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Problem adapted reduced models based on Reaction-Diffusion Manifolds (REDIMs)

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Thirty-Second International Symposium on Combustion,
Montreal, Canada, 3 - 8 August, 2008

- Problem Statement: Simulation of reacting flows and model reduction…
- Theoretical Background: Decomposition of motions, Invariant manifolds…
- Realization Strategies: ILDM, Tabulation, Generalized coordinates, REDIM…
- REDIM: Adaptation procedure

System of governing equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\, v) = 0$$

$$\frac{\partial \rho w_i}{\partial t} + \nabla \cdot (\rho\, v\, w_i) = \nabla \cdot (\rho\, D_{im}\, \nabla w_i) + s_i$$

$$\frac{\partial \rho v}{\partial t} + \nabla \cdot (\rho\, v \otimes v) = -\nabla \cdot P - \rho\, g$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho\, v\, h) = \nabla \cdot (\lambda \nabla T) + \nabla \cdot \left(\rho \sum_{i=1}^{n_s} h_i\, D_{im} \nabla w_i \right)$$

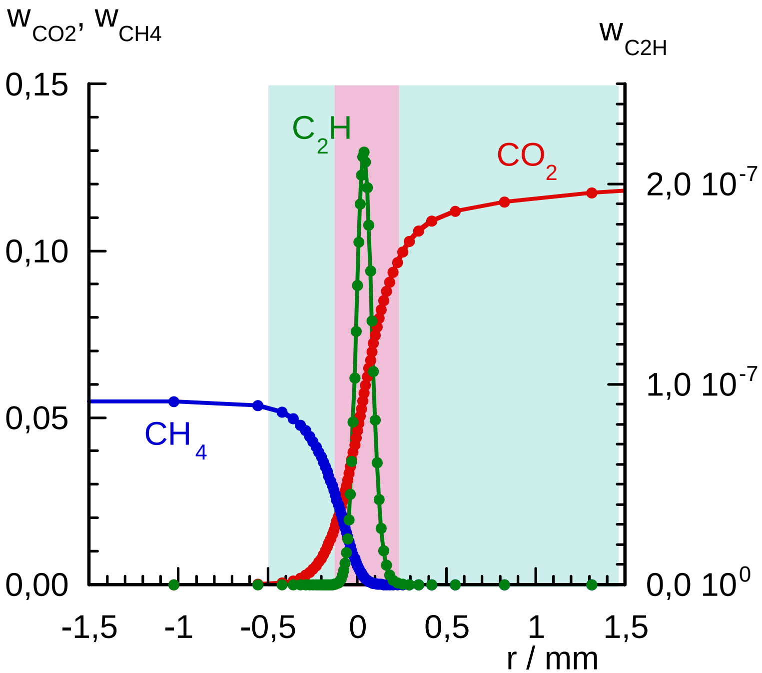
$$\frac{p}{\rho} = \frac{R\,T}{\overline{M}}$$

Composition space: $\psi = \left(h, p, \frac{w_1}{M_1}, \ldots, \frac{w_{n_s}}{M_{n_s}} \right)^T, \quad n = n_s + 2$

System in vector notation (scalar variables only)

$$\frac{\partial \psi}{\partial t} = F(\psi) - v\, \mathrm{grad}(\psi) - \frac{1}{\rho} \mathrm{div}(D \cdot \mathrm{grad}(\psi))$$

Detailed chemical kinetics



1-dimensional cut through a CH_4-air flame

Problems:

- extremely high dimension of the system!
- non-linear chemical source terms
- stiffness of the governing equation system
- different chemical time scales do not only introduce stiffness, but also cause the existence of very small length scales

Is it possible to decouple the fast chemical processes?

This would

- reduce the number of governing equations
- remove part of the scaling problems in space

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Theoretical Background: Decomposition

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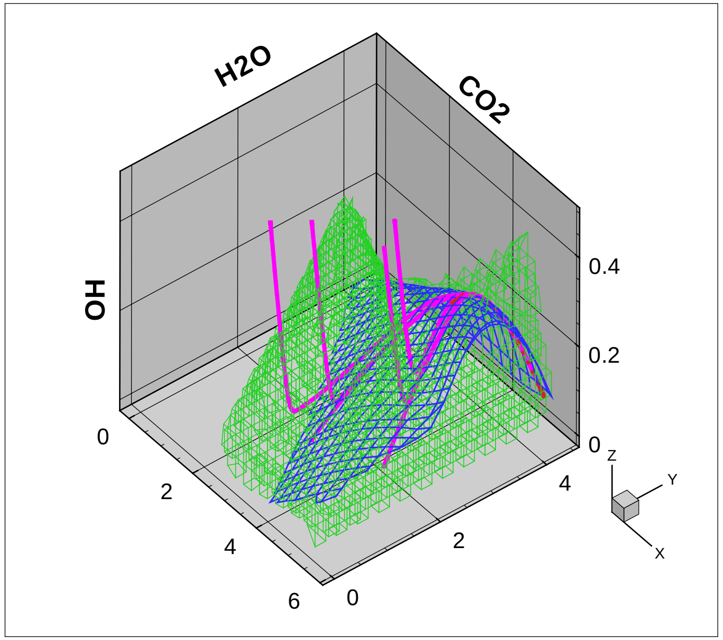
Pure homogeneous reaction system: $$\frac{d\psi}{dt} = F(\psi)$$

Jacobian decomposes into invariant subspaces of relatively large and small eigenvalues!

$$F_\psi = \left(Z_s \ Z_f\right)\begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix}\begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix}$$

ILDM equation: $$\boxed{M_s = \left\{\psi : \tilde{Z}_f F(\psi) = 0\right\}}$$

The manifold that annihilates sub-processes in the direction of the fast subspace!



Problem: Reaction source term analysis neglects coupling of reaction with transport processes in the reacting flow!

