Mechanism reduction methods based on time scale separation

2^{nd} part

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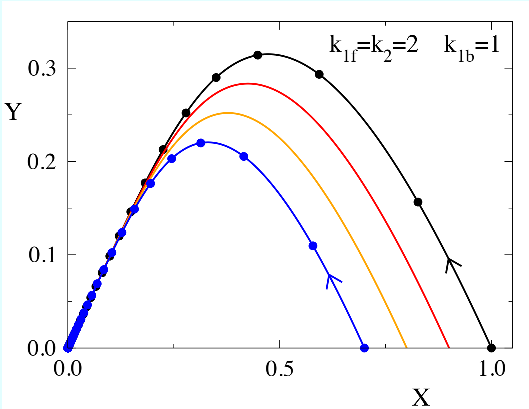
Outline

1. Mathematical background
2. Time scales
3. Traditional reduction tools and their limitations
4. New algorithmic tools
5. Various methodologies
6. Applications
7. Quasi steady-state and partial equilibrium approx.

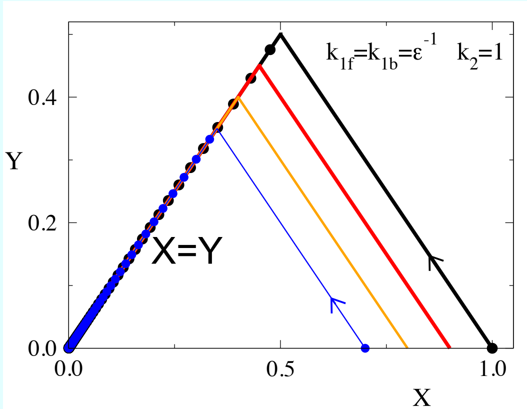
Some common features

$\varepsilon = 10^{-6}$

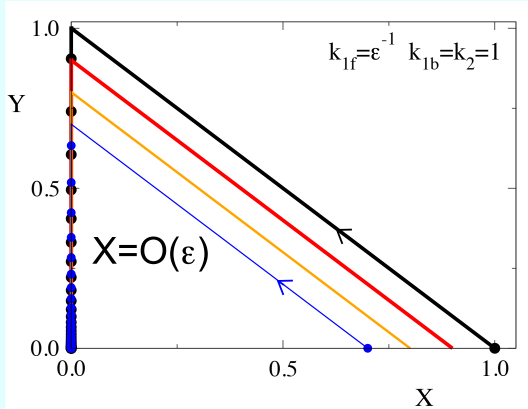
$\tau_1/\tau_2 = 0.25 \qquad \lambda_1 = -4$



$\tau_1/\tau_2 = \varepsilon/4 \qquad \lambda_1 = -2/\varepsilon$

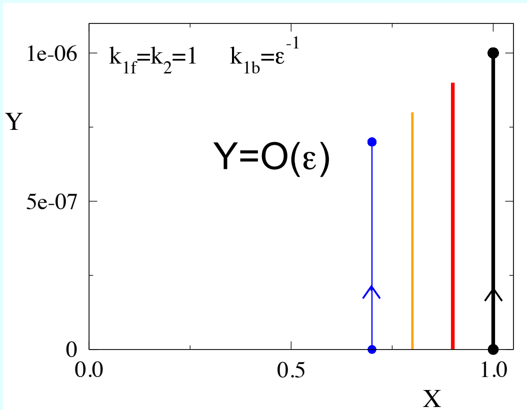


$\tau_1/\tau_2 = \varepsilon \qquad \lambda_1 = -1/\varepsilon$

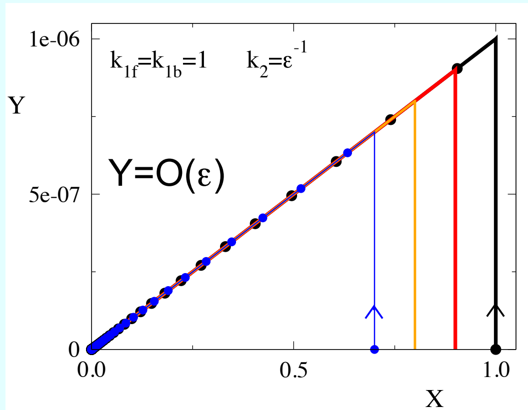


1. Time scale gaps
2. Dissipative time scales
3. Fast/slow behavior
4. Structures in phase space

$\tau_1/\tau_2 = \varepsilon^2 \qquad \lambda_1 = -1/\varepsilon$



$\tau_1/\tau_2 = \varepsilon \qquad \lambda_1 = -1/\varepsilon$



Obstacles for a successful asymptotic analysis

Given a system in dimensional form: $$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y};\mathbf{k})$$

When using the traditional tools a researcher must:

1. find all applicable *non-dimensional forms* of the system
2. transform all systems in *normal form*
3. determine the *sub-domain in phase space* where each system is valid
4. proceed with the *proper expansion* of variables
5. find a way to *match* the solution of the various systems

Theory of Singular Perturbations

Poincare, Stieltjes (1886, celestial mechanics)

Prandtl (1904, fluid mechanics)

Van der Pol (1920, circuits)

Tikhonov (1948), Levinson (1949)

Bogolubov, Carrier, Cole, van Dyke, Dorodnitsyn, Eckhaus, Hirsch, Holmes,

Fenichel, Friedrichs, Jones, Kaplun, Keller, Kevorkian, Lagerstrom, Mitropolsky,

O'Malley, Vasil'eva, Vehulst (from the 50's)

Geometrical Singular Perturbations

Hirsch, Fenichel, Pugh, Shub, Jones

Goals:

- Identify central dynamical *structures* in phase space
- Exploit their *properties*, such as fast slow decompositions

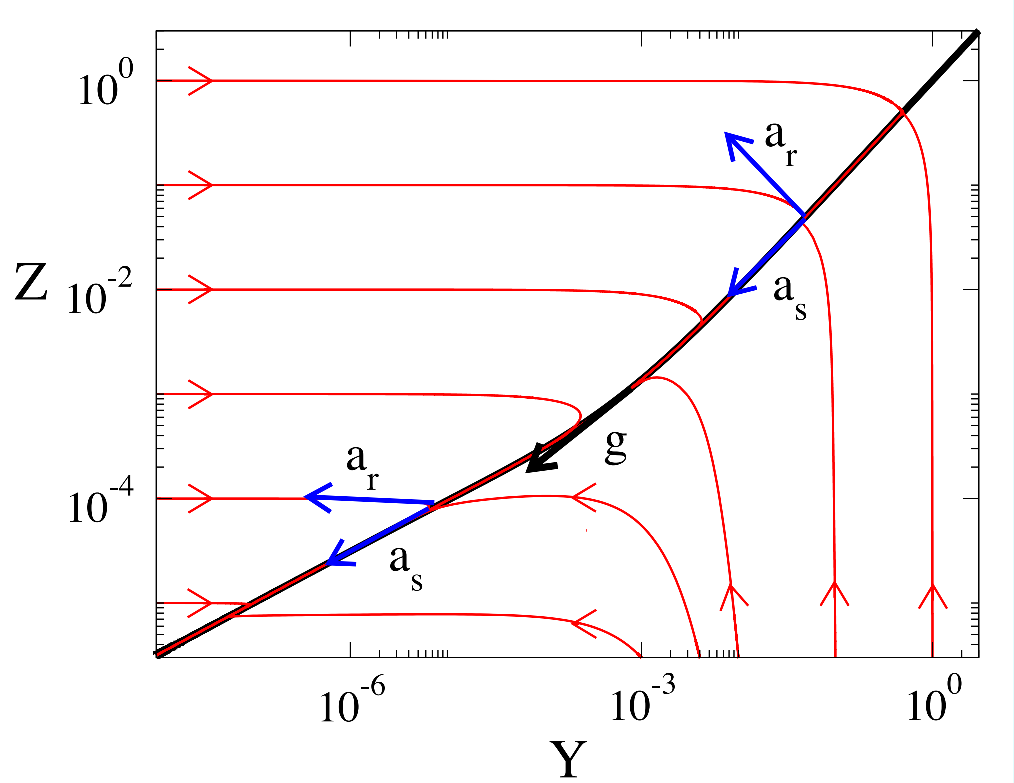
Basic tools:

- The *tangent space (the tangent bundle)*
- Fast and slow *sub-domains* of tangent space

(Tasso Kaper, AMS 1999)

The tangent space; its fast slow sub-domains

Lindemann, $k_{1f}=10^3$, $k_{1b}=10^3$, $k_2=1$



$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} +1 \\ -1 \end{bmatrix}\frac{z^2}{\varepsilon} + \begin{bmatrix} -1 \\ +1 \end{bmatrix}\frac{yz}{\varepsilon} + \begin{bmatrix} -1 \\ 0 \end{bmatrix} y$$

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y};\mathbf{k})$$

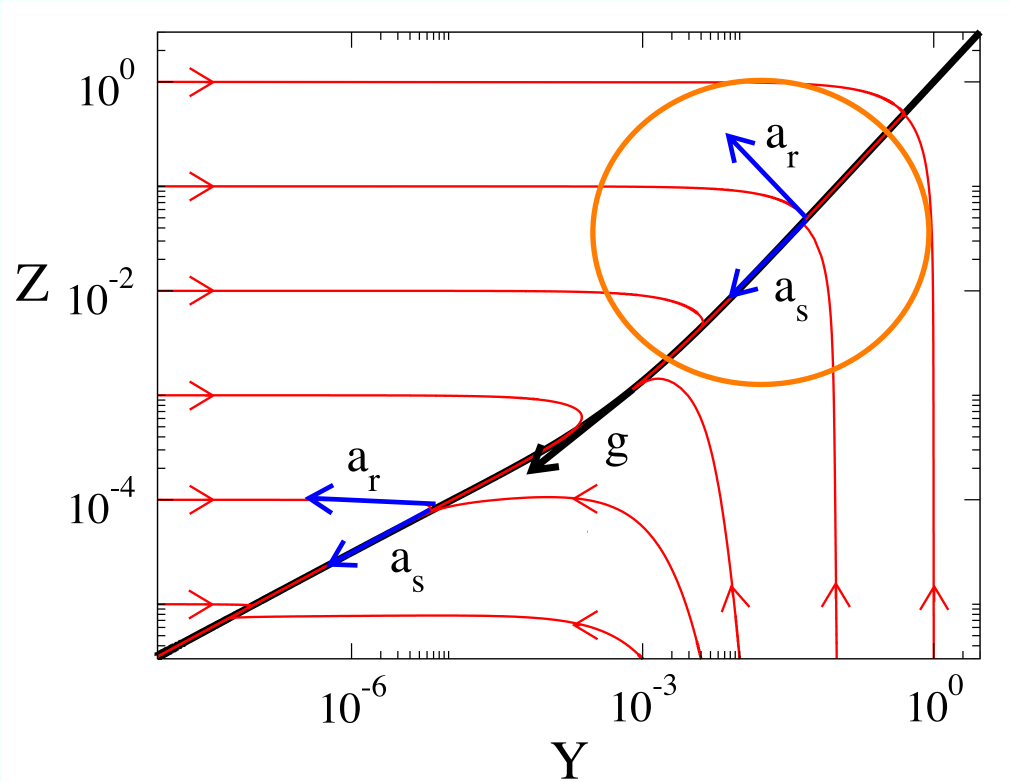
$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_r f^r + \mathbf{a}_s f^s$$

$$f^r \approx 0 \qquad \frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s f^s$$

Reduced Model

The tangent space; its fast slow sub-domains

Lindemann, $k_{1f}=10^3$, $k_{1b}=10^3$, $k_2=1$



$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} +1 \\ -1 \end{bmatrix}\frac{z^2}{\varepsilon} + \begin{bmatrix} -1 \\ +1 \end{bmatrix}\frac{yz}{\varepsilon} + \begin{bmatrix} -1 \\ 0 \end{bmatrix} y$$

$$\mathbf{a}_r = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \qquad \mathbf{a}_s = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} -1 \\ 1 \end{bmatrix} f^r + \begin{bmatrix} -1 \\ -1 \end{bmatrix} f^s$$

$$f^r = \frac{1}{\varepsilon}\left(yz - z^2 + \varepsilon\frac{y}{2}\right) \qquad f^s = \frac{y}{2}$$

$$f^r \approx 0 \quad \Rightarrow$$

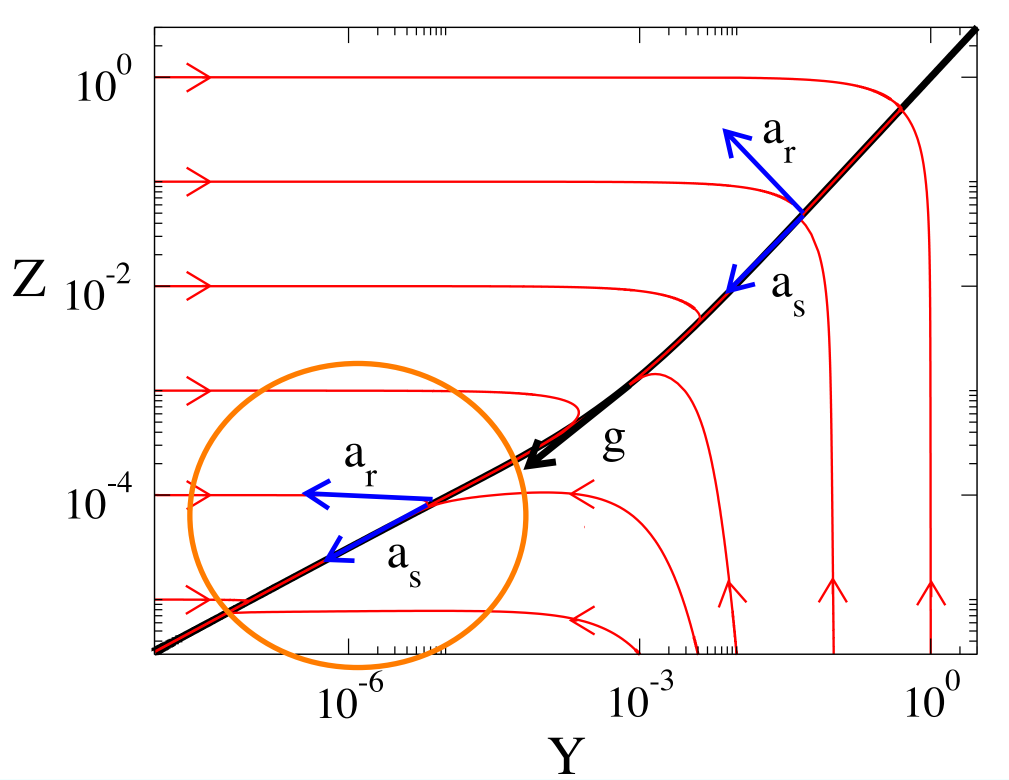
$$y \approx z$$

$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} \approx \begin{bmatrix} -1 \\ -1 \end{bmatrix} f^s$$

Reduced model

The tangent space; its fast slow sub-domains

Lindemann, $k_{1f}=10^3$, $k_{1b}=10^3$, $k_2=1$



$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} +1 \\ -1 \end{bmatrix}\frac{z^2}{\varepsilon} + \begin{bmatrix} -1 \\ +1 \end{bmatrix}\frac{yz}{\varepsilon} + \begin{bmatrix} -1 \\ 0 \end{bmatrix} y$$

$$\mathbf{a}_r = \begin{bmatrix} -1 \\ 0 \end{bmatrix} \qquad \mathbf{a}_s = \begin{bmatrix} -2z \\ -1 \end{bmatrix}$$

$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \end{bmatrix} f^r + \begin{bmatrix} -2z \\ -1 \end{bmatrix} f^s$$

$$f^r = (1+2\varepsilon z)z\left(y - \frac{z}{\varepsilon}\right) + \frac{y}{\varepsilon}$$

$$f^s = z^2 - \varepsilon yz$$

$$f^r \approx 0 \quad \Rightarrow$$

$$y \approx z^2$$

$$\frac{d}{dt}\begin{bmatrix} y \\ z \end{bmatrix} \approx \begin{bmatrix} -2z \\ -1 \end{bmatrix} f^s$$

