sets of tables with varying density, sampled from 50 or 100 detailed chemistry trajectories
- Number of exhausted modes ranging from 4 to 47
- Table storage ranging from 289MB to 2.4GB

The CSP integrator approximates the detailed kinetics solution well



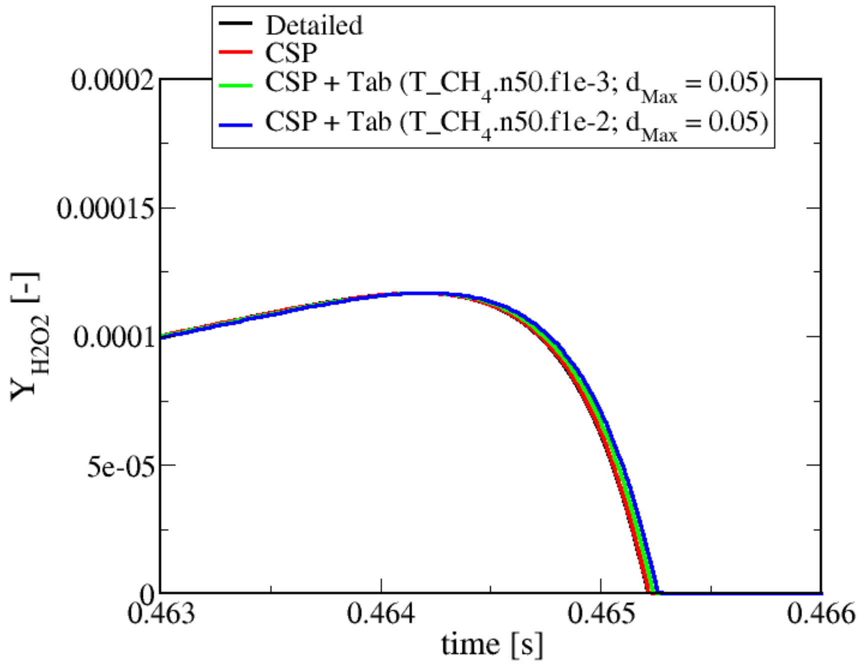
- Tabulation based on 50 design trajectories
- T profiles nearly identical, shifted by small error in ignition time
  - CSP without tabulation nearly on top of detailed chemistry
  - CSP with tabulation ignition time errors less than 5×10^{-5}s

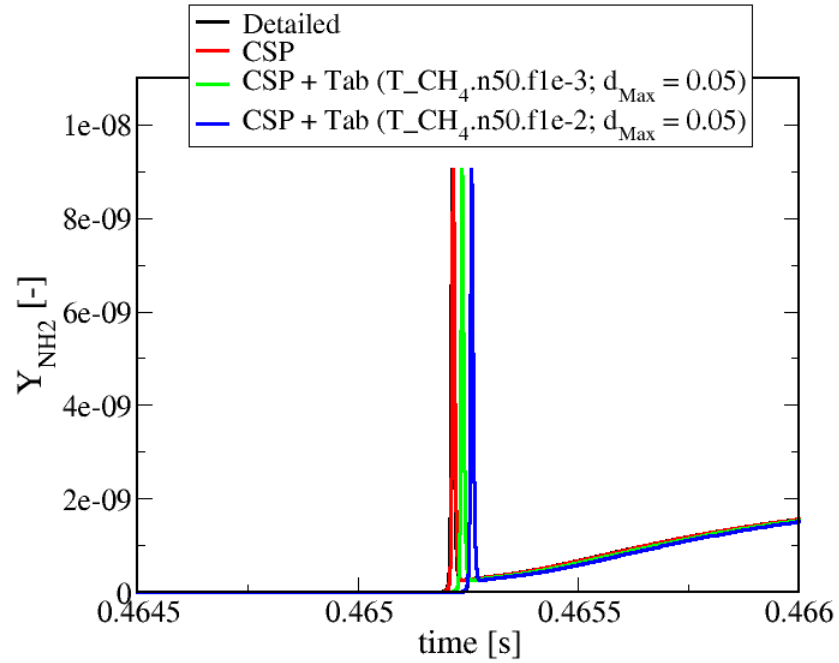
Other species equally well approximated



- CSP approximations shift CH_4 and O_2 profiles by small error in ignition time

Good accuracy is achieved for trace species as well





- Similar small shift in H_2O_2 and NH_2 profiles as before
- Magnitudes of trace species mass fractions accurately predicted

The accuracy of the CSP approximations is computed relative to the detailed chemistry

- Relative error in ignition time

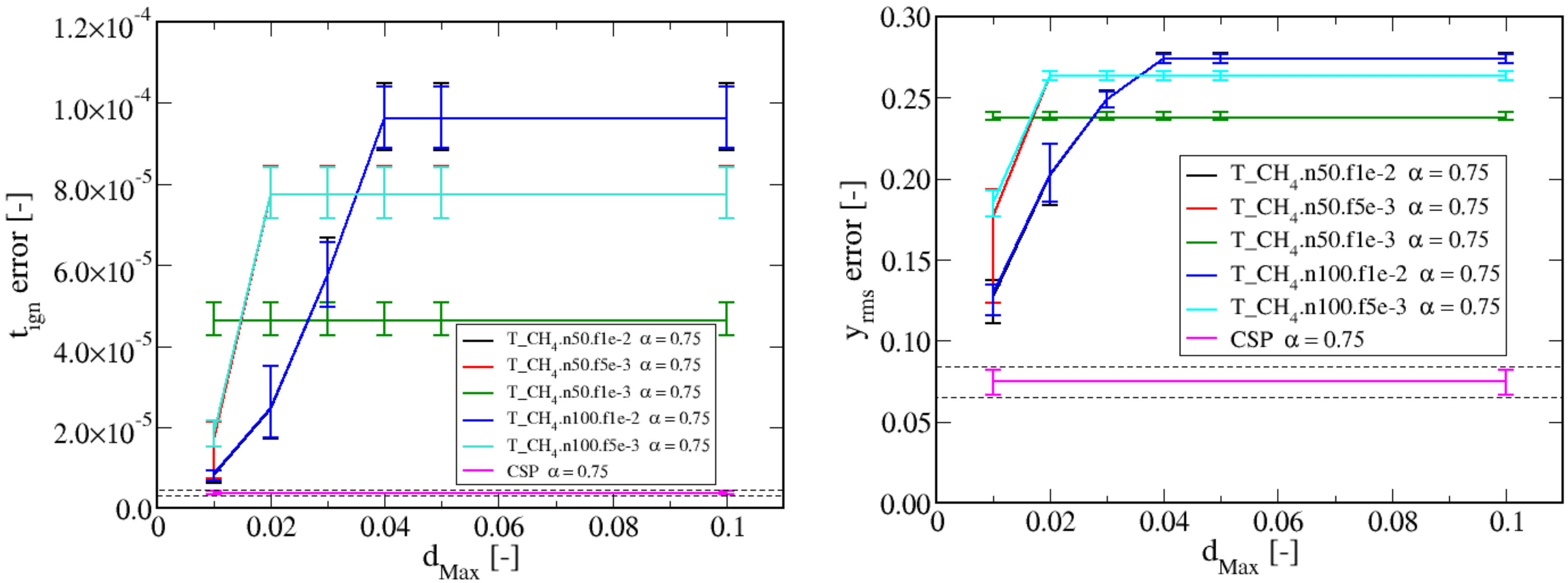
$$t_{\text{ign}} = t\left(T_{\text{ini}} + 0.5\left(T_{\text{final}} - T_{\text{ini}}\right)\right)$$

$$\varepsilon_{t_{\text{ign}}} = \frac{\left|t_{\text{ign}}^{\text{CSP}} - t_{\text{ign}}^{\text{det}}\right|}{t_{\text{ign}}^{\text{det}}}$$

