On the Spatial Dependence of REDIM Based Reduced Models of Reacting Flows

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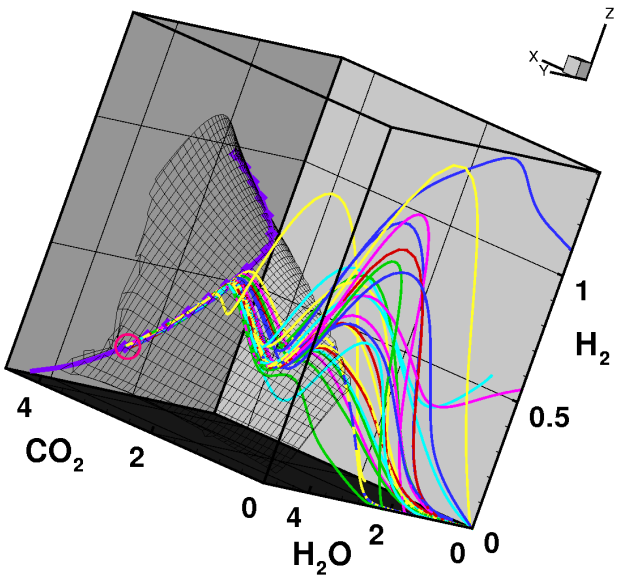


Overview

- Models of Reaction Flows
- Reacting Flows in Composition Space
- Reaction/Diffusion Manifolds
- Boundaries of REDIM
- Analysis of the gradient estimates
- Conclusions

Reacting flows

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

$$\frac{\partial \psi}{\partial t} = \underset{\text{chemistry}}{F(\psi)} + \underset{\text{convection}}{v \cdot \operatorname{grad}\psi} + \frac{1}{\rho}\underset{\text{transport}}{\operatorname{div} D \operatorname{grad}\psi} = F(\psi) + \Xi\left(\psi, \nabla\psi, \nabla^2\psi\right)$$

- **Thermokinetic state is a function of spatial coordinate and time**

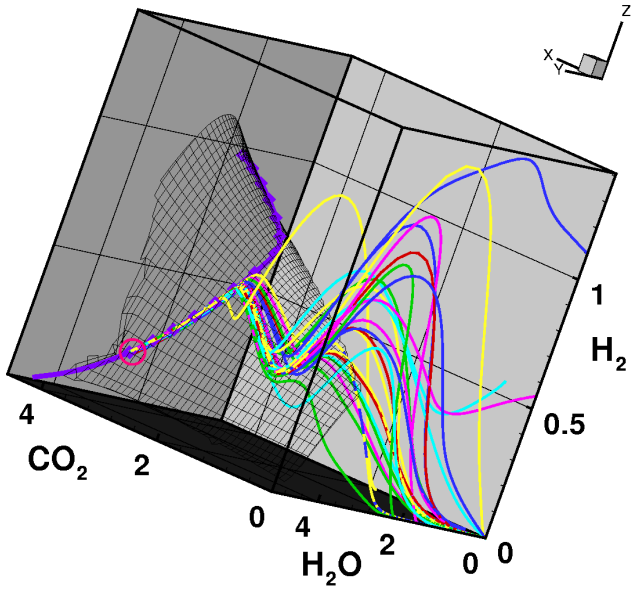
$$\psi = \psi = \psi\left(\vec{r}, t\right)$$

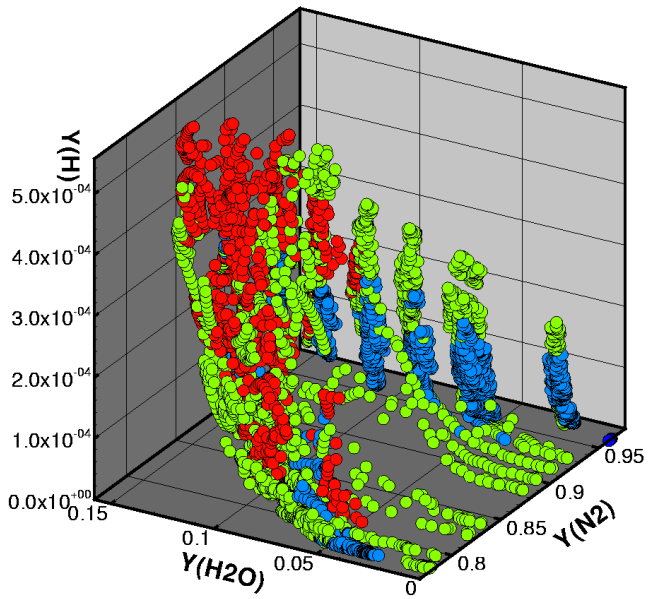
- **For general 3D flows: ψ depends on 3+1 variables**

- **Notation in the following:**

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

Behaviour in Composition Space





dynamics of homogeneous combustion systems, successive relaxation to lower dimensional manifolds

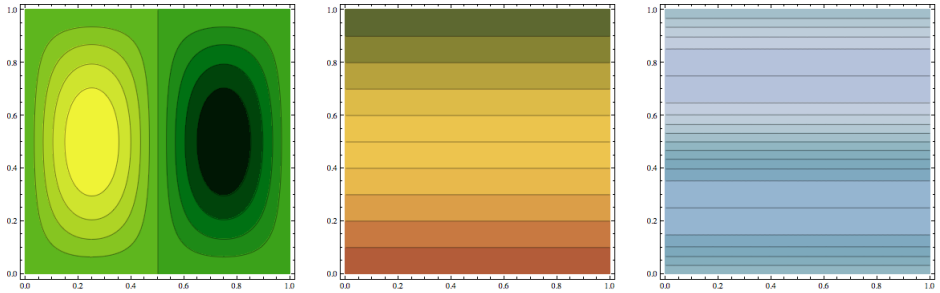
Results of a direct numerical simulation in composition space

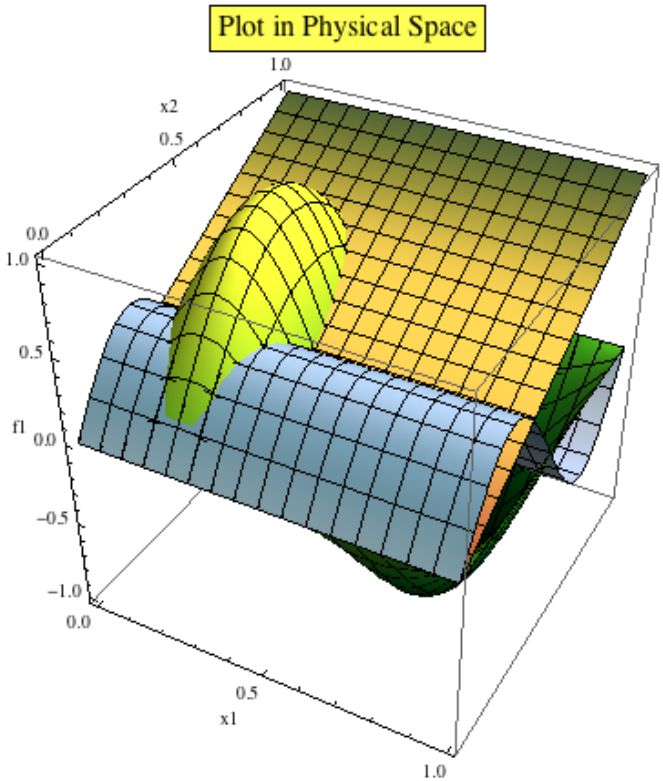
- **Both chemistry and transport processes cause the existence of low-dimensional attractors in composition space!**
- **But: Forget for the moment about manifold methods and just look at arbitrary reacting flows.**