Theoretical Background: Invariant manifolds

invariant manifold in an explicit form:

$$M = \left\{ \psi = \psi(\theta) \,\middle|\, \psi : R^m \to R^n \right\}$$

PDEs system's vector field:

$$\Phi = F(\psi) - v\,\mathrm{grad}(\psi) - \frac{1}{\rho}\mathrm{div}(D \cdot \mathrm{grad}(\psi))$$

INVARIANCE

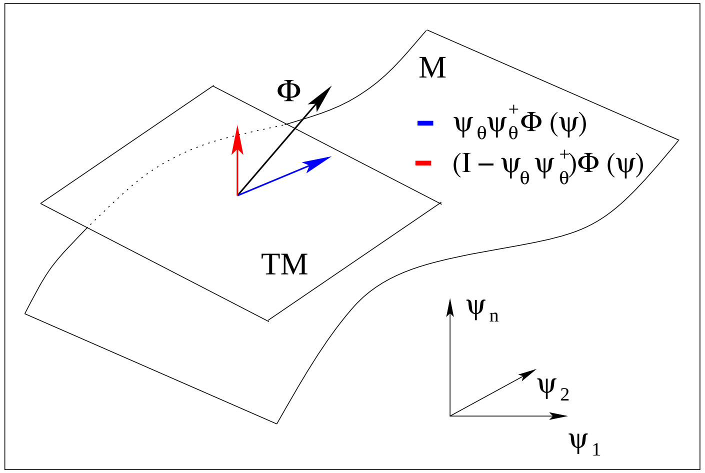
$$\boxed{\Phi \in TM \Rightarrow \left(\psi_\theta^\perp\right)^T \cdot \Phi(\psi) = 0}$$

The question: How to obtain the invariant system manifold?

projector: $P = I - \psi_\theta \psi_\theta^+$

relaxation method:

$$\boxed{\frac{\partial \psi(\theta)}{\partial t} = \left(I - \psi_\theta \psi_\theta^+\right)\Phi(\psi(\theta))}$$



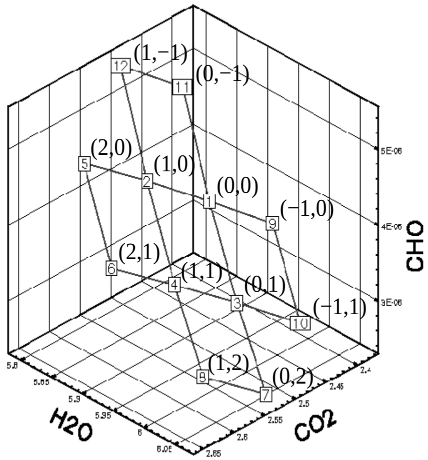
Generalized coordinates

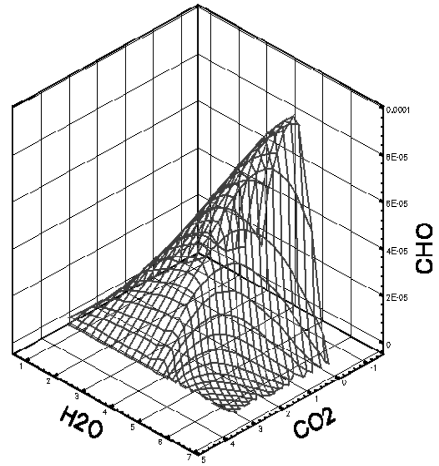
slow manifold is parameterized and tabulated by indices of mesh points:

$$M_s = \left\{\psi = \psi(\theta) : \tilde{Z}_f F(\psi(\theta)) \equiv 0\right\}$$

at any grid point we tabulate the state space with tangent subspace defined in this point:

$$\boxed{\psi(\theta_0), \quad \psi_\theta(\theta_0)}$$





then, the system can be projected on the manifold by using normal subspace

$$\frac{\partial\theta}{\partial t} = \tilde{F}(\theta), \quad \tilde{F}(\theta) = \psi_\theta^+(\theta) F(\theta)$$

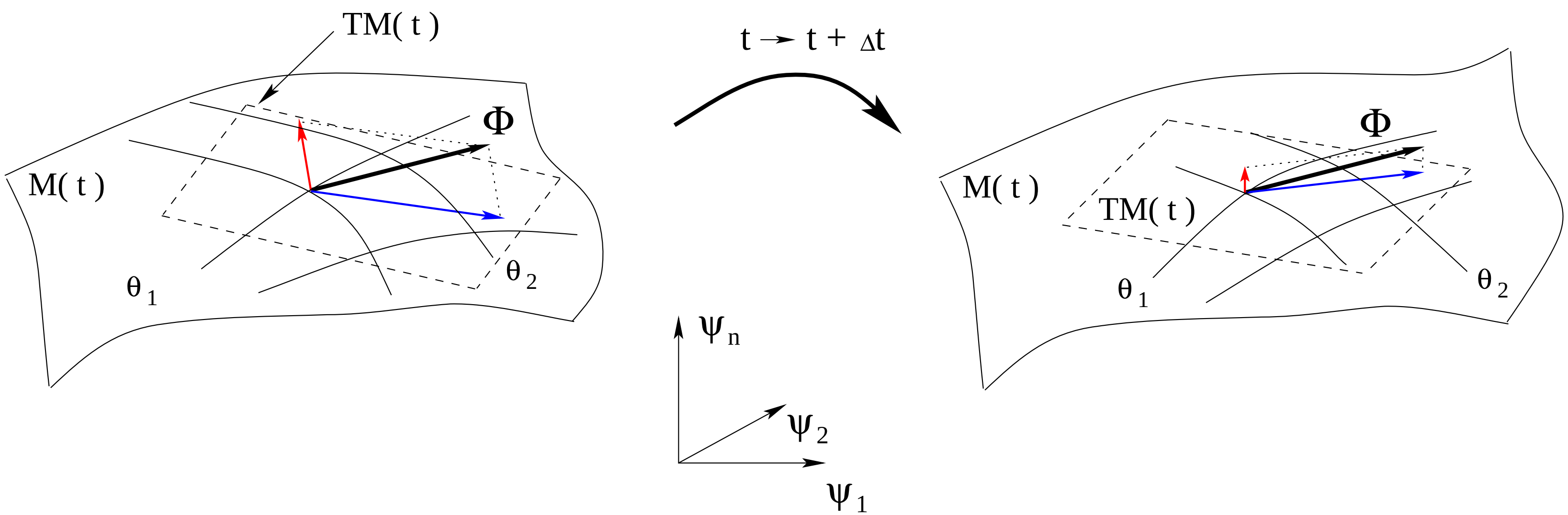
Moore-Penrose pseudo-inverse: $\psi_\theta^+ = \left(\psi_\theta^T \psi_\theta\right)^{-1} \psi_\theta^T$

