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On Global Quasi Linearization (GQL) in Model Reduction of Chemical Kinetics

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Mathematics of Model Reduction, Leicester, UK
28-30 August, 2007

Overview

- Chemical kinetics in reacting flows
- System/model reduction by decomposition
- Singularly Perturbed Vector Fields (SPVF)
- General case

  - generic toy example

  - standard SPS system
- Linear case

  - global quasi-linearization (GQL)

  - algorithm and implementation

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System of governing equations

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

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

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

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

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

Gas phase chemistry:
Arrhenius law
$$r_l = A_l\, T^{\beta_l} \exp\left(-E_{a,l} / R\,T\right) \prod_{j=1}^{n_s} c_j^{a_{j,l}}$$

$$s_i = \sum_{l=1}^{n_r} r_l \left(\tilde{a}_{i,l} - a_{i,l} \right)$$

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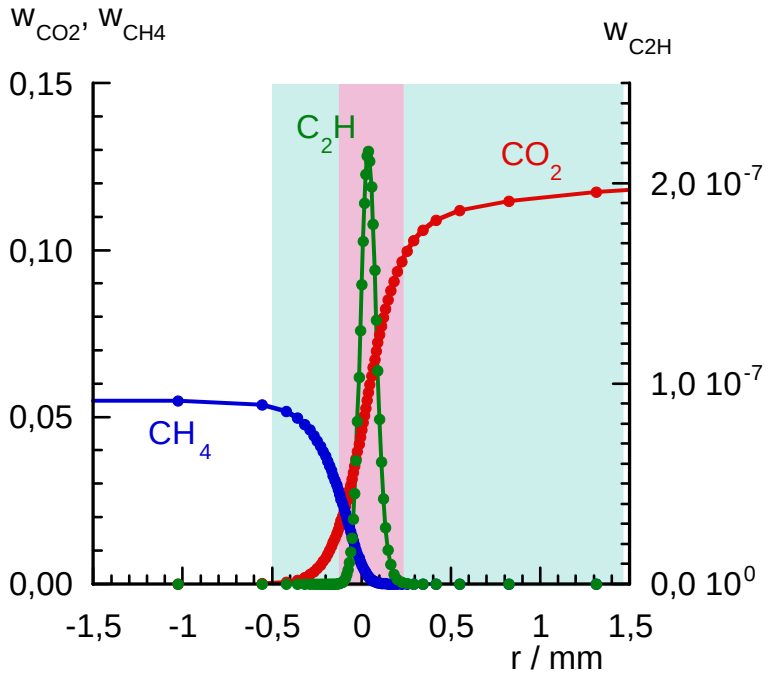
Detailed Chemical Kinetics



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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Concept: Dimension Reduction

