Hierarchical concepts for model reduction for reacting flows based on low-dimensional manifolds

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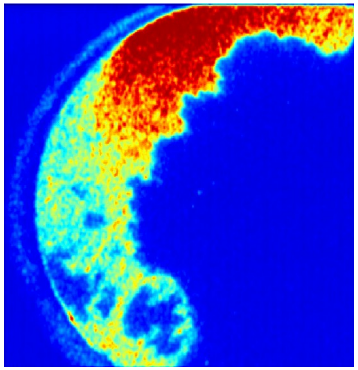
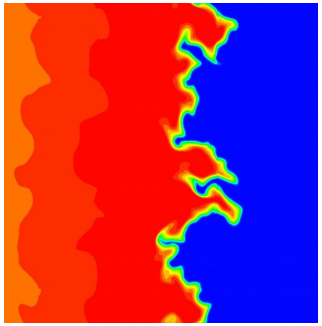
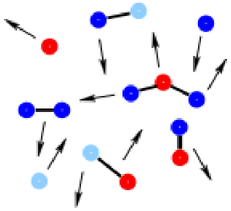






Motivation

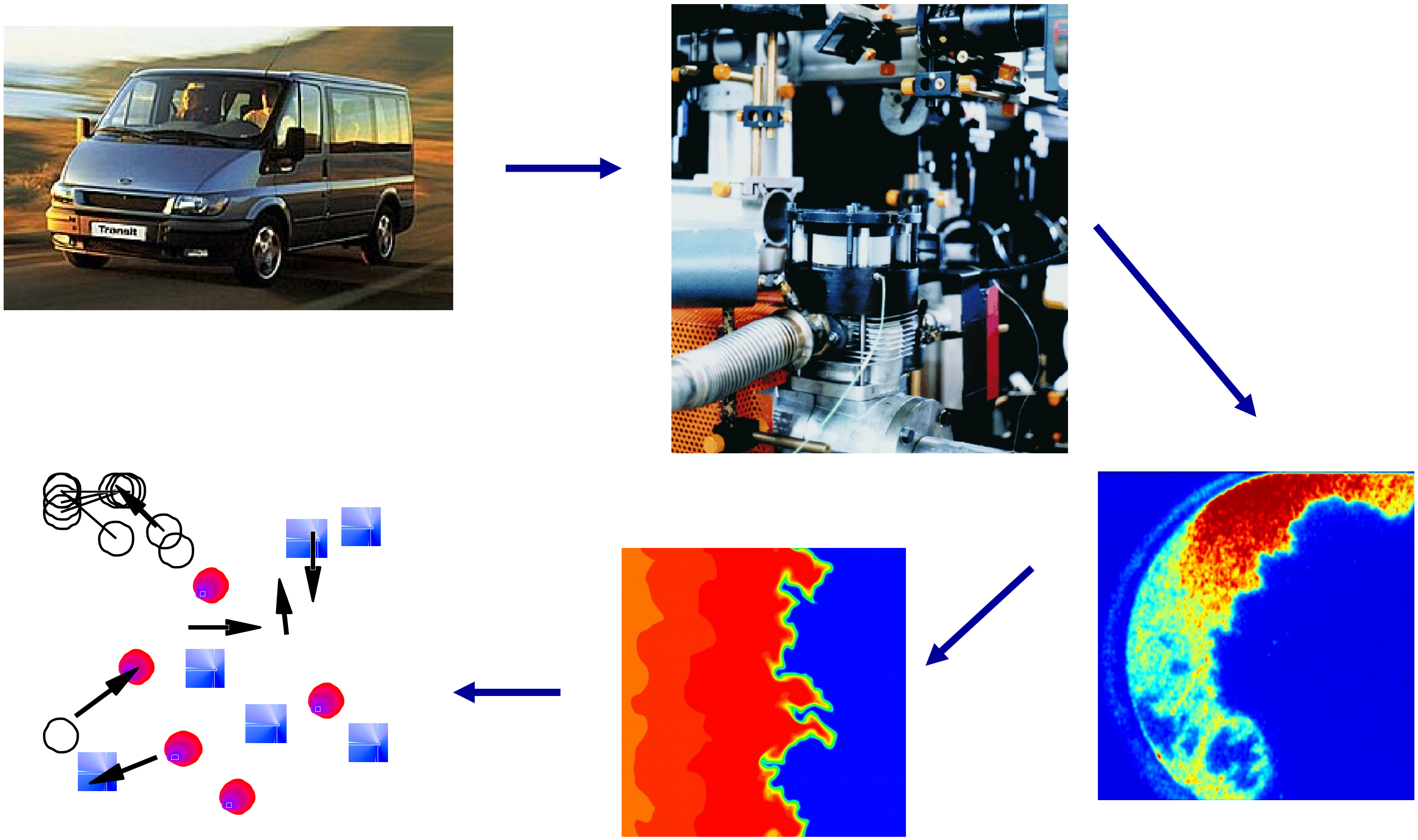
Principles and problems of modeling

Hierarchical concepts for model reduction

- Behavior of the system in state space
- Low-Dimensional manifolds
- Implementation

Conclusions

Scaling Problems



Which degree of detail is necessary for a reliable description of technical processes?

Conservation Equations

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governing equations

$$
\begin{aligned}
&\partial_t \boldsymbol{\rho} &&+ \mathrm{div}\,(\rho \vec{v}) && &&= 0 \\
&\partial_t (\boldsymbol{\rho} \vec{v}) &&+ \mathrm{div}\,(\rho \vec{v} \otimes \vec{v}) &&+ \mathrm{div}\,\overline{\overline{P}} &&= \rho\,\vec{g} \\
&\partial_t (\boldsymbol{\rho} u) &&+ \mathrm{div}\,(\rho u \vec{v}) &&+ \mathrm{div}\,\vec{j}_q + \overline{\overline{P}} : \mathrm{grad}\,\vec{v} &&= q \\
&\partial_t (\boldsymbol{\rho} w_i) &&+ \mathrm{div}\,(\rho w_i \vec{v}) &&+ \mathrm{div}\,\vec{j}_i &&= M_i\,\dot{\omega}_i \qquad i = 1, \ldots, n_s
\end{aligned}
$$

closure of the equation system

$$\vec{j} = \overline{\overline{\Delta}}^{\xi}\,\mathrm{grad}\,\xi + \overline{\overline{\Delta}}^{T}\,\mathrm{grad}\,T + \overline{\overline{\Delta}}^{\pi}\,\mathrm{grad}\,\pi$$

$$\vec{j}_q = \overline{\overline{H}}^{\xi}\,\mathrm{grad}\,\xi + \overline{\overline{H}}^{T}\,\mathrm{grad}\,T + \overline{\overline{H}}^{\pi}\,\mathrm{grad}\,T$$

$$\overline{\overline{\Pi}} = -\mu \left\{ (\mathrm{grad}\,\vec{v}) + (\mathrm{grad}\,\vec{v})^{T} - \frac{2}{3} (\mathrm{div}\,\vec{v})\,\overline{\overline{E}} \right\}$$

$$p = \pi(\eta, \rho_1, \rho_2, \ldots, \rho_{\Sigma})$$

$$\omega_i = \omega_i(T, p, w_1, w_2, \ldots, w_S)$$

$$r_l = A_{\lambda} T^{\beta_{\lambda}} \exp(-E_{a,\lambda} / \mathcal{R}\,T) \prod_{\varphi=1}^{\nu_{\sigma}} \chi_{\varphi}^{\alpha_{\varphi\lambda}}$$

$$\dot{\omega}_i = \sum_{l=1}^{n_r} r_l\,(\tilde{a}_{i,l} - a_{i,l})$$

Gas Phase Chemistry

Arrhenius law

$$r_l = A_\lambda T^{\beta_\lambda} \varepsilon\xi\pi\left(-E_{\alpha,\lambda} / \mathrm{P}\, T\right) \prod_{\varphi=1}^{\nu_\sigma} \chi_\varphi^{\alpha_{\varphi\lambda}}$$

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

- 37 elementary reactions in the H_2-O_2 system, $n_s = 8$
- 74 elementary reactions in the CO-H_2-O_2 system, $n_s = 13$

  •

  •

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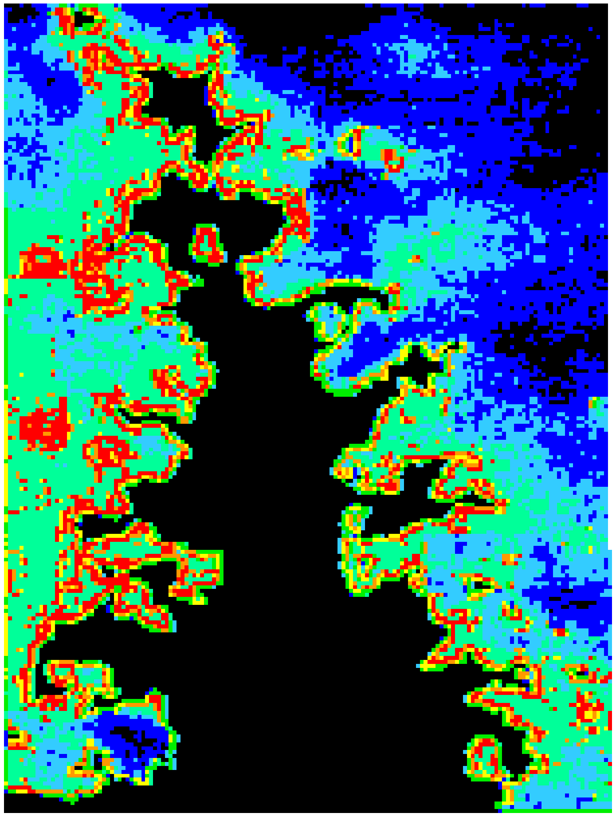
- 7000 elementary reactions in the low-temperature oxidation of higher hydrocarbons (Chevalier et al. 1992), $n_s > 1000$

Problems: many species, different time scales, highly non-linear

Problems



LIF image of a turbulent flame,
Dinkelacker et al.

Scaling problems

- length scales

system dimensions	(m)
reaction zone thickness	(mm)
turbulent length scales	(mm)
shock thickness	(μm)

- velocity scales

flame speeds	(cm/s)
speed of sound	(330 m/s)
detonation velocities	(> 1000 m/s)

- time scales

chemical time scales (10^{-10} - 10 s)!

extreme number of different chemical species

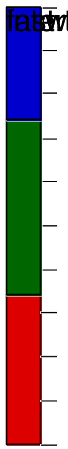
How Can the Problems be Overcome?

Exploit capabilities of modern computers (vectorization, parallelization).

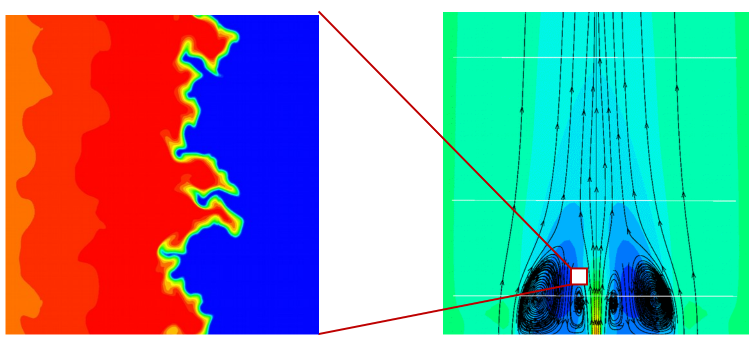
Use adaptive numerical methods (adaptive in space and time).

Exploit the hierarchical structure!

different levels of time scales



different levels of spatial structures



The overall process can only be understood if the underlying sub-processes are known adequately!