Invariant manifolds: relaxation process

Initial guess for a manifold $$M = \left\{ \psi = \psi(\theta) \,\middle|\, \psi : R^m \rightarrow R^n \right\}$$

$$\frac{\partial \psi(\theta)}{\partial t} = \left(I - \psi_\theta \psi_\theta^+ \right) \Phi\left(\psi(\theta)\right)$$

The manifold changes locally to satisfy INVARIANCE condition!



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REDIM: Coordinates dependence

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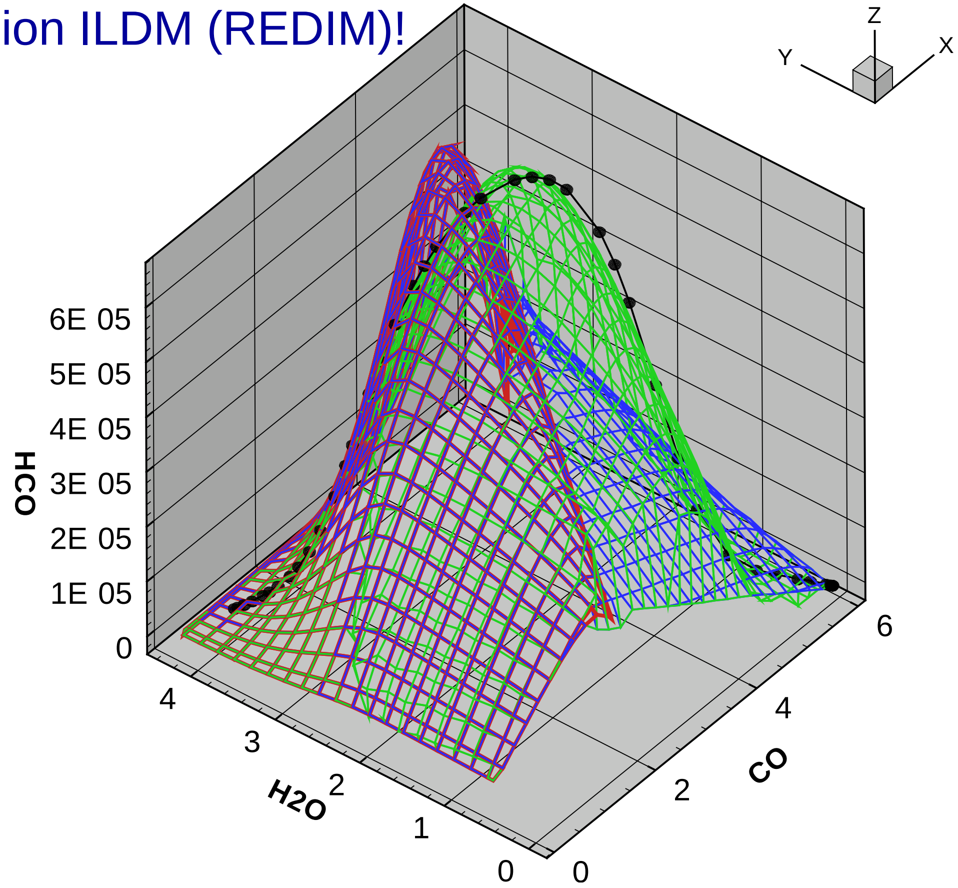
an extended ILDM can be used as an initial guess in relaxation process to a reaction-diffusion ILDM (REDIM)!

$$\begin{cases} \dfrac{\partial \psi}{\partial t} = \left(I - \psi_\theta \psi_\theta^+\right)\{F + G\} \\ \psi\big|_{t=0} = \psi_{ILDM}^{ex}(\theta) \end{cases}$$

$$G = -\frac{d}{\rho}\psi_{\theta\theta} \circ \mathrm{grad}(\theta) \circ \mathrm{grad}(\theta)$$