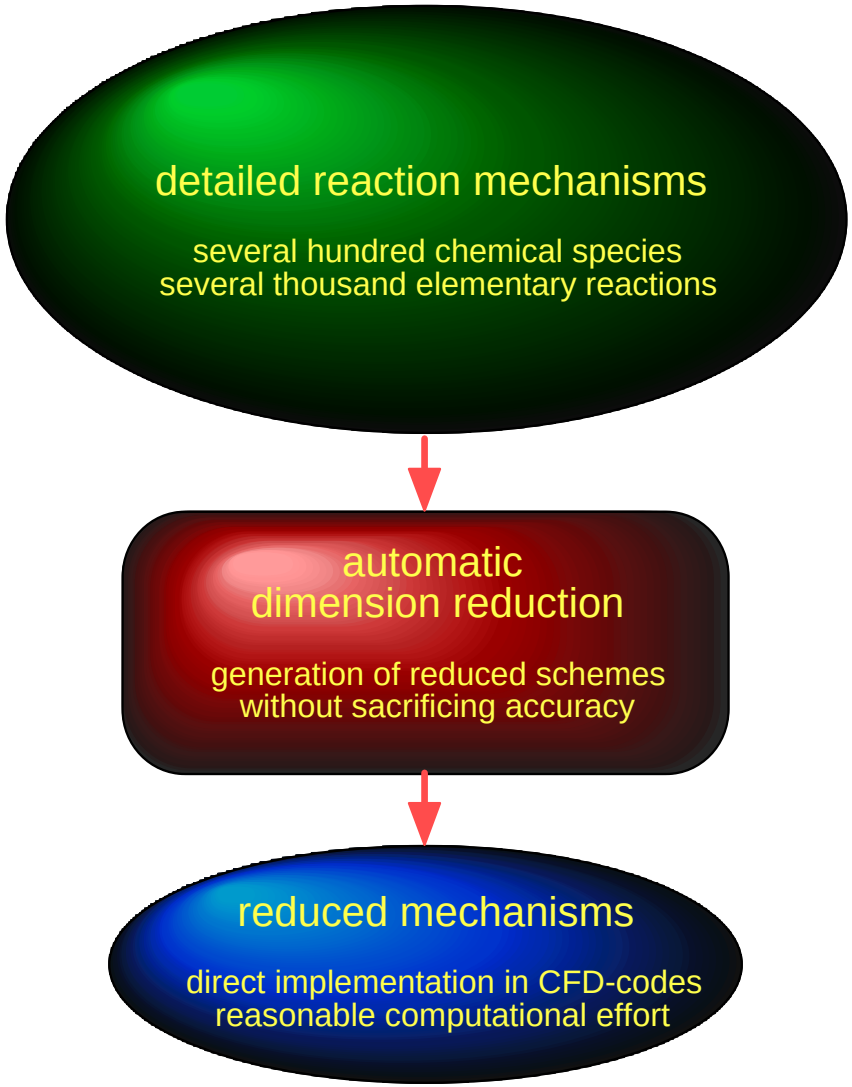
Problems of detailed chemical kinetics:

- several hundred chemical species
- several thousand elementary reactions
- stiffness of the governing equation system

But: only few reactions are rate limiting!

Fundamental questions:

- Does the chemical kinetics exhibit a hierarchical structure?
- How much detail is needed for the description of the chemical kinetics?
- Is it really necessary to solve for hundreds of chemical species?
- How can the information of detailed models be condensed to yield reduced models?



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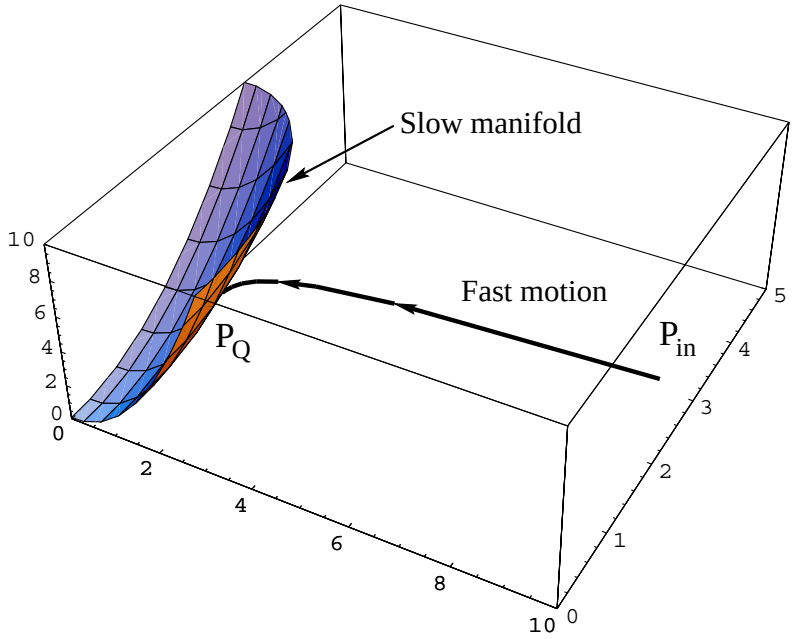
Model reduction by decomposition

multi-scale phenomena are widely spread in the nature, most complex processes have this special type of behavior!



Observations:

the system accesses only a small domain of the state space,

after a short time the system is relaxed onto a low dimensional manifold.

Idea: Reduce the dimension of the system by using “fast” / “slow” invariant manifolds!