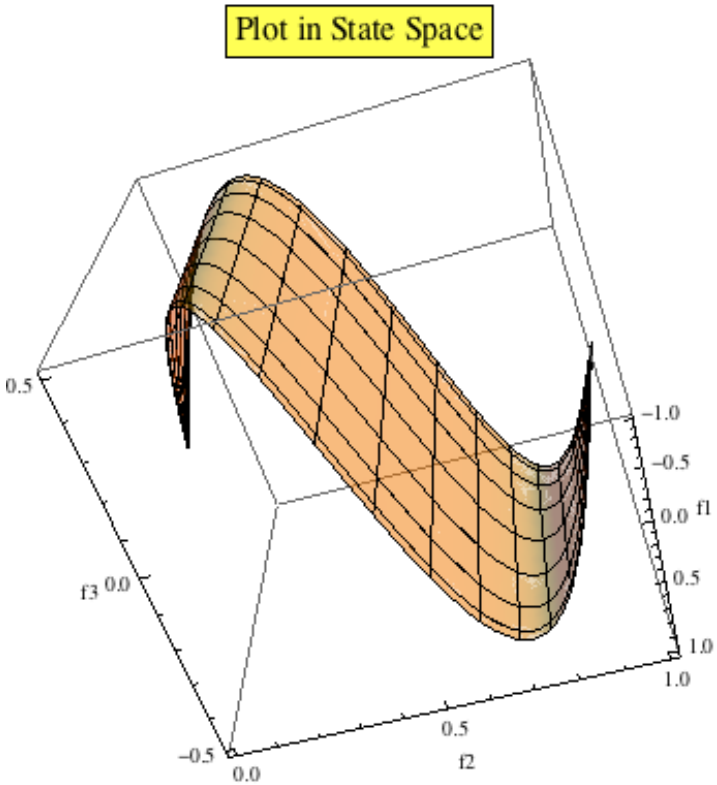
From physical to Composition Space

- **Toy example:**

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







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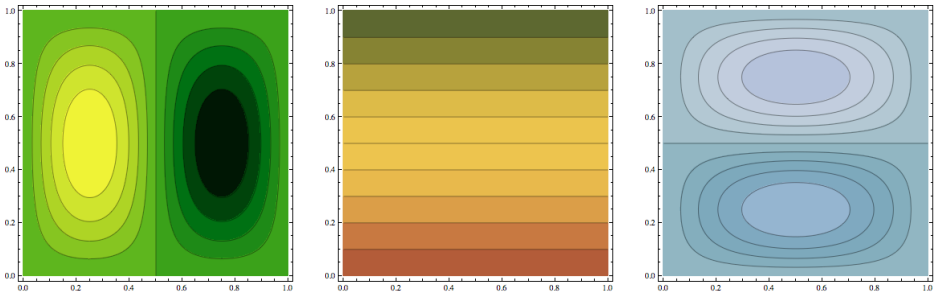
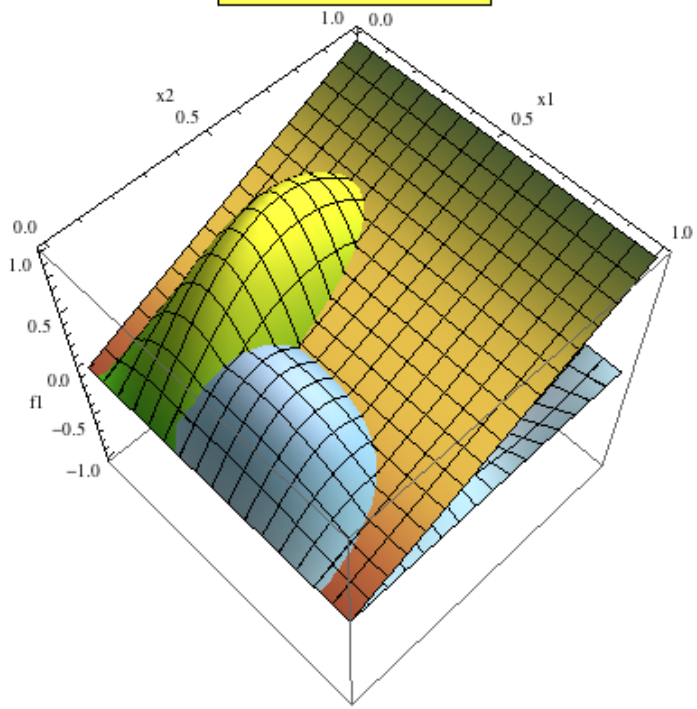
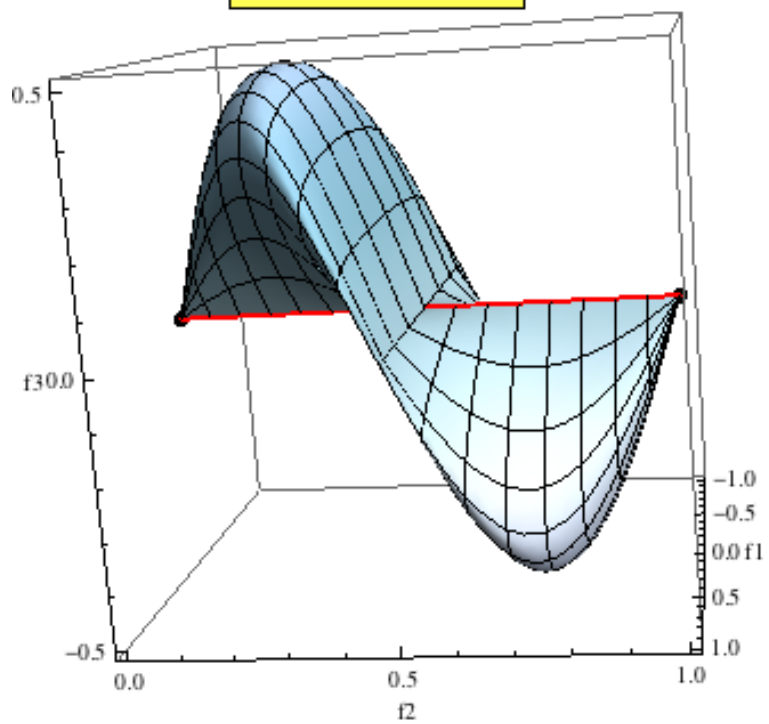