Reduced model

Lindemann mechanism: the fast and slow basis vectors

$$A + A \underset{k_{1b}}{\overset{k_{1f}}{\Leftrightarrow}} B + A \qquad B \overset{k_2}{\Rightarrow} P$$

$$\frac{d}{dt}\begin{bmatrix}[B]\\ \\ [A]\end{bmatrix} = \begin{bmatrix}+1\\ \\ -1\end{bmatrix} k_{1f}[A]^2 + \begin{bmatrix}-1\\ \\ +1\end{bmatrix} k_{1b}[B][A] + \begin{bmatrix}-1\\ \\ 0\end{bmatrix} k_2[B]$$

$$\mathbf{a}_1 = \begin{bmatrix}1\\ -\delta_1\end{bmatrix} \qquad \mathbf{a}_2 = \begin{bmatrix}-\delta_1\delta_2\\ -1\end{bmatrix}$$

$$\delta_1 = \left(1 + \frac{k_2}{k_{1b}[A]}\right)^{-1}$$

$$\delta_2 = 2\frac{k_{1f}}{k_{1b}} - \frac{[B]}{[A]}$$

Lindemann mechanism: the reduced model

$$A + A \underset{k_{1b}}{\overset{k_{1f}}{\Leftrightarrow}} B + A \qquad B \overset{k_2}{\Rightarrow} P$$

$$\frac{d}{dt}\begin{bmatrix}[B]\\ [A]\end{bmatrix} = \begin{bmatrix}+1\\ -1\end{bmatrix} k_{1f}[A]^2 + \begin{bmatrix}-1\\ +1\end{bmatrix} k_{1b}[B][A] + \begin{bmatrix}-1\\ 0\end{bmatrix} k_2[B]$$

$$(1+\delta_1\delta_2)^{-1}(k_{1f}[A]^2 - k_{1b}[B][A]) - k_2[B] \approx 0$$

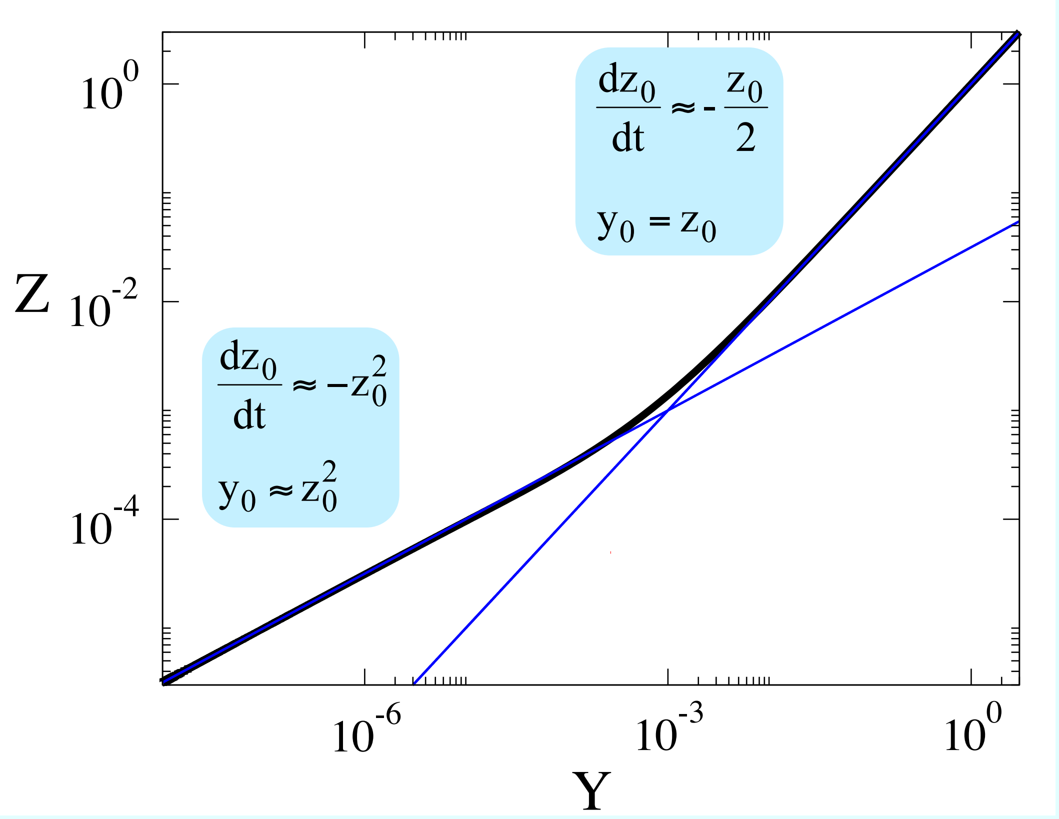
$$\frac{d}{dt}\begin{bmatrix}[B]\\ [A]\end{bmatrix} \approx \begin{bmatrix}-\delta_1\delta_2\\ -1\end{bmatrix} \frac{\delta_1}{1+\delta_1^2\delta_2} \frac{k_{1f}}{k_{1b}} k_2[B]$$

$$\delta_1 = \left(1 + \frac{k_2}{k_{1b}[A]}\right)^{-1}$$

$$\delta_2 = 2\frac{k_{1f}}{k_{1b}} - \frac{[B]}{[A]}$$

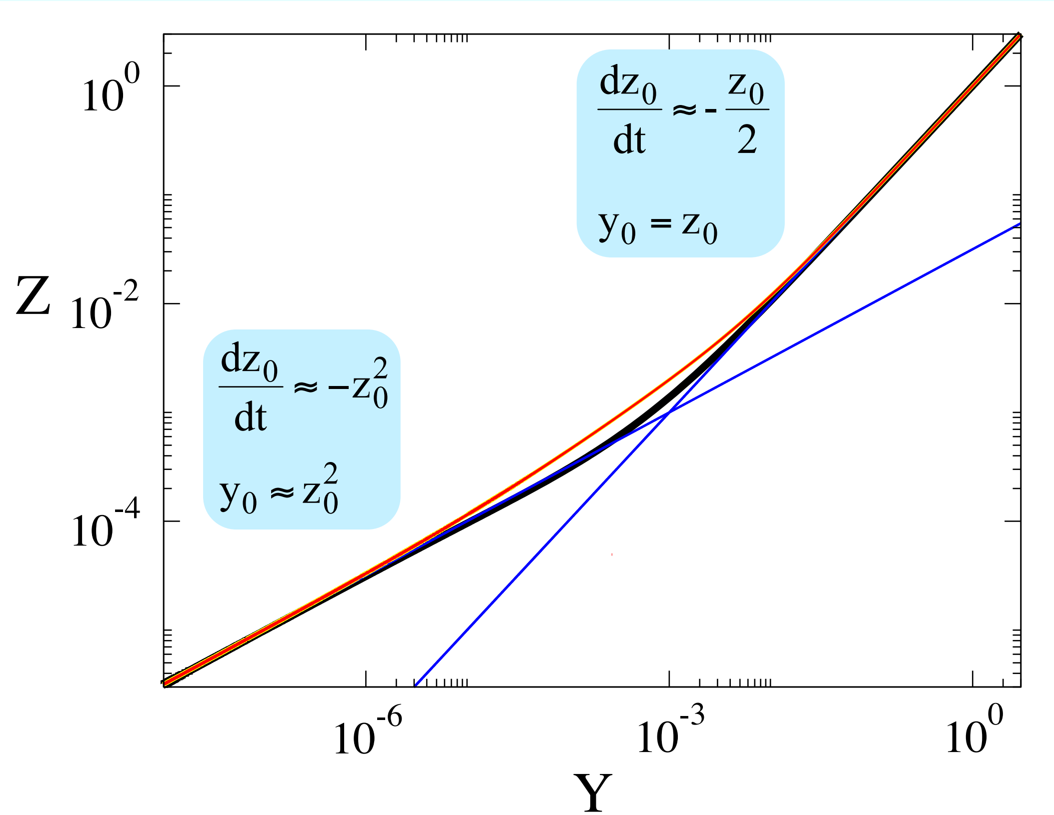
Traditional vs new asymptotics

$k_{1f}=10^3$ $k_{1b}=10^3$ $k_2=1$



Traditional vs new asymptotics

$k_{1f}=10^3 \quad k_{1b}=10^3 \quad k_2=1$



$$\frac{k_{1f}[A]^2 - k_{1b}[B][A]}{1+\delta_1\delta_2} - k_2[B] \approx 0$$

$$\frac{d}{dt}\begin{bmatrix}[B]\\ [A]\end{bmatrix} \approx \begin{bmatrix}-\delta_1\delta_2\\ -1\end{bmatrix}\frac{\delta_1}{1+\delta_1^2\delta_2}\frac{k_{1f}}{k_{1b}}k_2[B]$$

Removing obstacles for a successful asymptotic analysis

Given a system in dimensional form: $$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y};\mathbf{k})$$

When using the new algorithms a researcher does not have to:

1. find all applicable *non-dimensional forms* of the system
2. transform all systems in *normal form*
3. determine the *sub-domain in phase space* where each system is valid
4. proceed with the *proper expansion* of variables
5. find a way to *match* the solution of the various systems

Instead, he has to:

1. find the *fast and slow basis vectors* of the tangent space
2. find ways to *efficiently* use them

Model reduction

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = [\mathbf{a}_1 \;\; .. \;\; \mathbf{a}_M]\left(\begin{bmatrix} \mathbf{b}^1 \\ : \\ \mathbf{b}^M \end{bmatrix}\mathbf{g}(\mathbf{y})\right) + [\mathbf{a}_{M+1} \;\; .. \;\; \mathbf{a}_N]\left(\begin{bmatrix} \mathbf{b}^{M+1} \\ : \\ \mathbf{b}^N \end{bmatrix}\mathbf{g}(\mathbf{y})\right) = \mathbf{a}_r\mathbf{f}^r + \mathbf{a}_s\mathbf{f}^s$$

$$\left|\boldsymbol{\tau}\,\mathbf{a}_r\mathbf{f}^r\right| < \mathbf{y}_{error} = \varepsilon_{rel}\mathbf{y} + \varepsilon_{abs} \qquad \boldsymbol{\tau} = \left(\mathbf{b}^r\mathbf{J}\mathbf{a}_r\right)^{-1}$$

$$\mathbf{f}^r = \mathbf{b}^r\mathbf{g}(\mathbf{y})$$

$$\mathbf{f}^s = \mathbf{b}^s\mathbf{g}(\mathbf{y})$$

Reduced model

$$\mathbf{f}^r \approx 0$$

$$\frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s\mathbf{f}^s$$

Structures in tangent space

Slow model

Problems

1. Complex structures
2. Variation of M with time/space
3. Evaluation of $\mathbf{a}_i$
4. Solving the algebraic eqs.

Model reduction

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = \begin{bmatrix}\mathbf{a}_1 & .. & \mathbf{a}_M\end{bmatrix}\left(\begin{bmatrix}\mathbf{b}^1 \\ : \\ \mathbf{b}^M\end{bmatrix}\mathbf{g}(\mathbf{y})\right) + \begin{bmatrix}\mathbf{a}_{M+1} & .. & \mathbf{a}_N\end{bmatrix}\left(\begin{bmatrix}\mathbf{b}^{M+1} \\ : \\ \mathbf{b}^N\end{bmatrix}\mathbf{g}(\mathbf{y})\right) = \mathbf{a}_r\mathbf{f}^r + \mathbf{a}_s\mathbf{f}^s$$

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Structures in tangent space

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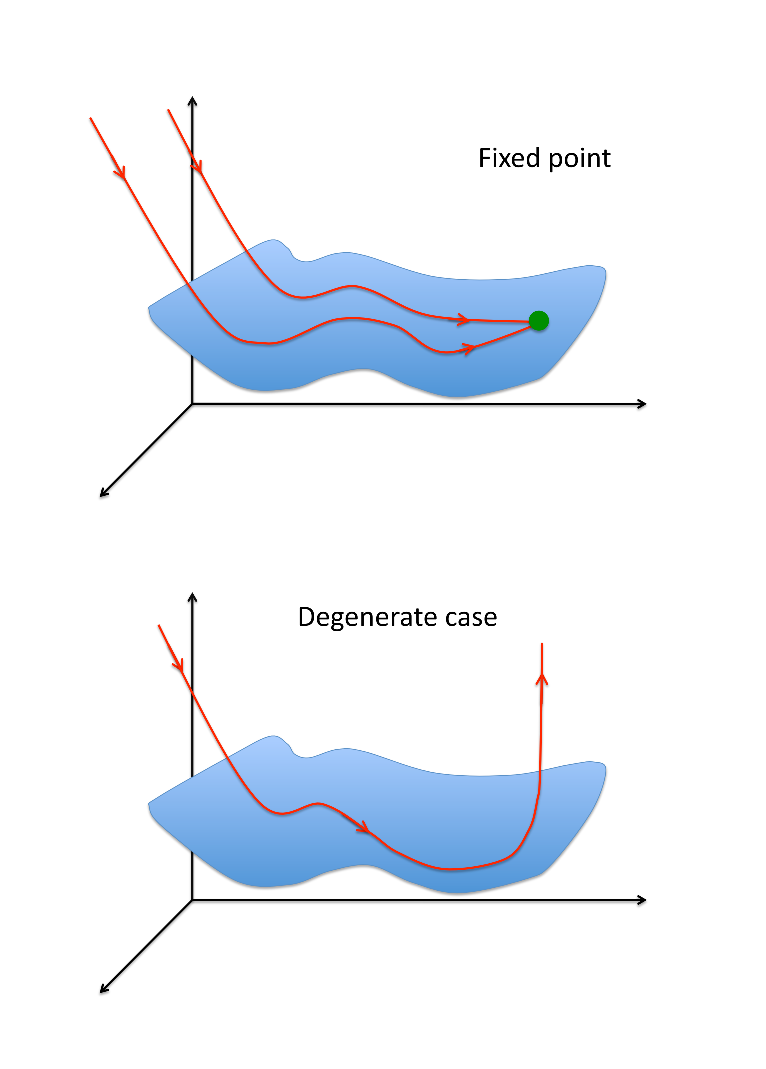
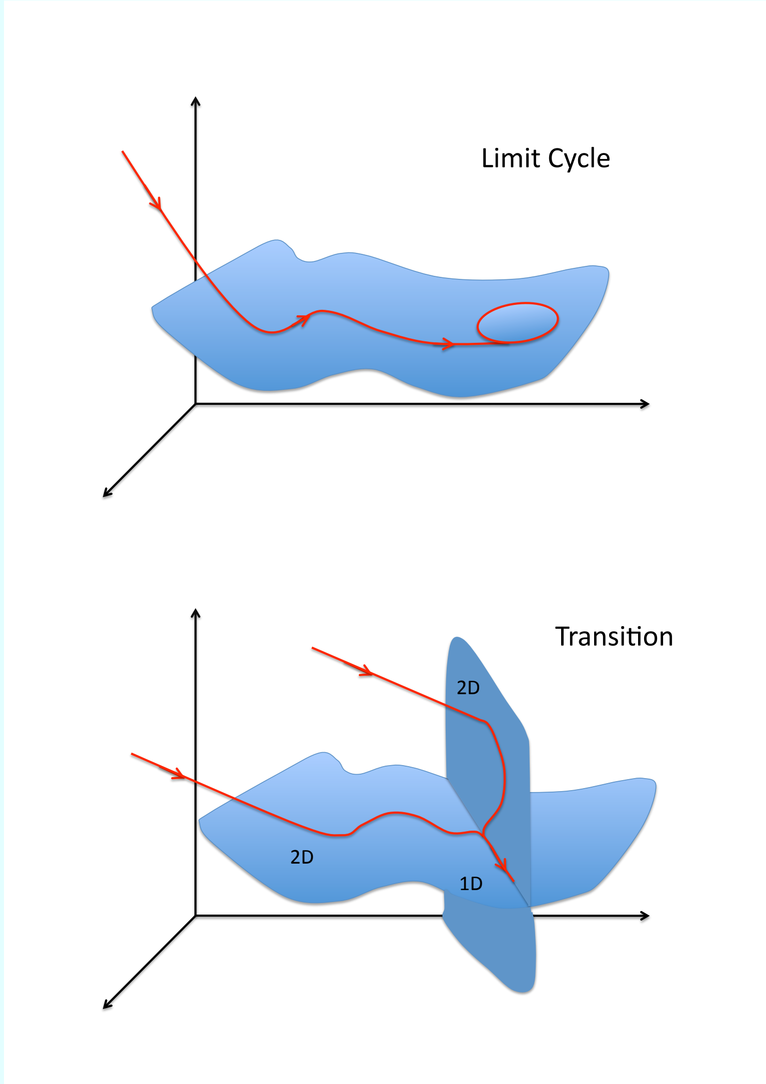
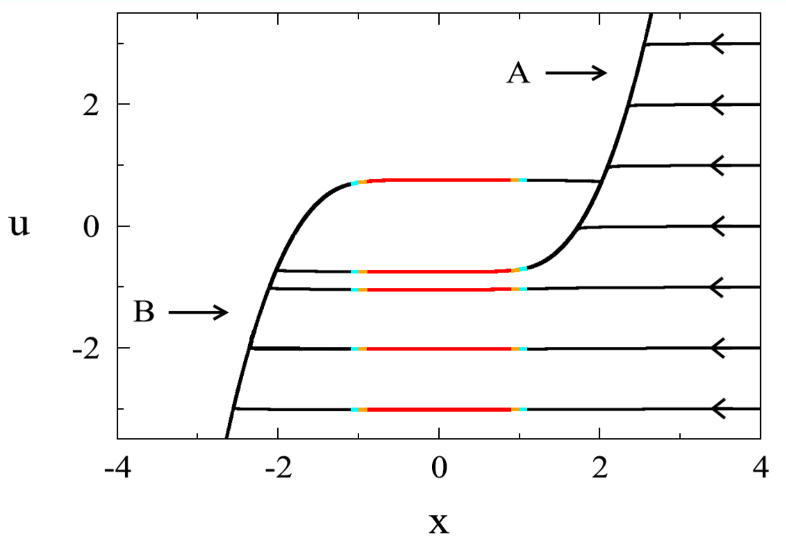
Structures in tangent space