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Singularly Perturbed System (SPS)

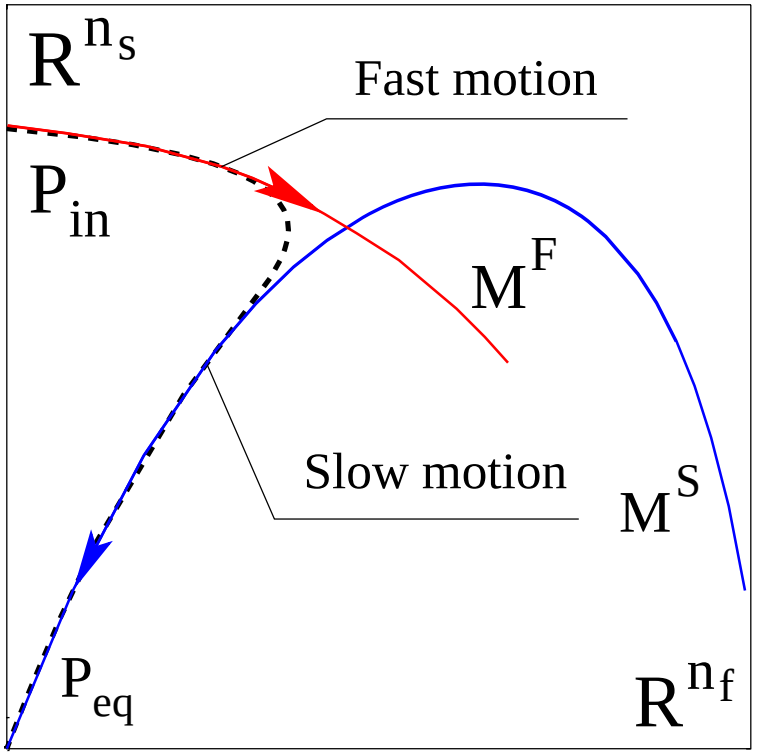
simplest mathematical model for multi-scale phenomena is a
Singularly Perturbed System (SPS)

The system with two different time scales are modeled by using small system parameter given explicitly

$$\frac{dX}{dt} = \frac{1}{\varepsilon} F(X, Y), \quad X \in R^{n_f}$$

$$\frac{dY}{dt} = G(X, Y), \quad Y \in R^{n_s}$$

$$n_f + n_s = n, \quad \varepsilon << 1$$



Idea: It allows to separate motions and decompose the system!

System in general form

consider a system that exhibits multi-scale phenomena

$$z' = \Phi(z, \varepsilon) \quad \Phi : \Omega \to R^n$$

Assumptions:

-The system has two different time scales
-There is a small system parameter controlling the scales
-The system can be transformed to the standard SPS form:

$$\frac{dX}{dt} = \frac{1}{\varepsilon} F(X, Y), \quad X \in R^{n_f}$$

$$\frac{dY}{dt} = G(X, Y), \quad Y \in R^{n_s}$$

$$n_f + n_s = n, \quad \varepsilon << 1$$

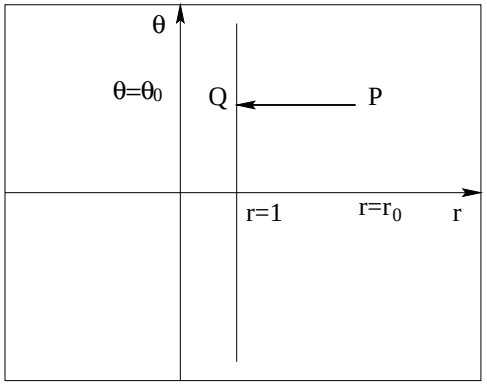
Question: How can this special representation be found?