- Scaled RMS error over all species and time points

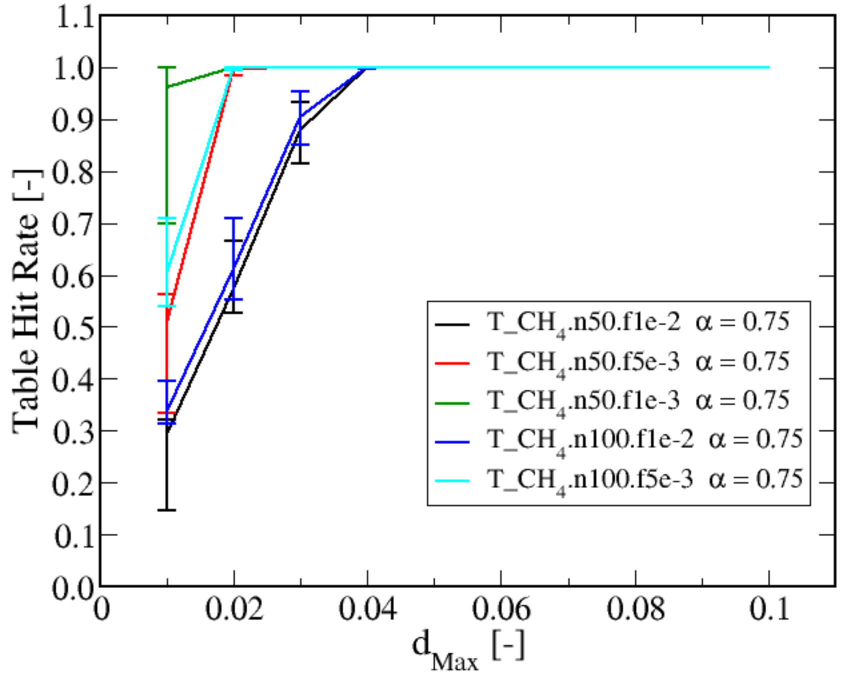
$$\varepsilon_{\text{RMS}} = \sqrt{\frac{1}{N_t N} \sum_{i=1}^{N} \sum_{j=1}^{N_t} \frac{\left(y_i^{\text{CSP}}\left(t_j\right) - y_i^{\text{det}}\left(t_j\right)\right)^2}{\left(\Delta y_i\right)^2}}$$

Accuracy decreases with increasing limit on distance to nearest neighbor



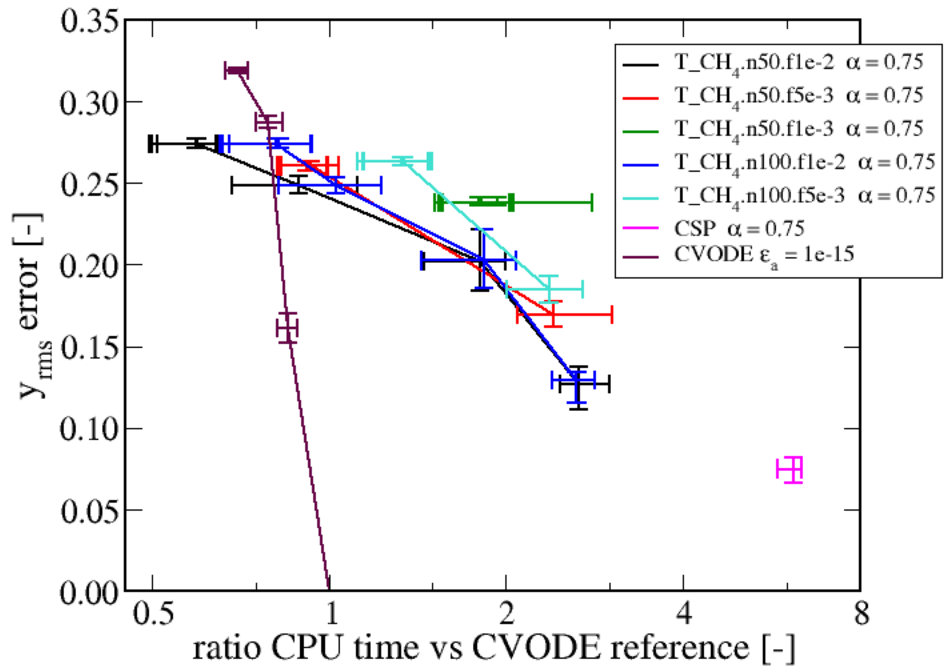
- Averaged over 100 conditions, randomly sampled from same range as initial table design points
- Error insensitive to d_{Max} for large d_{Max}
- Number of samples along time trajectories more important for accuracy than number of design point trajectories

Table usage increases with limit on distance to nearest neighbor



- Usage measured by ratio of table hits over total number of table lookups
- For small d_{Max}, table usage drops dramatically, unless table sufficiently dense
- Averaged over 100 conditions sampled from same range as initial table design points

CPU time performance relative to implicit integration of detailed kinetics



- Objective CPU time comparison by making CVODE integrate between same time points as CSP
  - Representative of comparing either CVODE or CSP for chemical source term in operator split scheme for reacting flows
- CSP with tabulation 10 times faster than regular CSP and up to 40% faster than CVODE

Conclusions and ongoing work

- CSP integrator provides good accuracy while reducing stiffness
- Tabulation is needed to reduce its computational cost
  - Effective dimensionality reduction (*N* - *M* non-radical species)
  - Nonparametric representation of each manifold; tree-based nearest-neighbor queries for local regression
  - Tabulation factor 10 faster than regular CSP for CH_4
- CSP integrator with tabulation competitive with implicit time integrator for complex chemistries
  - up to 40% faster than CVODE for CH_4
- Ongoing work:
  - Relationship between distance in table and accuracy
  - Performance testing on more complex systems
  - On-the-fly nonparametric table construction with effective table resolution control
  - Extension to reacting flows

Extra material

Model Problem example: 3-species kinetic system

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$

$$\frac{d\mathbf{y}}{dt} = \mathbf{g} = \begin{bmatrix} -\frac{5\,y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} + y_2 y_3 + \frac{5\,y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} - y_1 \\ 10\frac{y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - 10\frac{y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} + y_1 \\ \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - \frac{y_3}{\varepsilon} + y_1 \end{bmatrix}$$

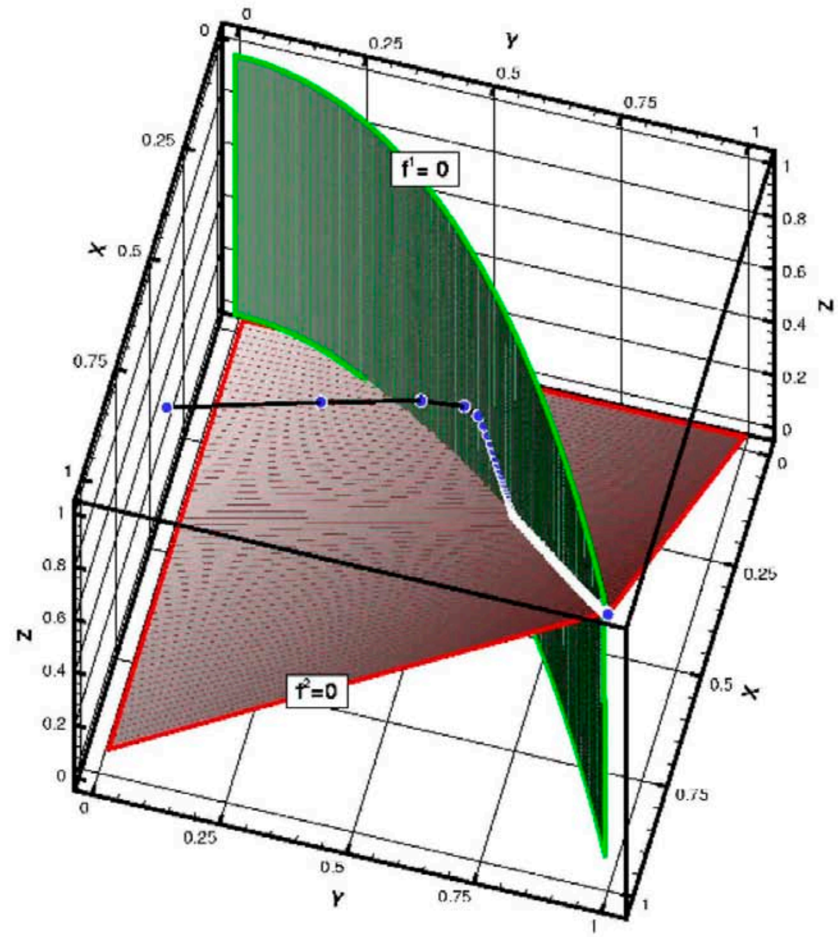
$\varepsilon \ll 1$ controls stiffness

- Project states onto the manifold using iterated applications of the homogeneous correction