- Motivation
- Principles and problems of modeling
- Hierarchical concepts for model reduction
  - Behavior of the system in state space
  - Low-Dimensional manifolds
  - Implementation
- Conclusions

Reacting flows

Starting point: equation for the scalar field $\psi = (h, p, w_1, w_2, \ldots, w_{n_s})^T$

$$\frac{\partial \psi}{\partial t} = F(\psi) + v \cdot \text{grad}\psi + \frac{1}{\rho}\text{div}D\,\text{grad}\psi = F(\psi) + \Xi(\psi, \nabla\psi, \nabla^2\psi)$$

⇑ •chemistry ⇑ •convection ⇑ •transport

Thermokinetic state is a function of spatial coordinate and time

$$\psi = \psi = \psi(\vec{r}, t)$$

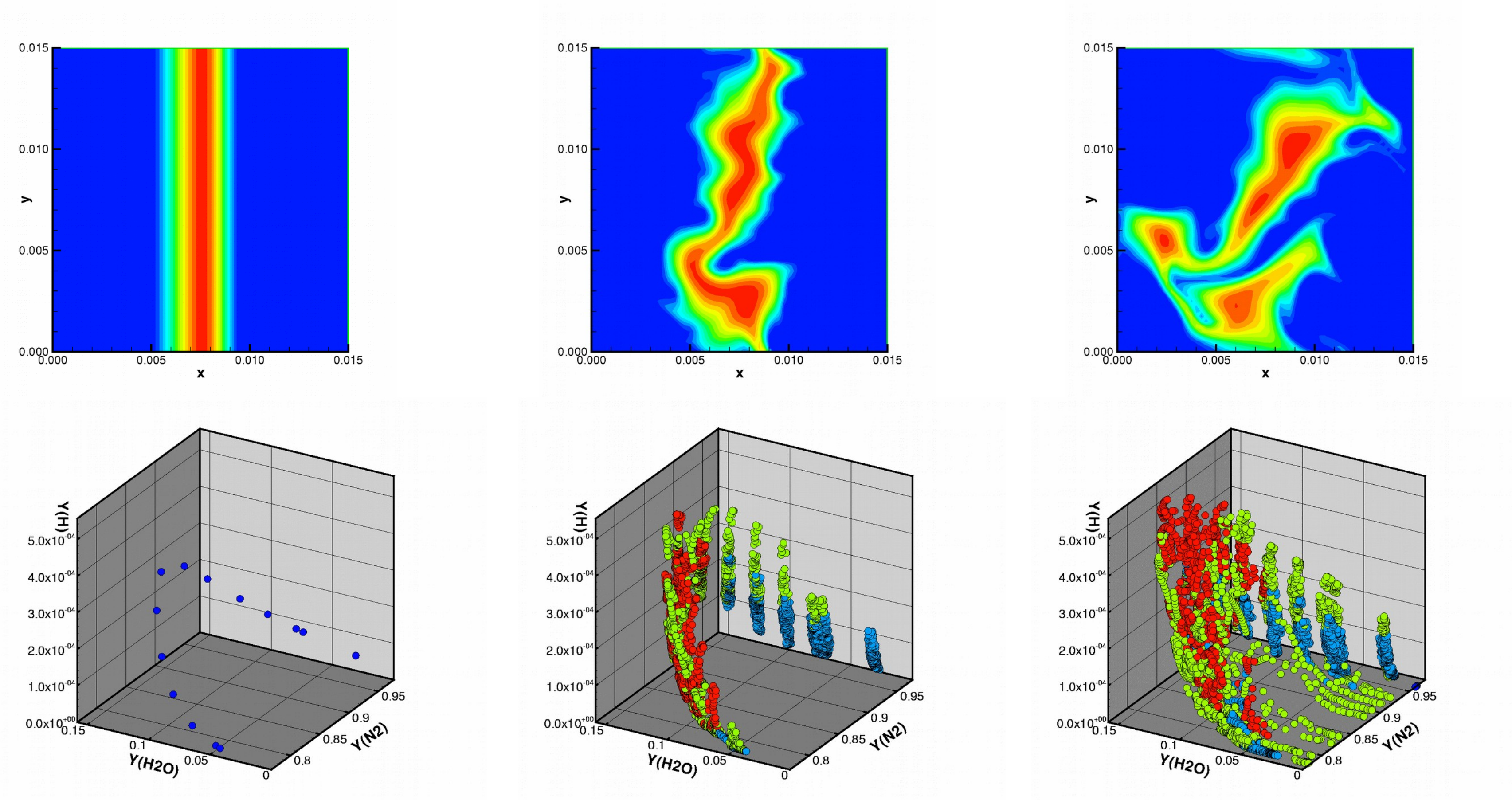
For general 3D flows: ψ depends on 3+1 variables

Notation in the following:

$$\psi_\theta = \begin{pmatrix} \frac{\partial \psi_1}{\partial \theta_1} & \cdots & \frac{\partial \psi_1}{\partial \theta_m} \\ \frac{\partial \psi_2}{\partial \theta_1} & \cdots & \frac{\partial \psi_2}{\partial \theta_m} \\ \vdots & \ddots & \\ \frac{\partial \psi_n}{\partial \theta_1} & \cdots & \frac{\partial \psi_n}{\partial \theta_m} \end{pmatrix}$$

Note: "Dimension" is used here for the number of variables

Consequences



Maas & Thévenin 1998

Observations:

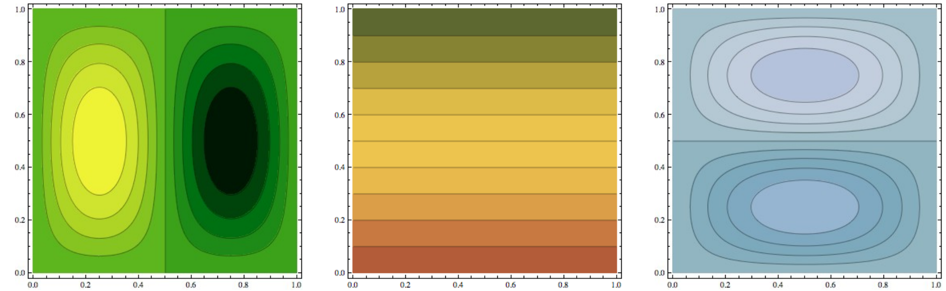
Only a small subspace is actually accessed.

In addition the accesed space is confined to low-dimensional manifolds.

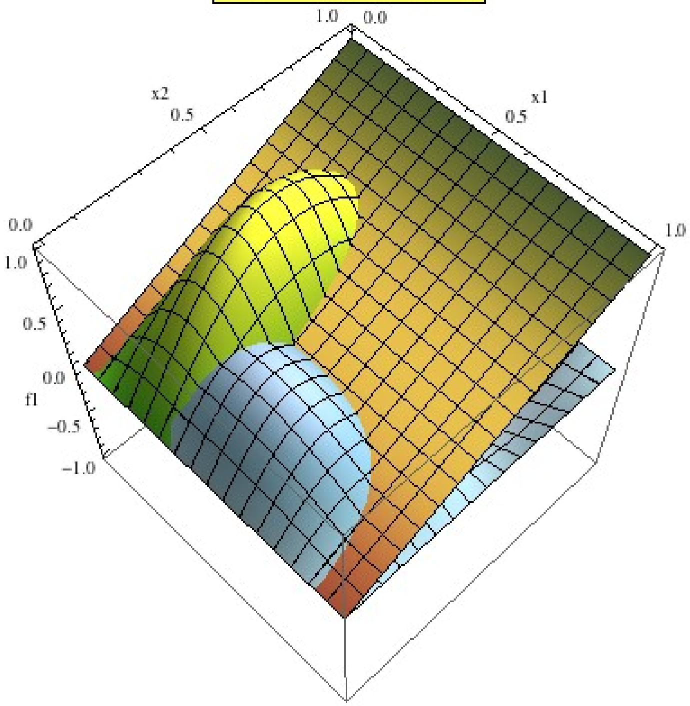
From physical to Composition Space

Toy example:

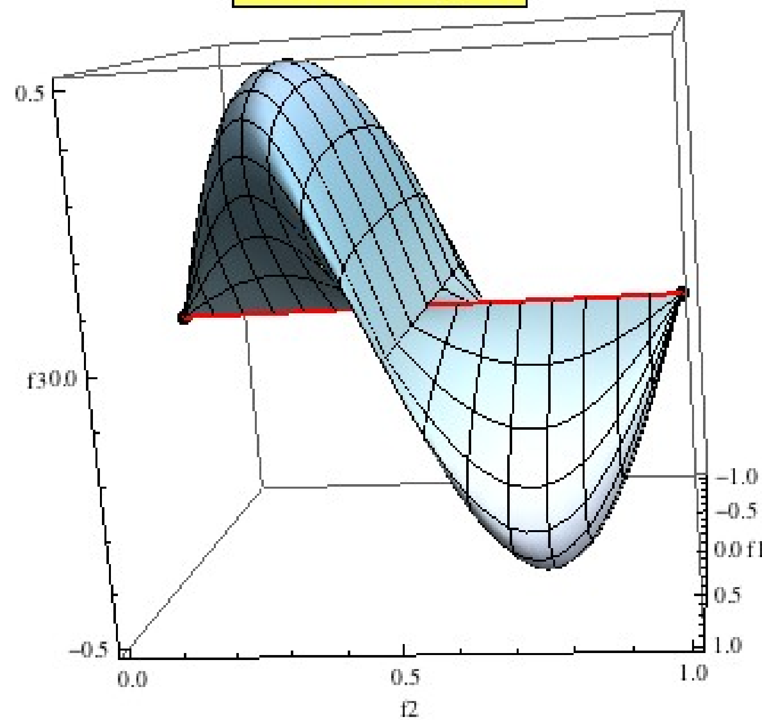
$$\psi(x,y) = \begin{pmatrix} \sin(2\pi x)\sin(\pi y) \\ y \\ \sin(\pi x)\sin(\pi y)\cos(\pi y) \end{pmatrix}$$



Plot in Physical Space



Plot in State Space



Evolution of the Manifold in Composition Space

Starting point: $$\frac{\partial\psi}{\partial t} = F(\psi) + v\cdot\mathrm{grad}\psi + \frac{1}{\rho}\mathrm{div}D\,\mathrm{grad}\psi \qquad \psi = \psi(\theta,\alpha)$$

Evolution of a point in composition space

$$\frac{\partial\psi(\theta)}{\partial t} = F(\psi(\theta)) - \vec{v}\,\psi_\theta \mathrm{grad}\theta + \frac{1}{\rho}\left(\mathrm{D}(\theta)\psi_\theta \mathrm{grad}\theta\right)_\theta$$

Projection onto the orthogonal space

$$\frac{\partial\psi(\theta)}{\partial t} = (I - \psi_\theta\psi_\theta^{+})\cdot\left\{F(\psi(\theta)) + \frac{1}{\rho}\left(\mathrm{D}(\theta)\psi_\theta \mathrm{grad}\theta\right)_\theta\right\}$$

Evolution in Composition Space

At any time *t* the scalar field of a reacting flow defines a manifold of dimension *d* ≤ 3.

$$\psi = \psi(\vartheta(\vec{r})) \qquad \psi = \psi(\vartheta(\vec{r}))$$

A *d** ≤ 4-dimensional manifold is describes the whole time evolution

$$\psi = \psi(\vartheta^*(\vec{r},t))$$

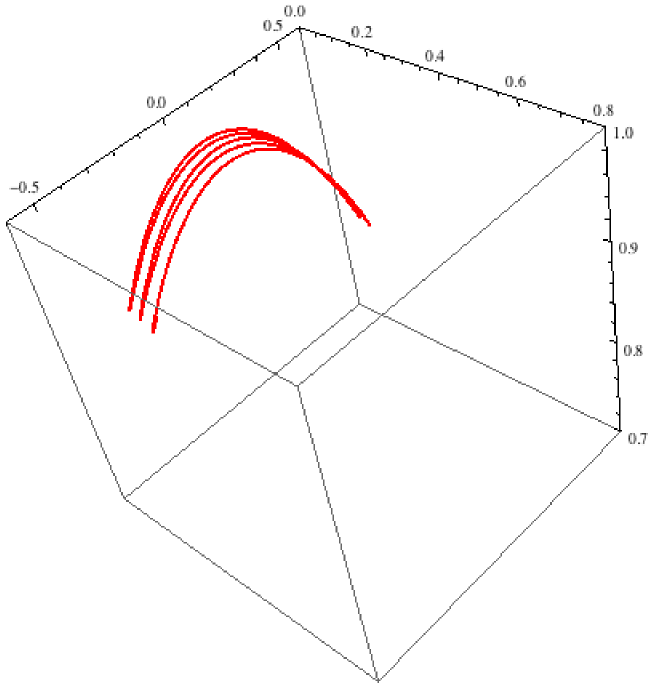
One could imagine to devise a method, which calculates the evolution of the manifold and its parameters separately!