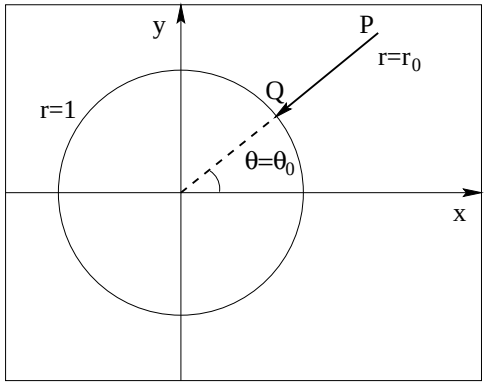
Toy example - motivation

Example 1. Standard SPS system in polar coordinates

$$\begin{cases} \varepsilon\, r' = 1 - r \\ \theta' = -\theta \end{cases} \Rightarrow \begin{aligned} x &= r\cos(\theta) \\ y &= r\sin(\theta) \end{aligned}$$

$$\begin{cases} x' = -\dfrac{y}{x^2+y^2} + \dfrac{1}{\varepsilon}\dfrac{x\left(1-\sqrt{x^2+y^2}\right)}{\left(x^2+y^2\right)^{3/2}} \\ y' = \dfrac{x}{x^2+y^2} + \dfrac{1}{\varepsilon}\dfrac{y\left(1-\sqrt{x^2+y^2}\right)}{\left(x^2+y^2\right)^{3/2}} \end{cases}$$





Idea: Choice of a suitable coordinate system representing the system in the decomposed form as the standard SPS!

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Singularly Perturbed Vector Field (SPVF)

informal definition: parametric family of vector fields

$$z' = \Phi(z, \varepsilon) \quad z \in \Omega \subset R^n$$

is a singular perturbed one, if for any fixed z the limiting vector field belongs to a priory fixed linear subspace of smaller dimension:

$$\Phi(z,0) \in L_f(z), \quad \dim(L_f(z)) = n_f < n$$

Moreover, the dimension does not depend on the point. Then, a fast manifold M_f associated with z satisfies

$$\Phi(z,0) \in TM_f$$

and a slow manifold given by $M_s = \{z : \Phi(z,0) = 0\}$

(See e.g. “Singularly Perturbed Vector Fields” Bykov, Goldfarb, Gol’dshtein, 2006)

It is obvious that this construction is almost useless in applications if there is no efficient algorithm to identify the fast manifold!

Singularly Perturbed Vector Field (SPVF)

formal definition: $$z' = \Phi(z, \varepsilon) \quad z \in \Omega \subset R^n$$

-Fiber bundle that structures the domain: Suppose there is a fiber bundle $\xi = \{E, p, \psi\}$:

$$p : E \to \Omega, \quad E \subset R^n$$

$$F_z^{\xi} = p^{-1}(z) - \text{affine subspace}$$

$$\forall z \in \Omega \quad \exists U : z \in U \,\big|\, \psi : p^{-1}(U) \to U \times R^{n_f}$$

-Family of fast manifolds: Suppose the domain is structured by ξ then the fast manifold (associated with a point z) is

$$M_f(z) \equiv \psi^{-1}\left(p^{-1}\left(\psi(z) \cap U\right)\right)$$

-Singular perturbed vector field: a parametric family Φ is a SPVF if

$$\lim_{\varepsilon \to 0} \Phi(z, \varepsilon) \in TM_f(z)$$

Minimal fiber bundle: there is no a proper sub-bundle such that the vector field is SPVF in the domain structured by this sub-bundle!

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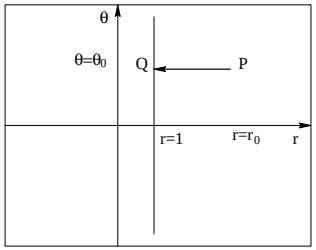
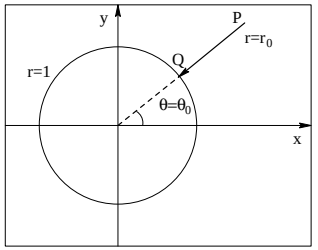
Toy example - decomposition

Example 1. SPS system in polar coordinates

$$\Phi = \frac{1}{\varepsilon}F + G \Rightarrow F = \begin{pmatrix} \dfrac{x\left(1-\sqrt{x^2+y^2}\right)}{\left(x^2+y^2\right)^{3/2}} \\ \dfrac{y\left(1-\sqrt{x^2+y^2}\right)}{\left(x^2+y^2\right)^{3/2}} \end{pmatrix}, \quad G = \begin{pmatrix} -\dfrac{y}{x^2+y^2} \\ \dfrac{x}{x^2+y^2} \end{pmatrix}$$





$$z' = G(z), \quad \frac{dx}{dy} = -\frac{y}{x} \Rightarrow x^2 + y^2 = \text{Const}$$

$$z' = F(z), \quad \frac{dx}{dy} = \frac{x}{y} \Rightarrow \frac{x}{y} = \text{Const}$$

$$M_s = \{z : F = 0\} = \left\{(x,y) : 1 - \sqrt{x^2+y^2} = 0\right\}$$

$$M_f(z_0) = \{(x,y) : y_0 x - x_0 y = 0\}$$

It means that the fast motion is realized along straight lines going through the origin and the slow motion follows circles!