Structures in tangent space

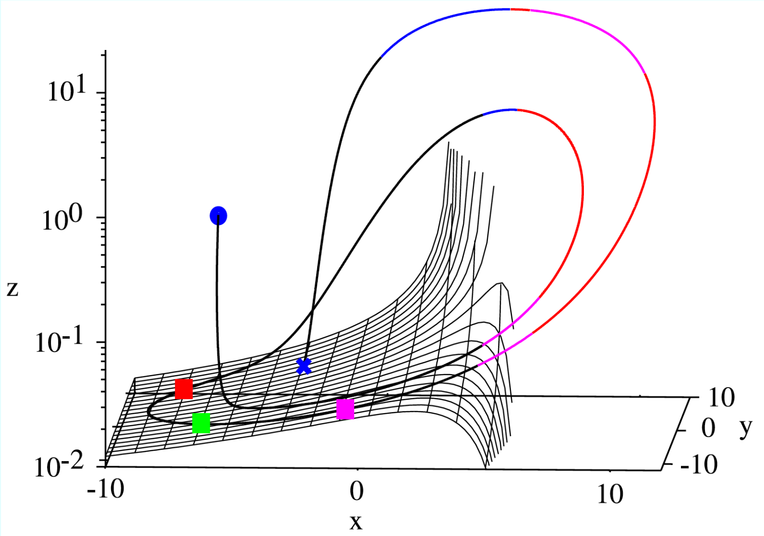
van der Pol



$$\frac{du}{dt} = -x$$

$$\frac{dx}{dt} = \frac{1}{\varepsilon}\left(u - x - \frac{x^3}{3}\right)$$

Rossler

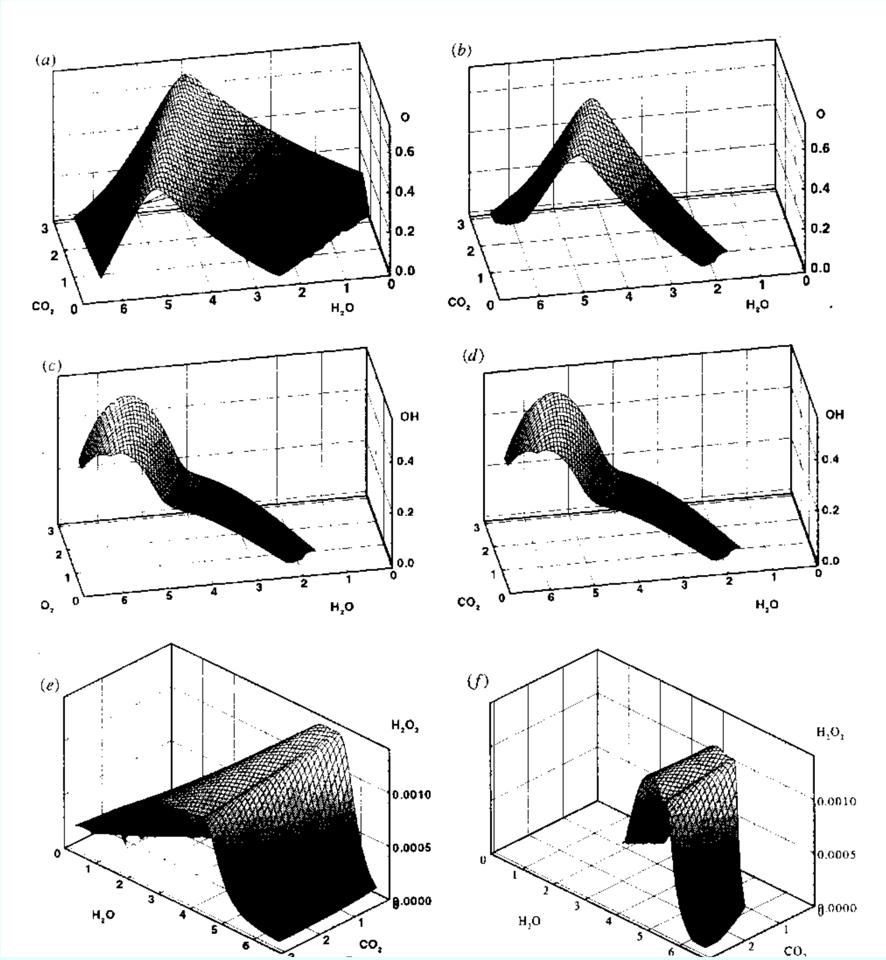


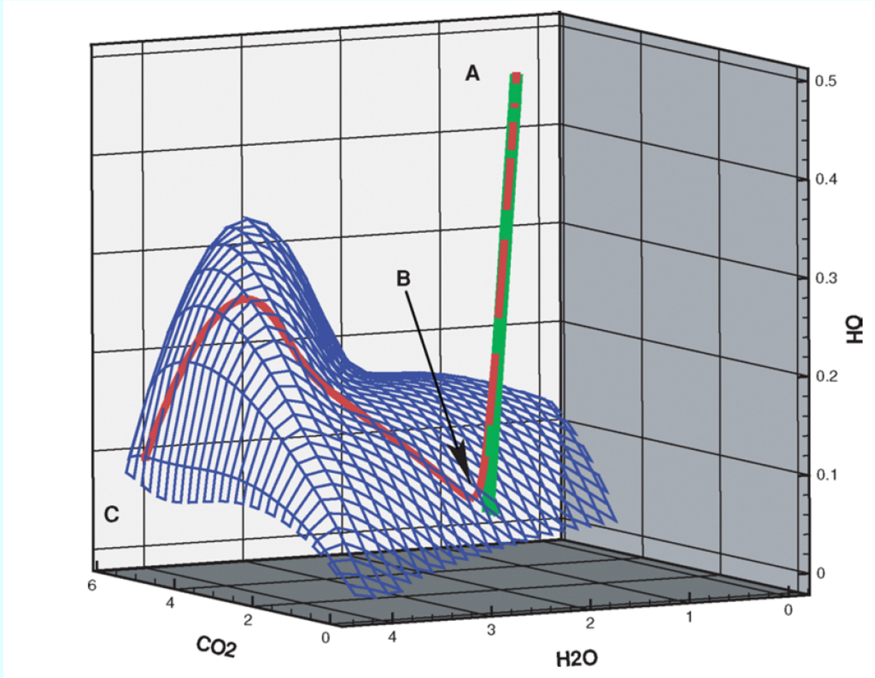
$$\frac{dx}{dt} = -y - z$$

$$\frac{dy}{dt} = x + \mathrm{a}y$$

$$\frac{dz}{dt} = b + \mathrm{z}(\mathrm{x} - \mathrm{c})$$

Structures in tangent space





Bykov & Maas, CTM 2007

Model reduction

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = [\mathbf{a}_1 \;\; .. \;\; \mathbf{a}_M]\left(\begin{bmatrix}\mathbf{b}^1\\ :\\ \mathbf{b}^M\end{bmatrix}\mathbf{g}(\mathbf{y})\right) + [\mathbf{a}_{M+1} \;\; .. \;\; \mathbf{a}_N]\left(\begin{bmatrix}\mathbf{b}^{M+1}\\ :\\ \mathbf{b}^N\end{bmatrix}\mathbf{g}(\mathbf{y})\right) = \mathbf{a}_r\mathbf{f}^r + \mathbf{a}_s\mathbf{f}^s$$

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$$\mathbf{f}^r = \mathbf{b}^r\mathbf{g}(\mathbf{y})$$

$$\mathbf{f}^s = \mathbf{b}^s\mathbf{g}(\mathbf{y})$$

Reduced model

$$\mathbf{f}^r \approx 0$$ ← Structures in tangent space

$$\frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s\mathbf{f}^s$$ ← Slow model

Problems

1. Complex structures
2. Variation of M with time/space
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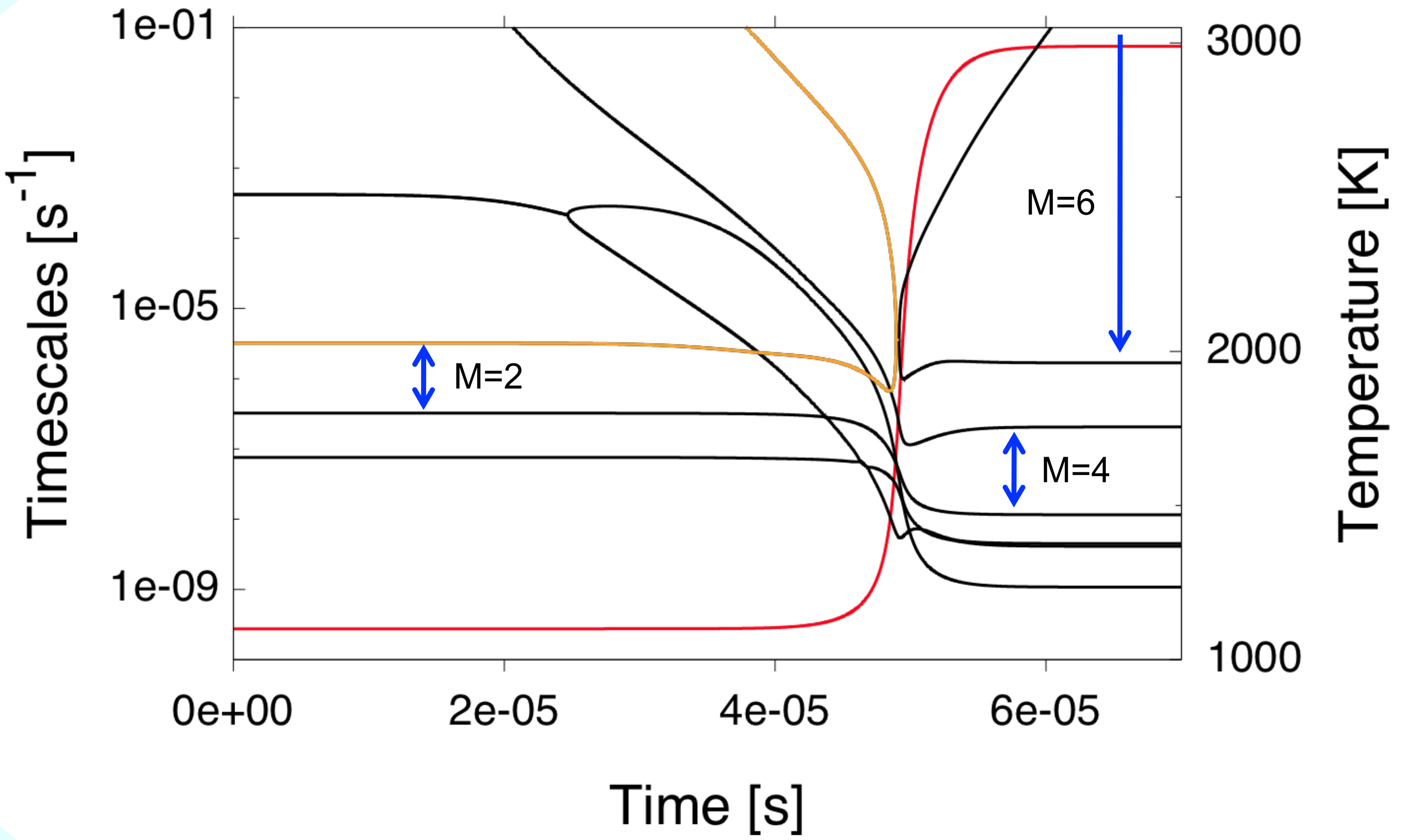
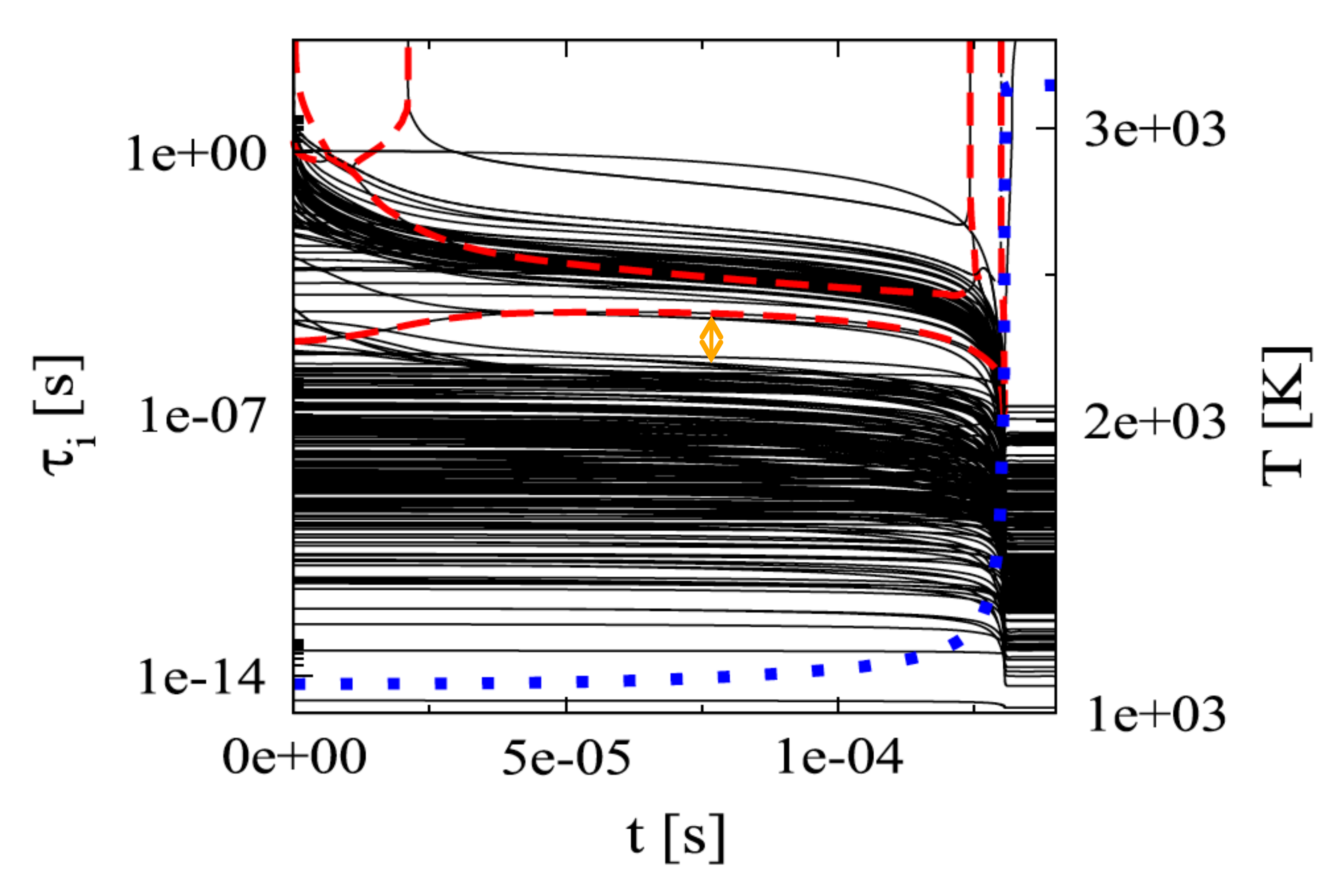
Number of fast time scales H_2/air