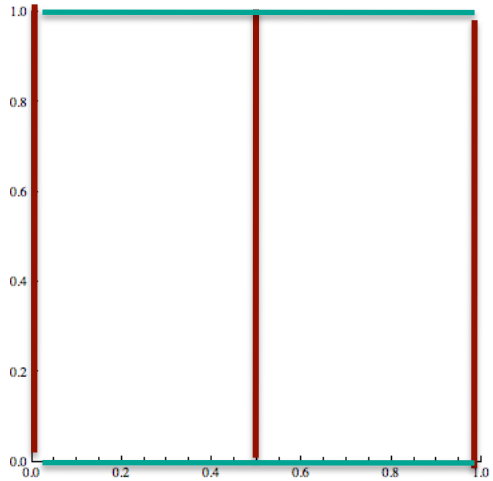
Plot in Physical Space

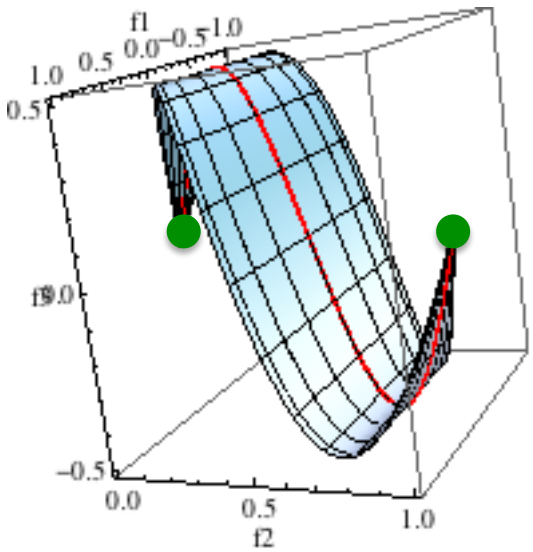


Plot in State Space



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

Evolution in Composition Space

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

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

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

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

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

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

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

Evolution in Composition Space

- **Evolution equations for the manifold and the parameters:**

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

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

- **Problems: Equations are coupled**

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

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

- **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

- **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.**

- **Consequences**
  - **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.**

Reaction-Diffusion-Manifolds (REDIM)

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

Evolution of a manifold according to reaction and diffusion

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

$$\xi = \mathrm{grad}\,\theta$$

Assumption: ξ **depends only on** θ **but not on** $\vec{r}, t$

Remaining equations in physical space

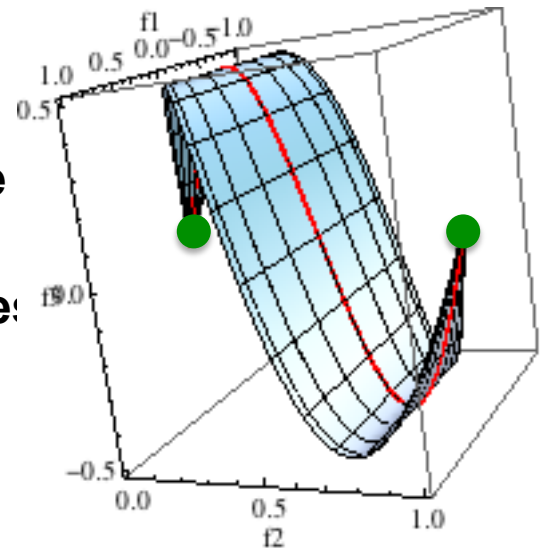
$$\frac{\partial \theta}{\partial t} = S(\theta) + \vec{v}\ \mathrm{grad}\,\theta + \frac{1}{\rho} P\,\mathrm{div}\left(\overline{\overline{D}}^{*}\ \mathrm{grad}\,\theta\right)$$

$$\theta = (\theta_1, \theta_2, \ldots, \theta_m)^T \qquad m \le 3 \ll n_s + 2$$

Questions to be answered

- How can the boundary (and its evolution) in composition space be described?
- How well is the dynamics characterized by a gradient estimate that depends only on the location in the composition space and not on the location in physical space?
- How can the reduced model dimension be defined?

Boundary Conditions



- **Diriclet boundaries in physical space**
  - **Diriclet boundaries in physical space are boundaries in composition space.**
  - **They might, however, be inner boundaries**
- **Van Neumann boundaries** $\mathrm{grad}\,\psi = c$
  - **Have to be treated separately**
  - **Are obtained simply by using** $\mathrm{grad}\,\psi = c$ **at the boundary in the evolution equation**
- **Mixed boundary conditions** $\mathrm{grad}\,\psi = F(\psi)$**: future work**
- **But what about the boundaries of the manifold, which do not represent boundaries in physical space?**

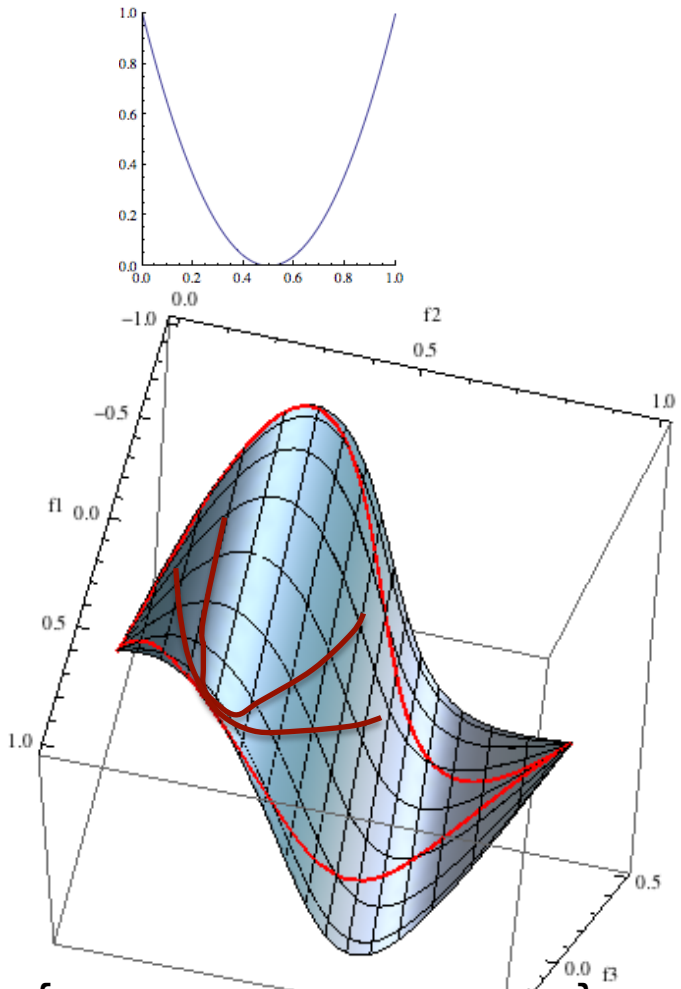
Boundary Conditions

- A curve in physical space is represented by a curve in composition space.
- The curves are not allowed to leave the manifold.
- Conditions for the gradients at the boundaries:

$$\mathrm{grad}\,\psi \parallel M$$

$$\mathrm{grad}\,\psi \parallel \partial M$$

- Transform into a local coordinate system at the boundary
- Reformulate evolution equation on the boundary