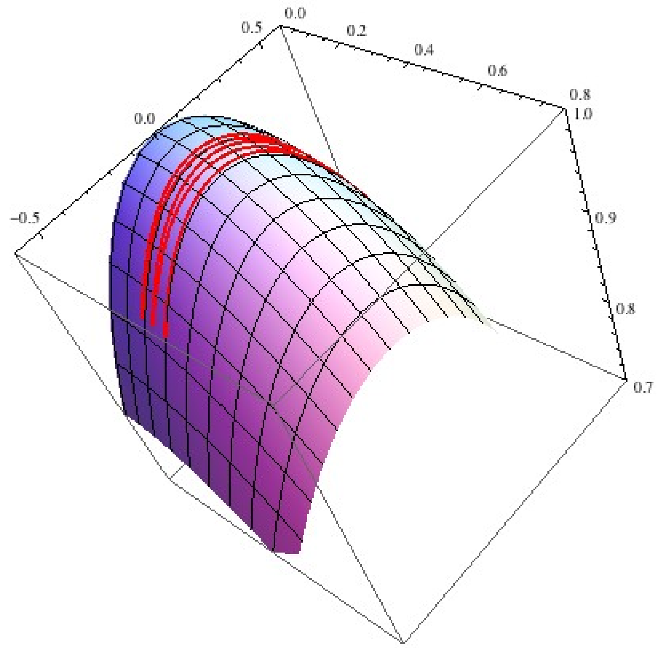
$$\frac{\partial\psi}{\partial t} = G(\psi,\psi_\theta,\psi_{\theta\theta})$$

$$\frac{\partial\theta}{\partial t} = H(\theta,\theta_r,\theta_{rr})$$

Problems of this approach

Low-dimensional manifold might become arbitrarily complicated

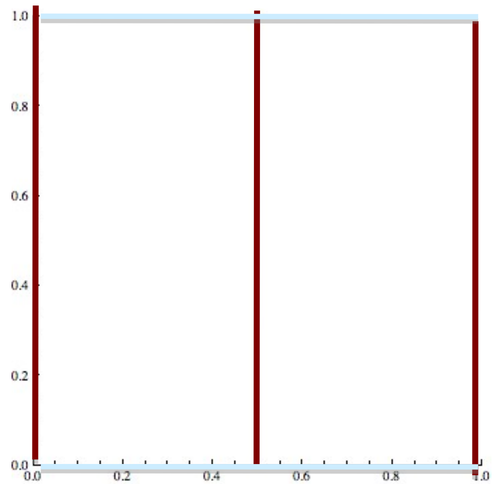


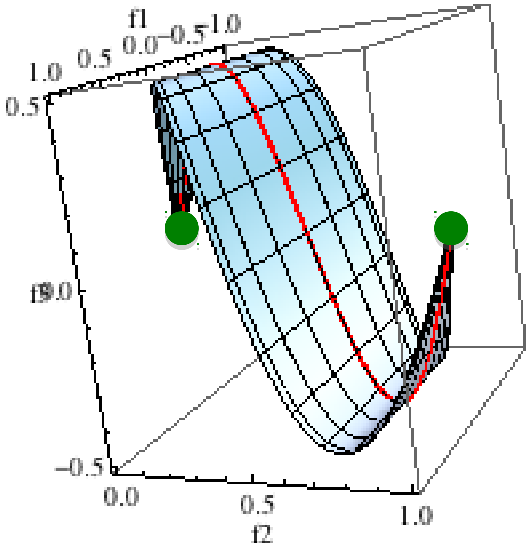


But: The geometry on the m+1 dimensional geometry looks much nicer.

An (m+1) dimensional manifold depends less on the gradients than an m-dimensional manifold.

Observations so Far





- the mapping is not injective (the same state vector can be found at different spatial locations,
  - This means: At the same location in state space the gradients might be different!
- boundaries in the physical space do not need to correspond to boundaries in composition space.
  - This means: We have to devise an evolution equation for the boundary
- Problems: Although the manifolds are at most 4-dimensional, each realization of a particular reacting flow might correspond to a different one.

Motivation

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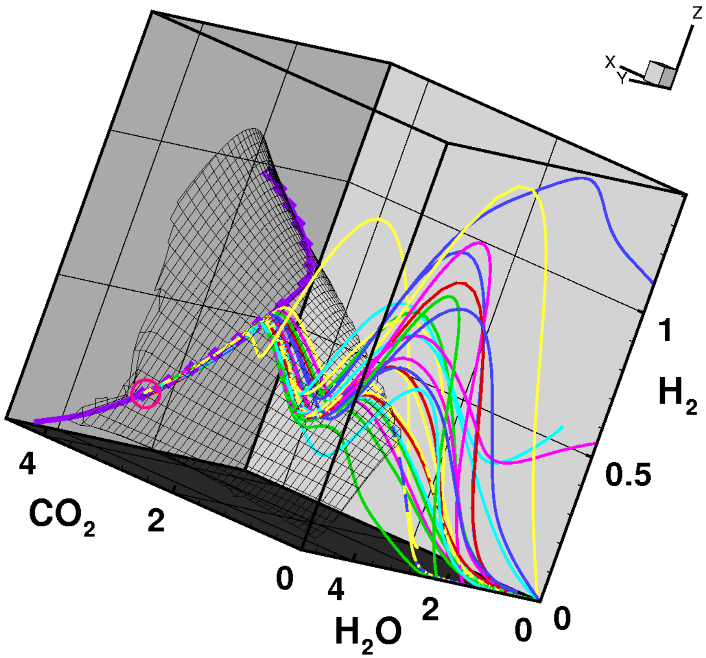
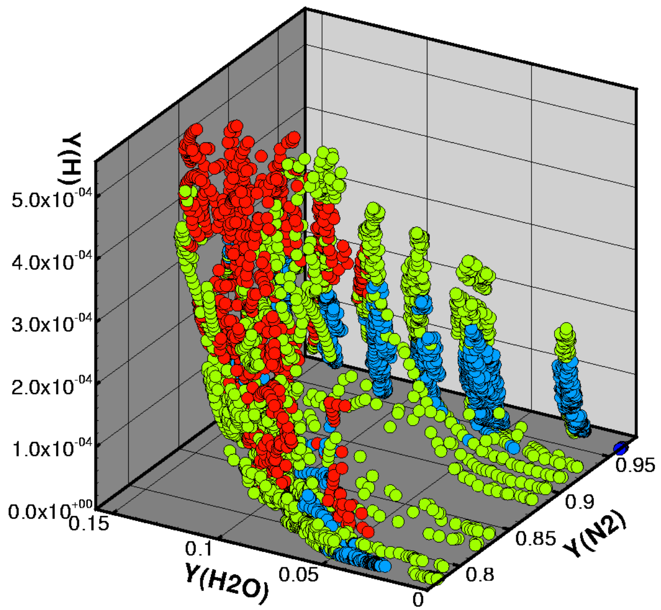
Conclusions

Observation:

Stiff chemical kinetics as well as molecular transport processes cause the existence of attractors in composition space



ILDMs of higher hydrocarbons



Correlation analysis of DNS-Data

Zel'dovich showed that there is a unique equilibrium: Ya. B. Zel'dovich, "A proof of the uniqueness of the solution of the equations for the law of mass action," Zh. Fiz. Khim. **115, 685–687 (**1938) in Russian.

Decomposition of Motions

$$\frac{\partial\psi}{\partial t} = F(\psi) + v\cdot\mathrm{grad}\,\psi + \frac{1}{\rho}\mathrm{div}D\,\mathrm{grad}\,\psi = F(\psi) + \Xi(\psi,\nabla\psi,\nabla^2\psi)$$

⇧ chemistry ⇧ convection ⇧ transport

Decomposition into "very slow, intermediate and fast subspaces"

$$F_\psi = (Z_c \quad Z_s \quad Z_f)\cdot\begin{pmatrix} N_c & & \\ & N_s & \\ & & N_f \end{pmatrix}\cdot\begin{pmatrix}\tilde{Z}_c \\ \tilde{Z}_s \\ \tilde{Z}_f\end{pmatrix}$$

$$\left|\lambda_i(N_c)\right| < \tau_c$$

$$\lambda_i^{\mathrm{real}}(N_f) < \tau_s < \lambda_i^{\mathrm{real}}(N_s)$$

$$\tilde{Z}_c\frac{\partial\psi}{\partial\tau} = \tilde{Z}_\chi\Phi(\psi) - \tilde{Z}_\chi\varpi\cdot\gamma\rho\alpha\delta\,\psi + \tilde{Z}_\chi\frac{1}{\rho}\delta\iota\varpi\Delta\,\gamma\rho\alpha\delta\,\psi$$

$$\tilde{Z}_\sigma\frac{\partial\psi}{\partial\tau} = \tilde{Z}_\sigma\Phi(\psi) - \tilde{Z}_\sigma\varpi\cdot\gamma\rho\alpha\delta\,\psi + \tilde{Z}_\sigma\frac{1}{\rho}\delta\iota\varpi\Delta\,\gamma\rho\alpha\delta\,\psi$$

diffusion-convection equation for "quasi conserved" variables evolution along the LDM

$$\tilde{Z}_\phi\frac{\partial\psi}{\partial\tau} = \tilde{Z}_\phi\Phi(\psi) - \tilde{Z}_\phi\varpi\cdot\gamma\rho\alpha\delta\,\psi + \tilde{Z}_\phi\frac{1}{\rho}\delta\iota\varpi\Delta\,\gamma\rho\alpha\delta\,\psi$$

ILDM-equations

Low-Dimensional Manifold Concepts

system equation	manifold equation
$\frac{\partial \psi}{\partial t} = F(\psi)$	$\tilde{Z}_f(\psi)\,\Phi(\psi) = 0$

QSSA (Bodenstein 1913)

Set right hand side for qss species to zero

$$\tilde{Z}_f = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

ILDM (Maas & Pope 1992)

Use eigenspace decomposition of Jacobian

$$F_\psi = (Z_\sigma \quad Z_\phi) \cdot \begin{pmatrix} N_\sigma & 0 \\ 0 & N_\phi \end{pmatrix} \cdot \begin{pmatrix} \tilde{Z}_\sigma \\ \tilde{Z}_\phi \end{pmatrix}$$

GQL (Bykov et al. 2007)

Use eigenspace decomposition of global quasilinearization matrix

$$T = \begin{pmatrix} | & & | \\ \Phi(\psi_1) & \Lambda & \Phi(\psi_\nu) \\ | & & | \end{pmatrix} \begin{pmatrix} | & & | \\ \psi_1 & \Lambda & \psi_\nu \\ | & & | \end{pmatrix}^{-1}$$

Many other strategies can be found in the literature!

