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 \( \psi = \left( h, \rho, w_1, w_2, \ldots, w_{n_s} \right)^T \)

\[
\frac{\partial \psi}{\partial t} = F(\psi) + \nu \cdot \text{grad} \psi + \frac{1}{\rho} \text{div} D \text{grad} \psi = F(\psi) + \Xi \left( \psi, \nabla \psi, \nabla^2 \psi \right)
\]

- Thermokinetic state is a function of spatial coordinate and time

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

- For general 3D flows: \( \psi \) depends on 3+1 variables

- Notation in the following:

\[
\psi_\theta = \left( \begin{array}{c}
\frac{\partial \psi_1}{\partial \theta_1} & \cdots & \frac{\partial \psi_1}{\partial \theta_m} \\
\frac{\partial \psi_2}{\partial \theta_1} & \cdots & \frac{\partial \psi_2}{\partial \theta_m} \\
\vdots & \ddots & \vdots \\
\frac{\partial \psi_n}{\partial \theta_1} & \cdots & \frac{\partial \psi_n}{\partial \theta_m}
\end{array} \right)
\]
Behaviour in Composition Space

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

- 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.

Results of a direct numerical simulation in composition space
From physical to Composition Space

Toy example:

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

Plot in Physical Space

Plot in State Space
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
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
At any time $t$ the scalar field of a reacting flow defines a manifold of dimension $d \leq 3$.

$$\psi = \psi \left( \vartheta \left( \bar{r} \right) \right) \quad \psi = \psi \left( \vartheta \left( \bar{r} \right) \right)$$

A $d^* \leq 4$-dimensional manifold is describes the whole time evolution

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

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

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

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

Evolution equations for the manifold and the parameters:

\[
\begin{align*}
\frac{\partial \psi (\theta)}{\partial t} &= \left( I - \psi_\theta \psi_\theta^+ \right) \cdot \left\{ F(\psi(\theta)) + \frac{1}{\rho} \left( D(\theta) \psi_\theta \text{grad} \theta \right) \psi_\theta \right\} \\
\frac{\partial \theta}{\partial t} &= S(\theta) + \bar{v} \text{ grad} \theta + \frac{1}{\rho} P \text{ div} \left( D^* \text{ grad} \theta \right)
\end{align*}
\]

Problems: Equations are coupled

\[
\begin{align*}
\frac{\partial \psi}{\partial t} &= G(\psi, \psi_\theta, \psi_{\theta\theta}, \theta_r, \theta_{rr}) \\
\frac{\partial \theta}{\partial t} &= H(\psi, \psi_\theta, \theta, \theta_r, \theta_{rr})
\end{align*}
\]

If \( \theta_r, \theta_{rr} \) were functions of \( \theta \) 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 $\theta$ 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)

\[
\frac{\partial \psi}{\partial t} = F(\psi) - \nabla \cdot \text{grad} \psi + \frac{1}{\rho} \text{div} D \text{grad} \psi
\]

Evolution of a manifold according to reaction and diffusion

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

\[\xi = \text{grad} \theta\]

Assumption: \( \xi \) depends only on \( \theta \) but not on \( \bar{r}, t \)

Remaining equations in physical space

\[
\frac{\partial \theta}{\partial t} = S(\theta) + \bar{\nu} \text{grad} \theta + \frac{1}{\rho} P \text{div} \left( \bar{D}^* \text{grad} \theta \right)
\]

\[\theta = (\theta_1, \theta_2, ..., \theta_m)^T \quad m \leq 3 \ll n_s + 2\]
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 \( \nabla \psi = c \)
  - Have to be treated separately
  - Are obtained simply by using \( \nabla \psi = c \) at the boundary in the evolution equation

- Mixed boundary conditions \( \nabla \psi = F(\psi) \): 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:
  \[ \nabla \psi \parallel M \]
  \[ \nabla \psi \parallel \partial M \]

- Transform into a local coordinate system at the boundary

- Reformulate evolution equation on the boundary
  \[
  \frac{\partial \psi(\theta)}{\partial \tau} = \left( I - \psi \theta \psi \theta^+ \right) \cdot \left\{ F(\psi(\theta)) + \left( D(\theta) \psi \hat{\theta} \hat{\xi} \right) \hat{\theta} \hat{\xi} \right\}
  \]
Boundary Conditions

- Typically the gradient estimate is given in terms of an estimate of gradients of some species
  \[ C \operatorname{grad} \psi = z \]

- Example:
  \[ \psi = \begin{pmatrix} w_{N_2}, w_{CO_2}, w_{H_2O}, \ldots \end{pmatrix}^T \]

Gradients of \( N_2 \) and \( CO_2 \) known:

\[ C\psi = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \end{pmatrix} \begin{pmatrix} w_{N_2}, w_{CO_2}, w_{H_2O}, \ldots \end{pmatrix}^T = \begin{pmatrix} z_{N_2}, z_{CO_2} \end{pmatrix}^T \]

- The gradient estimate is then given by:
  \[ \operatorname{grad} \psi = \eta = \psi_\theta \left( C\psi_\theta \right)^{-1} z \]

- and the components not tangential to the boundary can be removed by a projection
  \[ \hat{\eta} = \left( I - \psi_\theta^\dagger \left( \psi_\theta^\dagger \right)^+ \right) \psi_\theta \left( C\psi_\theta \right)^{-1} z \]

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

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- How can the reduced model dimension be defined?
Influence of the Gradient estimate

- Problems: One point in composition space may correspond to several points in physical space.
- Consequence: „Splitting of the surface“
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Influence of the Gradient estimate

- Low-dimensional manifold might become arbitrarily complicated
Influence of the Gradient estimate

- 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.
Influence of the gradients

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

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

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

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

\[
\psi_\theta^\perp (D(\theta) \psi_\theta)_{\theta} = 0
\]

- 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?

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

- 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
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

<table>
<thead>
<tr>
<th>$U_j$ (m/s)</th>
<th>$U_e$ (m/s)</th>
<th>Jet Comp.</th>
<th>Env. Comp.</th>
</tr>
</thead>
<tbody>
<tr>
<td>300</td>
<td>20</td>
<td>hot (1500K) burnt stoic. H$_2$/Air</td>
<td>cold stoic. H$_2$/Air</td>
</tr>
</tbody>
</table>

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. $\zeta=0.71$ 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 depend 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.

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