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

Boundary Conditions

- **Typically the gradient estimate is given in terms of an estimate of gradients of some species**

$$C\,\mathrm{grad}\,\psi = z$$

- **Example:** $\psi = \left(w_{N_2}, w_{CO_2}, w_{H_2O}, \ldots\right)^T$

Gradients of N_2 and CO_2 known:

$$C\psi = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \end{pmatrix} \left(w_{N_2}, w_{CO_2}, w_{H_2O}, \ldots\right)^T = \left(z_{N_2}, z_{CO_2}\right)^T$$

- **The gradient estimate is then given by:** $\mathrm{grad}\,\psi = \eta = \psi_\theta \left(C\psi_\theta\right)^{-1} z$

- **and the components not tangential to the boundary can be removed by a projection**

$$\hat{\eta} = \left(\mathrm{I} - \psi_{\hat{\theta}}^{\perp}\left(\psi_{\hat{\theta}}^{\perp}\right)^{+}\right)\psi_\theta \left(C\psi_\theta\right)^{-1} z$$

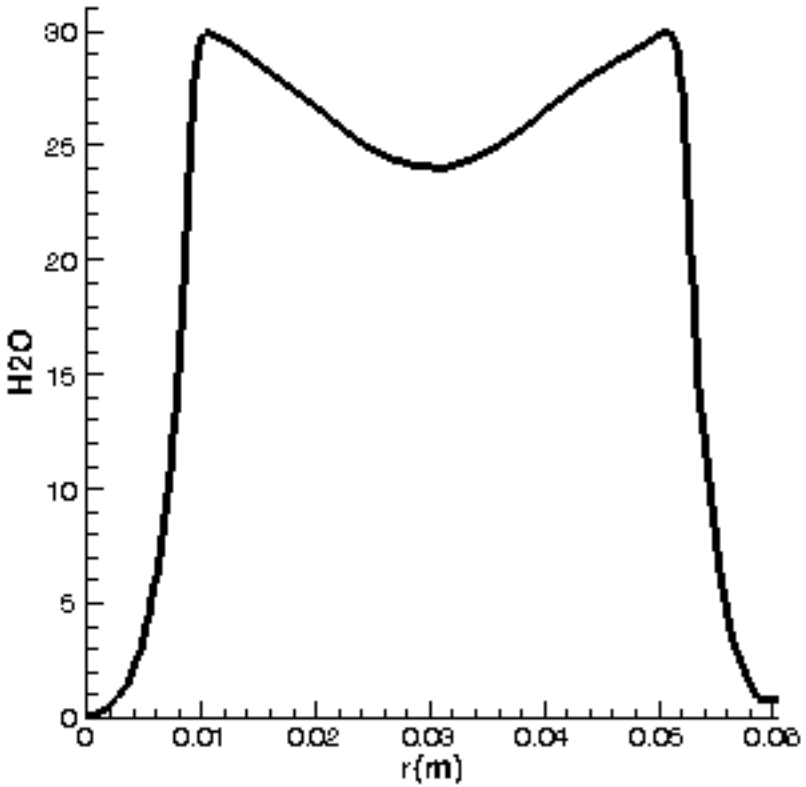
- **Note: This formulation allows an evolution of the boundary and a hierarchical generation of REDIM (publication in preparation)**

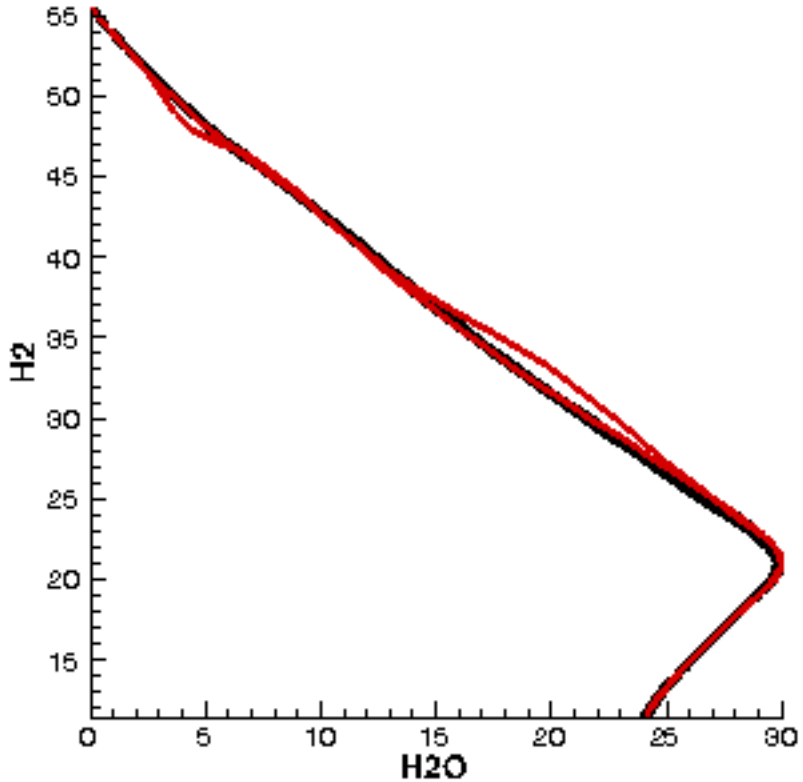
Questions to be answered

- How can the boundary (and its evolution) in composition space be described?
- **How well is the dynamics characterized by a gradient estimate that depends only on the location in the composition space and not on the location in physical space?**
- How can the reduced model dimension be defined?