Global Quasilinearization

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Idea: approximate the global behavior of the system by a linear approximation

For an n-dimensional system choose n different points and calculate their rates

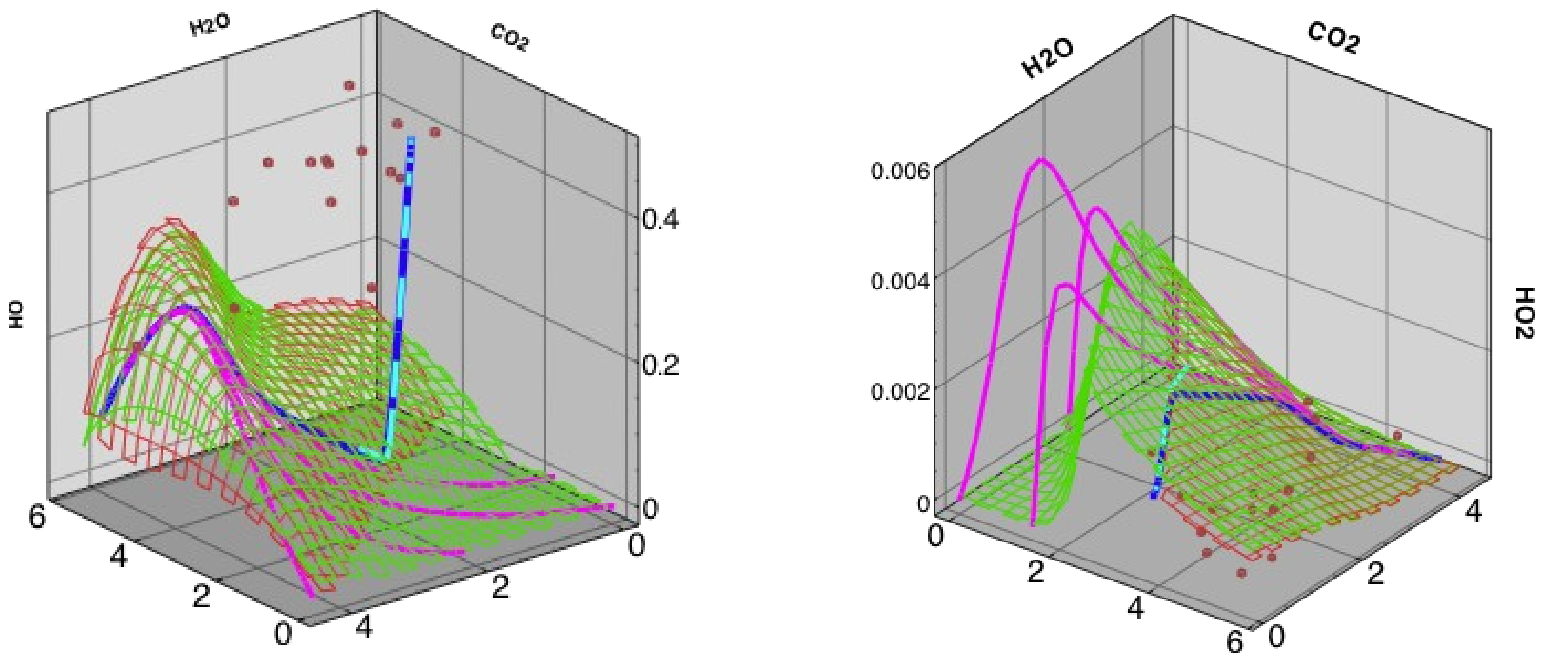
$$\overline{\overline{\psi}} = \begin{pmatrix} | & & | \\ \psi_1 & \cdots & \psi_n \\ | & & | \end{pmatrix} \qquad \overline{\overline{F}} = \begin{pmatrix} | & & | \\ F(\psi_1) & \cdots & F(\psi_n) \\ | & & | \end{pmatrix}$$

Approximate the non-linear system such that it is represented exactly at least for these n points

$$F_i(\psi) = T\psi_i \qquad \overline{\overline{\Phi}} = T\overline{\overline{\psi}} \qquad T = \overline{\overline{\Phi}}\,\overline{\overline{\psi}}^{-1}$$

Use this matrix T just like the Jacobian in the ILDM-context

GQL application



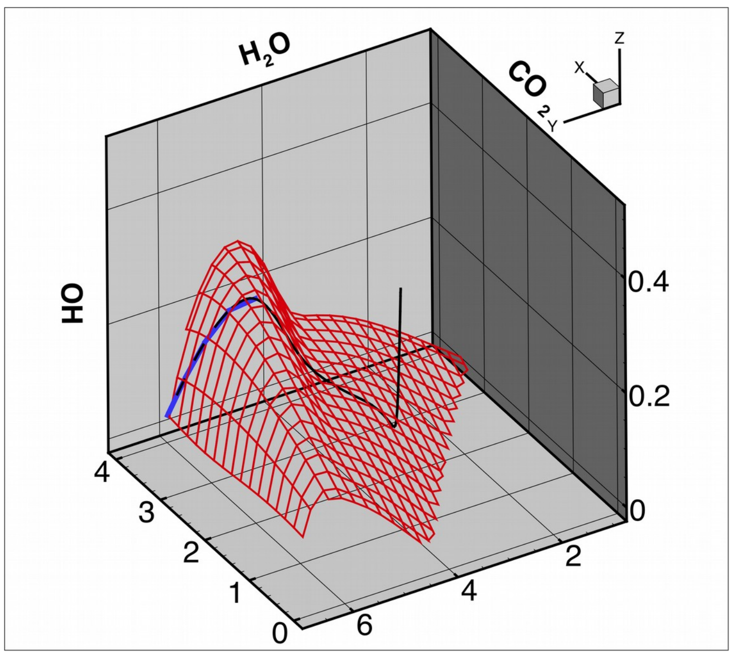
- red mesh: ILDM, green mesh: manifold, symbols: reference points
- blue curve: detailed system solution, cyan curve: fast subsystem solution
- magenta curves: detailed stationary system solution of flat flames
- Bykov, Goldshtein, Maas 2007

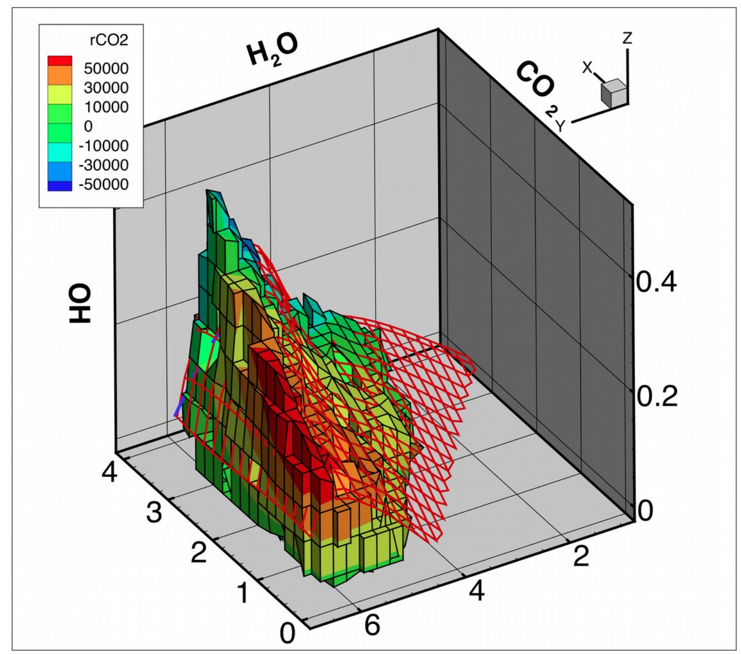
Hierarchy of Low-Dimensional Manifolds

It can be shown that QSS, ILDM, and GQL yield a hierarchy of low-dimensional mainfolds in composition space

$$M^m = \{\psi^\mu(\theta) \,|\, Z_\phi^\mu(\psi^\mu(\theta))\,\Phi(\psi^\mu(\theta)) = 0\}$$

$$M^1 \subset M^2 \subset \Lambda \subset M^\nu$$





Problems

Strong coupling of reaction and Diffusion

But there is no reason not to solve the manifold eqution and the equation for the reduced coordinates simultaeously

Evolution in Composition Space

Evolution equations for the manifold and the parameters:

$$\frac{\partial \psi(\theta)}{\partial t} = (I - \psi_\theta \psi_\theta^{+}) \cdot \left\{ F(\psi(\theta)) + \frac{1}{\rho} (\mathrm{D}(\theta) \psi_\theta \operatorname{grad}\theta)_\theta \right\}$$

$$\frac{\partial \theta}{\partial t} = S(\theta) + \vec{v} \operatorname{grad}\theta + \frac{1}{\rho} P \operatorname{div}\left(\overline{\overline{D}}^{*} \operatorname{grad}\theta\right)$$

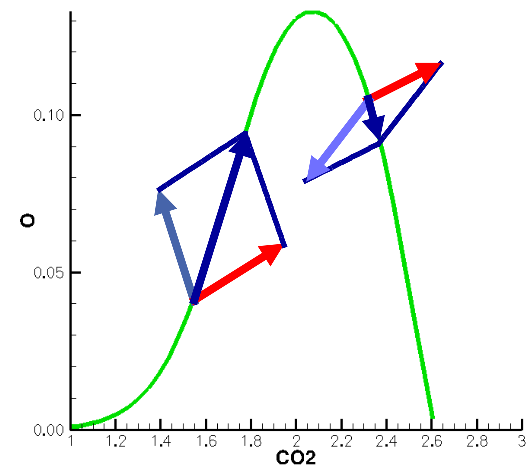
Proble...

$$\frac{\partial \psi}{\partial t} = G(\psi, \psi_\theta, \psi_{\theta\theta}, \theta_r, \theta_{rr})$$

$$\frac{\partial \theta}{\partial t} = H(\psi, \psi_\theta, \theta, \theta_r, \theta_{rr})$$

If θ_r, θ_{rr} were functions of θ only it would be simple!

This is the basis of the REDIM method!



Basic Assumptions and Consequences

$$\frac{\partial \psi(\theta)}{\partial \tau} = (I - \psi_\theta \psi_\theta^{+}) \cdot \left\{ F(\psi(\theta)) + \frac{1}{\rho} (\mathrm{D}(\theta) \psi_\theta \xi)_\theta \, \xi \right\}$$

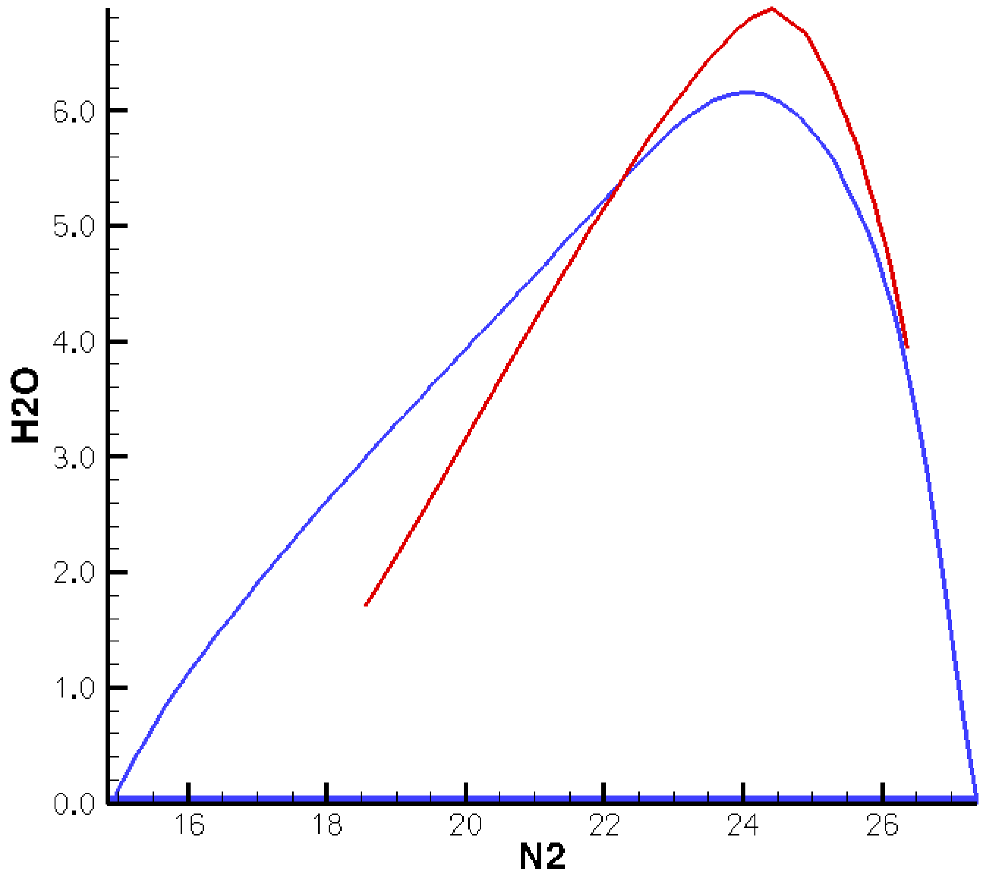
Assumptions

- The gradients, although they depend on the spatial location, can be estimated based on the value of θ only.
- Due to fast relaxation processes the steady solution of the evolution equation represents the manifold.