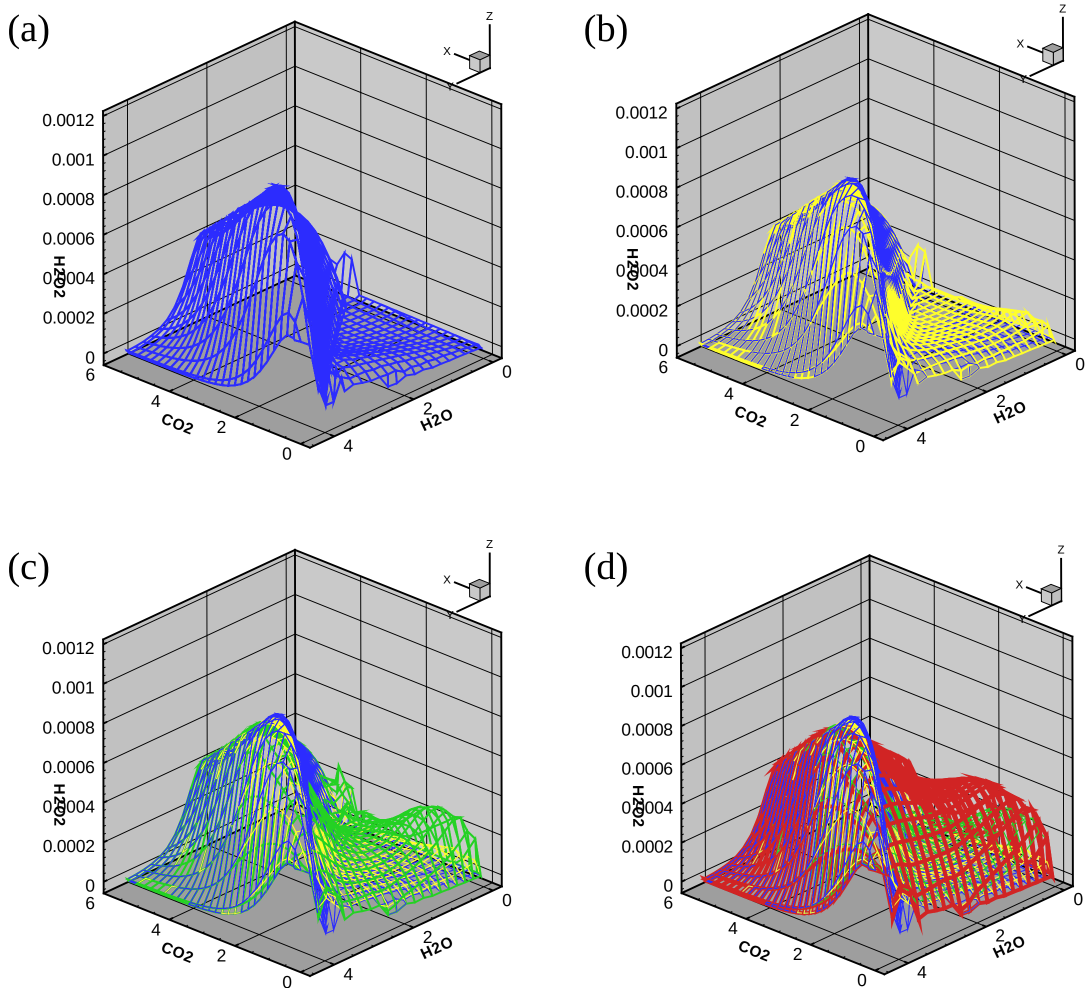


2D ILDM extended (red mesh), REDIM (blue) and a stationary solution (black).

Reference: V.Bykov, U.Maas. 2007, CTM, 11(6), 839 - 862

REDIM relaxation

$$\begin{cases} \dfrac{\partial \psi}{\partial t} = \left(I - \psi_\theta \psi_\theta^+\right)\left\{F + G^*\right\} \\ \psi\big|_{t=0} = \psi_{ILDM}^{ex}(\theta) \end{cases}$$



Simple approach

$$G^* = -\frac{d}{\rho}\left\|\mathrm{grad}(\theta)\right\|^2 \frac{1}{m} \mathrm{Tr}\left(\psi_{\theta\theta}\right)$$

$$G^* \sim -\frac{d}{\rho}\psi_{\theta\theta} \circ \mathrm{grad}(\theta) \circ \mathrm{grad}(\theta)$$

(a) – initial guess, (b) – after 10 iterations, (c) – 200, (d) - 700

REDIM relaxation

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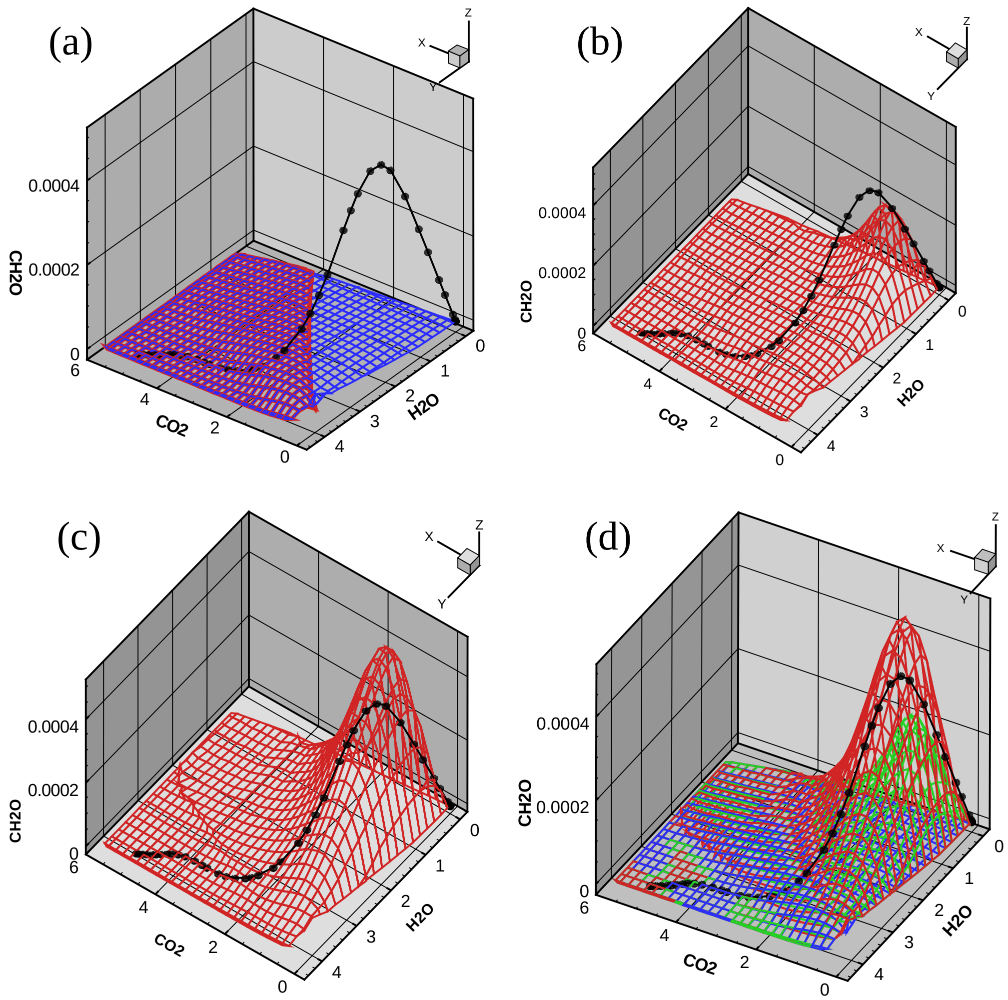