Influence of the Gradient estimate

- **Problems: One point in composition space may correspond to several poins in physical space**
- **Consequence: „Splitting of the surface“**





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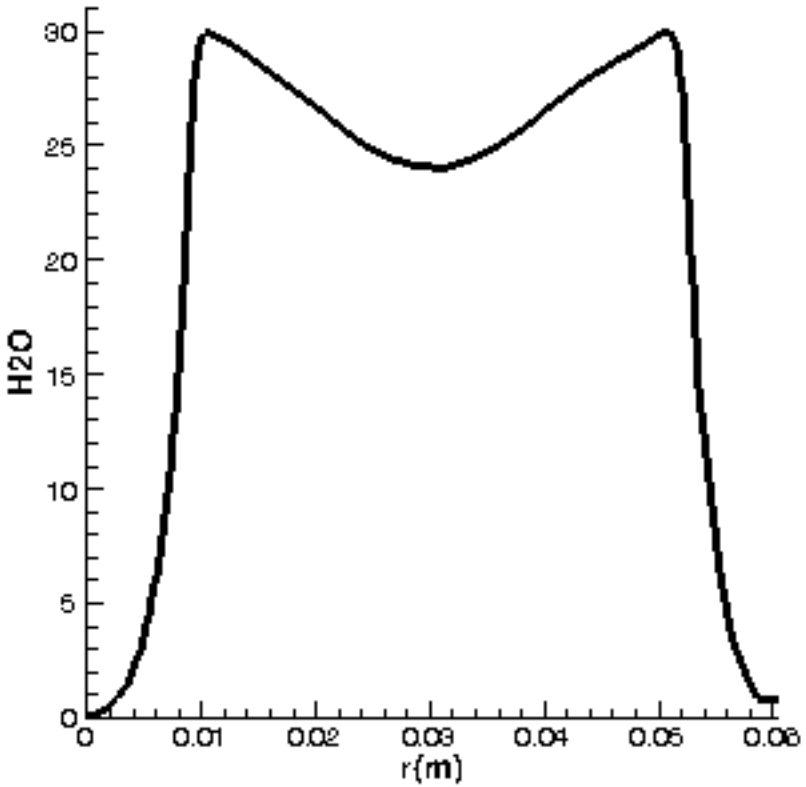
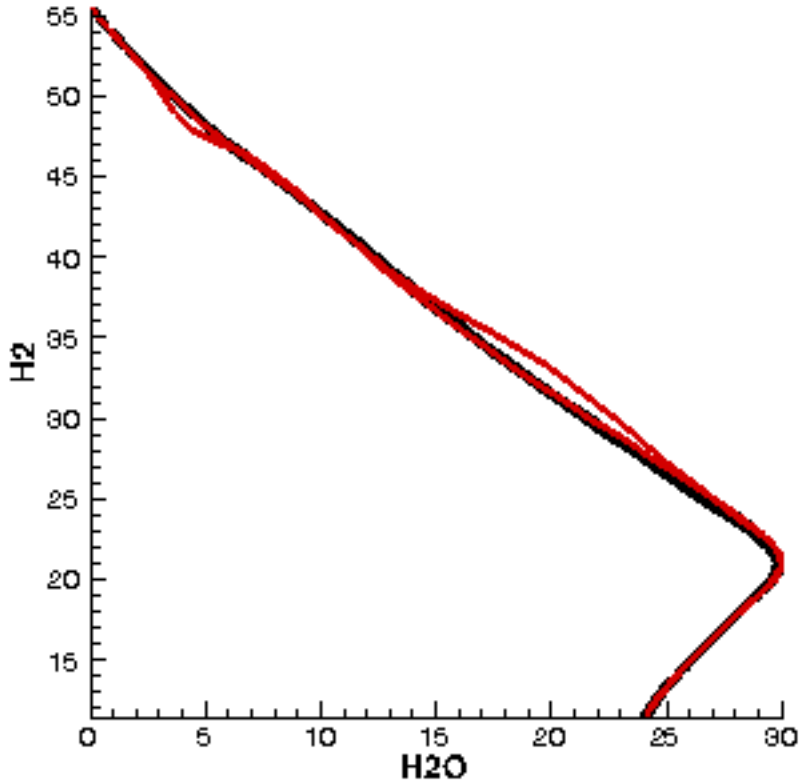
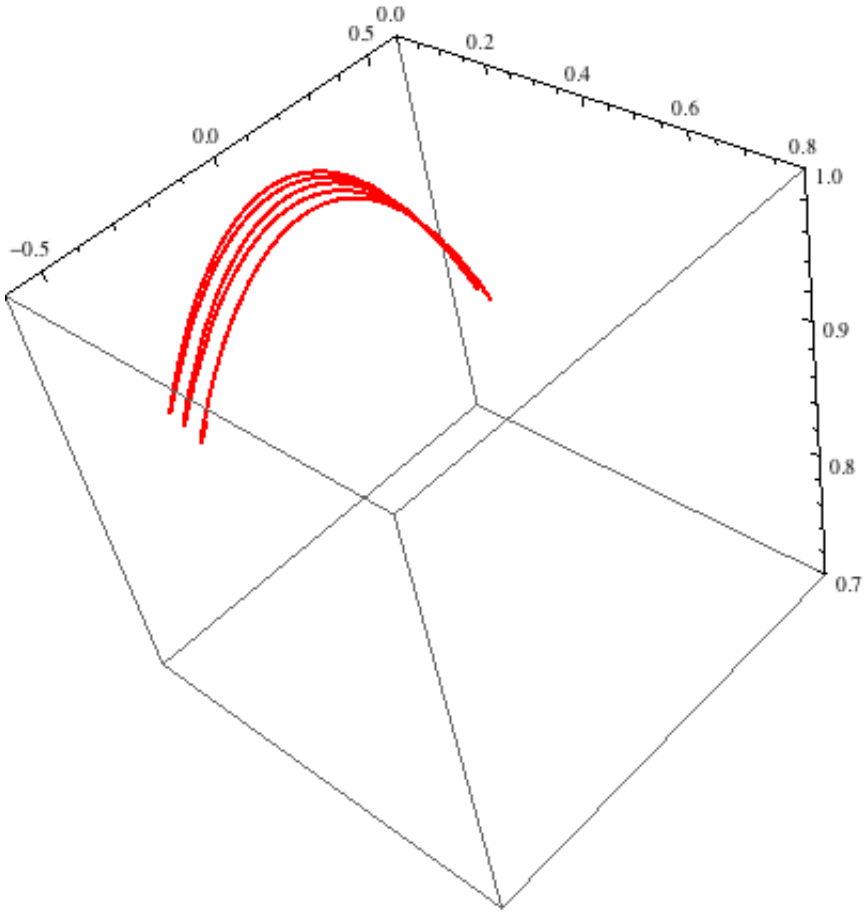