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

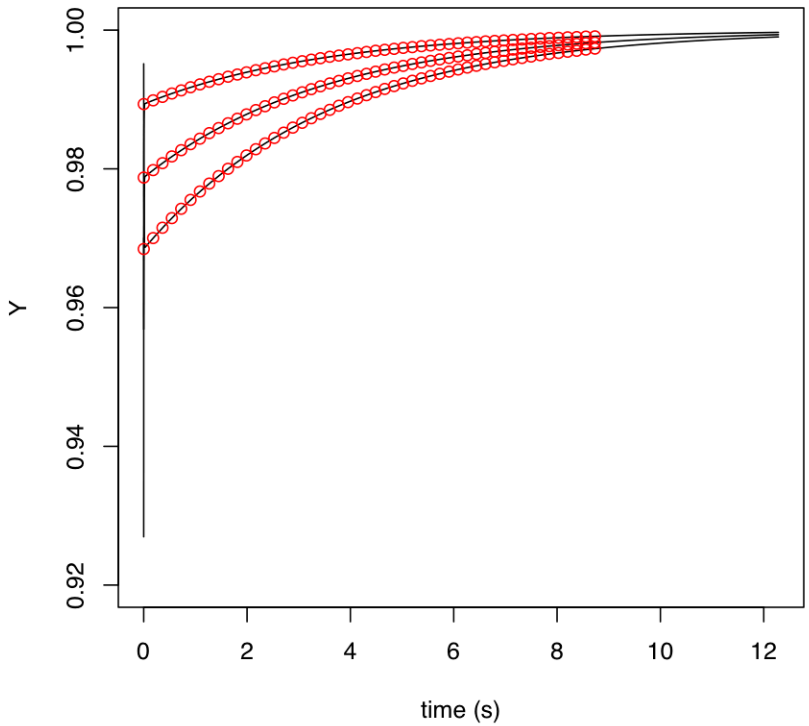
Manifolds for *M* = 1 and *M* = 2 are obtained by setting the fast modes to 0

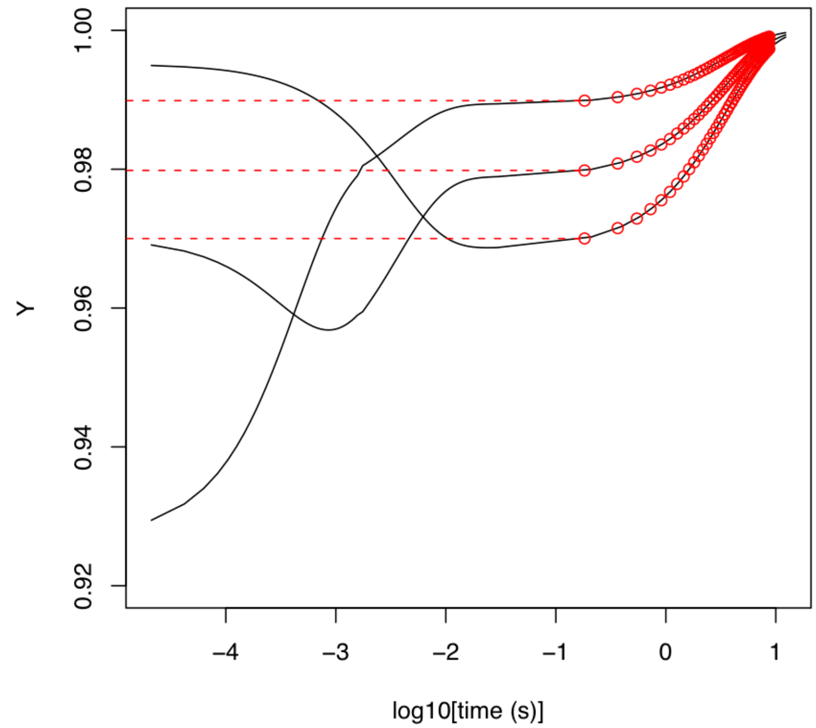
- After fast transients, the system follows the slow manifold
- State can be projected directly onto manifold using homogeneous corrections



The CSP time integrator resolves the time scales on the order of the first active mode

***M* = 2**



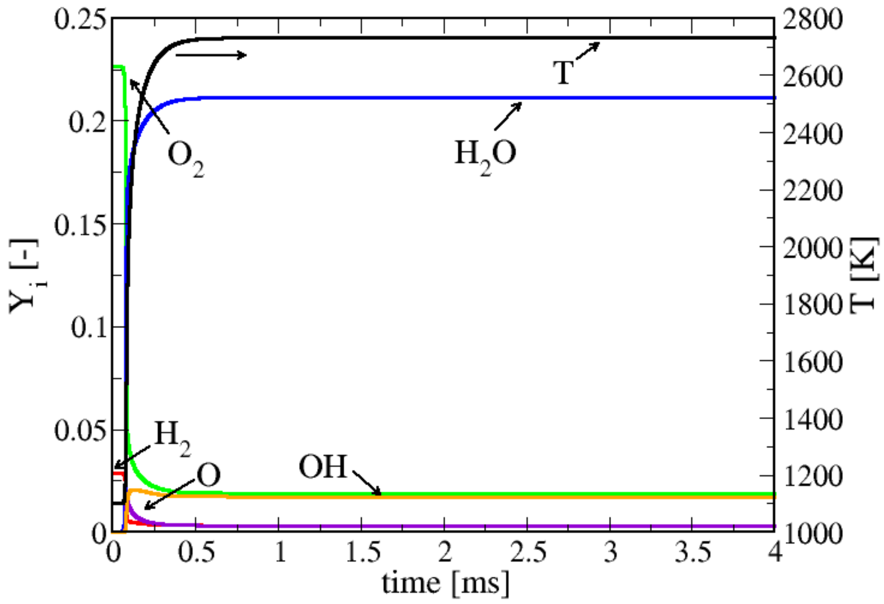


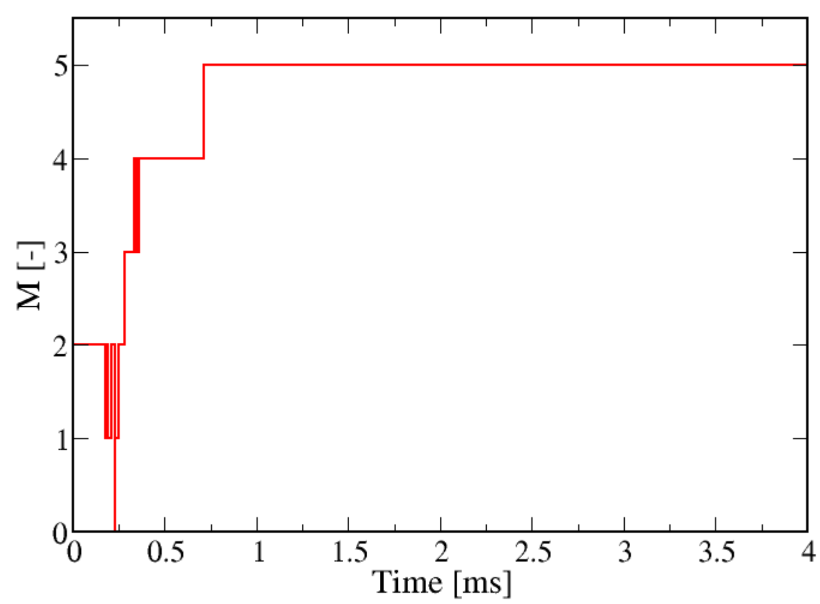
- ***a***, ***b*** as a function of the $Y_{N\text{-}M} = \{y_3\}$ non-radical species
- Driving time scale *O*(0.1)

CSP with tabulation expected to gain competitive edge for more complex chemistries in reacting flows

- Fuels with more complex chemistry tend to have more exhausted modes
  - Greater potential for speed-up by removing stiffness
  - Tabulation of CSP information in *(N-M)* dimensions offers advantage over other N-dimensional tabulation as *N* increases
- Reacting flows likely to offer better re-use of previously computed states
  - E.g. similar conditions occur as reaction front sweeps through computational domain