Note:

- If the gradient estimation is bad or the relaxation is not fast enough, then the dimension needed to describe the system might be higher than 3 + 1.
- A method is needed that estimates the influence of the gradient estimate.

Principle of the Evolution equation



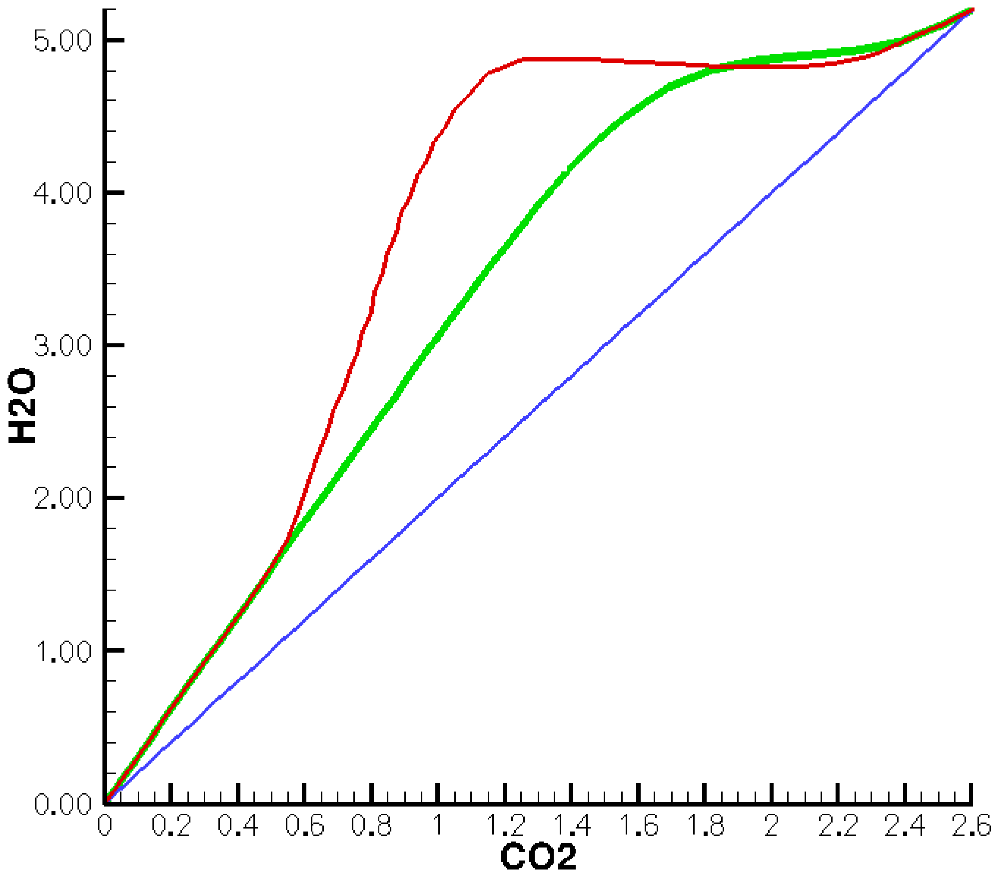
$$\frac{\partial \psi}{\partial \tau} = (I - \psi_\theta \psi_\theta^+) F(\psi(\theta))$$

- equilibrium curve

$$\frac{\partial \psi}{\partial \tau} = (I - \psi_\theta \psi_\theta^+) d \; \xi \circ \psi_{\theta\theta} \circ \xi$$

- mixing line

Principle of the Evolution equation



$$\frac{\partial \psi}{\partial \tau} = (I - \psi_\theta \psi_\theta^+) F(\psi(\theta))$$

- slow manifold

$$\frac{\partial \psi}{\partial \tau} = (I - \psi_\theta \psi_\theta^+) d\ \xi \circ \psi_{\theta\theta} \circ \xi$$

- mixing line

Principle of the Evolution Equation

Basic Procedure:

formulate initial guess

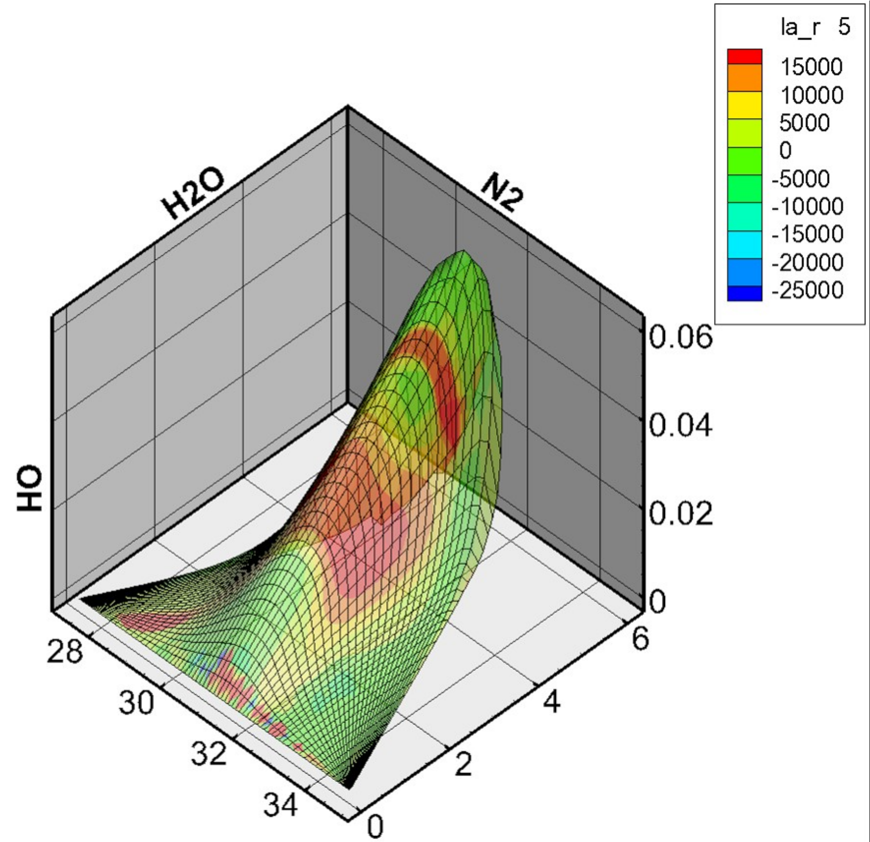
specify boundary conditions

estimate the gradient

(it has been shown that a good estimate gets more and more unimportant for increasing dimension)

solve the evolution equation (PDE)

stationary solution yields the REDIM



Influence of the gradients

A detailed analysis of the influence of the gradients is quite lengthy

But: The principle can be understood very easily

$$\frac{\partial \psi(\theta)}{\partial \tau} = (I - \psi_\theta \psi_\theta^{+}) \cdot \left\{ F(\psi(\theta)) + \frac{1}{\rho} (\mathrm{D}(\theta) \psi_\theta \xi)_\theta \, \xi \right\}$$

1. What is the sensitivity if the reactions are very slow?

$$\frac{\partial \psi(\theta)}{\partial \tau} = (I - \psi_\theta \psi_\theta^{+}) \cdot \left\{ \frac{1}{\rho} (\mathrm{D}(\theta) \psi_\theta \xi)_\theta \, \xi \right\} \quad \text{for} \quad \tau \to \infty$$

$$\psi_\theta^{\perp} (\mathrm{D}(\theta) \psi_\theta)_\theta = 0$$

Solution is a minimal surface and does not depend on the gradient

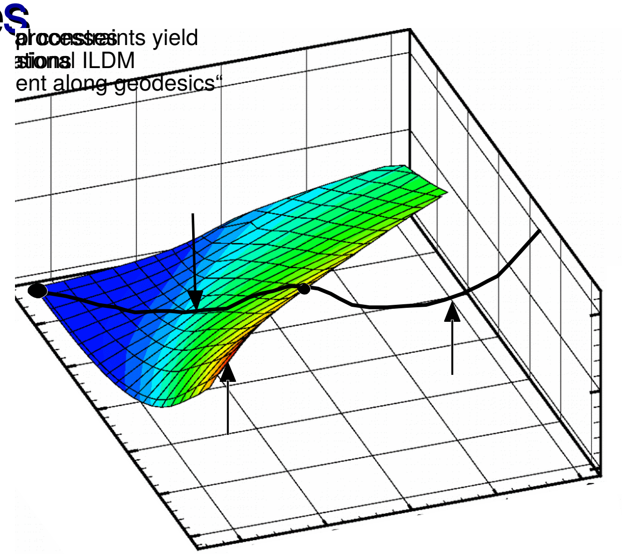
Influence of the gradients

2. What is the sensitivity if the reactions are very fast?

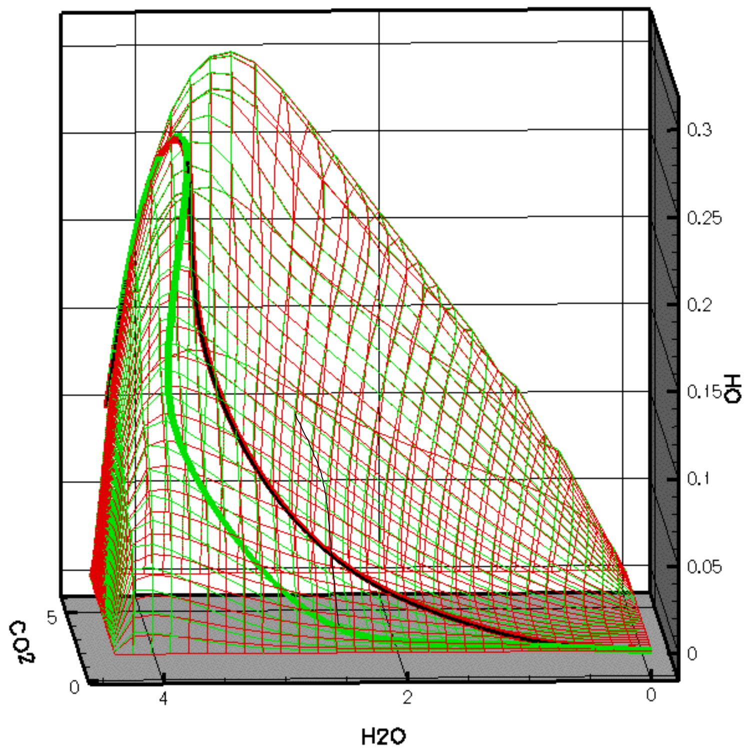
$$\frac{\partial \psi(\theta)}{\partial \tau} \approx (I - \psi_{\theta}\psi_{\theta}^{+}) \cdot \{F(\psi(\theta))\}$$