Explosive/Dissipative Temperature

PhD thesisKourdis 2013

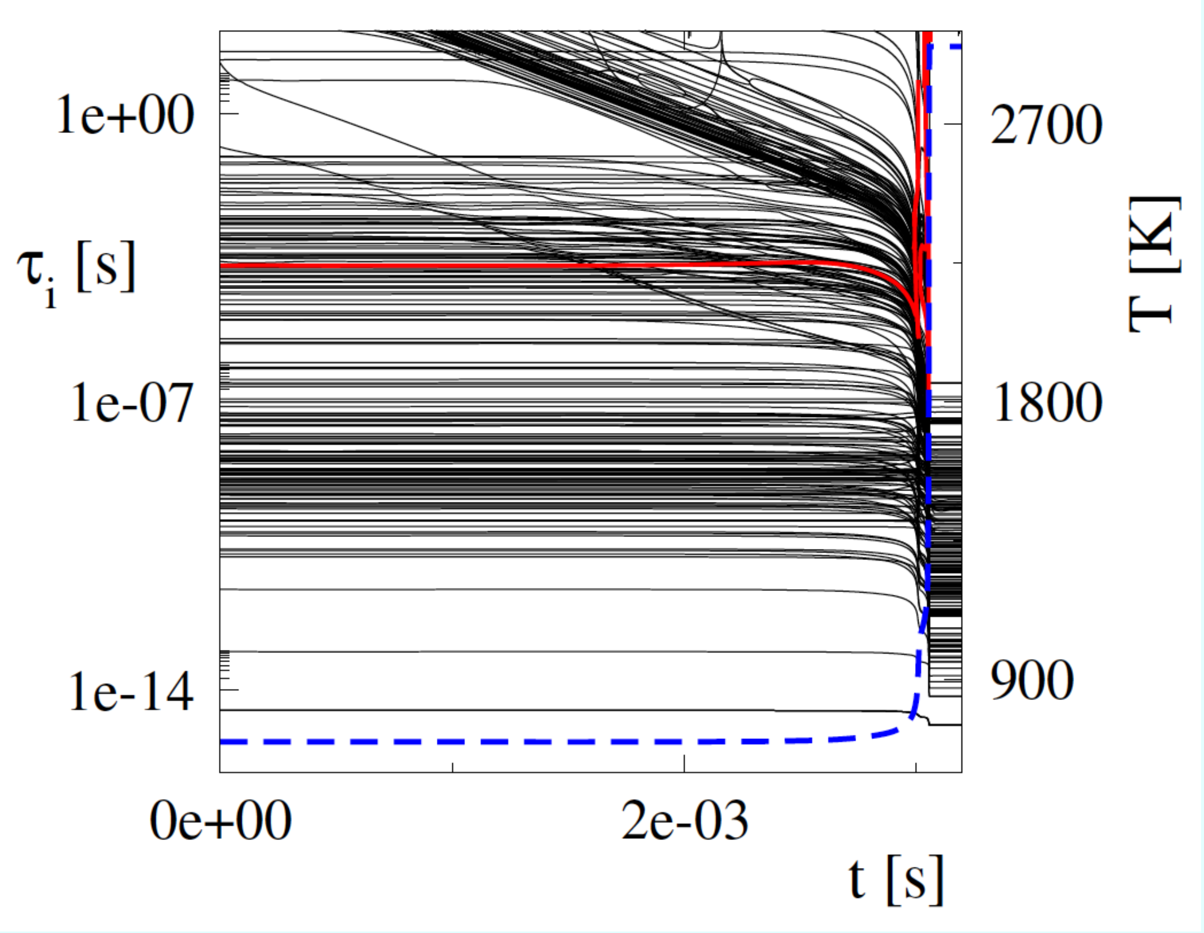
Number of fast time scales DME/air (1100K)



Explosive/Dissipative Temperature

Tigas et al C&F 2015

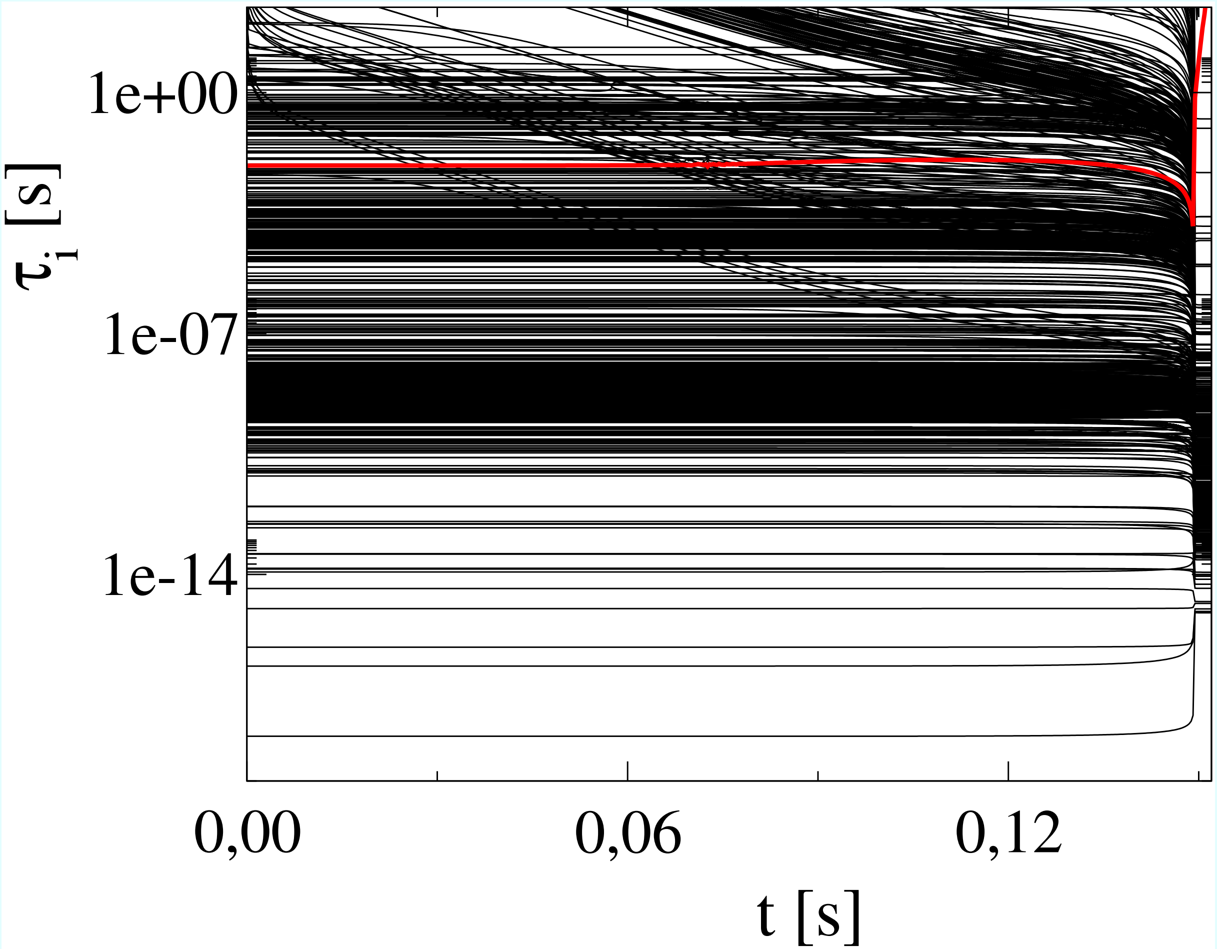
Number of fast time scales   DME/air (900K)



Explosive/Dissipative   Temperature

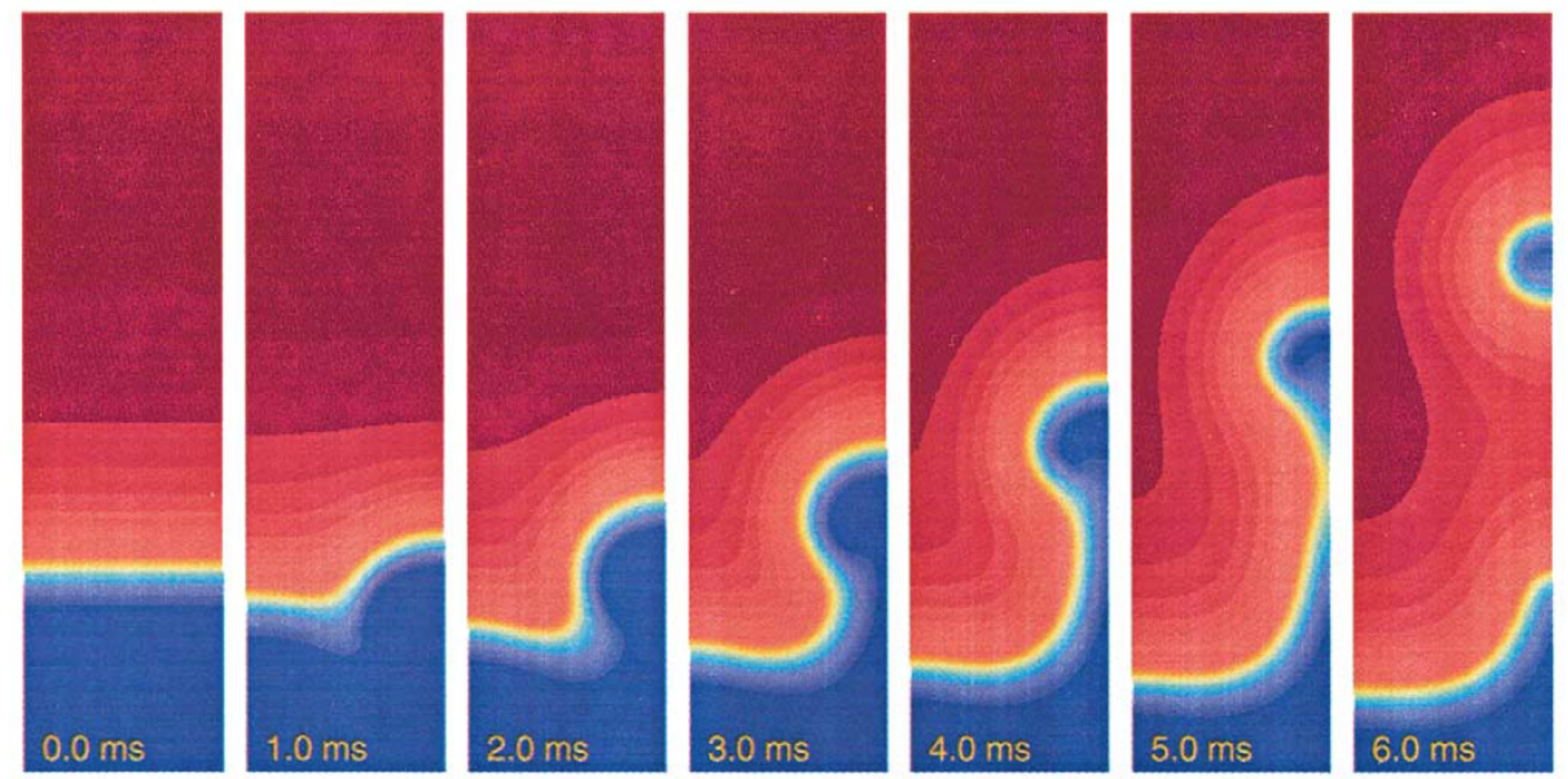
Tigas et al Fuel 2015

Number of fast time scales n-hexane/air (600K)