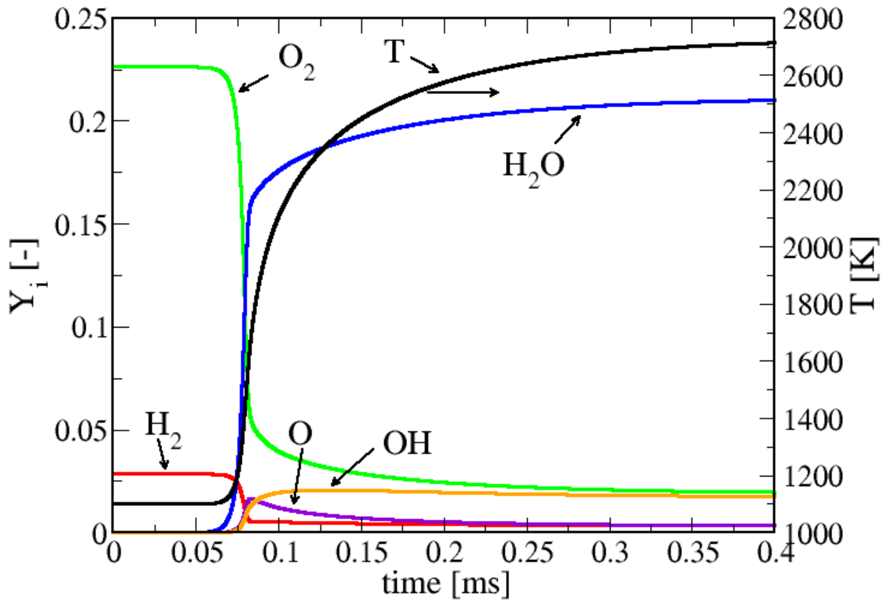
Application to H_2-air ignition

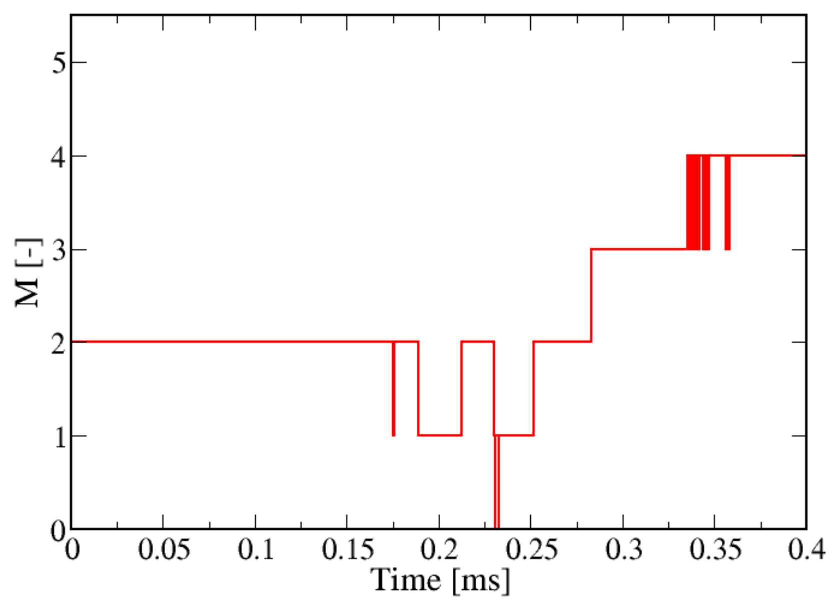




- Yetter, Dryer, & Rabitz, CST, 1991
- N = 10 (9 species + T), 19 reactions
- Initial conditions:
  - T_0 = 1100K, stoichiometric
  - No N_2 dilution, 1 atm
- Exhausted modes allow dimensionality reduction

Application to H_2-air ignition





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  - T_0 = 1100K, stoichiometric
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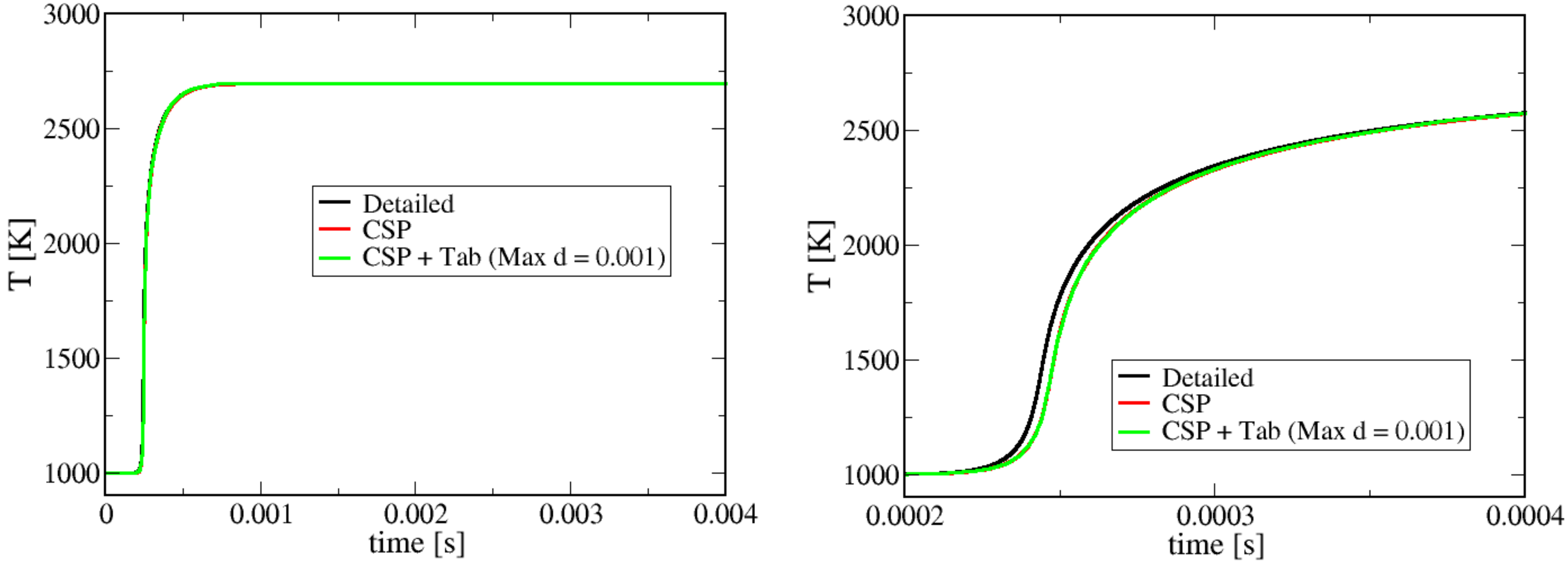
- Exhausted modes allow dimensionality reduction

Multiple tables with varying density were constructed from sampled detailed chemistry ignition simulations.

Table	n_ϕ	n_T	# manifolds	$M_{\min}$	$M_{\max}$	# points
T_H_2.n400.f1e-2	40	10	11	1	5	62549
T_H_2.n400.f1e-3	40	10	11	1	5	551602
T_H_2.n2500.f2e-2	100	25	11	1	5	202424
T_H_2.n2500.f1e-2	100	25	11	1	5	390799
T_H_2.n2500.f1e-3	100	25	11	1	5	3446175

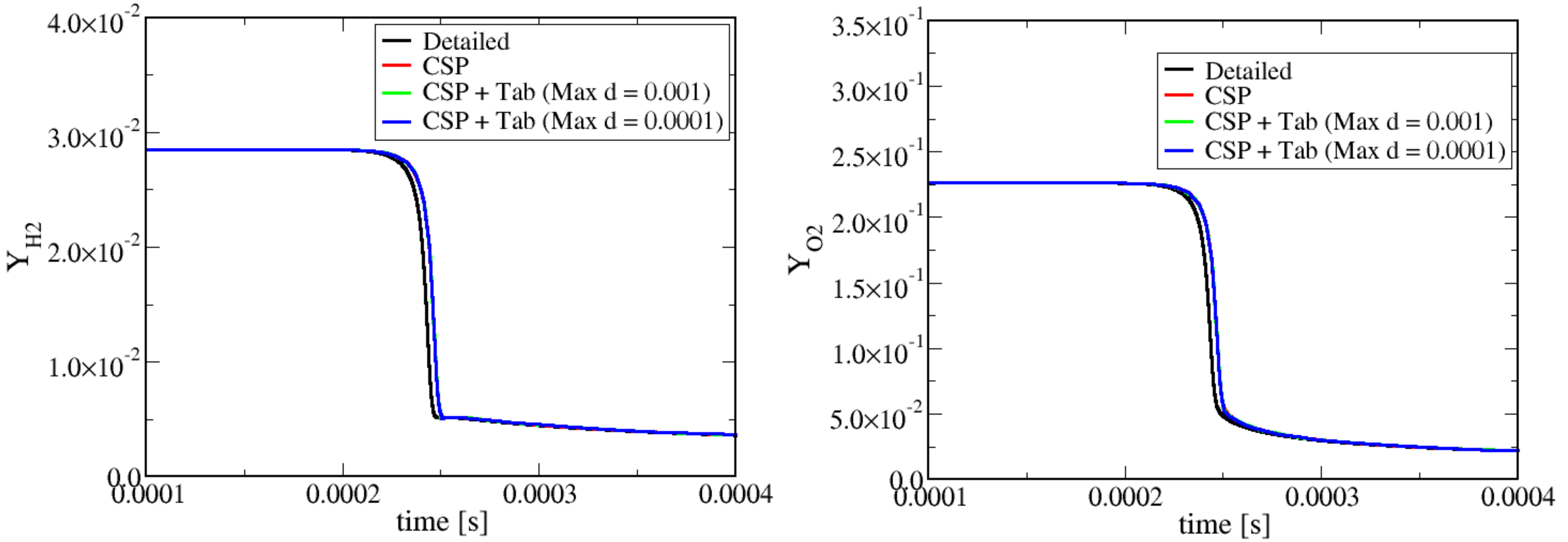
- Initial conditions sampled on uniform grid:
  - T ranging from 1000 to 1200 K
  - Φ ranging from 0.8 to 1.2
- Two sets of tables with varying density, sampled from 400 or 2500 detailed chemistry trajectories
- Number of exhausted modes ranging from 1 to 5