Example 2. SPS system

$$M_s = \{(x,y) : F(x,y) = 0\}$$

$$M_f(z_0) = \{(x,y) : y - y_0 = 0\}$$

Linearly decomposed SPVF

definition: parametric family of vector fields

$$z' = \Phi(z, \varepsilon) \quad \Phi : \Omega \to R^n$$

is a linearly decomposed singular perturbed vector field, iff

$$M_f(z) = \{z\} + L_f$$

It means there exists constant matrix Q such that

$$\begin{pmatrix} u \\ v \end{pmatrix} = Q\, z : \quad \begin{pmatrix} u \\ v \end{pmatrix}' = \begin{pmatrix} \frac{1}{\varepsilon} F \\ G \end{pmatrix}$$

Purpose: Develop the algorithm, which allows to identify fast manifolds or a linear subspace of fast motions!

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Global Quasi-linearization (GQL) method!

In a fixed domain we approximate the vector field by a linear map:

$$T = \Phi^* \; Z^{-1} \qquad T : z_i \mapsto \Phi(z_i)$$

$$\Phi^* = [\Phi(z_1),\ldots,\Phi(z_n)],\; Z = [z_1,\ldots,z_n]$$

Reference point's choice:

-"initial set" is formed by quasi-stochastic uniform distribution:

$$S_N = \{\psi_1,\ldots,\psi_N\}$$

-refinance set has to satisfy the following conditions:

$$Z = \left\{ z_i \in \Omega : \|\Phi(z_i)\| > \|\overline{\Phi}\| \right\}, \quad \overline{\Phi} = \frac{1}{N}\sum_{i=1}^{N} \Phi(z_i)$$

$$\mathrm{Det}(Z) \geq \delta > 0$$

"Global Quasi Linearization (GQL) for the automatic reduction of chemical kinetics"
Bykov, Gol'dshtein, Maas, 2007

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Hierarchy analysis based on GQL!

There is a gap between eignevalues of the GQL

$$T = \left(Q_s \; Q_f\right) \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \begin{pmatrix} \tilde{Q}_s \\ \tilde{Q}_f \end{pmatrix}$$

$$N_s = \begin{pmatrix} \lambda_1(T) & & \\ & \dots & \\ & & \lambda_{m_s}(T) \end{pmatrix} \quad N_f = \begin{pmatrix} \lambda_{m_s+1}(T) & & \\ & \dots & \\ & & \lambda_n(T) \end{pmatrix} \quad \Rightarrow \quad \varepsilon = \left(\frac{\left|\lambda_{m_s+1}(T)\right|}{\left|\lambda_{m_s}(T)\right|} \right)^{-1}$$

The system small parameter is estimated by the gap of the GQL matrix decomposition!

Thus, the suggested algorithm allows at the same time

- Check the system hierarchy!
- Estimate the reduced dimension!
- Approximate the fast linear subspace!
- Decompose the system!

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Slow manifold approximation

homogenous ODE system $$\frac{dz}{dt} = \Phi(z)$$

Global approach: GQL matrix decomposition into invariant subspaces

Local approach: Jacobi matrix decomposition into invariant subspaces - ILDM

$$T = \begin{pmatrix} Q_s & Q_f \end{pmatrix} \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \begin{pmatrix} \tilde{Q}_s \\ \tilde{Q}_f \end{pmatrix} \qquad \Phi_z = \begin{pmatrix} Q_s & Q_f \end{pmatrix} \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \begin{pmatrix} \tilde{Q}_s \\ \tilde{Q}_f \end{pmatrix}$$

Manifold equation $$M_s = \left\{ z(\theta) : R^{n_s} \rightarrow R^n, \tilde{Q}_f F(z) = 0 \right\}$$

The manifold that annihilates the fast subspace!