Explosive/Dissipative Temperature

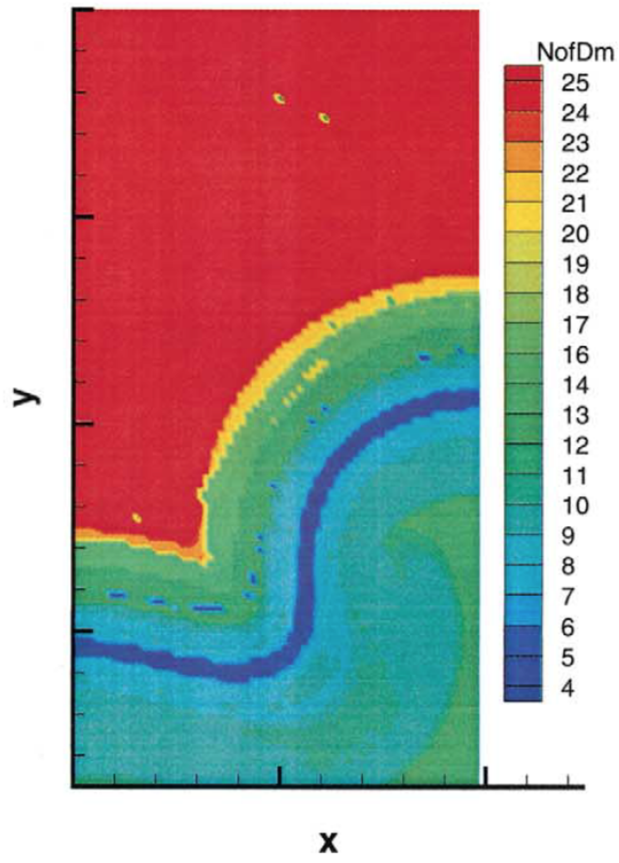
Number of fast time scales CH_4/air



Temperature

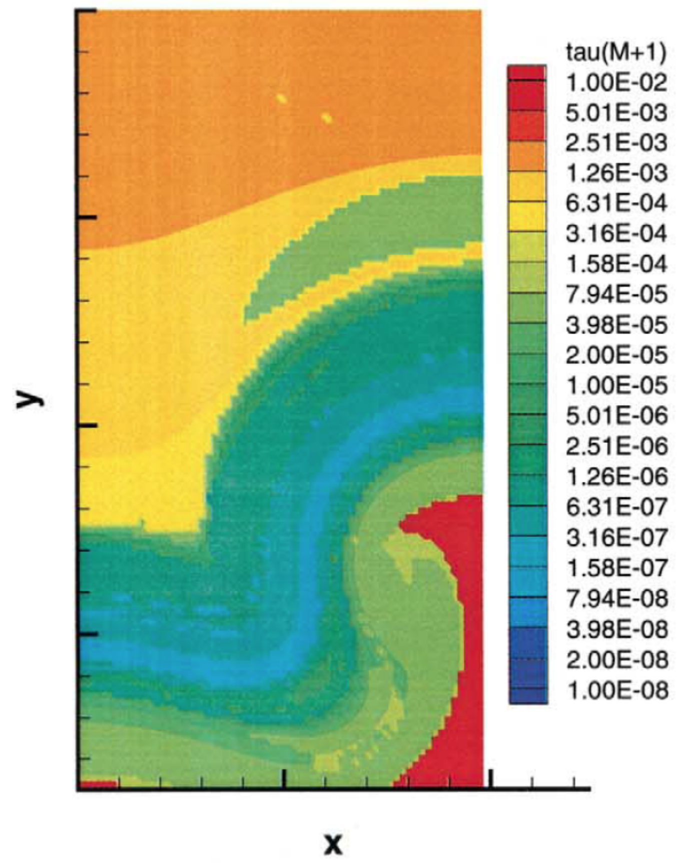
Valorani et al, C&F 2003

Number of fast time scales CH_4/air



(a) Time 1.8 ms

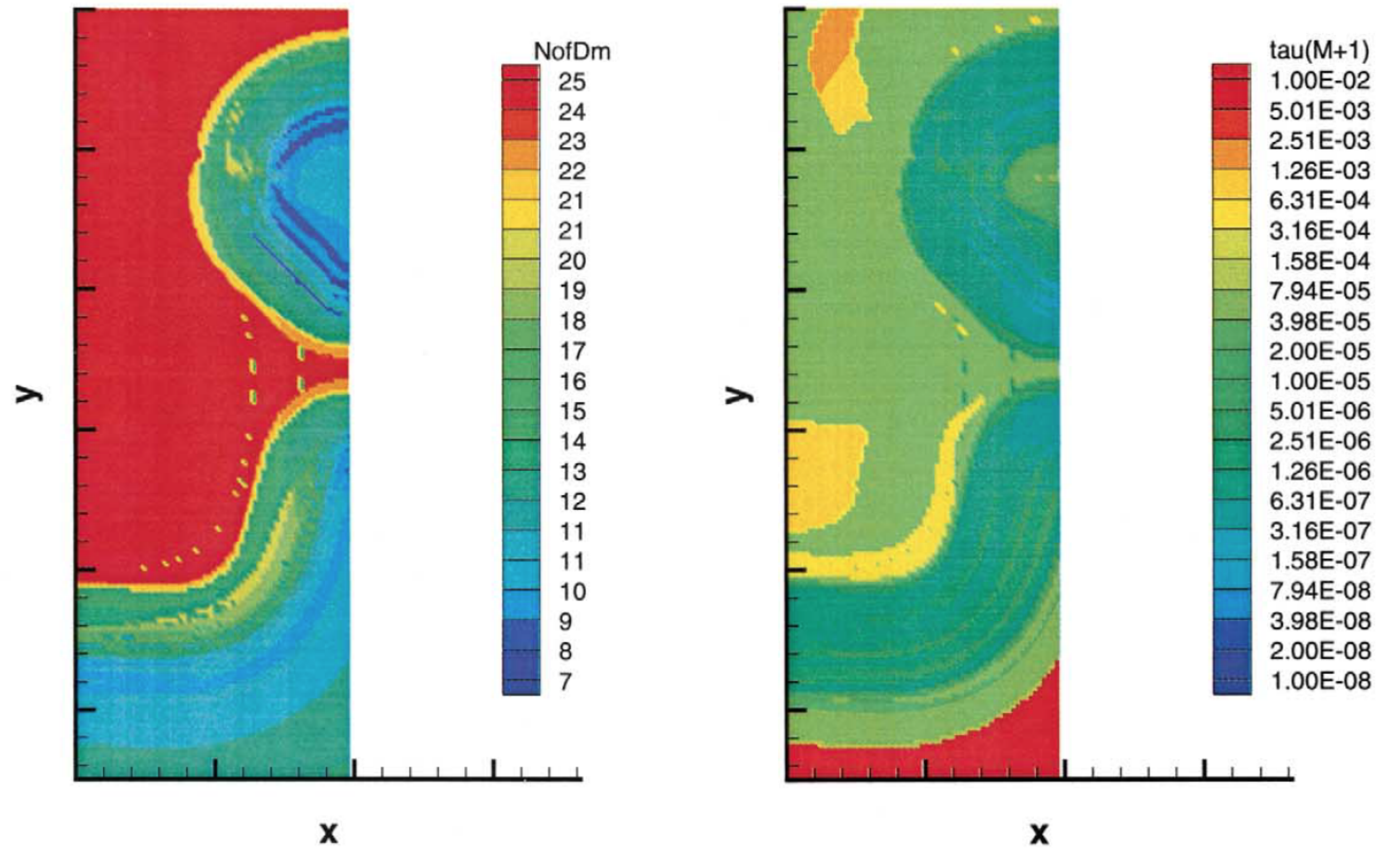
No. of fast time scales



(a) Time 1.8 ms

Characteristic time scale

Number of fast time scales CH_4/air



(b) Time 5.0 ms

(b) Time 5.0 ms

No. of fast time scales

Characteristic time scale

Model reduction

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = [\mathbf{a}_1 \;\; .. \;\; \mathbf{a}_M]\left(\begin{bmatrix}\mathbf{b}^1 \\ : \\ \mathbf{b}^M\end{bmatrix}\mathbf{g}(\mathbf{y})\right) + [\mathbf{a}_{M+1} \;\; .. \;\; \mathbf{a}_N]\left(\begin{bmatrix}\mathbf{b}^{M+1} \\ : \\ \mathbf{b}^N\end{bmatrix}\mathbf{g}(\mathbf{y})\right) = \mathbf{a}_r\mathbf{f}^r + \mathbf{a}_s\mathbf{f}^s$$

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$$\mathbf{f}^r = \mathbf{b}^r\mathbf{g}(\mathbf{y})$$

$$\mathbf{f}^s = \mathbf{b}^s\mathbf{g}(\mathbf{y})$$

Reduced model

$$\mathbf{f}^r \approx 0$$ ← Structures in tangent space

$$\frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s\mathbf{f}^s$$ ← Slow model

Problems

1. Complex structures
2. Variation of M with time/space
3. Evaluation of $\mathbf{a}_i$
4. Solving the algebraic eqs.

Finding the fast and slow basis vectors

Fenichel, Indiana Univ. Math. J., 23:1109-1137 (1971)
J. Differential Equations, 31:53-98 (1979)

Lam and Goussis CSP (1988)

Maas and Pope ILDM (1992)

Valorani et al. NTDB (2006)

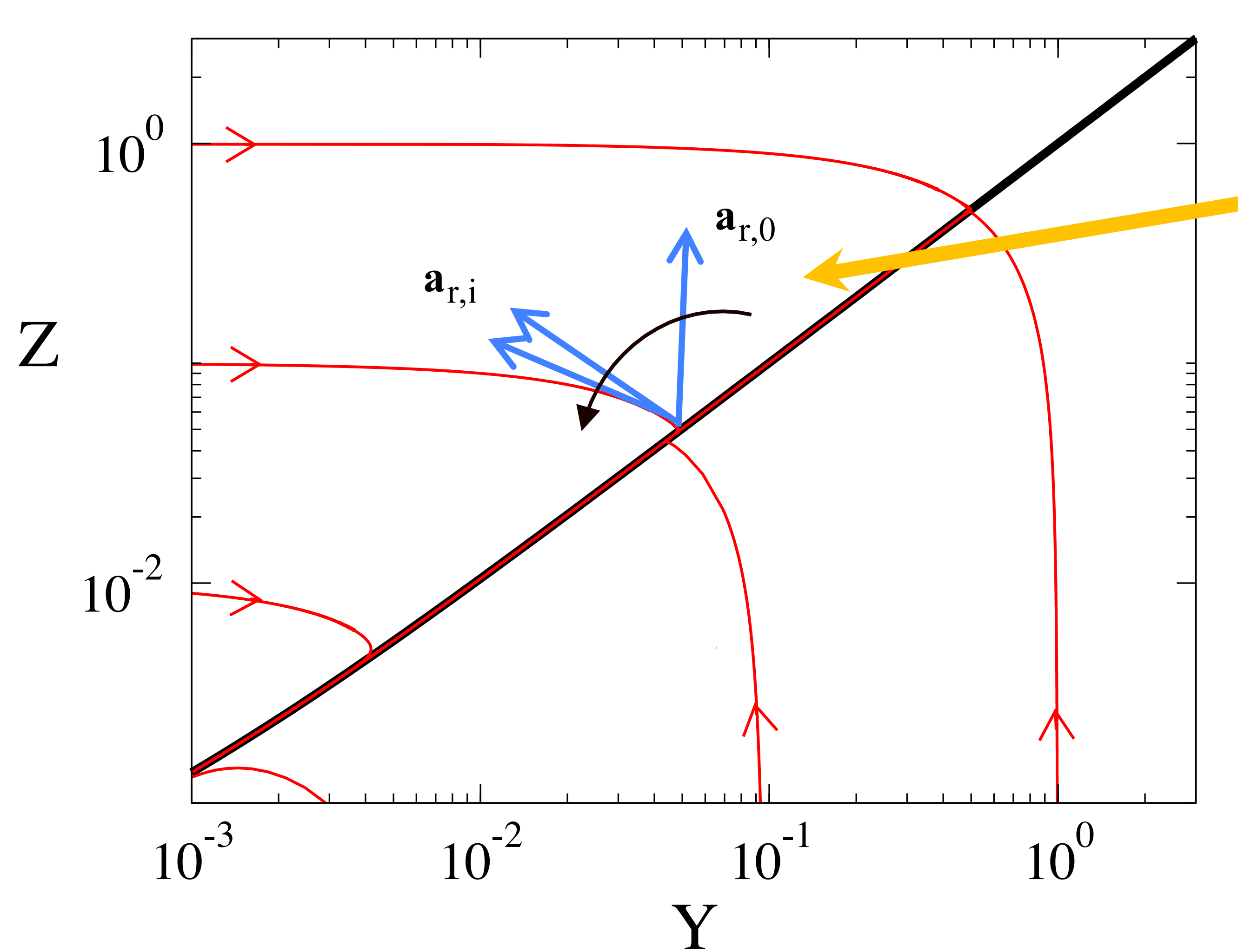
Roussel and Fraser (1988) [Goussis and Valorani (2006)]

Gear and Kevrekidis (2005) [Zagaris, Kaper and Kaper (2005)]

Gorban and Karlin (2003)

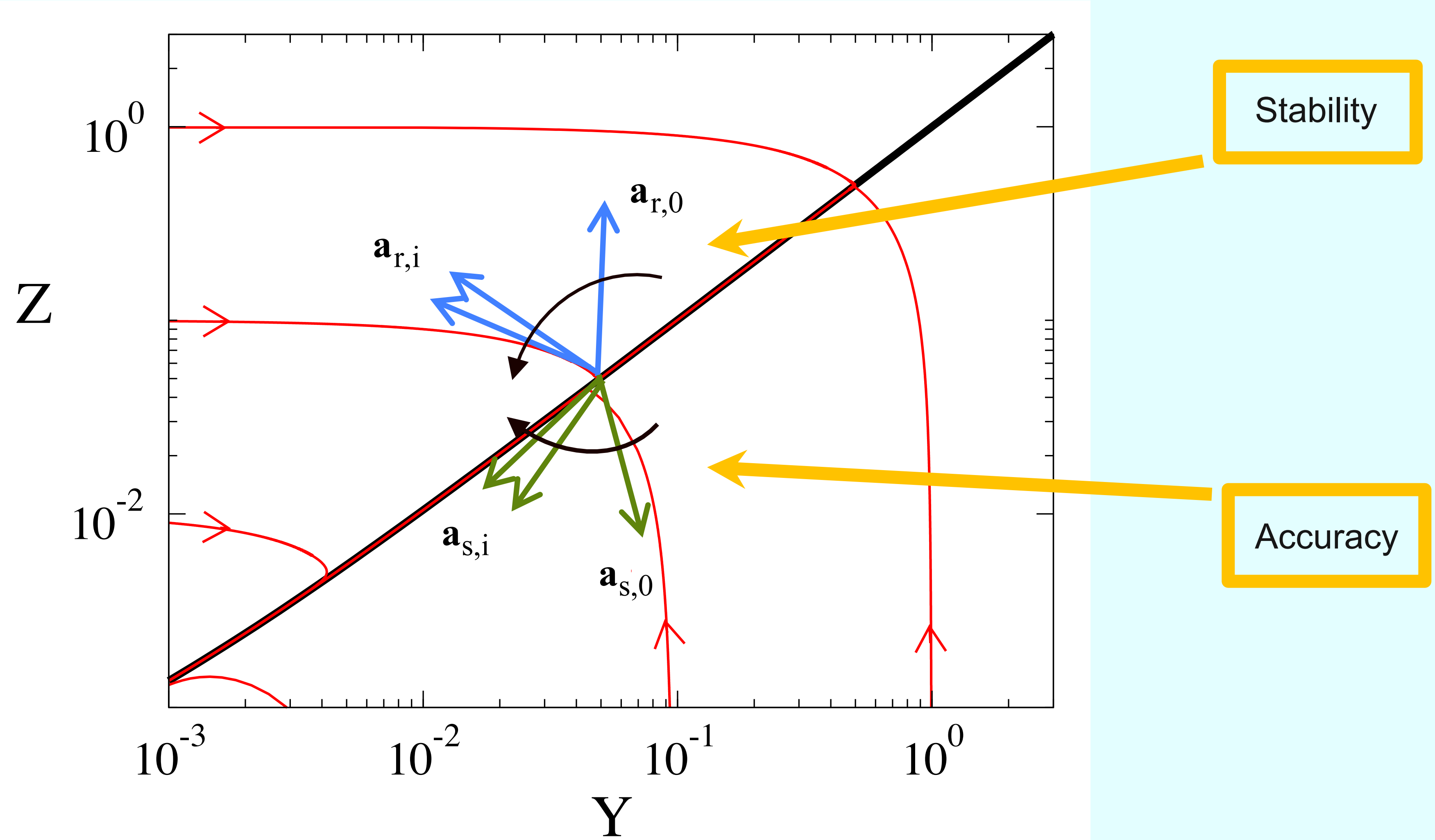
Contou and Daoutidis (2008)