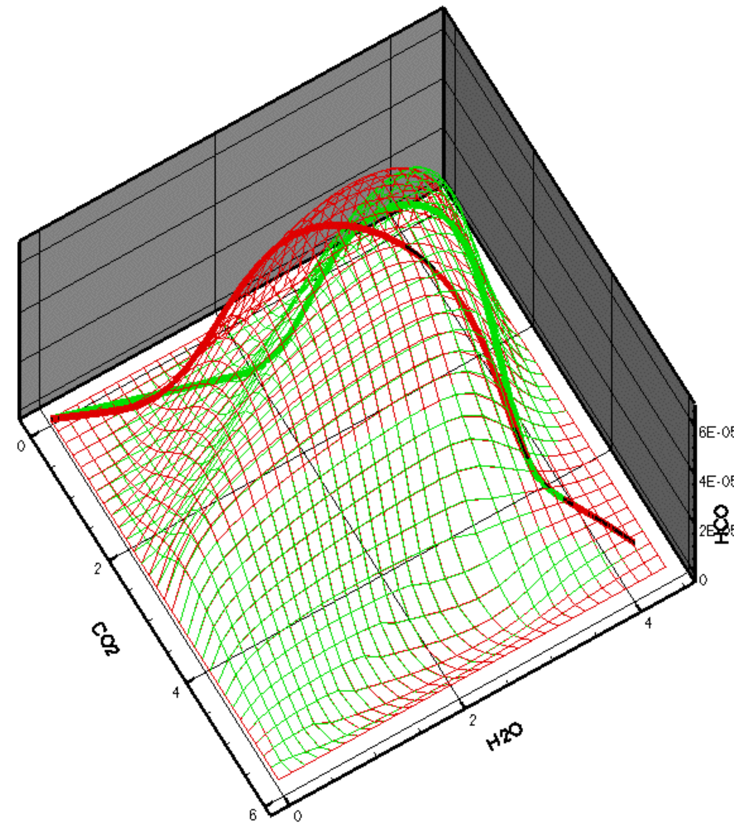
- Solution does not depend on the gradient! (in fact:if it is 0, then the solution are slow invariant manifolds

In principle the REDIM defines minimal sub-surfaces on the nonlinear surface of fast chemical processes



Influence of the gradients



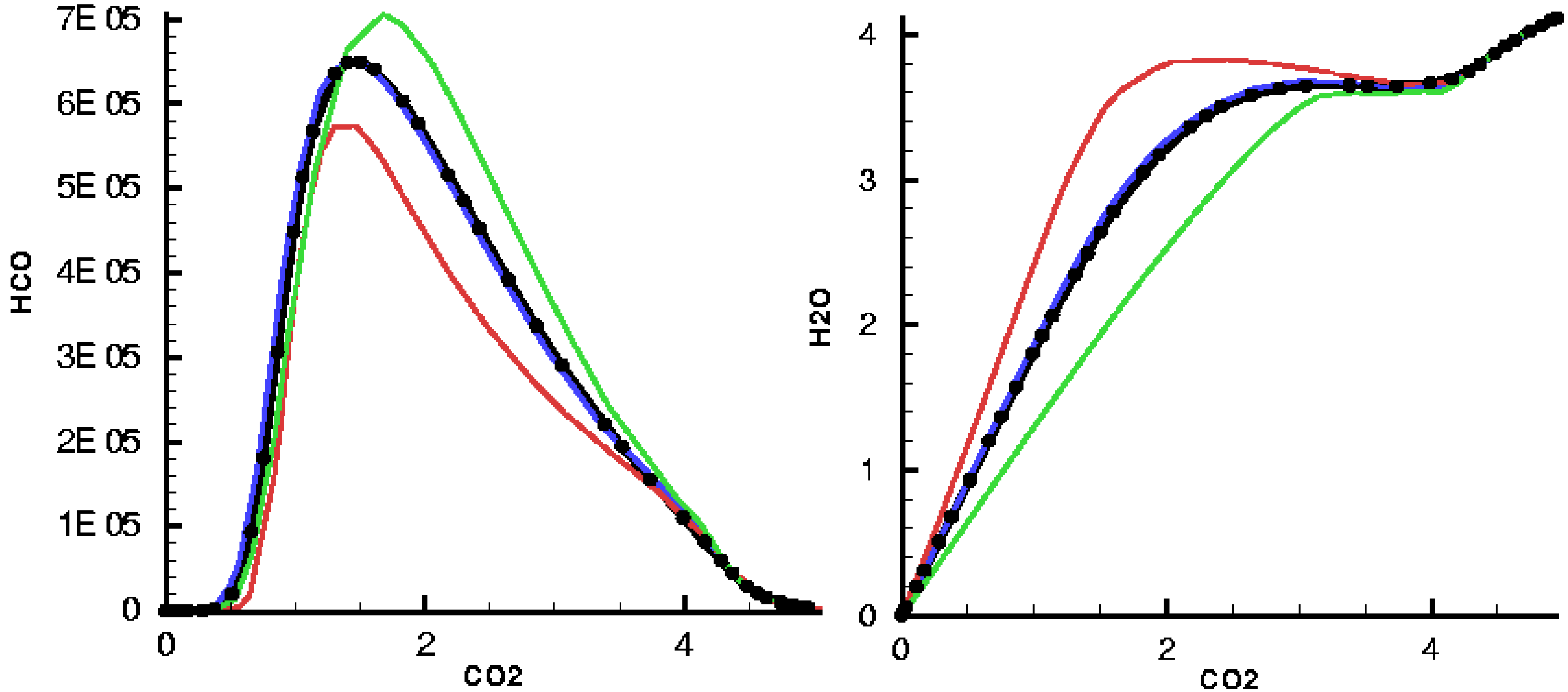


•1D (curves) and 2D (mesh) REDIMs

•red: estimate from 1-D flat flame, green: gradient estimated one order of magnitude lower

•black curve: exact solution for a flat flame

1D-REDIM:
Dependence on Gradient Estimate



flame structures in composition space

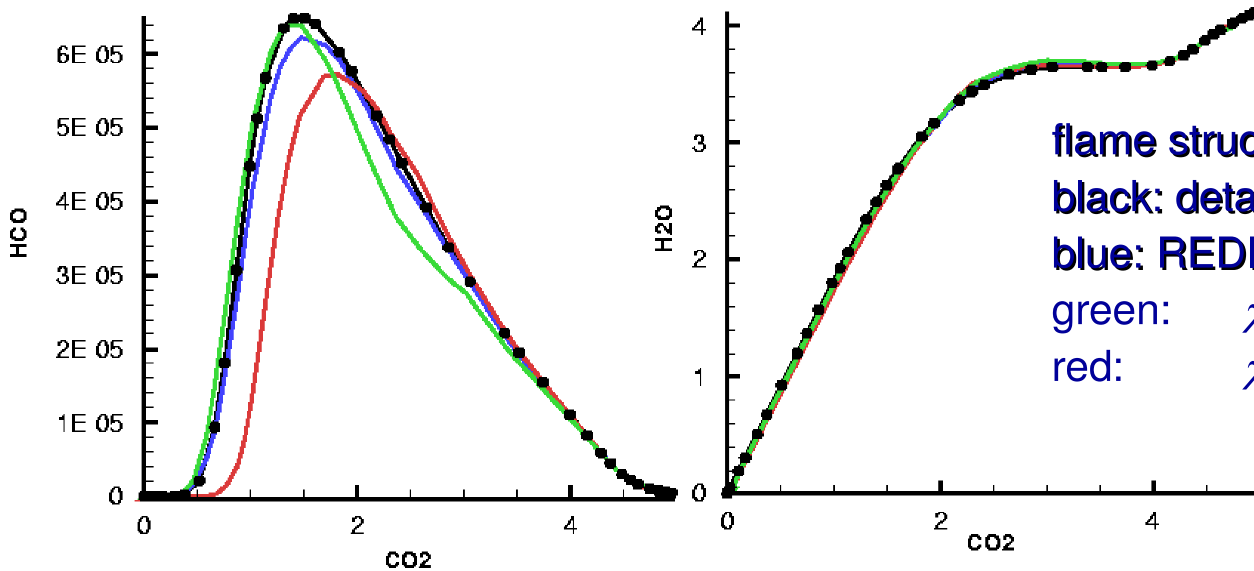
black: detailed solution

blue: REDIM for gradients from flamelet: $\chi(\theta) = \chi^{\Phi}(\theta)$

green: $\chi(\theta) = 10\ \chi^{\Phi}(\theta)$

red: $\chi(\theta) = 0.1\ \chi^{\Phi}(\theta)$

2D-REDIM: Dependence on Gradient Estimate



flame structures in composition space

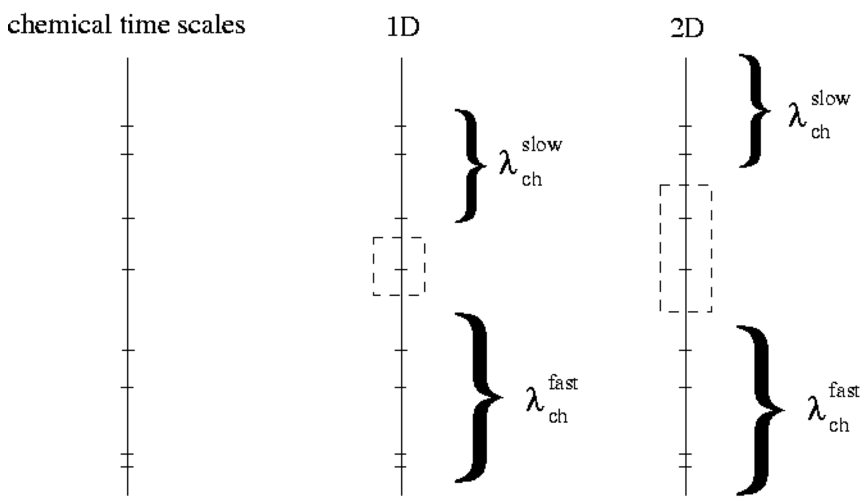
black: detailed solution

blue: REDIM for gradients from flamelet

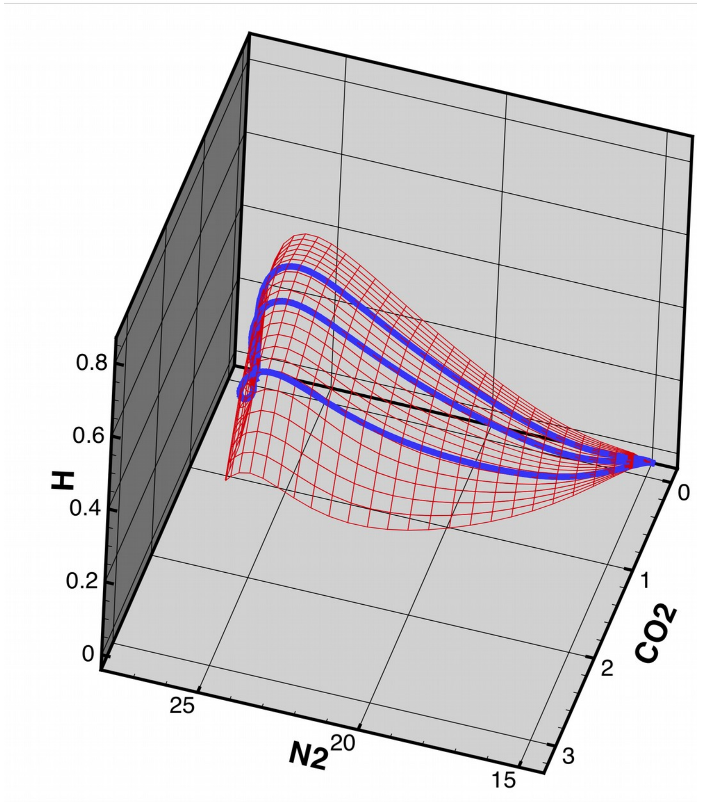
green: $\chi(\theta) = 10\ \chi^{\Phi}(\theta)$