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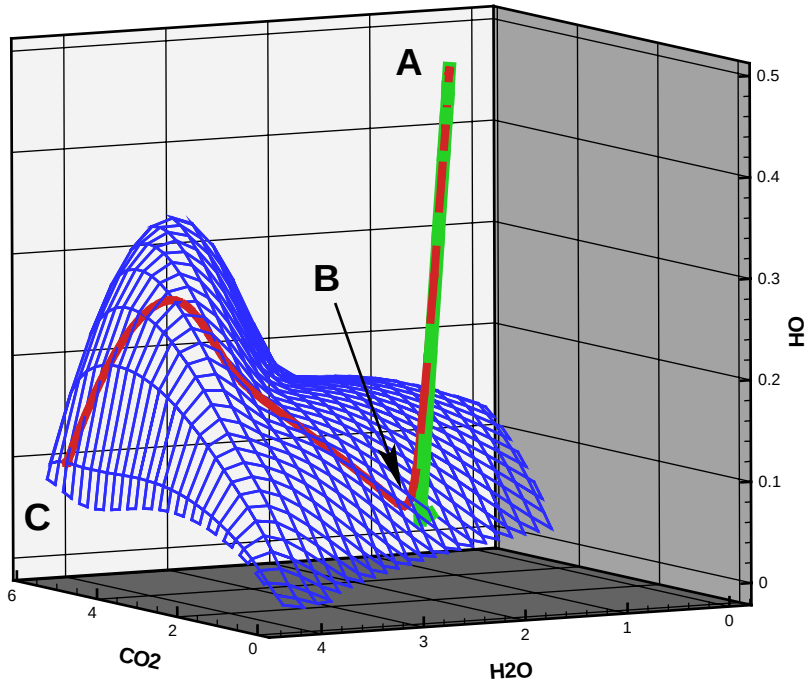
Reduction - decomposition of motions

the system is transformed into fast/slow subsystems

fast subsystem:

$$\begin{cases} \dfrac{dz}{dt} = Q_f \tilde{Q}_f F(z) \\ \tilde{Q}_s z = \tilde{Q}_s z_0 \end{cases}$$



slow subsystem:

$$\begin{cases} \dfrac{dz}{dt} = Q_s \tilde{Q}_s F(z) \\ \tilde{Q}_f F(z) = 0 \end{cases}$$

Projection of the state space of the CO-H_2-O_2 system

Reduction - decomposition of motions

Advantages:

- the numerical solution of the manifold equations is significantly simplified because the computationally expensive decomposition into invariant subspaces is not longer needed for each step of the manifold's tabulation

- the fixed decomposition permits the identification of a fast subsystem behavior such that a correct projection becomes available

- relatively simple manifold's equations; in principle only the transformation matrix is needed to reduce the system!

Disadvantages:

- less accurate, if the system small parameter is not small enough, then one can get large errors!