Influence of the Gradient estimate

- **Low-dimensional manifold might become arbitrarily complicated**



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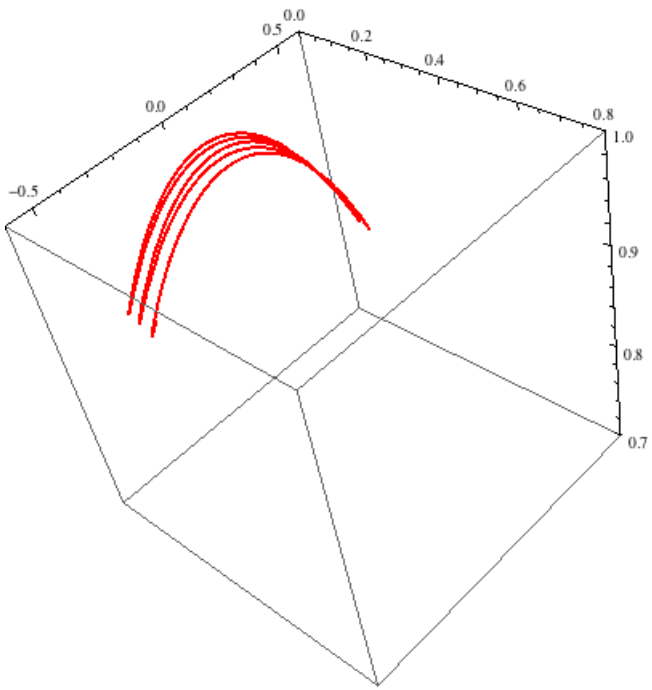
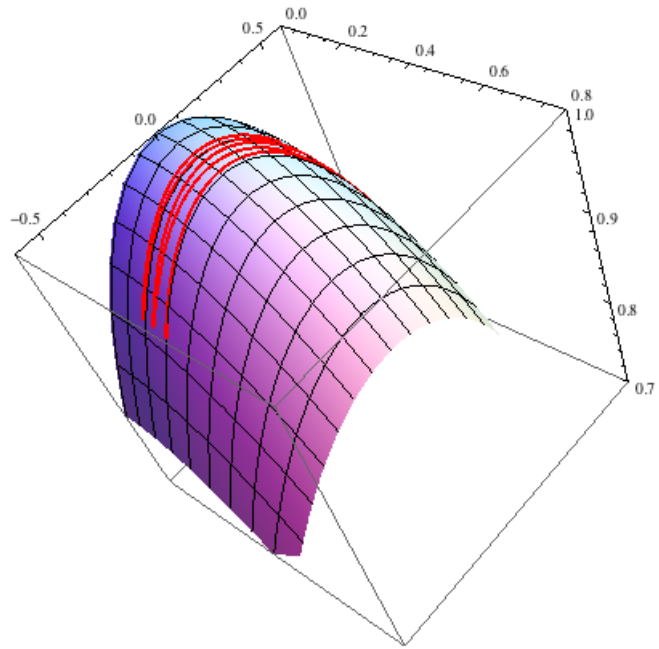




- **But: The geometry on the m+1 dimensional geometry looks much nicer.**
- **An (m+1) dimensional manifold depends less on the gradients than an m-dimensional manifold.**

Influence of the gradients

- A detailed analysis of the influence of the gradients is quite lengthy
- But: The principle can be understood very easily

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

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

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

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

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

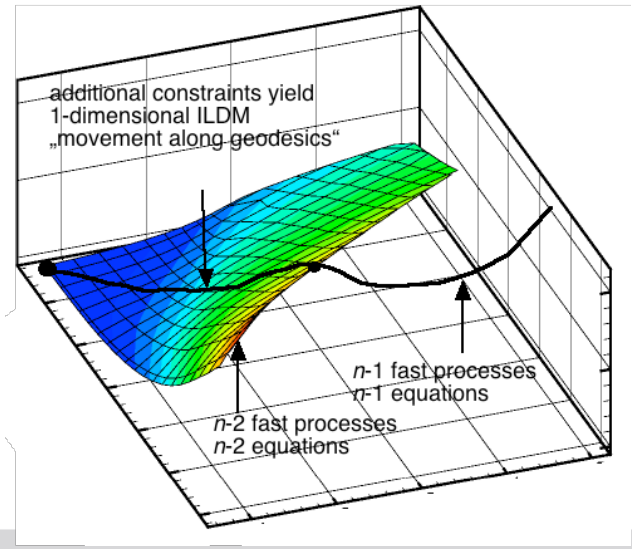
Influence of the gradients

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

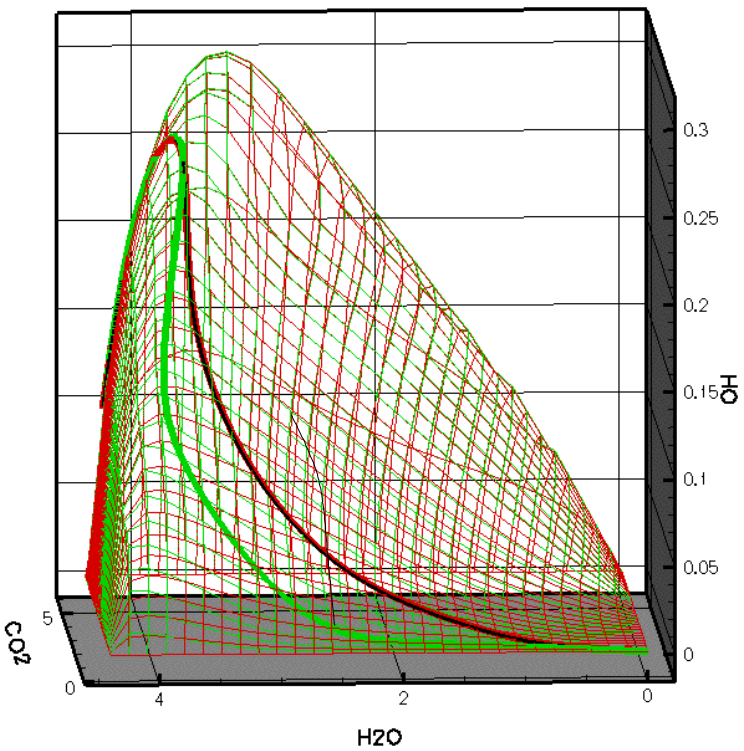
$$\frac{\partial \psi(\theta)}{\partial \tau} \approx \left(I - \psi_\theta \psi_\theta{}^+\right) \cdot \left\{F\left(\psi(\theta)\right)\right\}$$