The CSP integrator approximates the detailed kinetics solution well



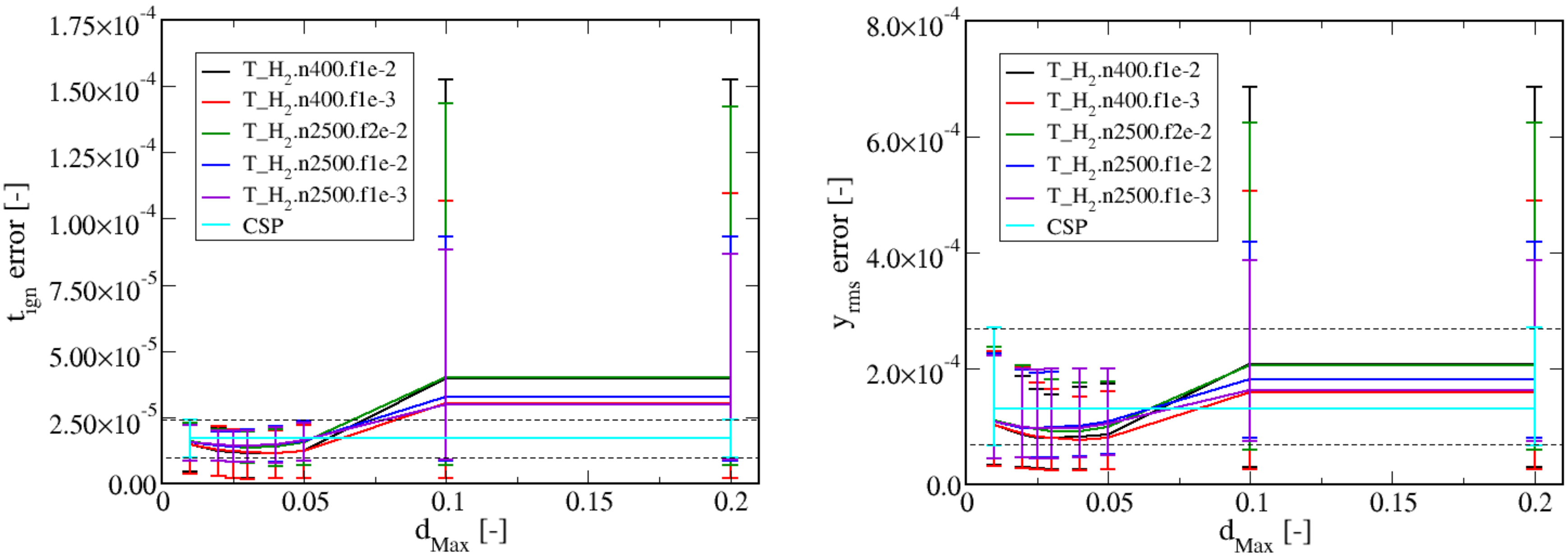
- Small shift due to ignition time error

Comparison for H_2 and O_2



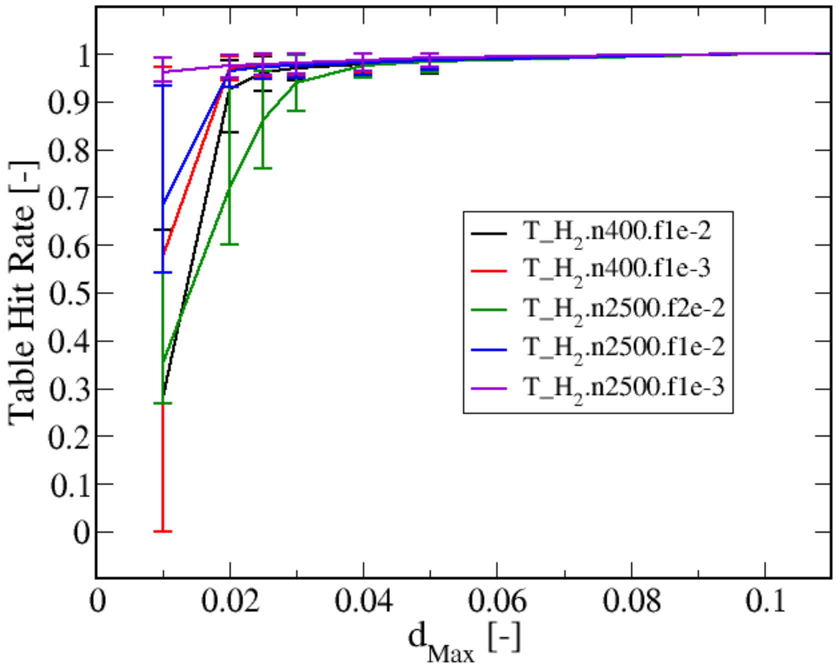
- Major species well represented with CSP and tabulation

Accuracy decreases with increasing limit on distance to nearest neighbor



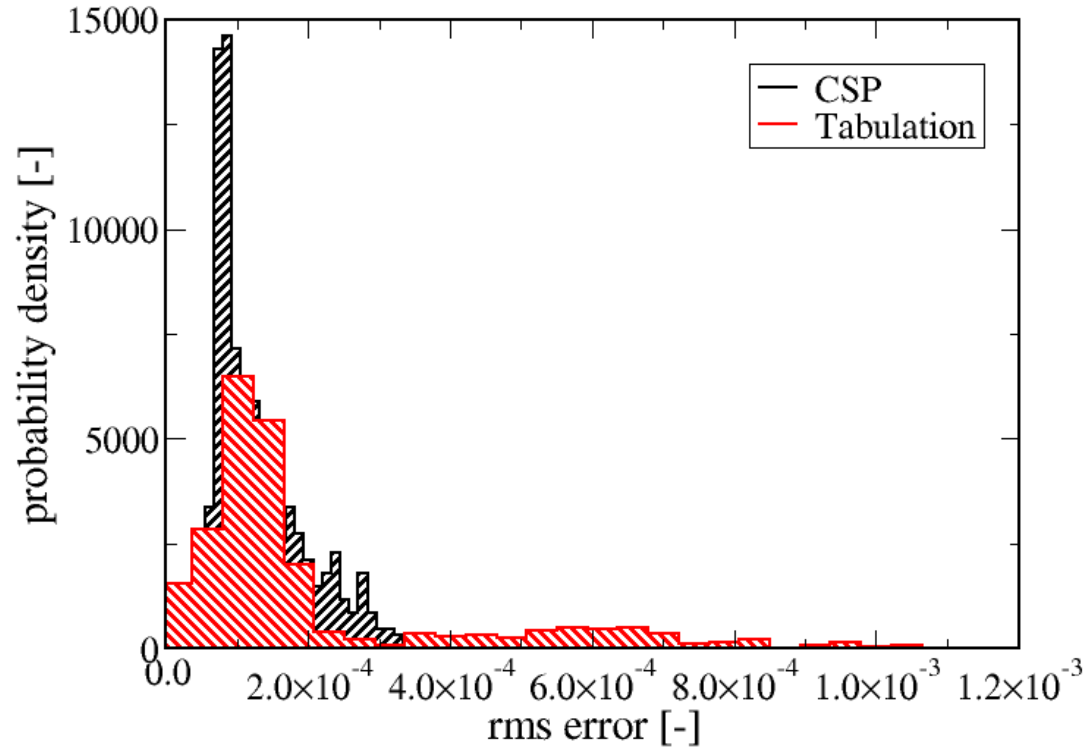
- Averaged over 1000 conditions sampled from same range as initial table design points
- Error insensitive to d_{Max} for large d_{Max}
- At small d_{Max}, tabulation results approach CSP accuracy