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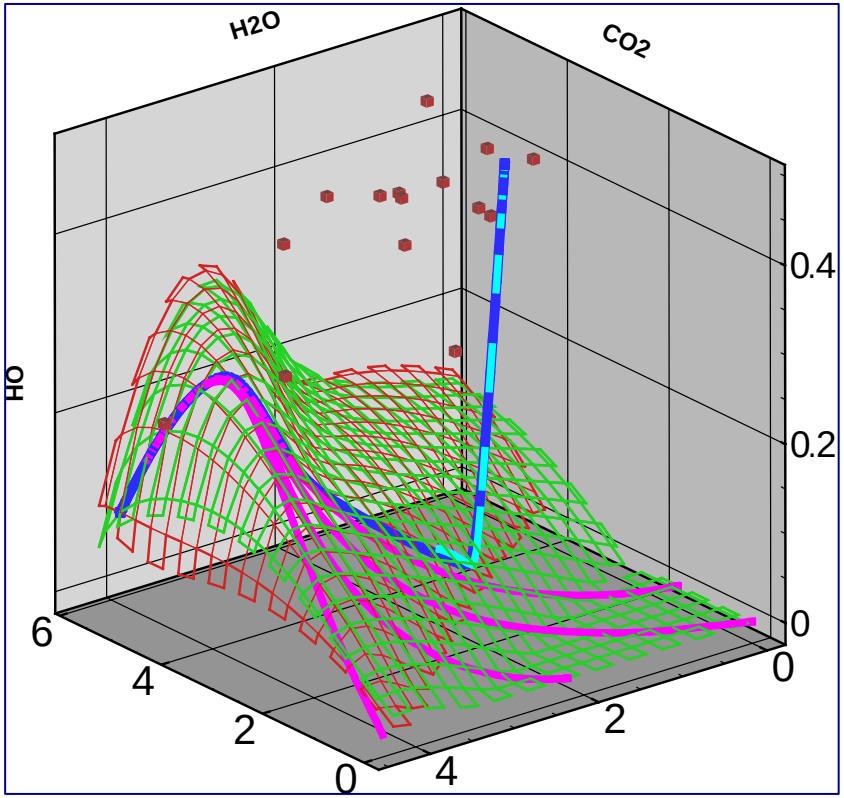
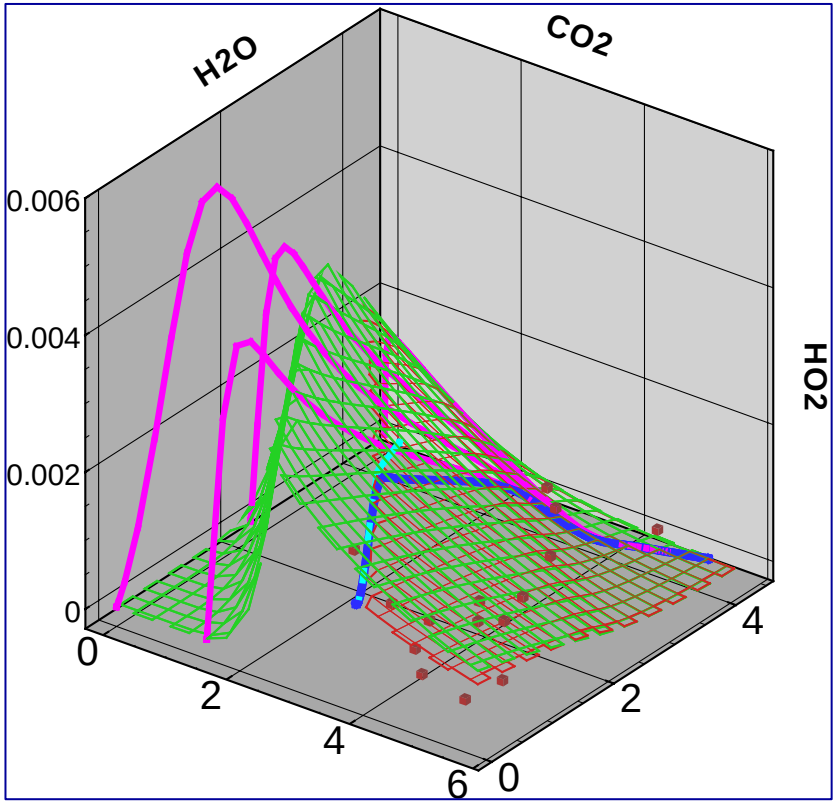
GQL application

In the projections: Red mesh is the ILDM, Green mesh is the GQL manifold, Deep blue solid line shows the detailed system solution, Blue line is the fast subsystem solution, Red cubes are the reference points and Red lines present detailed stationary system solution of flat flames.