Computing the fast and slow basis vectors



Stability

Computing the fast and slow basis vectors



Model reduction

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$$\mathbf{f}^r = \mathbf{b}^r \mathbf{g}(\mathbf{y})$$

$$\mathbf{f}^s = \mathbf{b}^s \mathbf{g}(\mathbf{y})$$

Reduced model

$$\mathbf{f}^r \approx 0$$

$$\frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s \mathbf{f}^s$$

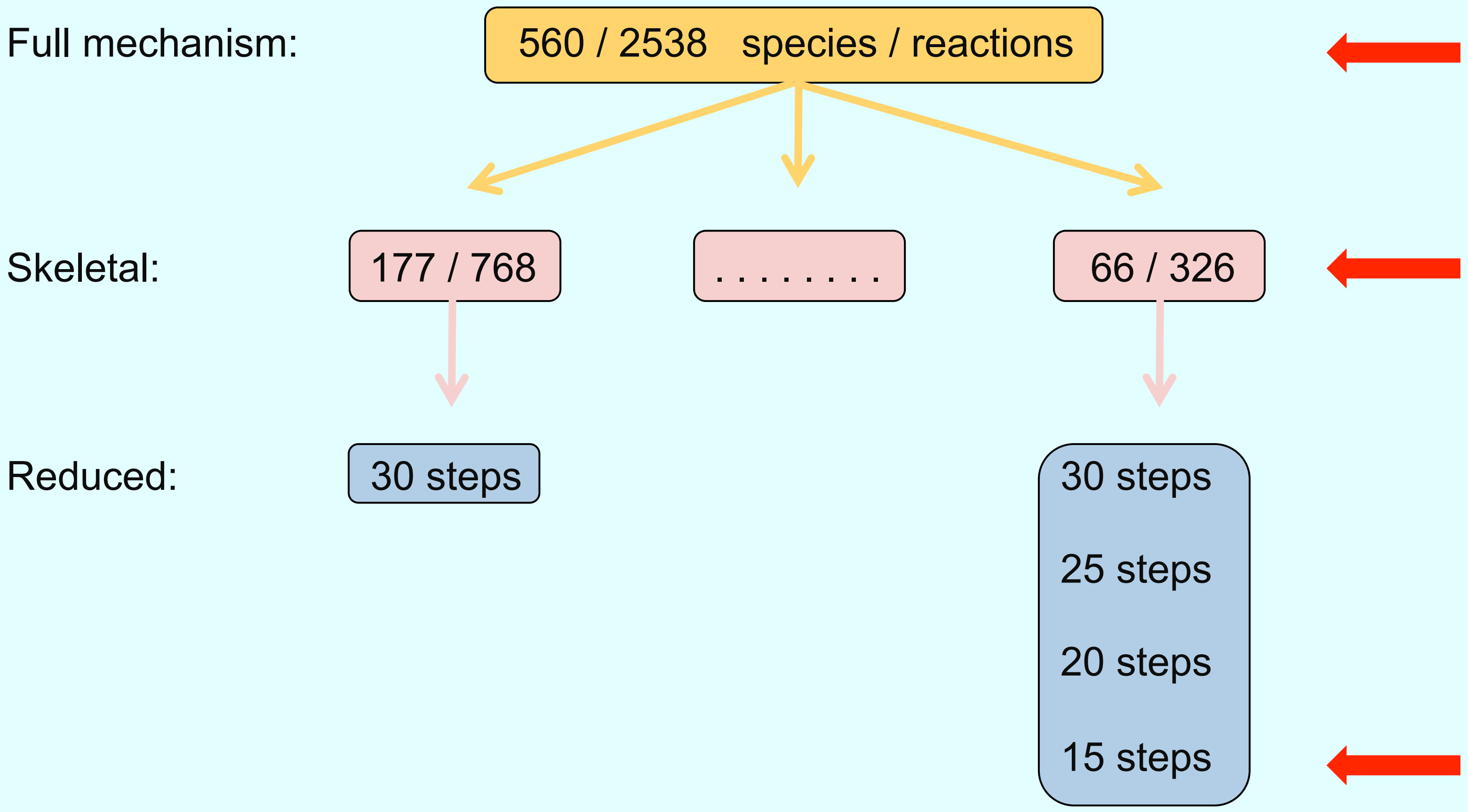
Structures in tangent space

Slow model

Problems

1. Complex structures
2. Variation of M with time/space
3. Evaluation of $\mathbf{a}_i$
4. Solving the algebraic eqs.

n-heptane

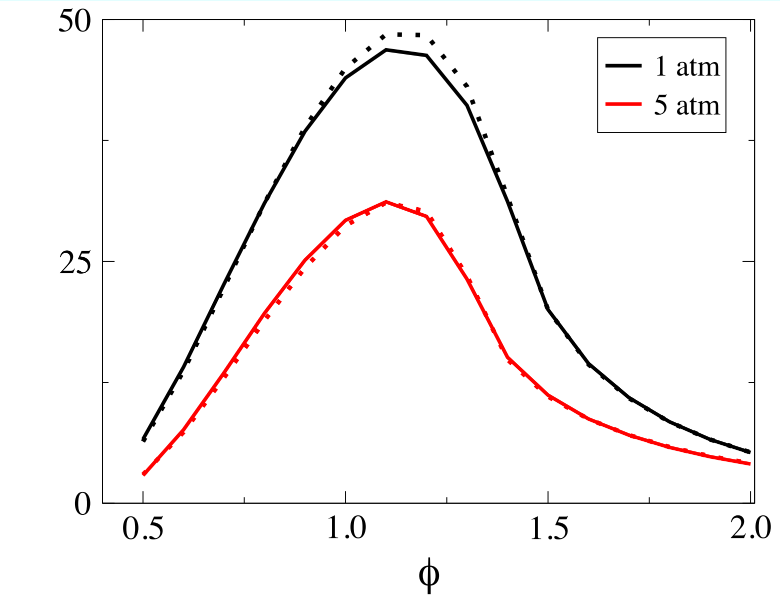


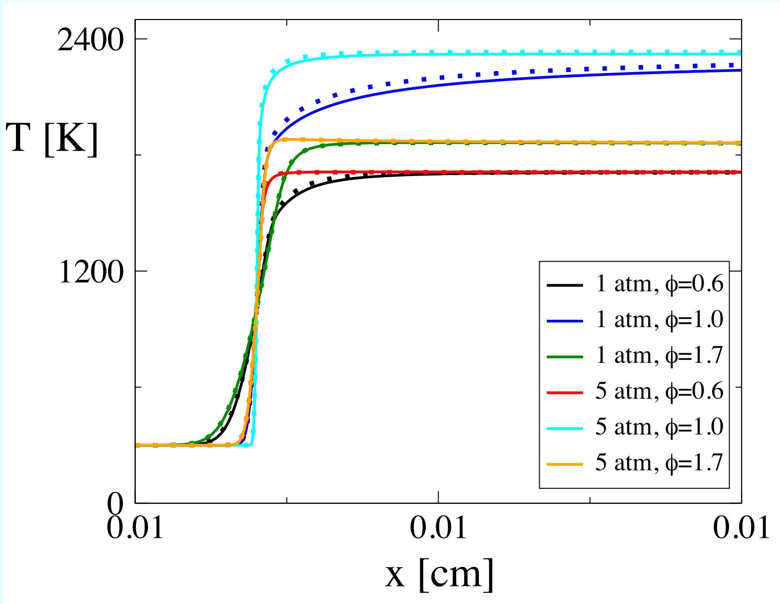
66-15-5 = **46** algebraic relations

Constant basis vectors

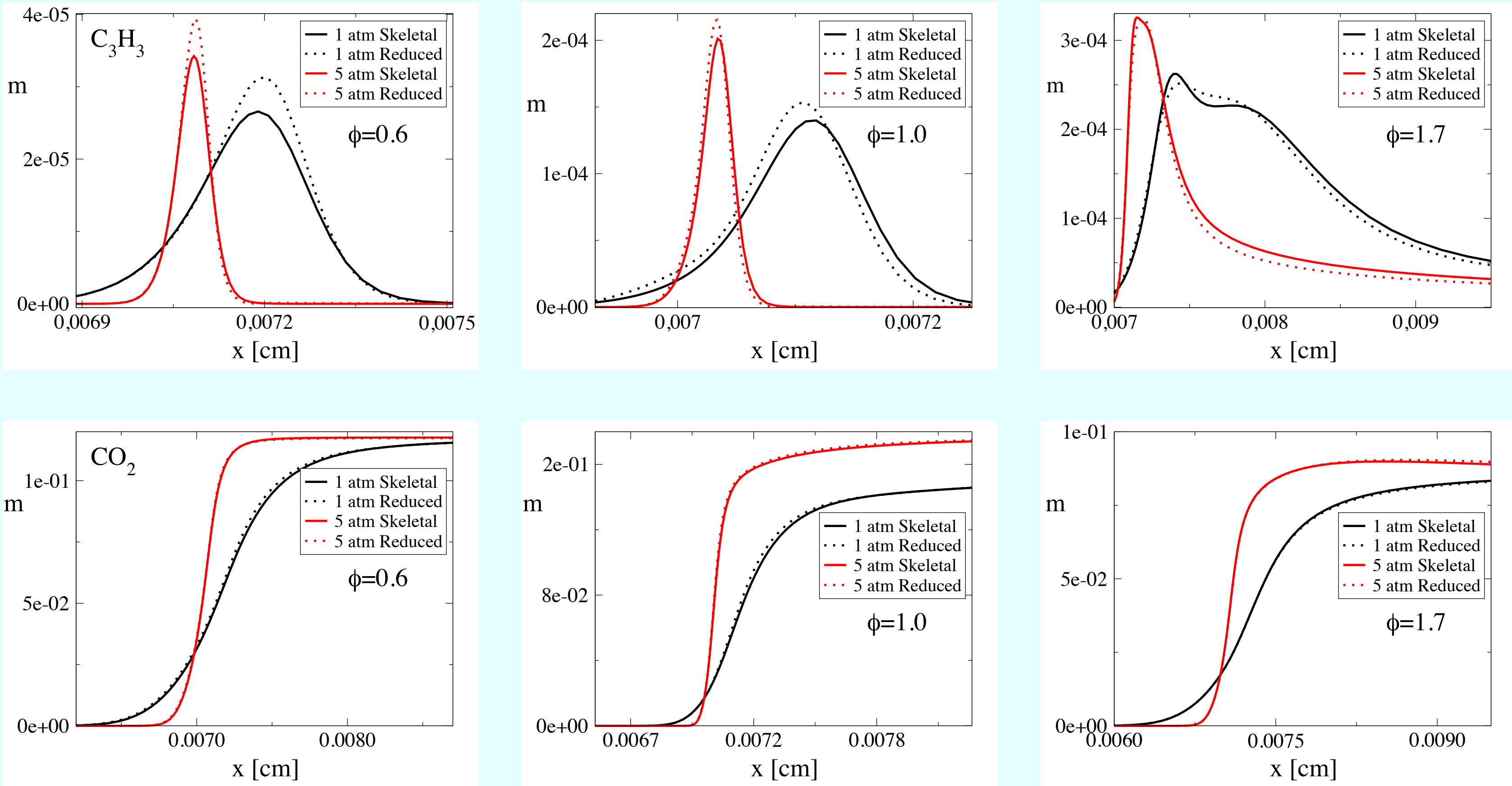
Tigas MsThesis 2014

Premixed flames: skeletal vs reduced

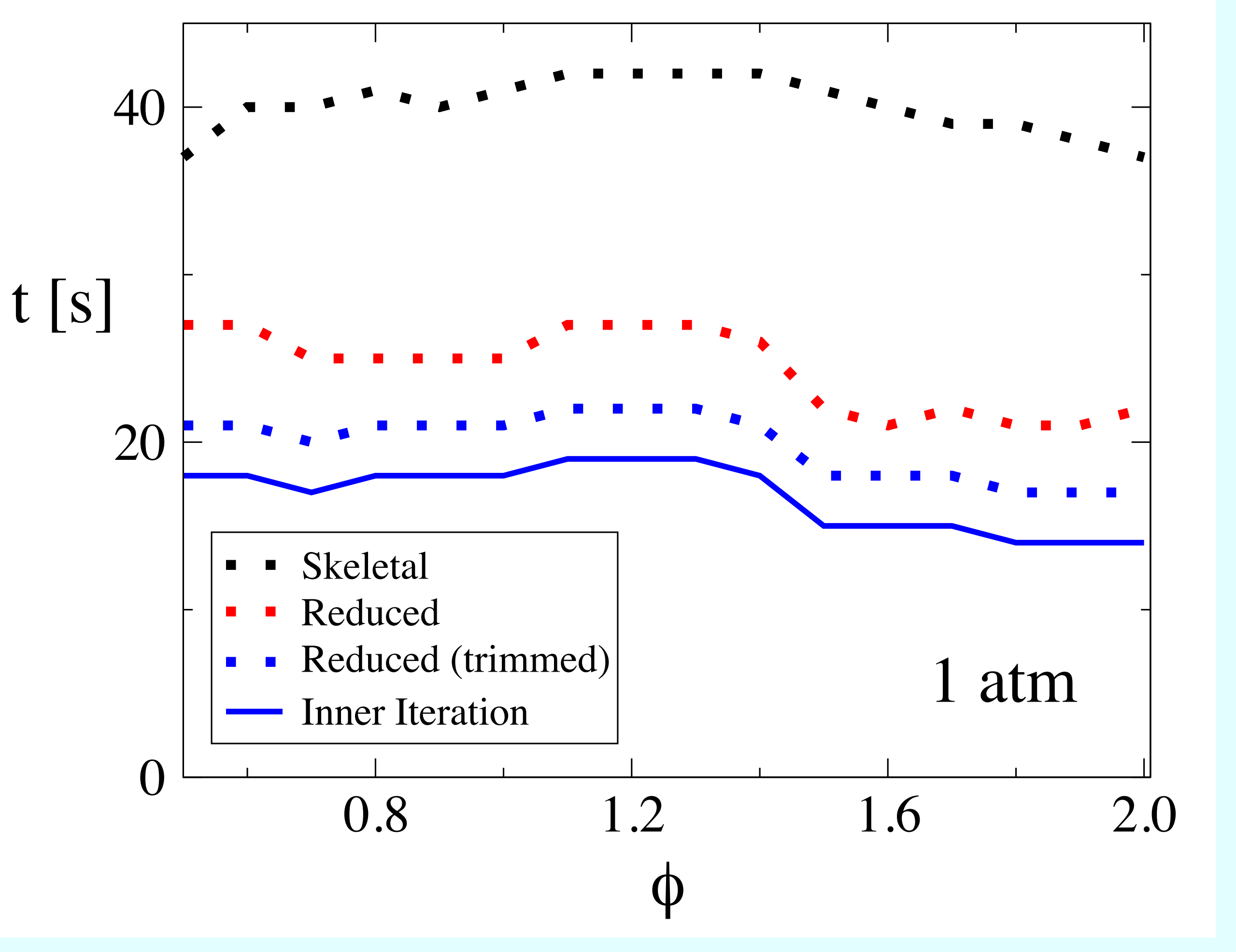




Premixed flames: skeletal vs reduced



Run time



40
20
0
t [s]
0.8
1.2
1.6
2.0
ϕ
Skeletal
Reduced
Reduced (trimmed)
Inner Iteration
1 atm

Model reduction

$$\frac{d\mathbf{y}}{dt} = \mathbf{g}(\mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = [\mathbf{a}_1 \;\; .. \;\; \mathbf{a}_M]\left(\begin{bmatrix}\mathbf{b}^1\\ :\\ \mathbf{b}^M\end{bmatrix}\mathbf{g}(\mathbf{y})\right) + [\mathbf{a}_{M+1} \;\; .. \;\; \mathbf{a}_N]\left(\begin{bmatrix}\mathbf{b}^{M+1}\\ :\\ \mathbf{b}^N\end{bmatrix}\mathbf{g}(\mathbf{y})\right) = \mathbf{a}_r\mathbf{f}^r + \mathbf{a}_s\mathbf{f}^s$$

$$\left|\tau\,\mathbf{a}_r\mathbf{f}^r\right| < \mathbf{y}_{error} = \varepsilon_{rel}\mathbf{y} + \varepsilon_{abs}$$

$$\mathbf{f}^r = \mathbf{b}^r\mathbf{g}(\mathbf{y})$$

$$\mathbf{f}^s = \mathbf{b}^s\mathbf{g}(\mathbf{y})$$

Reduced model

$$\mathbf{f}^r \approx 0$$

$$\frac{d\mathbf{y}}{dt} \approx \mathbf{a}_s\mathbf{f}^s$$

← Structures in tangent space

← Slow model

Problems

1. Complex structures
2. Variation of M with time/space
3. Evaluation of $\mathbf{a}_i$
4. Solving the algebraic eqs.

Diagnostics

$$\frac{d\mathbf{y}}{dt} = \mathbf{S}_1 R^1 + \mathbf{S}_2 R^2 + \ldots + \mathbf{S}_K R^K = \mathbf{g}(\mathbf{y})$$