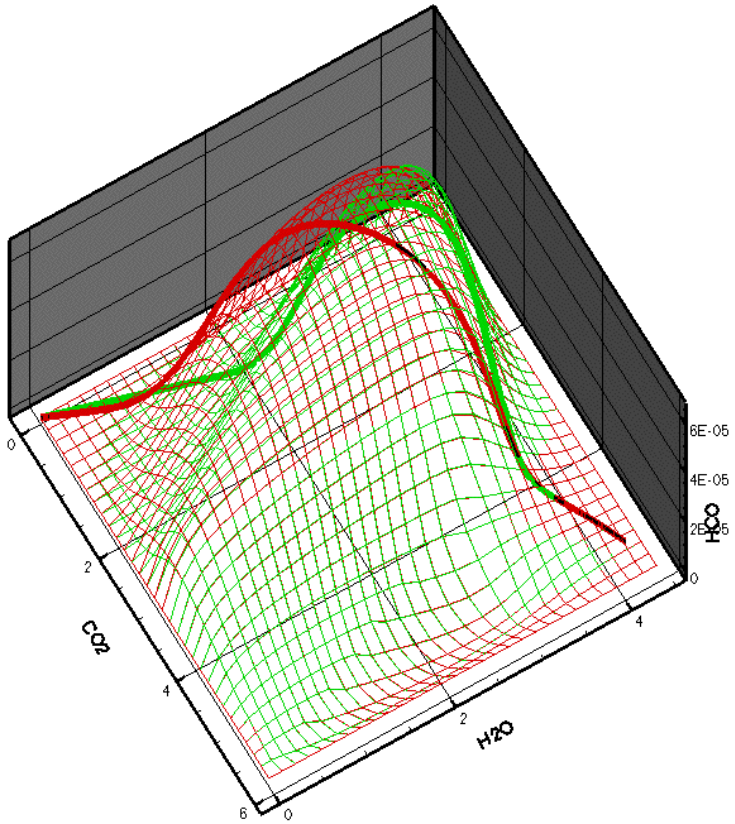
  - **Solution does not depend on the gradient! (in fact:if it is 0, then the solution are slow incariant manifolds**

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



Influence of the gradients





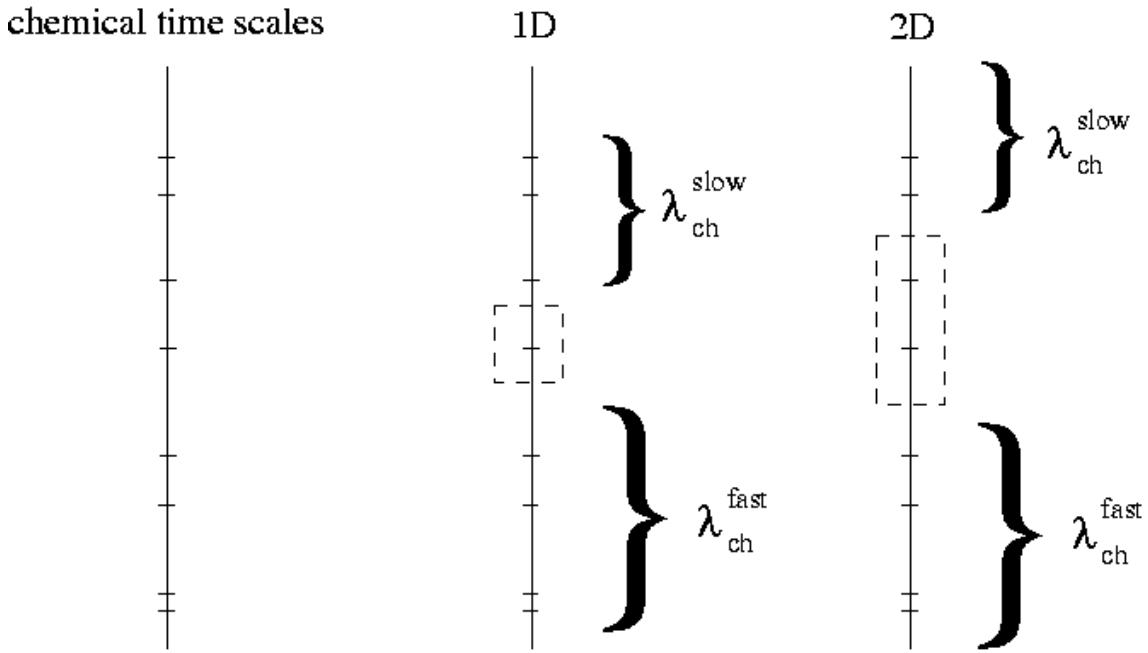
1D (curves) and 2D (mesh) REDIMs

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

black curve: exact solution for a flat flame

Optimal choice of the dimension

- **The quality of the description of transient processes will depend on the dimension of the manifold.**
- **Chemistry and Transport must be analyzed in a coupled way**

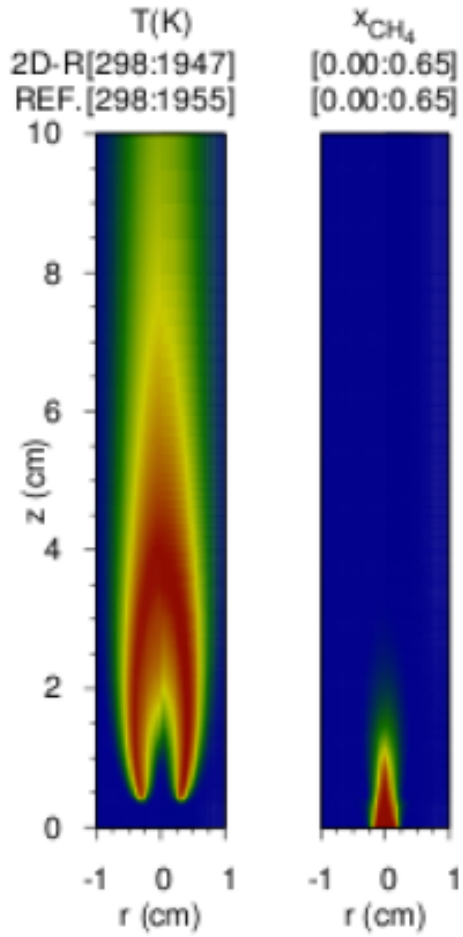


Use in „Real Life“

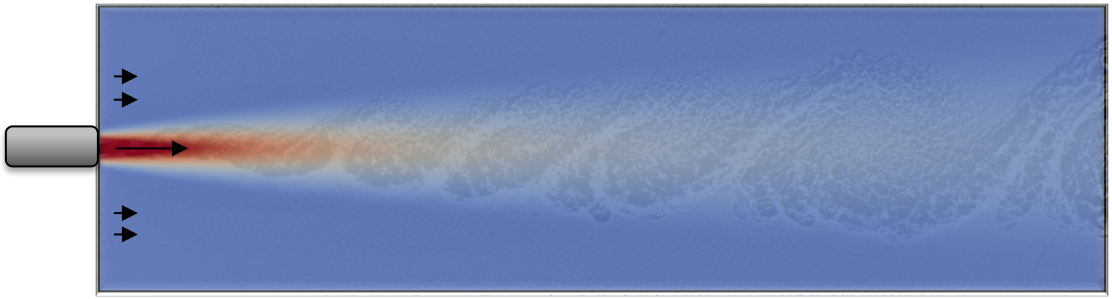
- Various applications

- 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.)