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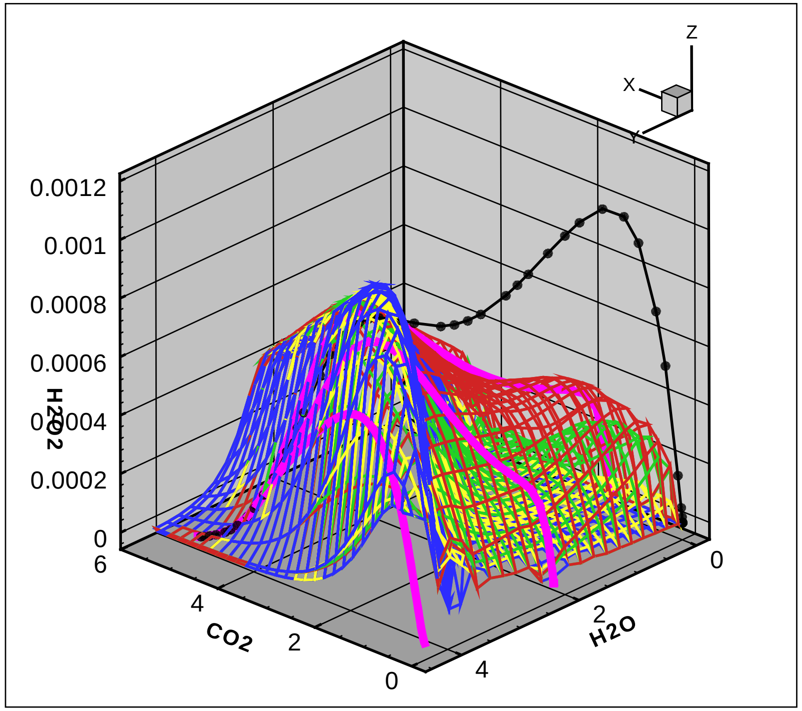
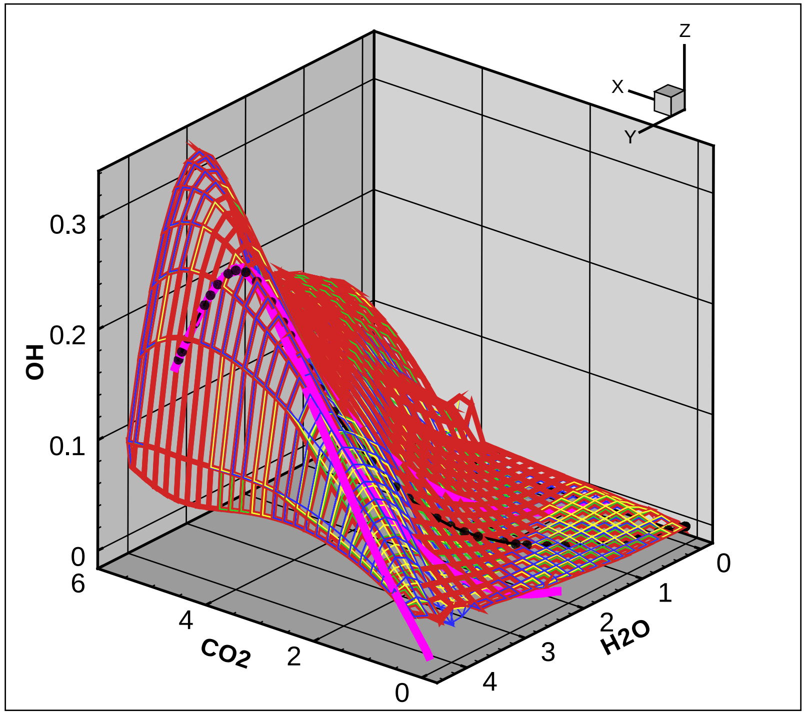
REDIM relaxation

relaxation process in projection to minor and major species specific mole numbers!