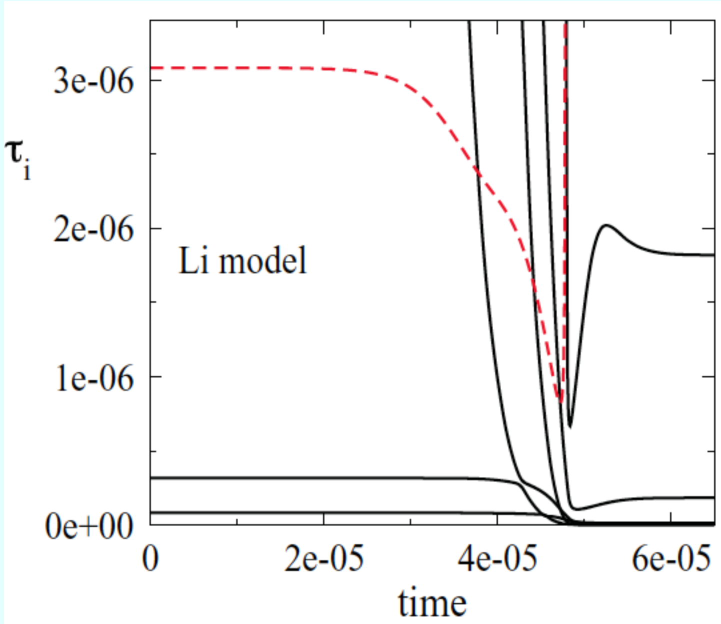
$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_r \mathbf{f}^r + \mathbf{a}_s \mathbf{f}^s = \underbrace{\left(\mathbf{a}_1 f^1 + \ldots + \mathbf{a}_M f^M\right)}_{=0} + \left(\mathbf{a}_{M+1} f^{M+1} + \ldots + \mathbf{a}_N f^N\right) \qquad f^i = \mathbf{b}^i . \mathbf{g}$$

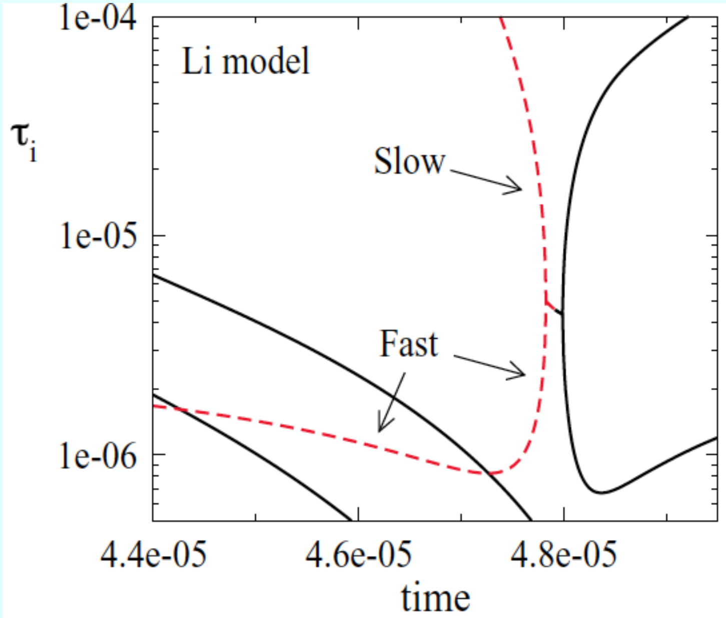
$$f^i = \left(\mathbf{b}^i . \mathbf{S}_1\right) R^1 + \left(\mathbf{b}^i . \mathbf{S}_2\right) R^2 + \ldots + \left(\mathbf{b}^i . \mathbf{S}_K\right) R^K = 0 \qquad i = 1, M$$

$$f^i = \left(\mathbf{b}^i . \mathbf{S}_1\right) R^1 + \left(\mathbf{b}^i . \mathbf{S}_2\right) R^2 + \ldots + \left(\mathbf{b}^i . \mathbf{S}_K\right) R^K \neq 0 \qquad i = M+1, N$$

$$\tau_i = \left(\mathbf{b}^i . \mathbf{S}_1\right)\left(\nabla R^1 . \mathbf{a}_i\right) + \ldots + \left(\mathbf{b}^i . \mathbf{S}_K\right)\left(\nabla R^K . \mathbf{a}_i\right) \qquad i = 1, N$$

Diagnostics: H_2/air autoignition



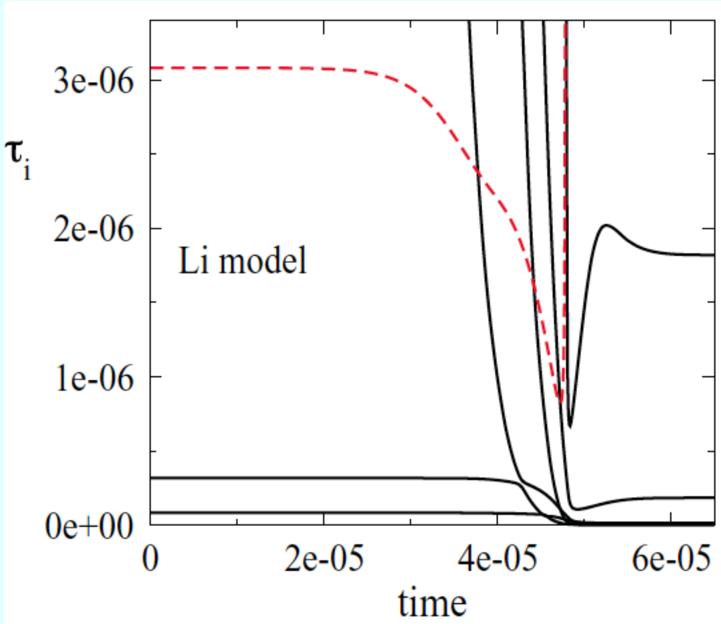


$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_r \mathbf{f}^r + \mathbf{a}_s \mathbf{f}^s = \underbrace{\left(\mathbf{a}_1 f^1 + .. + \mathbf{a}_M f^M\right)}_{=\ 0} + \left(\mathbf{a}_{M+1} f^{M+1} + .. + \mathbf{a}_N f^N\right) \qquad f^i = \mathbf{b}^i . \mathbf{g}$$

Explosive mode

Diamantis et al, CTM 2015

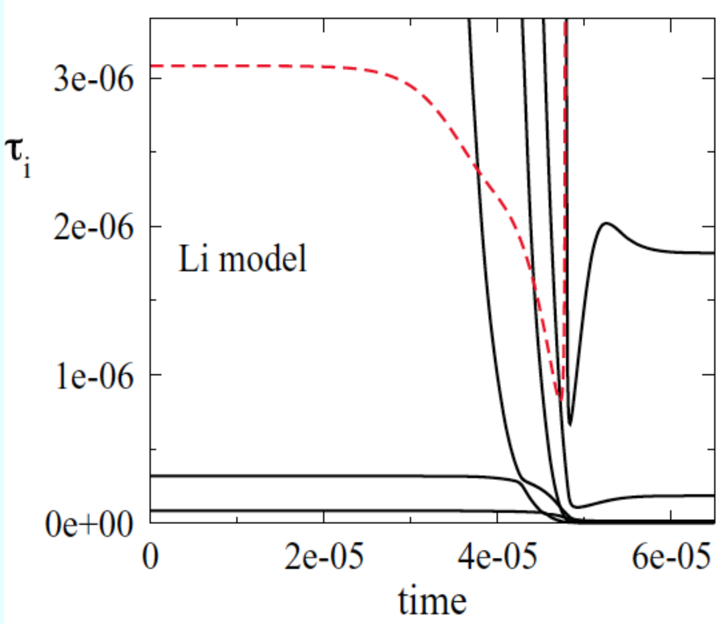
Diagnostics: H_2/air autoignition



	$t = 0.0 \times 10^{-6}$ s $T = 1100$ K $\lambda = 3.245 \times 10^5\ s^{-1}$	$t = 3.0 \times 10^{-6}$ s $T = 1100$ K $\lambda = 3.245 \times 10^5\ s^{-1}$
TPI	$1f$: + 0.6273 $2f$: + 0.0739 $3f$: + 0.0183 $9f$: − 0.2792	$1f$: + 0.6273 $2f$: + 0.0739 $3f$: + 0.0183 $9f$: − 0.2792
API	$10b$: + 1.0000	$1f$: + 0.4987 $10b$: + 0.2100 $2f$: + 0.0543 $3f$: + 0.0138 $9f$: − 0.2220
Po	H: +0.79 O: +0.17 OH: +0.04	H: +0.79 O: +0.17 OH: +0.04

$1f$ – EN	$H + O_2 \rightarrow O + OH$	$1b$ – EX	$H + O_2 \leftarrow O + OH$
$2f$ – EN	$O + H_2 \rightarrow H + OH$	$2b$ – EX	$O + H_2 \leftarrow H + OH$
$3f$ – EX	$OH + H_2 \rightarrow H + H_2O$	$3b$ – EN	$OH + H_2 \leftarrow H + H_2O$
$8f$ – EX	$H + OH(+M) \rightarrow H_2O(+\ M)$	$9f$ – EX	$H + O_2(+M) \rightarrow HO_2(+\ M)$
$10f$ – EX	$H + HO_2 \rightarrow H_2 + O_2$	$10b$ – EN	$H + HO_2 \leftarrow H_2 + O_2$
$11f$ – EX	$H + HO_2 \rightarrow OH + OH$		

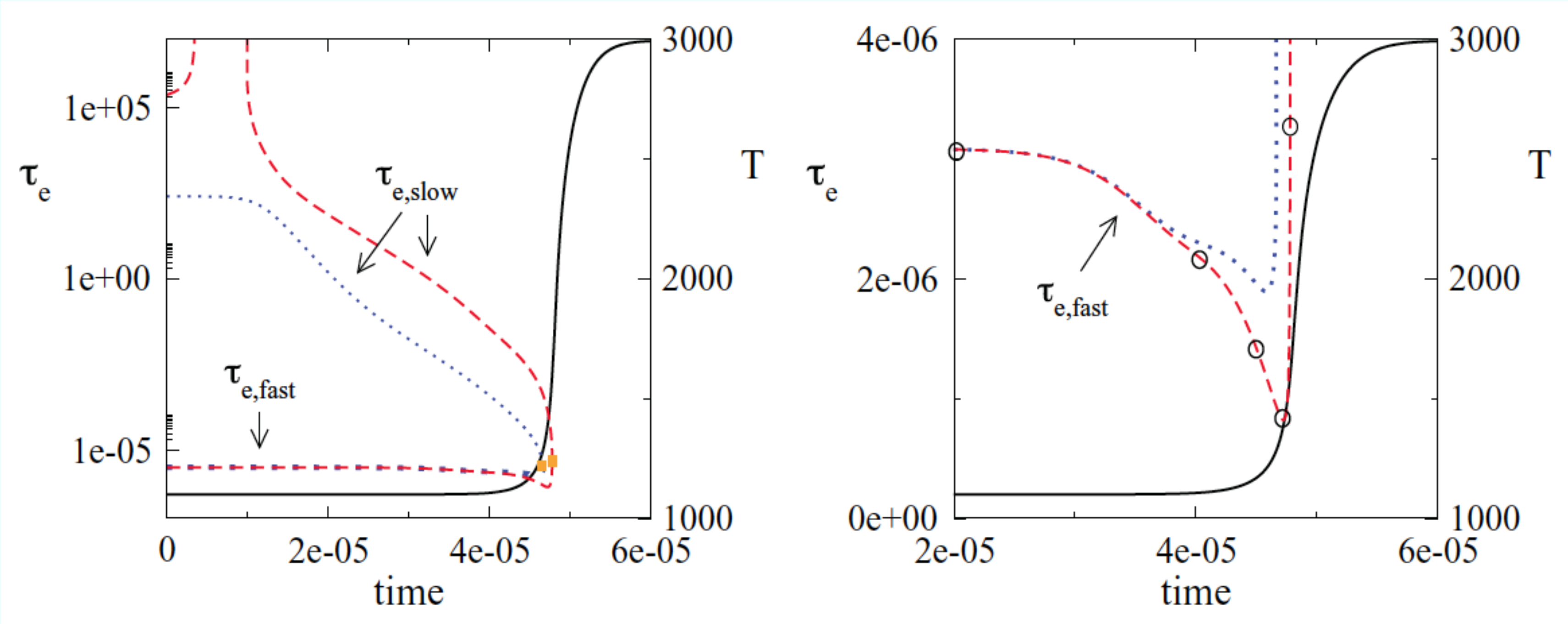
Diagnostics: H_2/air autoignition



	$t = 2.000 \times 10^{-5}$ s, $T = 1100$ K, $\lambda = 3.251 \times 10^{5}$ s^{-1}	$t = 4.500 \times 10^{-5}$ s, $T = 1168$ K, $\lambda = 7.014 \times 10^{5}$ s^{-1}	$t = 4.782 \times 10^{-5}$ s, $T = 1593$ K, $\lambda = 3.043 \times 10^{5}$ s^{-1}
TPI	1*f*: + 0.6265 2*f*: + 0.0740 3*f*: + 0.0184 9*f*: − 0.2785	1*f*: + 0.5959 2*f*: + 0.1430 3*f*: + 0.0886 11*f*: + 0.0543 10*f*: − 0.0316 1*b*: − 0.0304 8*f*: − 0.0210	1*f*: + 0.2652 2*f*: + 0.1607 3*f*: + 0.0569 8*f*: + 0.0277 1*b*: − 0.1581 2*b*: − 0.1244 3*b*: − 0.0853
API	1*f*: + 0.6265 2*f*: + 0.0740 3*f*: + 0.0184 9*f*: − 0.2785	1*f*: + 0.5823 2*f*: + 0.1408 3*f*: + 0.0972 11*f*: + 0.0723 10*f*: − 0.0414 1*b*: − 0.0173 8*f*: − 0.0126	1*f*: + 0.3389 2*f*: + 0.1646 3*f*: + 0.1432 9*f*: + 0.0704 8*f*: + 0.0598 1*b*: − 0.0838 2*b*: − 0.0515 3*b*: − 0.0366
Po	H: +0.79 O: +0.17	H: +0.65 *T*: +0.19 O: +0.13	*T*: +3.50 O_2: −2.60 H_2O: −2.45

1*f* – EN	$H + O_2 \rightarrow O + OH$	1*b* – EX	$H + O_2 \leftarrow O + OH$
2*f* – EN	$O + H_2 \rightarrow H + OH$	2*b* – EX	$O + H_2 \leftarrow H + OH$
3*f* – EX	$OH + H_2 \rightarrow H + H_2O$	3*b* – EN	$OH + H_2 \leftarrow H + H_2O$
8*f* – EX	$H + OH(+M) \rightarrow H_2O(+M)$	9*f* – EX	$H + O_2(+M) \rightarrow HO_2(+M)$
10*f* – EX	$H + HO_2 \rightarrow H_2 + O_2$	10*b* – EN	$H + HO_2 \leftarrow H_2 + O_2$
11*f* – EX	$H + HO_2 \rightarrow OH + OH$		

Diagnostics: H_2/air autoignition



Chemical vs thermal runaway regime

Algorithms

1. Computational Singular Perturbation (CSP)
2. Intrinsic Low-Dimensional Manifolds (ILDM)
3. In Situ Adaptive Tabulation (ISAT)
4. Reaction Diffusion Manifolds (REDIM)

CSP: *Proc. Combust. Inst., 22:931-941 (1988), Int. J. Chem. Kinet., 26:461-486 (1994)*

ISAT: *Combust. Theory Model., 1:41-63 (1977), J. Comp. Phys., 228:361-386 (2009)*

ILDM: *Proc. Combust. Inst., 24:103-112 (1992), Proc. Combust. Inst., 25:1349-1356 (1994)*

REDIM: *Proc. Combust. Inst., 31:465-472 (2007), Proc. Combust. Inst., 34:197-203 (2013)*

Computational Singular Perturbation (CSP) algorithm

$$\mathbf{a}_r^o = [\mathbf{a}_1^o \; . \; . \; . \; \mathbf{a}_N^o] \qquad \mathbf{a}_s^o = [\mathbf{a}_{M+1}^o \; . \; . \; . \; \mathbf{a}_N^o]$$

$$\mathbf{b}_o^r = \begin{bmatrix} \mathbf{b}_o^1 \\ : \\ \mathbf{b}_o^M \end{bmatrix} \qquad \mathbf{b}_o^s = \begin{bmatrix} \mathbf{b}_o^{M+1} \\ : \\ \mathbf{b}_o^N \end{bmatrix}$$

$$\begin{bmatrix} \mathbf{b}_o^r \\ \mathbf{b}_o^s \end{bmatrix} \begin{bmatrix} \mathbf{a}_r^o & \mathbf{a}_s^o \end{bmatrix} = \begin{bmatrix} \mathbf{I}_M^M & \mathbf{0}_{N-M}^M \\ \mathbf{0}_N^{N-M} & \mathbf{I}_{N-M}^{N-M} \end{bmatrix}$$

a$_r$ – refinement:

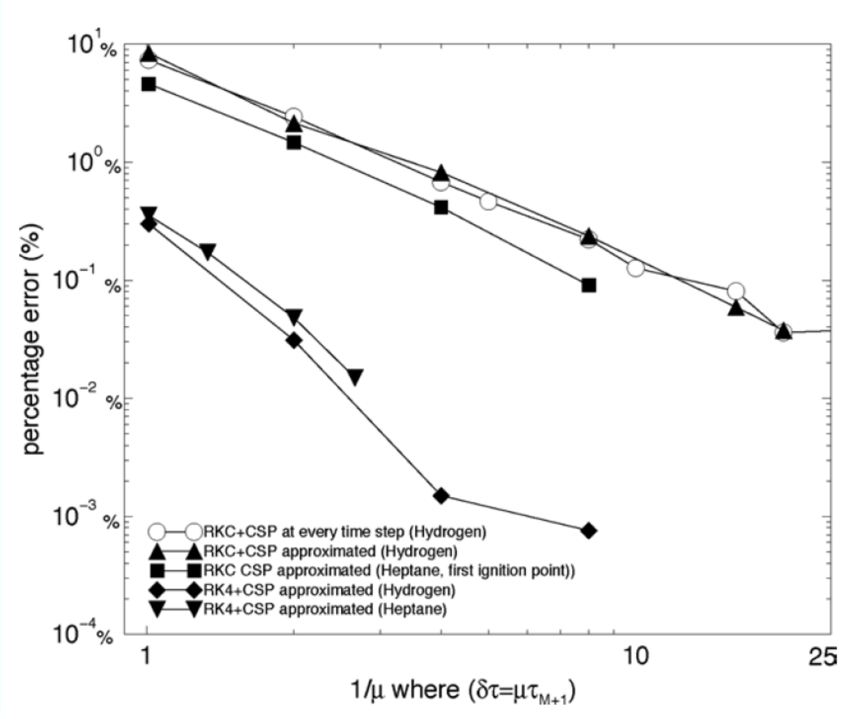
$$\mathbf{a}_r = \left(\frac{d\mathbf{a}_r^o}{dt} + \mathbf{J}\mathbf{a}_r^o \right) \mathbf{k}_\mathrm{r}^\mathrm{r}$$

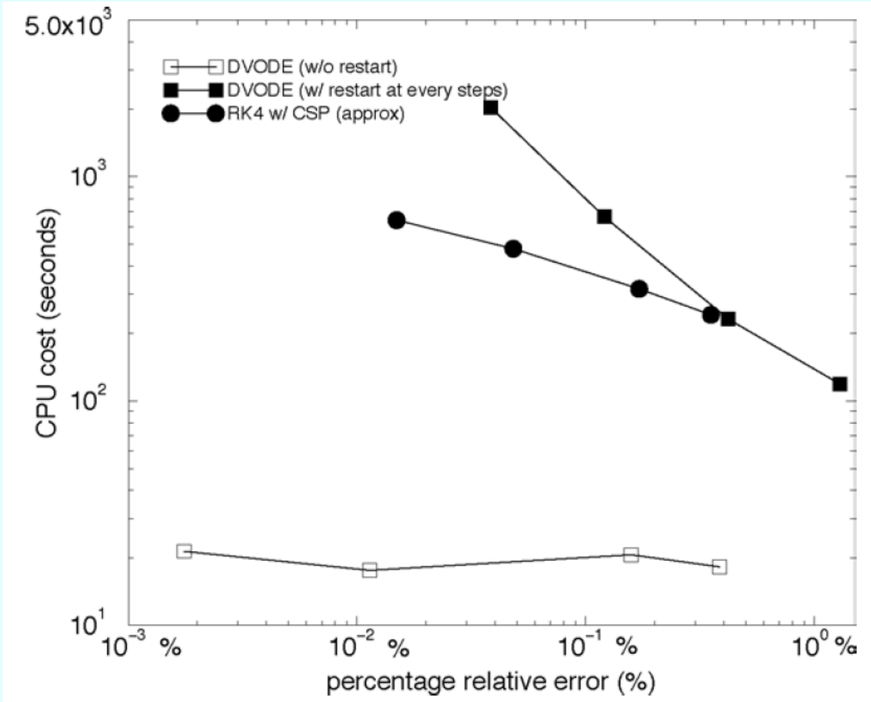
b^r- refinement:

$$\mathbf{b}^r = \mathbf{k}_\mathrm{r}^\mathrm{r} \left(\frac{d\mathbf{b}_o^r}{dt} + \mathbf{b}_o^r \mathbf{J} \right)$$

$$\mathbf{k}_\mathrm{r}^\mathrm{r} = \left[\mathbf{b}_o^r \left(\frac{d\mathbf{a}_r^o}{dt} + \mathbf{J}\mathbf{a}_r^o \right) \right]^{-1}$$

H2/air and n-heptane/air ignition





$$\frac{1}{\mu} = \frac{\tau_{ch}}{\Delta t}$$

Implicit Low Dimensional Manifolds (ILDM) algorithm

$\mathbf{a}_r$ – refinement:

$$\mathbf{a}_r = \left(\frac{d\mathbf{a}_r^o}{dt} + \mathbf{J}\mathbf{a}_r^o \right) \mathbf{k}_\mathrm{r}^\mathrm{r}$$

$\mathbf{b}^r$- refinement:

$$\mathbf{b}^r = \mathbf{k}_\mathrm{r}^\mathrm{r} \left(\frac{d\mathbf{b}_o^r}{dt} + \mathbf{b}_o^r \mathbf{J} \right)$$

$$\mathbf{k}_\mathrm{r}^\mathrm{r} = \left[\mathbf{b}_o^r \left(\frac{d\mathbf{a}_r^o}{dt} + \mathbf{J}\mathbf{a}_r^o \right) \right]^{-1}$$

$$\text{ignore} \quad d/dt$$

$$\mathbf{a}_r^o = \boldsymbol{\alpha}_r \qquad \mathbf{b}_o^r = \boldsymbol{\beta}^r$$

$$\mathbf{a}_r = \left(\mathbf{J}\mathbf{a}_r^o \right) \mathbf{k}_\mathrm{r}^\mathrm{r} = \left(\mathbf{J}\boldsymbol{\alpha} \right) \left[\boldsymbol{\beta}^r \mathbf{J}\boldsymbol{\alpha} \right]^{-1} = \left(\boldsymbol{\alpha}\boldsymbol{\lambda} \right) \left[\boldsymbol{\lambda} \right]^{-1} = \boldsymbol{\alpha}$$

Implicit Low Dimensional Manifolds (ILDM) algorithm

$$\mathbf{f}^{\mathrm{r}} = \boldsymbol{\beta}^{r}\mathbf{g} = 0$$ ← Solve for $\mathbf{y}^{M}$

$$\frac{d\mathbf{y}}{dt} = \boldsymbol{\alpha}_{s}\mathbf{f}^{\mathrm{S}} = \boldsymbol{\alpha}_{s}\boldsymbol{\beta}^{s}\mathbf{g} = \left[\mathbf{I} - \boldsymbol{\alpha}_{r}\boldsymbol{\beta}^{r}\right]\mathbf{g}$$ ← Solve for $\mathbf{y}^{N-M}$

$$\mathbf{y} = \begin{bmatrix} \mathbf{y}^{M} \\ \mathbf{y}^{N-M} \end{bmatrix}$$

Tabulate $\mathbf{y}^{M}$, $\boldsymbol{\alpha}_{r}$ and $\boldsymbol{\beta}^{r}$ in phase space of $\mathbf{y}^{N-M}$

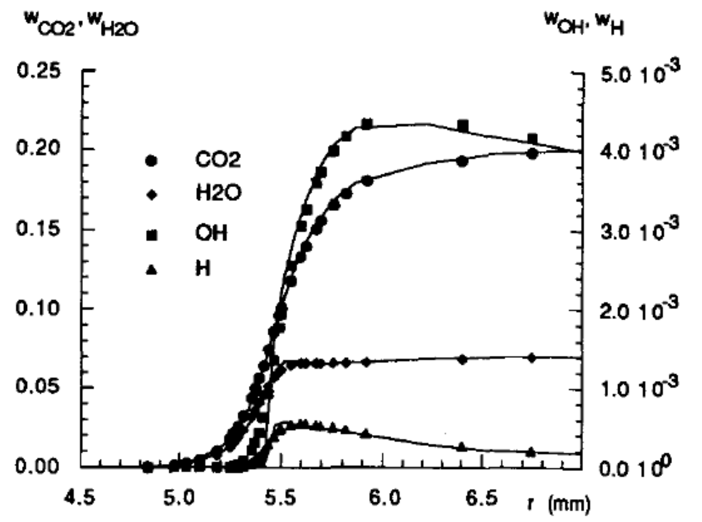


FIG. 4. Calculated structure of a syngas-air flame (points: reduced mechanism, lines: detailed mechanism).

Speed up by O(10)

Maas and Pope, Proc. CI, 1994

Transport

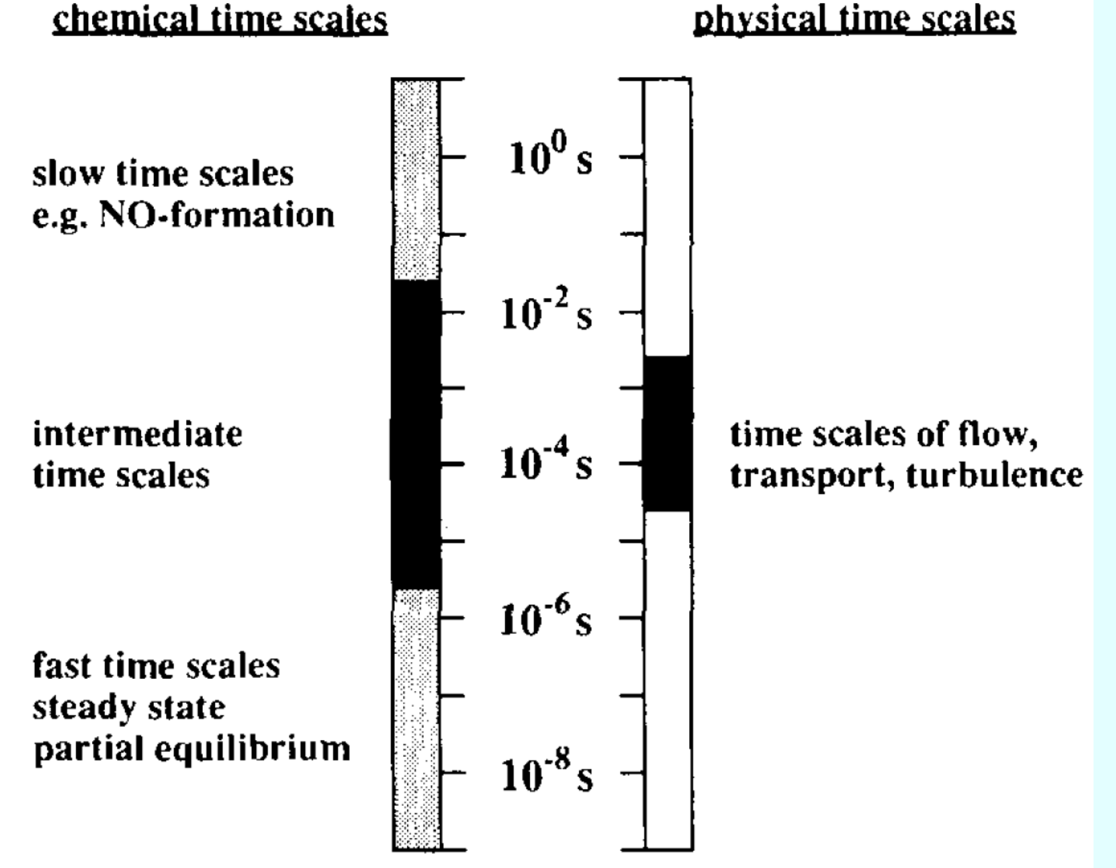


Fig. 1. Schematical illustration of the time scales governing a chemically reacting flow.

Maas & Pope, C&F 1992

Transport

$$\frac{d\mathbf{y}}{dt} = \mathbf{S}_1 R^1 + \mathbf{S}_2 R^2 + \ldots + \mathbf{S}_K R^K + \mathbf{q}\nabla^2\mathbf{y} = \mathbf{g}(\mathbf{y}) + \mathbf{q}\nabla^2\mathbf{y}$$

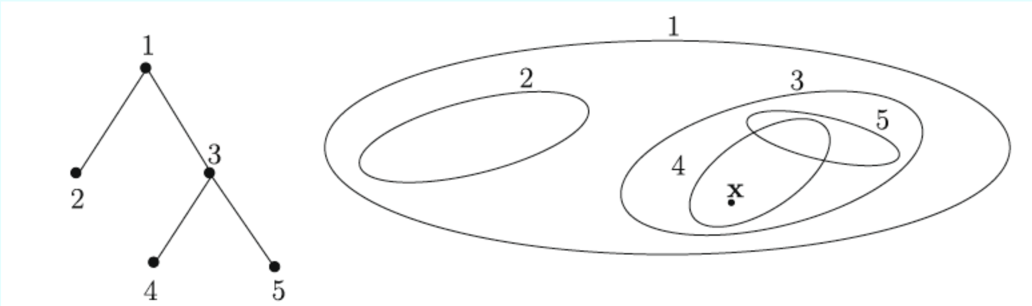
$$\frac{d\mathbf{y}}{dt} = \mathbf{a}_r \mathbf{f}^r + \mathbf{a}_s \mathbf{f}^s = \underbrace{\left(\mathbf{a}_1 f^1 + \ldots + \mathbf{a}_M f^M\right)}_{=\,0} + \left(\mathbf{a}_{M+1} f^{M+1} + \ldots + \mathbf{a}_N f^N\right)$$

$$f^i = \mathbf{b}^i \cdot \left(\mathbf{g} + \mathbf{q}\nabla^2\mathbf{y}\right)$$

Maas and Pope, Proc. CI, 1994
Hadjinicolaou and Goussis, SIAM MMS, 1998

In Situ Adaptive Calculation

Tabulate $\mathbf{y}^M$, $\boldsymbol{\alpha}_r$ and $\boldsymbol{\beta}^r$ in "useful" part of phase space of $\mathbf{y}^{N-M}$



Linear approximation of known quantity
or
Computation from full model

Pope, CTM, 1997
Tang and Pope, Proc. CI, 2002
Singer, Pope and Najm, CF, 2006
Lu and Pope, JCP, 2007

Conclusions

Model reduction is still an open field

[1] A. Tomlin, T. Turányi, and M. Pilling, *Mathematical tools for the construction, investigation and reduction of combustion mechanisms*, in *Low Temperature Combustion and Autoignition*, M. Pilling and G. Hancock, eds., Elsevier, Amsterdam, 1997, pp. 293–437.

[2] D.A. Goussis and U. Maas, *Model reduction for combustion chemistry*, in *Turbulent Combustion Modeling*, T. Echekki and E. Mastorakos, eds., Springer, New York, 2011, pp. 193–220.

[3] T. Lovas, *Model reduction techniques for chemical mechanisms*, in *Chemical Kinetics*, V. Patel, ed., InTech, Croatia, 2012, pp. 79–114.

[4] U. Maas and A.S. Tomlin, *Time-scale splitting-based mechanism reduction*, in *Cleaner Combustion – Green Energy and Technology*, F. Battin-Leclerc, J.M. Simmie, and E. Blurock, eds., Springer, London, 2013, pp. 467–484.

[5] T. Turányi and A.S. Tomlin, *Analysis of Kinetic Reaction Mechanisms*, Springer, Heidelberg, 2014.