Example: Ignition by a hot jet



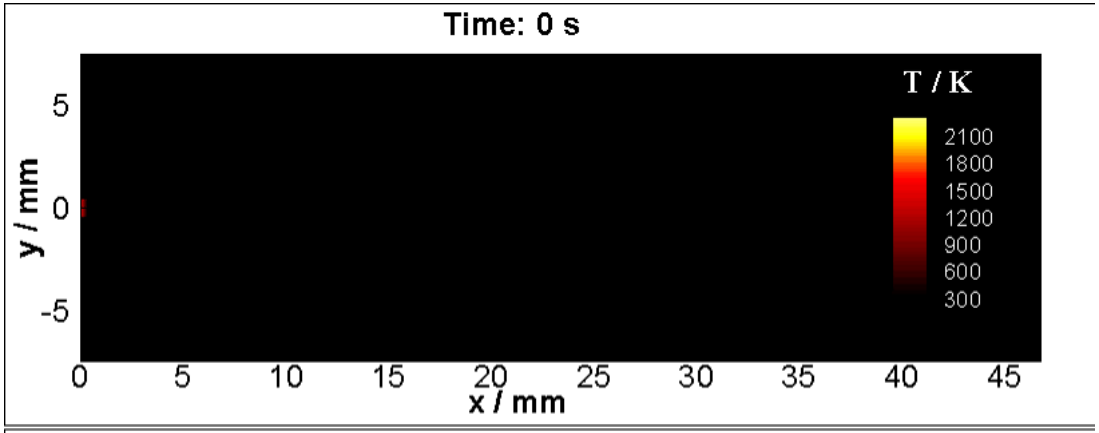
Hot jet of burned hydrogen/air mixture entering a cold hydrogen/air mixture.

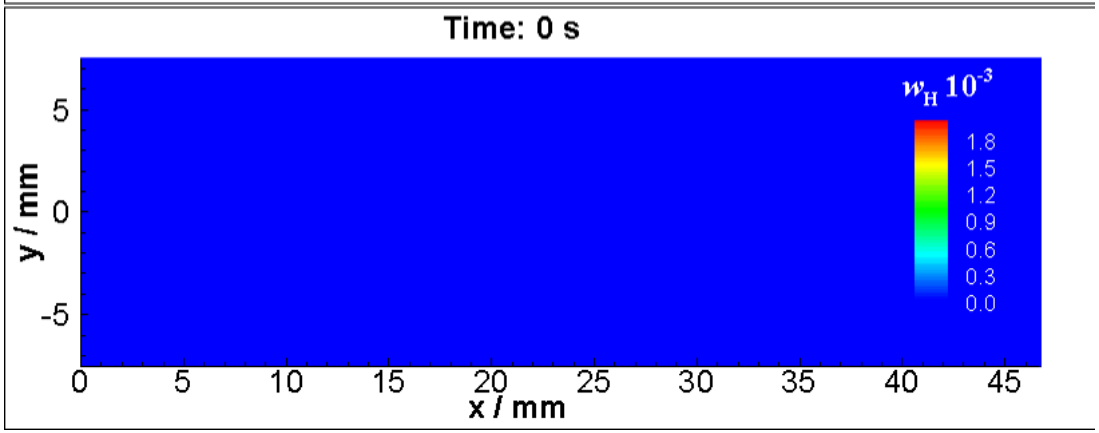
stand-alone Monte-Carlo-PDF-simulation

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



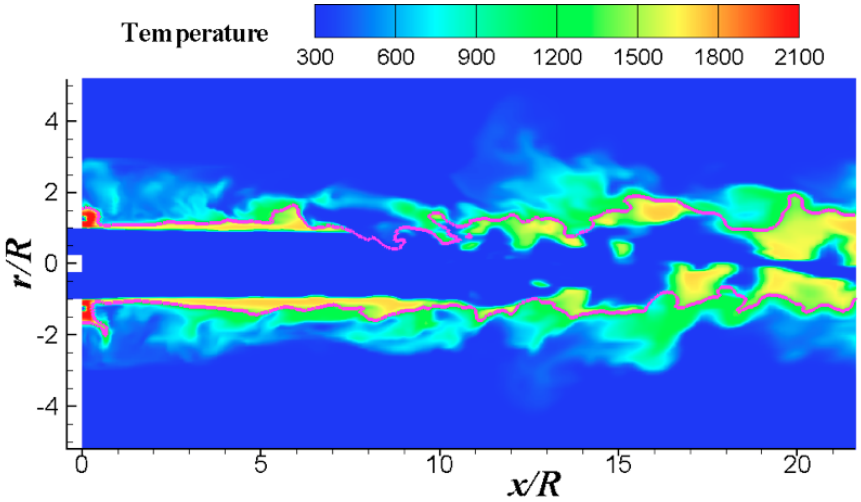


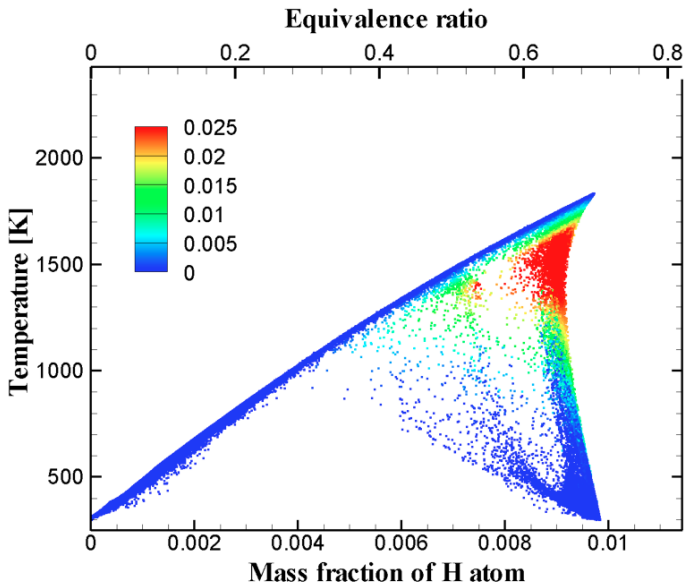
Ghorbani et al. 2014

Example: LES of a premixed flame

Large eddy simulation of a Methane-air flame coupled with an assumed PDF approach
REDIM reduced chemistry with two scalars

Wang et al.





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.

Conclusions

- Each reacting flow is represented by an ($m \leq 3+1$)-dimensional composition space, which despite the low dimension may have a complicated structure
- The concept of Reaction-Diffusion Manifolds (REDIM) allows to identify low-dimensional manifolds for reaction/diffusion systems
- Although gradients may dpend not only on the state but also on the spatial location, this dependence gets negligible for a sufficiently high dimension
- The concept can be applied to realistic systems
- Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.