Table usage increases with limit on distance to nearest neighbor



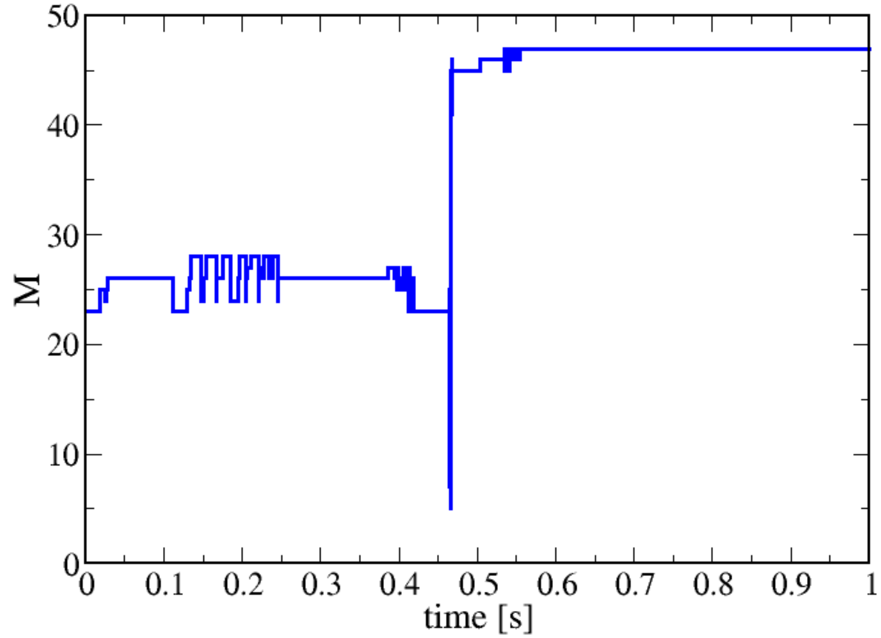
- Usage measured by ratio of table hits over total number of table lookups
- For small d_{Max}, table usage drops dramatically, unless table sufficiently dense
- Averaged over 1000 conditions sampled from same range as initial table design points

Tabulation induced errors are small in general but there are outliers



- Results for table T_H_2.n400.f1e-2 and d_{Max} = 0.1

Exhausted modes offer dimensionality reduction



- From full CSP
- M varies as simulation progresses
- M as high as 47 -> only 7 dimensional table needed

CSP projects the source term onto new basis vectors to decompose fast and slow components

- Decomposition of the source term:

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}) = \sum_{r=1}^{M} \mathbf{a}_r f^r + \sum_{s=M+1}^{N} \mathbf{a}_s f^s \qquad f^i = \mathbf{b}^i \cdot \mathbf{g}, \quad \mathbf{BA} = I \qquad \mathbf{y} \in R^N$$

where fast slow

$$\frac{df^m}{dt} = \sum_{n=1}^{N} \lambda_n^m f^n, \quad \lambda_n^m = \left[\frac{d\mathbf{b}^m}{dt} + \mathbf{b}^m \mathbf{J}\right]\mathbf{a}_n, \qquad \mathbf{J} = \frac{d\mathbf{g}}{d\mathbf{y}}$$

- Seek **a**, **b** such that Λ becomes block-diagonal
  - Eigenvalue problem, CSP refinements
- *Exhausted* modes: pick largest *M* such that $\left|\tau_{M+1} \sum_{r=1}^{M} \mathbf{a}_r f^r\right| < \mathbf{y}_{error}$
- $f^r \approx 0, \; r = 1 \ldots M$ describes slow manifold

Lam, Comb. Sci. Tech, 1993

The CSP integrator moves the system along the slow manifold

- After exhaustion of M fast modes: non-stiff reduced model:

$$\frac{d\mathbf{y}}{dt} \approx \sum_{s=M+1}^{N} \mathbf{a}_s f^s = \left(I - \sum_{r=1}^{M} \mathbf{a}_r \mathbf{b}^r \right) \mathbf{g} = \mathbf{P}\mathbf{g}$$

- Explicit *time-scale* splitting:
  - Slow dynamics along the manifold $\mathbf{y}(T+\Delta t) = \mathbf{y}(T) + \int_T^{T+\Delta t} \mathbf{P}\mathbf{g}\, dt$
  - Homogeneous correction (HC) to remain on manifold

$$\mathbf{y}(T+\Delta t) = \tilde{\mathbf{y}}(T+\Delta t) - \sum_{r,r'=1}^{M} \mathbf{a}_r \tau_{r'}^{r} f^{r'}$$ (τ_m^n *are entries of* $\mathrm{T} = \Lambda^{-1}$)

  - This elimination of fast time scales allows the use of explicit time integrators

Valorani, Goussis, J. Comp. Phys, 2001

Computational Singular Perturbation projects the source term onto new basis vectors to decompose fast and slow components

- Decomposition of the source term:

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}) = \underbrace{\sum_{r=1}^{M} \mathbf{a}_r f^r}_{\text{fast}} + \underbrace{\sum_{s=M+1}^{N} \mathbf{a}_s f^s}_{\text{slow}} \qquad f^i = \mathbf{b}^i \cdot \mathbf{g}, \quad \mathbf{BA} = I \qquad \mathbf{y} \in R^N$$

where

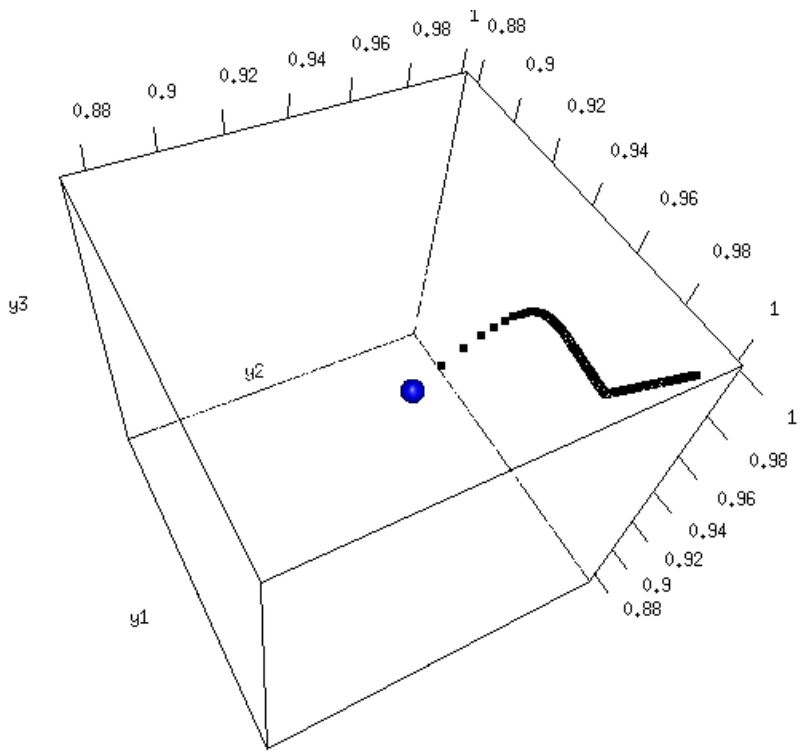
$$\frac{df}{dt} = \Lambda f, \quad \Lambda = \mathbf{B}(D\mathbf{g})\mathbf{A} + \frac{d\mathbf{B}}{dt}\mathbf{A}$$

- Seek **a**, **b** such that Λ becomes block-diagonal
  - Eigenvalue problem, CSP refinements