red: $\chi(\theta) = 0.1\ \chi^{\Phi}(\theta)$

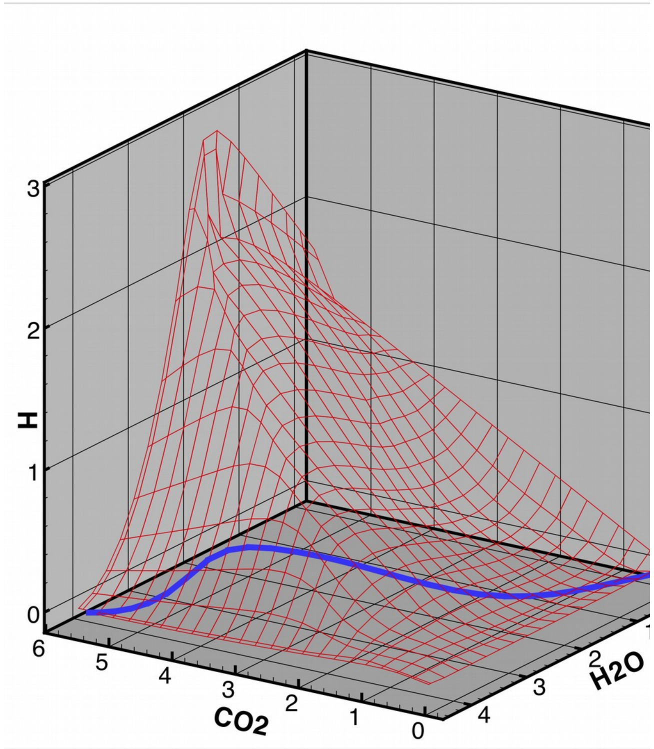
note: for typical flames $\chi(\theta)$ does not vary that much



Is there a hierarchy of LDMs?



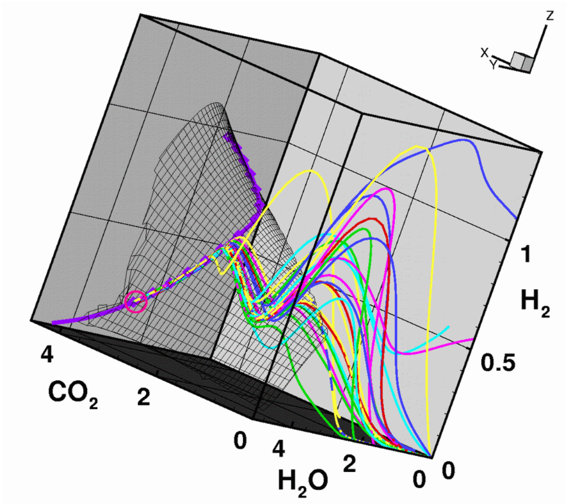
1D and 2D REDIMs of a non-premixed syngas/air system



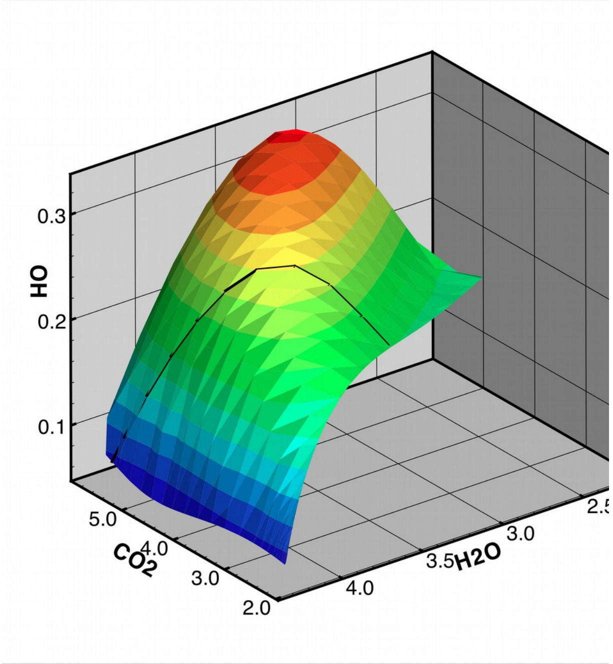
•1D and 2D REDIMs of a premixed syngas/air system

$$M_1^{REDIM} \subset M_2^{PE\Delta IM} \subset \Lambda \subset M_\nu^{PE\Delta IM}$$

Is there a hierarchy of LDMs?



- It can be shown for most manifold concepts that there is a hierarchy of manifolds of increasing dimension.



•1D and 2D ILDMs of a premixed syngas/air system

This hierarchy can be used for

- a hierarchical generation of LDMs
- an efficient implementation in reaction flow calculations
- an efficient error estimation
- an anlysis of the coupling of chemistry with molecular transport
- the developent of models for chemistry/turbulence coupling

Motivation

Principles and problems of modeling

Hierarchical concepts for model reduction

- Behavior of the system in state space
- Low-Dimensional manifolds
- Implementation

Conclusions

How can we use LDMs?

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Project governing equations onto the low-dimensional manifold

$$\psi = (h, p, w_1, w_2, \ldots, w_{n_s})^T = \psi(\theta)$$

$$\theta = (\theta_1, \theta_2, \ldots, \theta_m)^T \qquad m = n_s + 2$$

$$\frac{\partial \theta}{\partial t} = S(\theta) + \vec{v}\ \mathrm{grad}\theta + \frac{1}{\rho} P\, \mathrm{div}\left(\overline{\overline{D}}^{*}\ \mathrm{grad}\theta\right)$$

Note: The transport matrix is changed, too! This accounts for the coupling of kinetics with molecular transport.

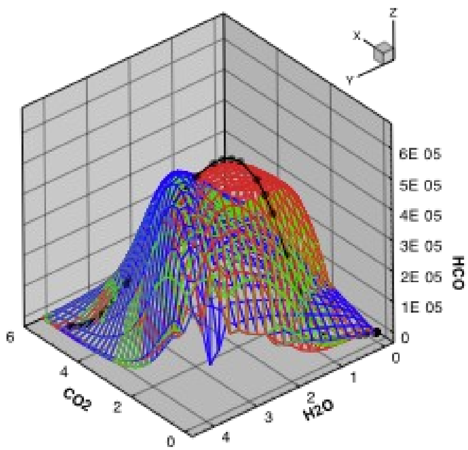
Implementation

reduced states $\theta, h, p, \nabla\theta, \nabla h, \tau$

ILDM

GQL

REDIM



CFD-code

reduced variables

$$\frac{\partial \theta}{\partial t} = S(\theta) + P\Xi\left(\psi(\theta), \nabla\psi(\theta), \nabla^2\psi(\theta)\right)$$

reaction transport

mass $\frac{\partial \rho}{\partial t} = K$

momentum $\frac{\partial \rho v}{\partial t} = K$

energy $\frac{\partial \rho u}{\partial t} = K$

interpolation

$S(\theta), \psi(\theta), T(\theta), \rho(\theta), \Pi(\theta)$

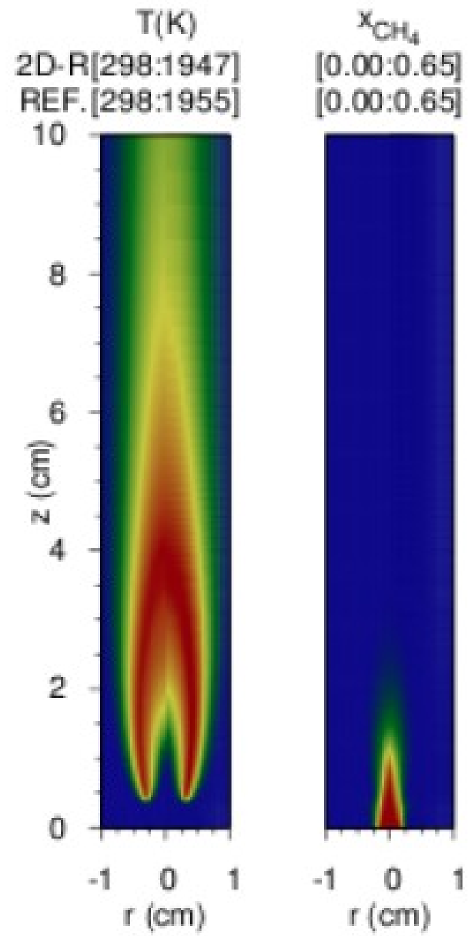
Use in „Real Life“

Various applications

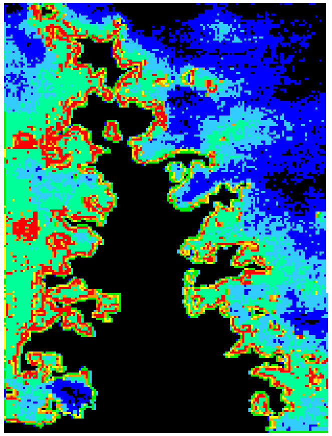
Tests with laminar flames

Example:

- Axi-symmetric methane/air flame
- Comparison of 2D-REDIM (right, Konzen et al.) with detailed simulations (left, Smooke et al.)



Deterministic and statistical models



Deterministic

Dinkelacker et al.

statistical

solve for ϕ and obtain $\langle\phi\rangle$ from a large number of calculations

extreme spatial and temporal resolution necessary

$$\frac{D\varphi}{Dt} = F(\varphi) + \frac{1}{\rho}\,\mathrm{div}\,D\,\mathrm{grad}\,\varphi$$

solve for $\langle\varphi\rangle$

only moderate spatial and temporal resolution needed

Is it really so simple? Problem: $\langle q(U,\varphi)\rangle \neq q(\langle U\rangle, \langle\varphi\rangle)$

Expectations can only be evaluated if the statistics is known!

Statistical Information

Averages of non-linear terms can be determined if the probability density function (PDF) is known.

$$\langle \omega_i \rangle = \int\int \omega_i(\psi, V) f(\psi, V; x, t) \, d\psi \, dV$$

$$f(\psi, \varsigma; \xi, \tau) \delta\psi \delta\varsigma = \Pi\rho o\beta\{\psi \leq \phi(\xi, \tau) < \psi + \delta\psi, \varsigma \leq Y(\xi, \tau) < \varsigma + \delta\varsigma\}$$

Advantages:

- $f(V, \psi; x, t)$ is time independent for statistically stationary problems
- $f(V, \psi; x, t)$ varies smoothly in space

Problem: How can $f(V, \psi; x, t)$ be determined?