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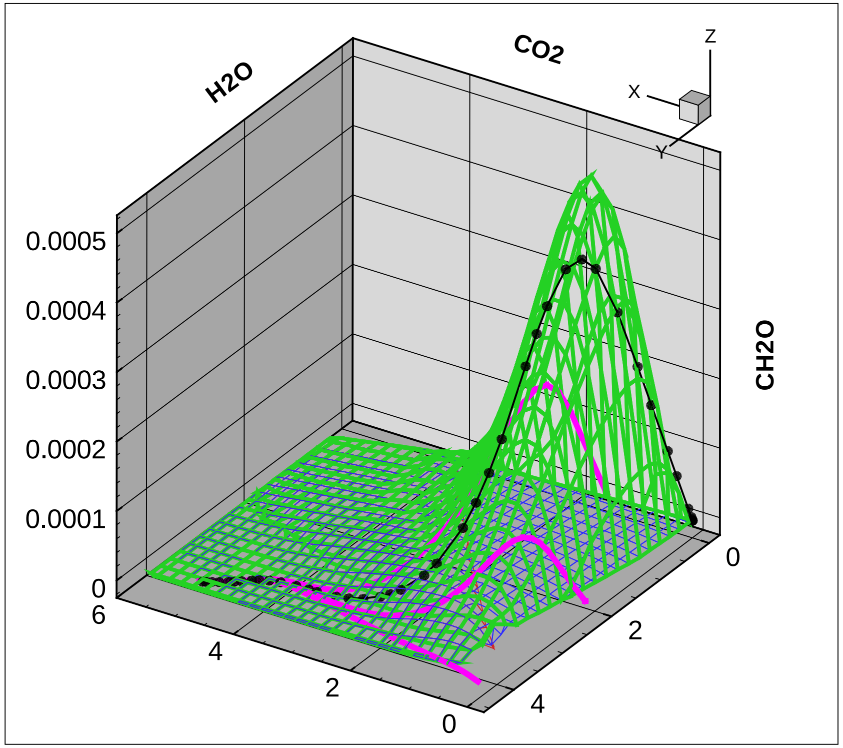
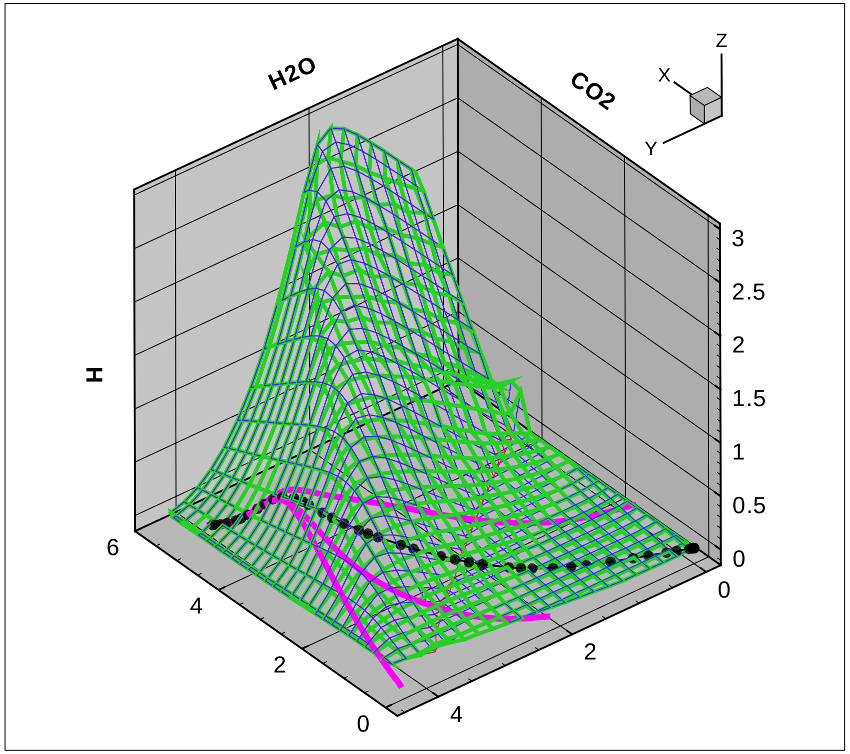
REDIM relaxation: Comparison

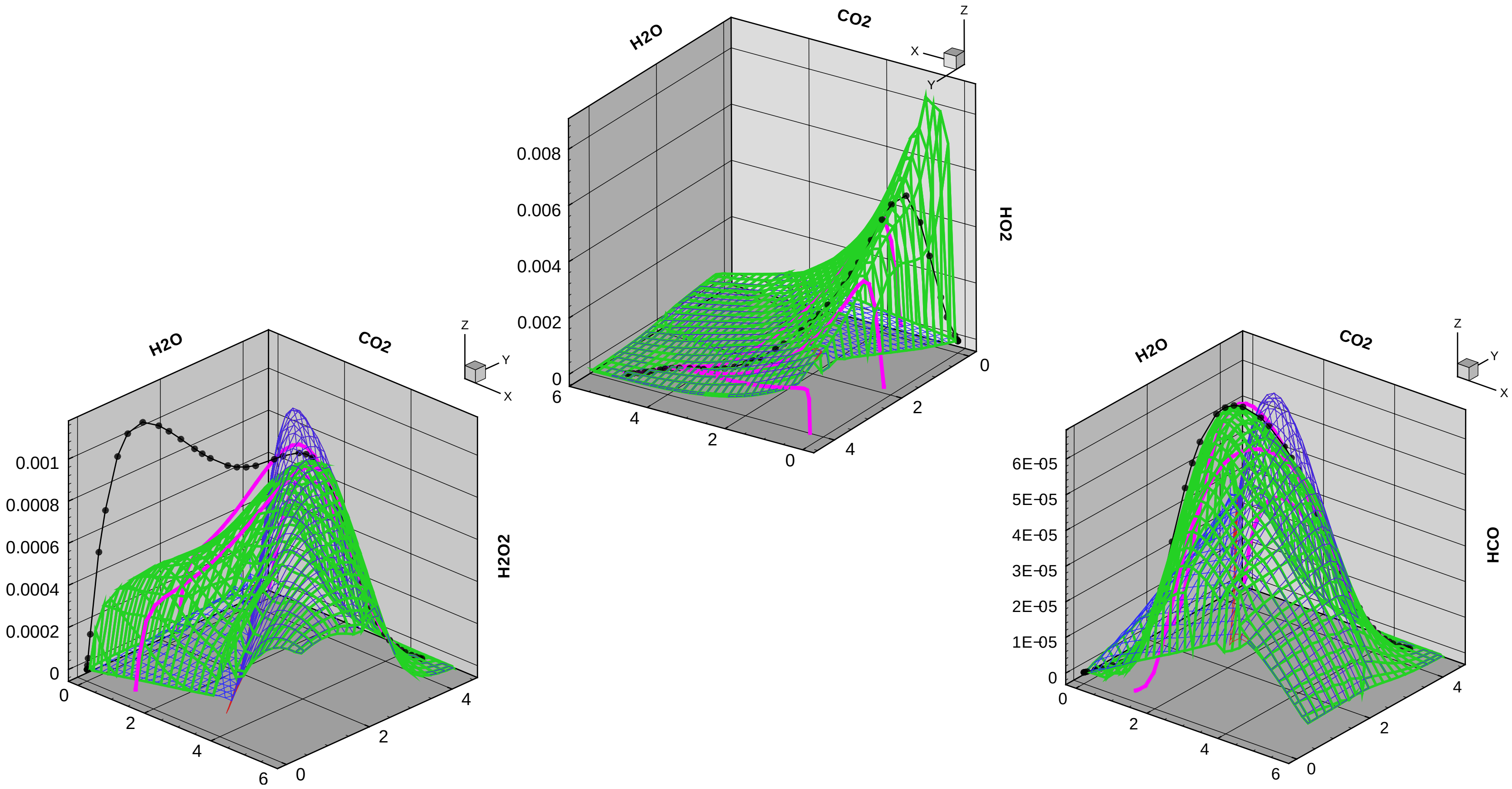
relaxation process in projection to minor and major species specific mole numbers!