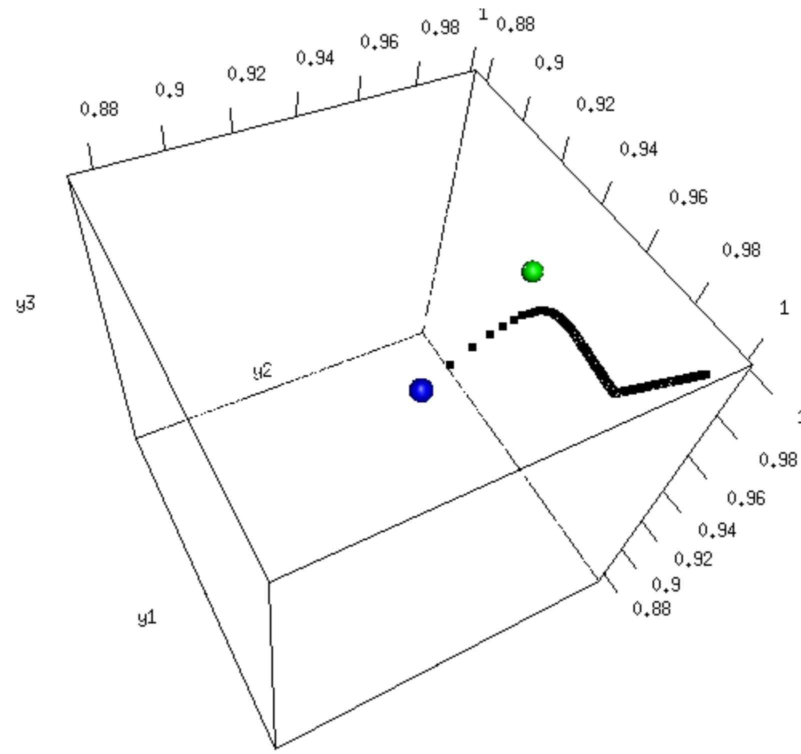
- $f^r \approx 0, \; r = 1 \ldots M$ describes slow manifold

- *Exhausted* modes: pick largest *M* such that $\left| \tau_{M+1} \sum_{r=1}^{M} \mathbf{a}_r f^r \right| < \mathbf{y}_{error}$

Homogeneous corrections project state onto slow manifold

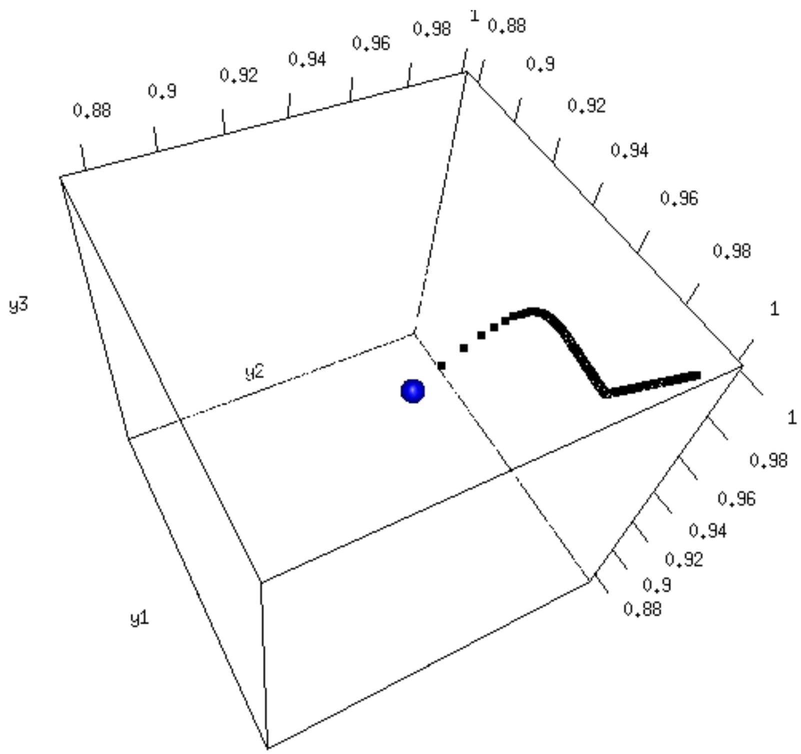


Full model trajectory

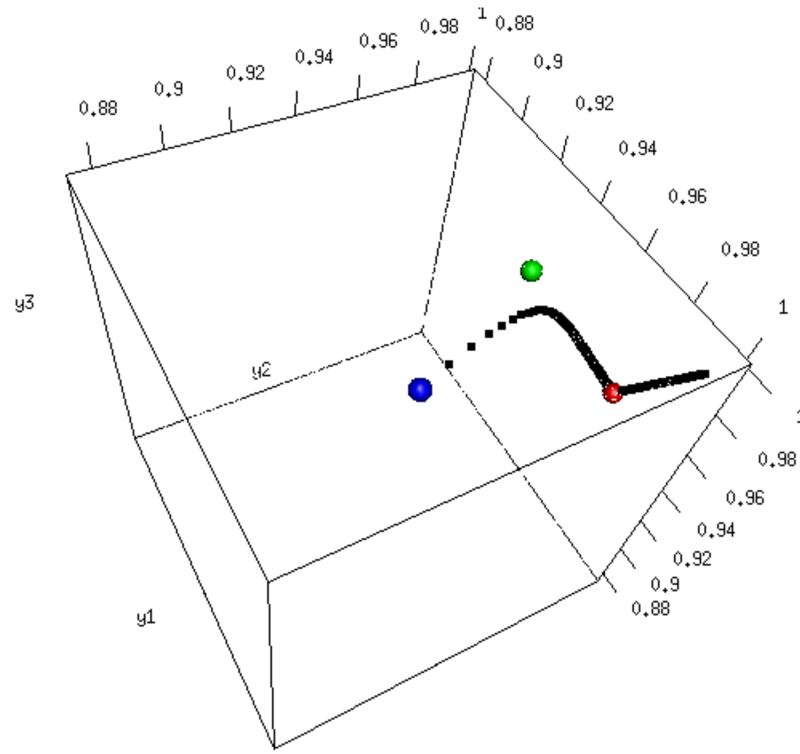


HC with ***M* = *1***

Homogeneous corrections project state onto slow manifold

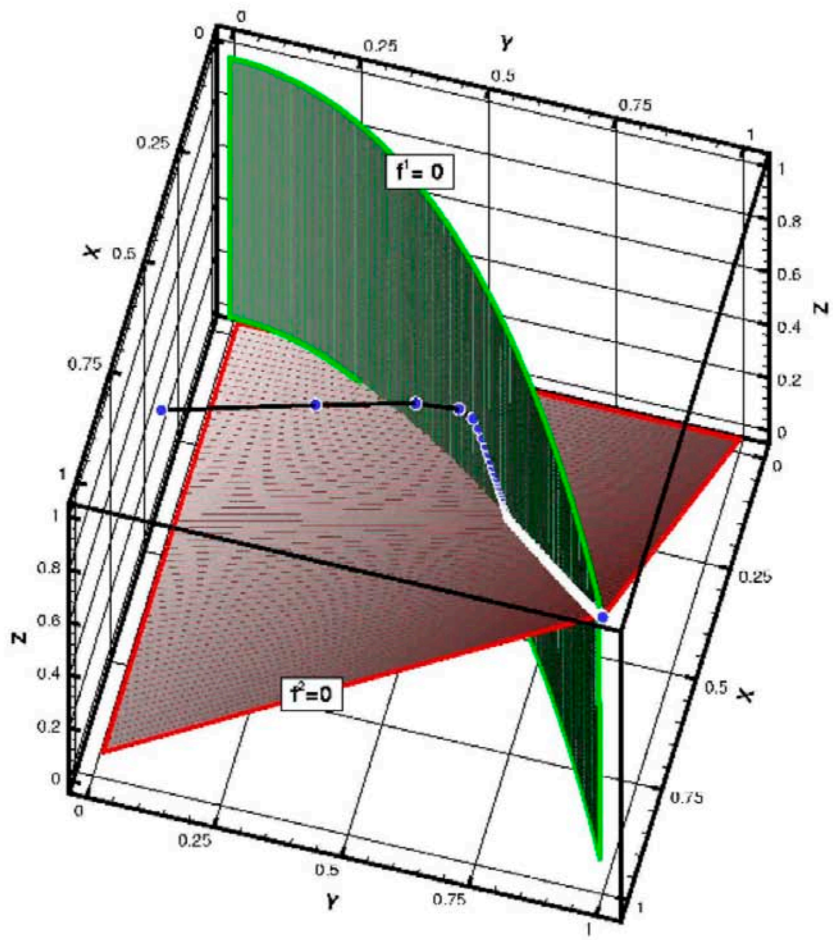


Full model trajectory



HC with ***M = 2***

Manifolds for *M* = 1 and *M* = 2 can be obtained by setting the fast modes to 0



CSP pointer $\boldsymbol{Q}_m$ identifies optimal choices of CSP radicals:

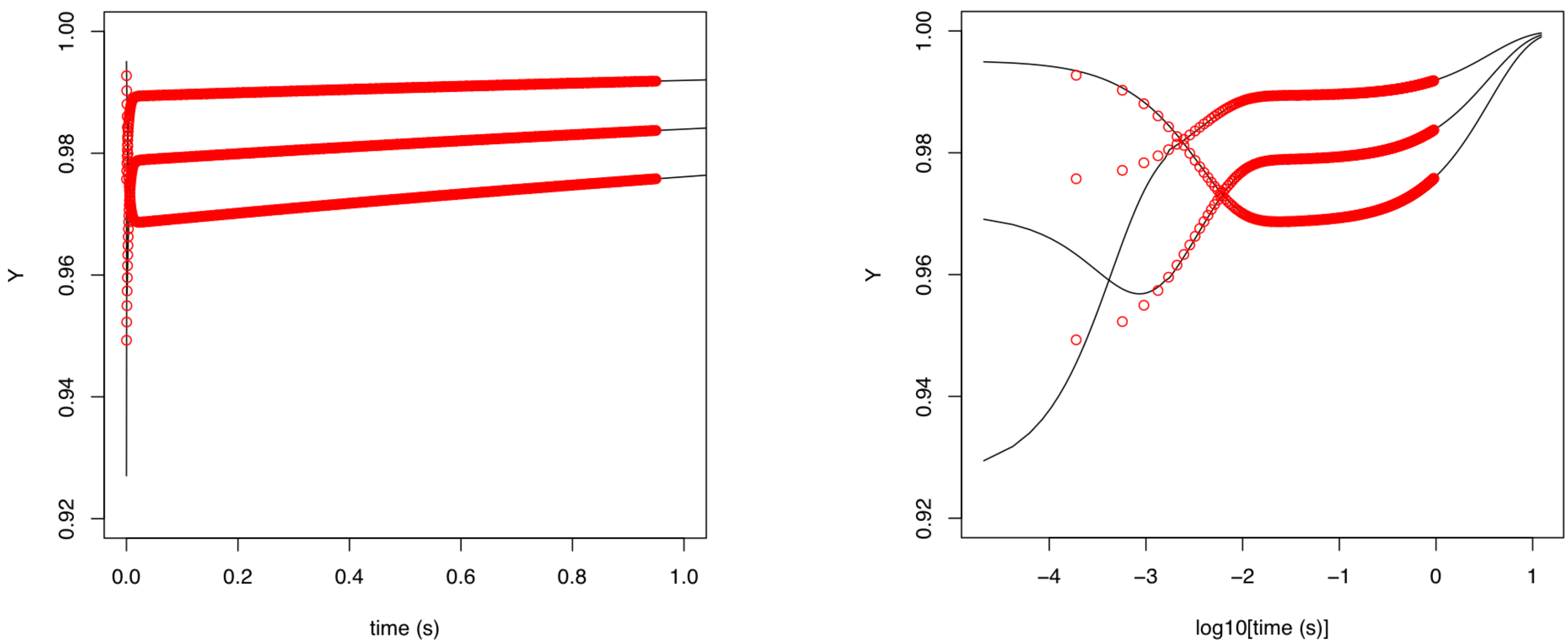
	Q_{m11}	Q_{m22}	Q_{m33}
$M = 1$	0.18	0.82	7.4E-04
$M = 2$	0.36	0.46	0.17

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

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

The CSP time integrator resolves the time scales on the order of the first active mode

***M* = 1**



- ***a***, ***b*** as a function of the $Y_{N\text{-}M} = \{y_3, y_1\}$ active species
- Driving time scale O(2e-4)

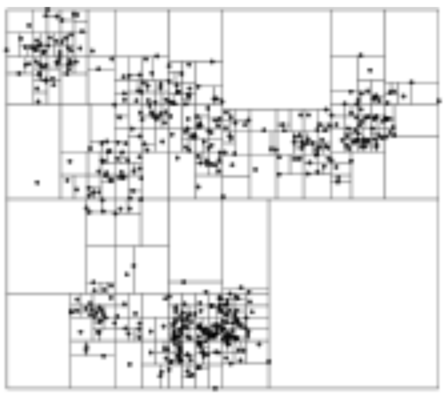
Application to H_2-air ignition problem

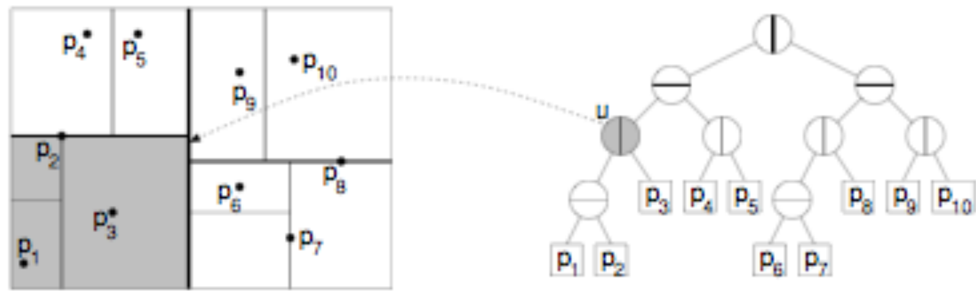
- Yetter, Dryer, & Rabitz, CST, 1991
- N = 10 (9 species + T)
- 19 reactions
- Initial conditions
  - T_0 = 1000K
  - Y_{H2} = 0.018
  - Y_{O2} = 0.2
  - Y_{N2} = 0.782
  - Φ = 0.714
  - Dilution: 0.15 extra mol N_2 per mol air
  - 1 atm

$$
\begin{aligned}
H + O_2 &\Leftrightarrow O + OH \\
O + H_2 &\Leftrightarrow H + OH \\
H_2 + OH &\Leftrightarrow H_2O + H \\
OH + OH &\Leftrightarrow O + H_2O \\
H_2 + M &\Leftrightarrow H + H + M \\
O + O + M &\Leftrightarrow O_2 + M \\
O + H + M &\Leftrightarrow OH + M \\
H + OH + M &\Leftrightarrow H_2O + M \\
H + O_2 + M &\Leftrightarrow HO_2 + M \\
HO_2 + H &\Leftrightarrow H_2 + O_2 \\
HO_2 + H &\Leftrightarrow OH + OH \\
HO_2 + O &\Leftrightarrow O_2 + OH \\
HO_2 + OH &\Leftrightarrow H_2O + O_2 \\
HO_2 + HO_2 &\Leftrightarrow H_2O_2 + O_2 \\
H_2O_2 + M &\Leftrightarrow OH + OH + M \\
H_2O_2 + H &\Leftrightarrow H_2O + OH \\
H_2O_2 + H &\Leftrightarrow HO_2 + H_2 \\
H_2O_2 + O &\Leftrightarrow OH + HO_2 \\
H_2O_2 + OH &\Leftrightarrow HO_2 + H_2O
\end{aligned}
$$

*k*d-Trees support efficient nearest neighbor queries

- How to perform NN or *k*-NN queries efficiently?
  - Use spatial data structures: ***k*d-trees** and variants





- Yet better scaling: ***approximate*** nearest neighbors [Mount & Arya]
  - *Return a point within relative error ε of the true nearest neighbor*
  - Storage = O(*dn*) space; preprocessing = O(*dn* log *n*) time
  - Per-query cost: O($c_{d,\varepsilon}$ log *n*) time, where $c_{d,\varepsilon} \le d\lceil 1 + 6d/\varepsilon \rceil^{d}$
  - And *d* = *N* - *M* always
- Easy to **add new points** to the tree ("online" learning)

Computational singular perturbation (CSP): a general method for analysis and reduction of dynamical systems

- Identify fast and slow modes in system

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y}) = \mathbf{g}_{fast} + \mathbf{g}_{slow}$$
$$= \mathbf{a}_1 f^1 + \mathbf{a}_2 f^2 + \ldots + \mathbf{a}_N f^N \qquad f^i = \mathbf{b}^i \mathbf{g}$$

- After relaxation of fast transients: M exhausted modes

$$f^i \approx 0, \qquad i = 1, \ldots, M$$
$$\mathbf{g}_{fast} = \sum_{r=1}^{M} \mathbf{a}_r f^r \approx 0$$
$$\mathbf{g}_{slow} = \sum_{s=M+1}^{N} \mathbf{a}_s f^s = \left(I - \sum_{r=1}^{M} \mathbf{a}_r \mathbf{b}^r \right) \mathbf{g} = \mathbf{P}\mathbf{g}$$

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}_{slow}$$

[Lam, Goussis, Valorani, Najm, 1988 – 2009]

- Automated analysis:
  - Stiffness removed
  - M algebraic constraints define slow manifold and enable system reduction