- detailed measurements
- statistical models

  presumed PDF - solve for moments $<\phi>$, $<\phi'^2>$, . . .

  solve PDF transport equation

Turbulent Flow Modeling using PDF-methods

- transport equation for the joint PDF (Pope 1985)

$$\rho(\psi)\frac{\partial f}{\partial t} + \underbrace{\rho(\psi)V_j\frac{\partial f}{\partial x_j}}_{\text{transport in physical space due to convection}} - \underbrace{\frac{\partial\langle p\rangle}{\partial x_j}\frac{\partial f}{\partial V_j}}_{\text{transport in velocity space due to mean pressure gradient}} + \underbrace{\frac{\partial}{\partial \psi_\alpha}\left[\rho(\psi)S_\alpha(\psi)f\right]}_{\text{transport in scalar space due to chemical reaction}}$$

$$= \underbrace{\frac{\partial}{\partial V_j}\left[\left\langle (\mathrm{div}\,\overline{\overline{P'}})_j \middle| V,\psi\right\rangle f\right]}_{\text{transport in velocity space due to friction and pressure fluctuations}} + \underbrace{\frac{\partial}{\partial \psi_\alpha}\left[\left\langle \mathrm{div}\,j_\alpha \middle| V,\psi\right\rangle f\right]}_{\text{transport in scalar space due to molecular mixing}}$$

- one-point processes are treated exactly
- two-point processes (which appear as conditional expectations) have to be modeled

Particle Method

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Problem: Each chemical species enters as an independent variable.

- high dimension of the equation system ⇒ reduce dimension
- solution using finite differences, volumes or elements not feasible

Solution: PDF represented by stochastic particles

$$f(V,\psi;\vec{\rho},\tau) = \sum_{\iota=1}^{N} \delta(\varsigma - Y^{\iota}(\tau))\,\delta(\psi - \phi^{\iota}(\tau))\,\delta(\vec{\rho} - \vec{\rho}^{\iota}(\tau))$$

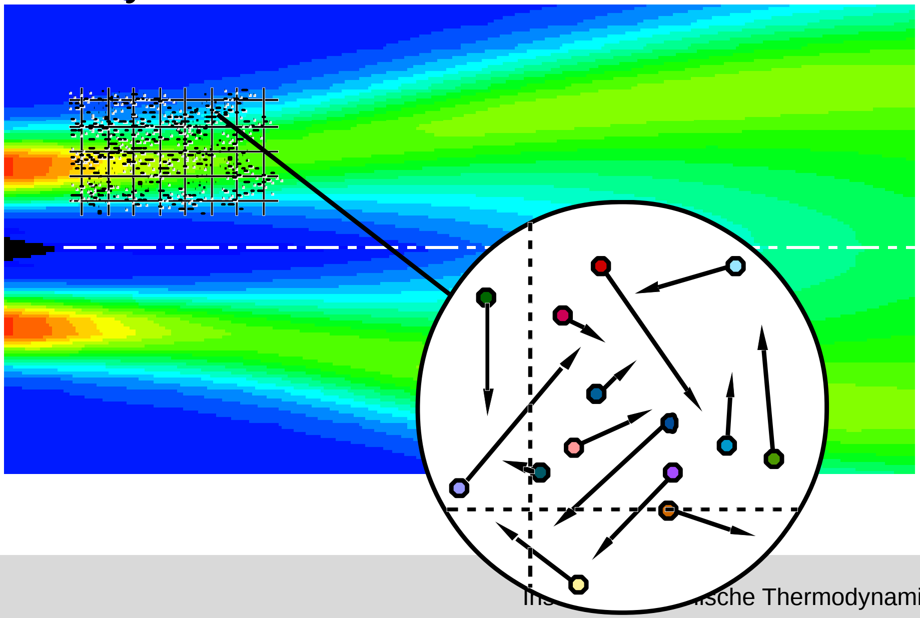
change of particle properties governed by ODEs

- example: convection

$$\frac{d\vec{r}^{\,i}(t)}{\delta\tau} = Y^{\iota}(\tau)$$

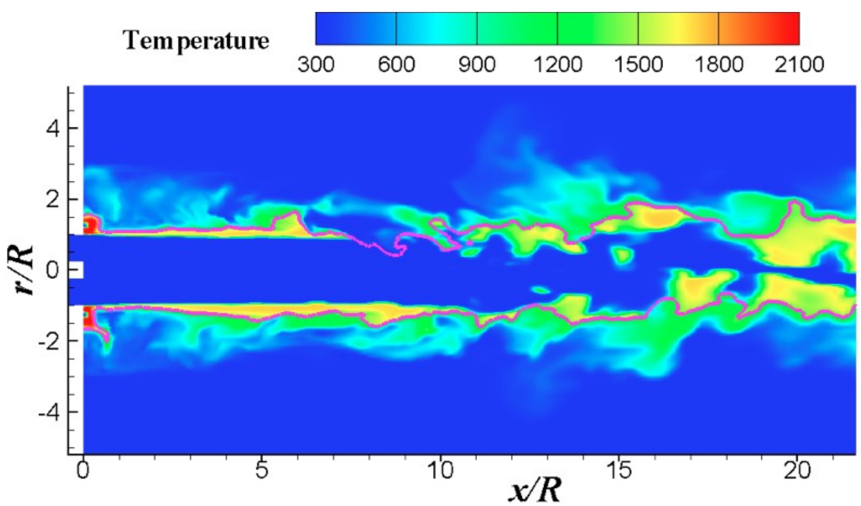
- example: reaction

$$\frac{d\phi^{\iota}(\tau)}{\delta\tau} = \Sigma^{\iota}(\phi^{\iota}(\tau))$$

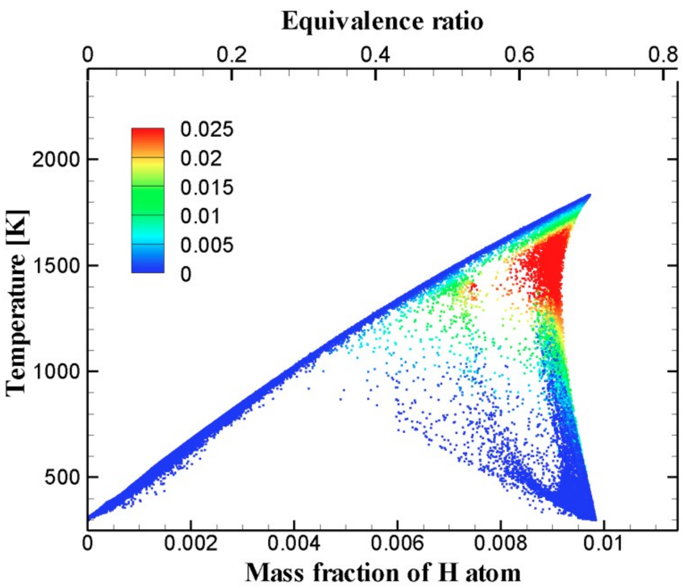


Example: LES of a premixed flame

Large eddy simulation coupled wirh an assumed PDF approach
REDIM reduced chemistry with two scalars



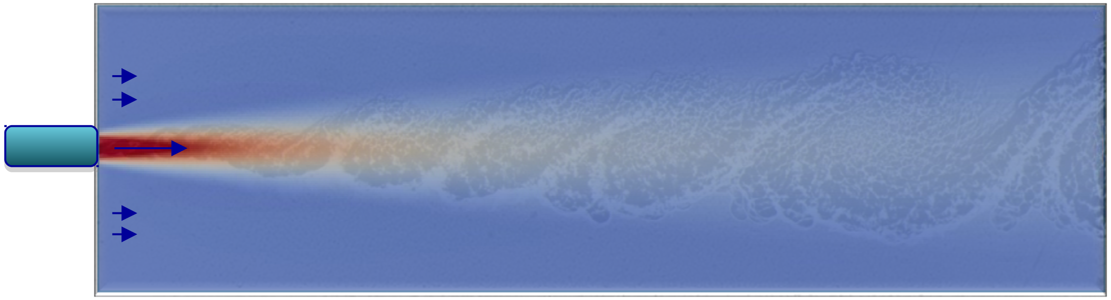
Instantaneous contours of temperature, red line: Z_H=0.7. An event of local extinction is seen around *x/R*=8, *r/R*=1.



Scatter plot of temperature vs. hydrogen mass fraction. ξ= 0.71 at one time step, calculated from LES resolved values.

P. Wang, F. Zieker, R. Schießl, N. Platova, J. Fröhlich, U. Maas, Proc Comb. Symp 2013

Example: Ignition by a hot jet



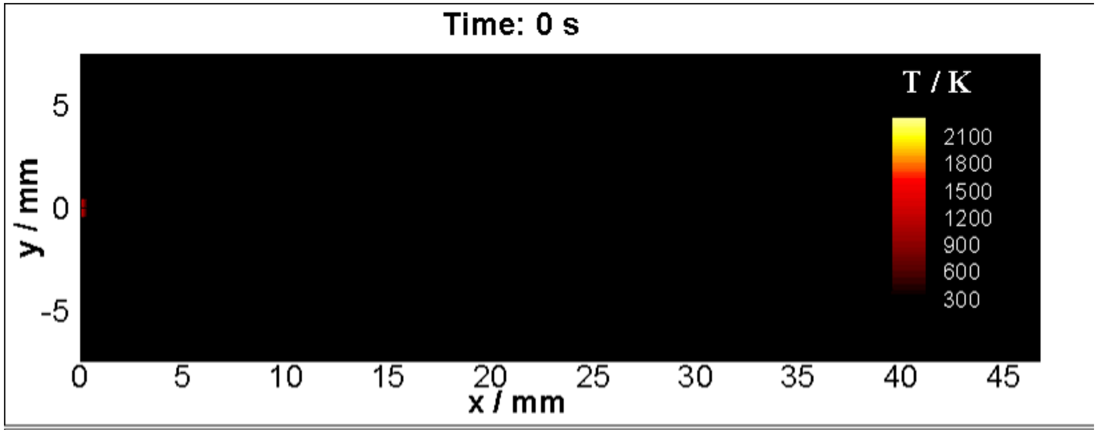
Hot jet of burned hydrogen/air mixture entering a cold hydrogen/air mixture.

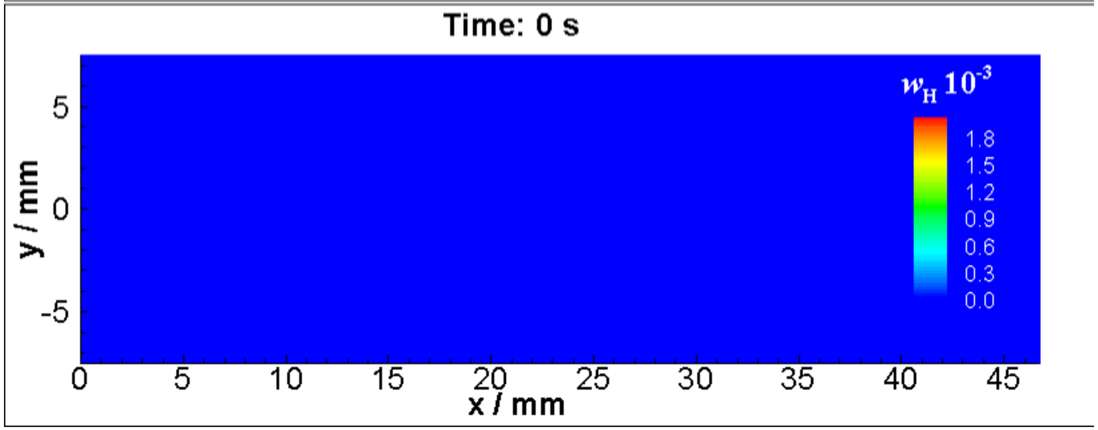
stand-alone Monte-Carlo-PDF-simulation

REDIM with two reduced variables

Example: Ignition by a hot jet

U_j (m/s)	U_e (m/s)	Jet Comp.	Env. Comp.
300	20	hot (1500K) burnt stoic. H_2/Air	cold stoic. H_2/Air





Ghorbani, Steinhilber, Markus, Maas 2014

Conclusions

Efficient methods for kinetic model reduction and its subsequent implementation in reacting flow calculations have been presented.

These methods can be coupled in an efficient way with deterministic or statistical methods for laminar and turbulent reacting flows

The dimension reduction reduces the number of equations to be solved considerably and at the same time it enters information on the chemistry-transport-coupling into the statistical models.

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