REDIM relaxation: Comparison

relaxation process in projection to minor and major species specific mole numbers!



REDIM Implementation

actual reduction is realized as a reformulation of the detailed system on the REDIM manifold

$$M_{REDIM} = \{\psi = \psi(\theta)\} \quad \Rightarrow \quad \psi(\theta_0), \quad \psi_\theta(\theta_0)$$

$$\psi_\theta \frac{\partial \theta}{\partial t} = F(\theta) - v\,\psi_\theta \cdot \mathrm{grad}(\theta) - \frac{1}{\rho}\mathrm{div}(D \cdot \psi_\theta \cdot \mathrm{grad}(\theta))$$

$$\Xi(\theta) = D \cdot \psi_\theta \qquad \tilde{F}(\theta) = \psi_\theta^+\left(F(\theta) - \frac{1}{\rho}\mathrm{div}(\Xi(\theta)\cdot \mathrm{grad}(\theta))\right)$$

$$\boxed{\frac{\partial \theta}{\partial t} = \tilde{F}(\theta) - v\,\mathrm{grad}(\theta)}$$

The evolution of the manifold parameter is calculated and then the whole state space is recovered by the REDIM table!

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Gradient's approximation: Adaptation

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suppose we have constructed a REDIM manifold, now, the question how this can be improved?

$$\mathrm{grad}(\theta) = \mathrm{Const} \quad \overset{???}{\Rightarrow} \quad \mathrm{grad}(\theta) = f(\theta)$$

here a test integration of the reduced model is suggested in order to incorporate the information about actual system gradients…

$$M^{i}_{\mathrm{REDIM}} = \left\{ \psi = \psi^{i}(\theta) \right\}$$

$$\left. \begin{aligned} &\frac{\partial \theta}{\partial t} = S(\theta) - v\,\mathrm{grad}(\theta) \quad \Rightarrow \quad \theta = \theta(x) \\ &\theta_* = \theta(x_*) \quad \Rightarrow \quad f^{i}(\theta_*) = \mathrm{grad}(\theta)\big|_{x = x_*} \end{aligned} \right\} \quad \Rightarrow \quad \mathrm{grad}(\theta) = f^{i}(\theta)$$

In this way an approximation is improved and can further be used in the relaxation REDIM procedure to yield more accurate manifold!

REDIM with improved gradients' estimate

A REDIM from the previous relaxation process can be used as a new initial guess…

$$\begin{cases} \dfrac{\partial \psi^{i+1}}{\partial t} = \left(I - \psi_\theta^{i+1}\left(\psi_\theta^{i+1}\right)^+\right)\left(F\left(\psi^{i+1}(\theta)\right) - \dfrac{d}{\rho}\left(\psi^{i+1}\right)_{\theta\theta} \circ f^i(\theta) \circ f^i(\theta)\right) \\ \psi\big|_{t=0} = \psi^i(\theta) \end{cases}$$

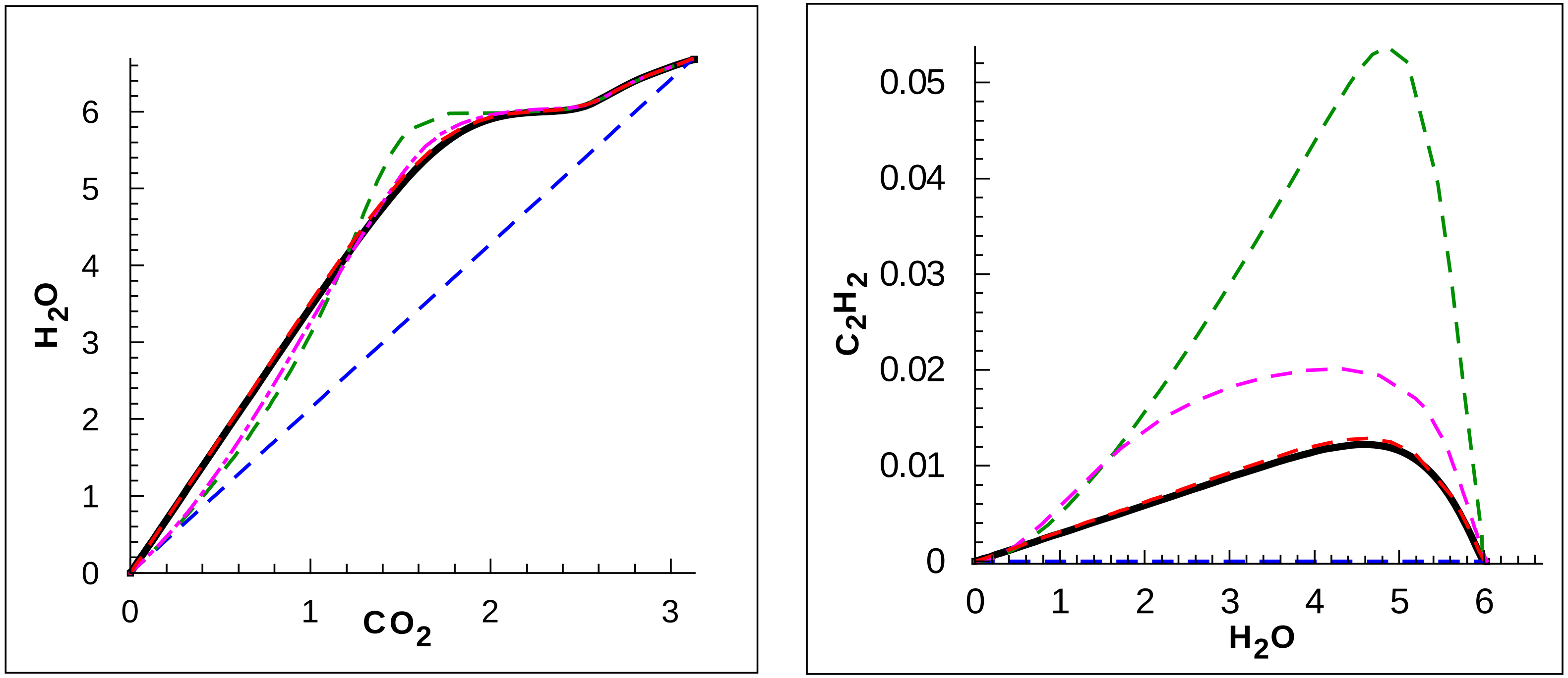
test integration of the reduced model based on the improved REDIM manifold yields enhanced gradients' estimate!