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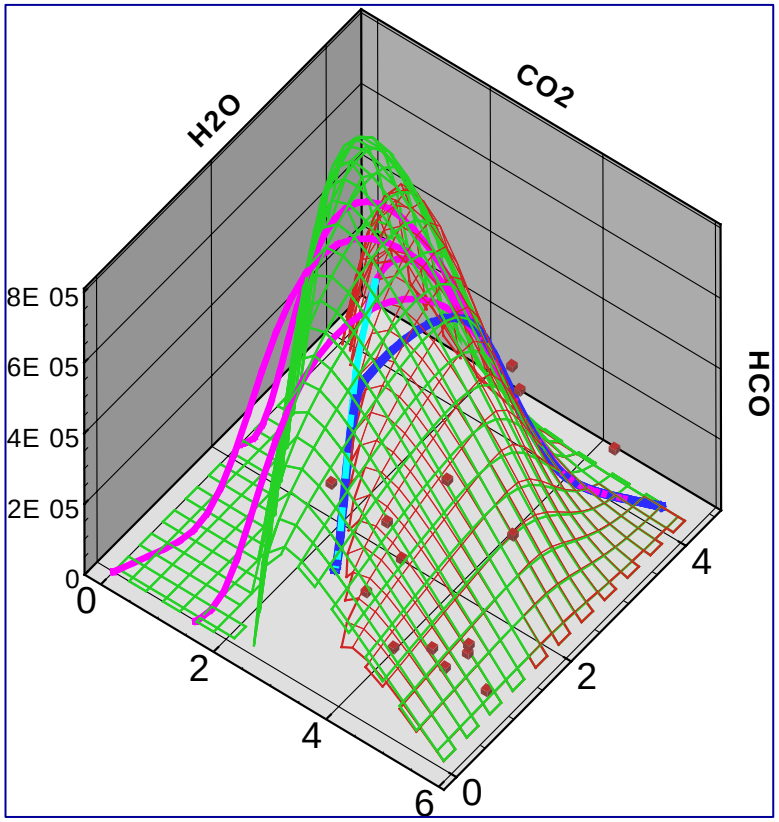

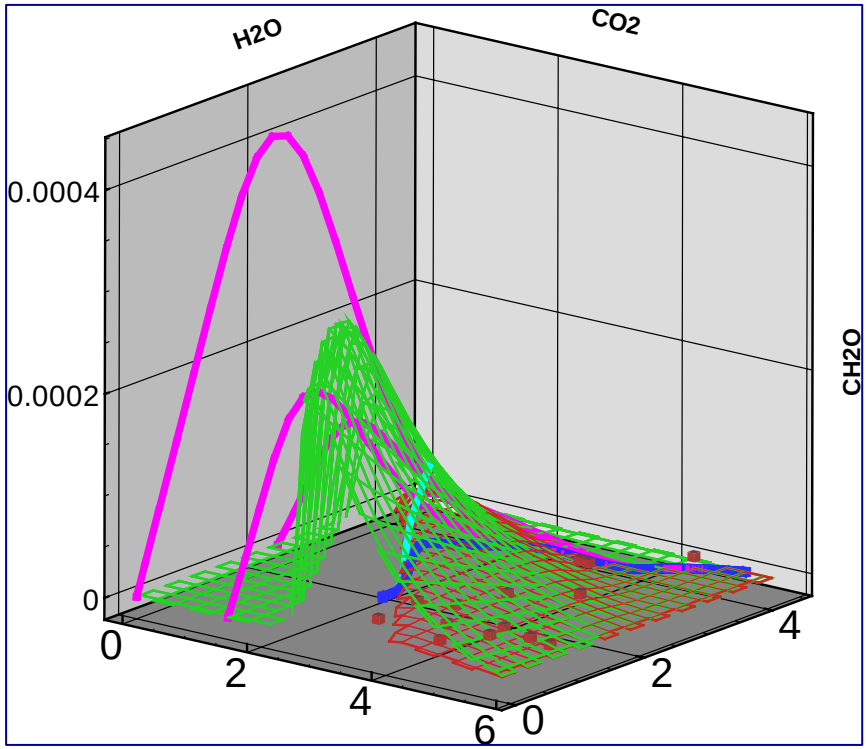

Conclusions

- An efficient method for kinetic model reduction and its subsequent implementation in reacting flow calculations has been presented.

- Reduced and detailed calculations have been performed in order to verify the method and compare it to the standard ILDM method.

- It has been shown that the SPVF approach can be used efficiently to resolve the structure of pressure driven flames.

Acknowledgments:
Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

Further studies: nonlinear decomposition, increasing the order of approximation of the decomposition, optimal domain definition, accuracy issues…

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