$$M_{REDIM}^{i+1} = \left\{\psi = \psi^{i+1}(\theta)\right\}$$

$$\left.\begin{array}{l} \dfrac{\partial \theta}{\partial t} = S(\theta) - v\,\mathrm{grad}(\theta) \quad \Rightarrow \quad \theta = \theta(x) \\ \theta_* = \theta(x_*) \quad \Rightarrow \quad f^{i+1}(\theta_*) = \mathrm{grad}(\theta)\big|_{x=x_*} \end{array}\right\} \quad \Rightarrow \quad \mathrm{grad}(\theta) = f^{i+1}(\theta)$$

REDIM with improved gradients' estimate

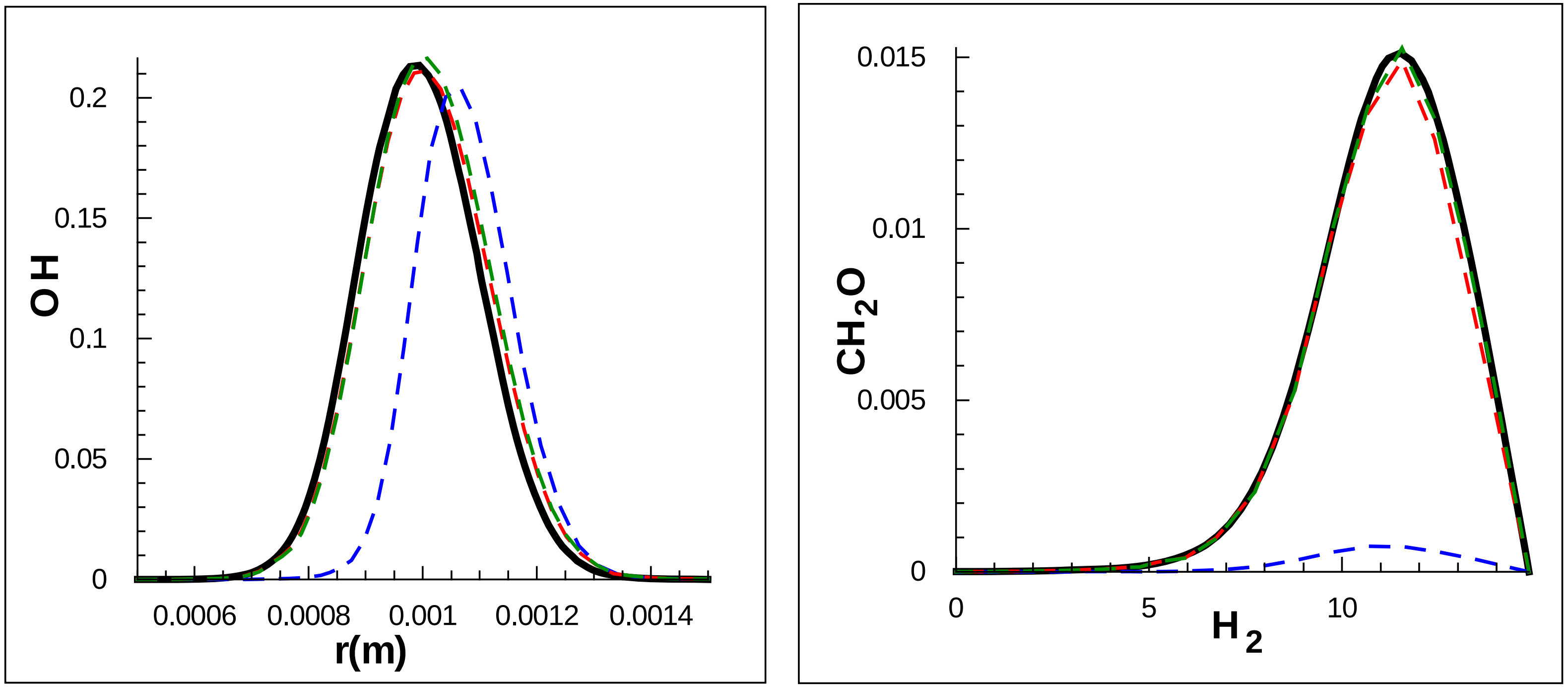
laminar premixed methane/air flame



Solid black line is the detailed stationary solution, blue line – initial guess, green line – result of the first iteration, the magenta line – second and red line the third one.

REDIM with improved gradients' estimate

non-premixed syngas/air diffusion flame



Solid black line is the detailed stationary solution, blue line – the result of the first iteration (constant gradient), green line – result of the second iteration, the red line represents the third one.

Conclusions

- A method for constructing of an approximation of the PDE reaction-diffusion system slow invariant manifold has been discussed.

- The method is based on the natural assumption of splitting of time scales and invariant manifolds concept.

- It allows to take into account the coupling of the reaction and transport processes in the reduced model.

Further studies: increasing of dimension… boundary conditions… detailed diffusion… accuracy issues…