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

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• 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

\[ \frac{\partial p}{\partial t} + \nabla \cdot (\rho \nu) = 0 \]

\[ \frac{\partial p w_i}{\partial t} + \nabla \cdot (\rho w_i v) = \nabla \cdot (\rho D_{im} \nabla w_i) + s_i \]

\[ \frac{\partial p v}{\partial t} + \nabla \cdot (\rho \otimes \nu) = -\nabla \cdot P - \rho g \]

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

\[ \frac{p}{\rho} = \frac{RT}{M} \]

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)

\[ \frac{\partial \psi}{\partial t} = F(\psi) - \nu \text{grad}(\psi) - \frac{1}{\rho} \text{div}(D \cdot \text{grad}(\psi)) \]
Detailed chemical kinetics

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

1-dimensional cut through a CH₄-air flame
Theoretical Background: Decomposition

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

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

\[ F_\psi = \begin{pmatrix} Z_s & Z_f \end{pmatrix} \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix} \]

ILDM equation:
\[ M_s = \{ \psi : \tilde{Z}_f F(\psi) = 0 \} \]

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:

\[ M = \{ \psi = \psi(\theta) \mid \psi : \mathbb{R}^m \to \mathbb{R}^n \} \]

PDEs system’s vector field:

\[ \Phi = F(\psi) - \nu \, \text{grad}(\psi) - \frac{1}{\rho} \, \text{div}(D \cdot \text{grad}(\psi)) \]

INVARINANCE

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

The question: How to obtain the invariant system manifold?

Projector:

\[ P = I - \psi_{\theta} \psi_{\theta}^+ \]

Relaxation method:

\[ \frac{\partial \psi(\theta)}{\partial t} = \left( I - \psi_{\theta} \psi_{\theta}^+ \right) \Phi(\psi(\theta)) \]
Generalized coordinates

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

\[ M_s = \{ \psi = \psi(\theta) : \tilde{Z}_f F(\psi(\theta)) \equiv 0 \} \]

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

\[ \psi(\theta_0), \quad \psi_\theta(\theta_0) \]

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:

\[ \psi_\theta^+ = \left( \psi_\theta^T \psi_\theta \right)^{-1} \psi_\theta^T \]
Initial guess for a manifold

\[ M = \{ \psi = \psi(\theta) \mid \psi : \mathbb{R}^m \rightarrow \mathbb{R}^n \} \]

\[ \frac{\partial \psi(\theta)}{\partial t} = (I - \psi_\theta \psi_\theta^+) \Phi(\psi(\theta)) \]

The manifold changes locally to satisfy INVARIANCE condition!
an extended ILDM can be used as an initial guess in relaxation process to a reaction-diffusion ILDM (REDIM)!

\[
\begin{align*}
\frac{\partial \psi}{\partial t} &= \left( I - \psi_\theta \psi_\theta^+ \right) \{ F + G \} \\
\psi_{t=0} &= \psi_{\text{ILDM}}^{\text{ex}}(\theta)
\end{align*}
\]

\[ G = -\frac{d}{\rho} \psi_{\theta\theta} \circ \text{grad}(\theta) \circ \text{grad}(\theta) \]

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

Reference: V. Bykov, U. Maas. 2007, CTM, 11(6), 839 - 862
\[
\begin{align*}
\frac{\partial \psi}{\partial t} &= \left( I - \psi_{\theta} \psi_{\theta}^* \right) \{ F + G^* \} \\
\psi|_{t=0} &= \psi_{\text{ILDM}}(\theta)
\end{align*}
\]

Simple approach

\[
G^* = -\frac{d}{\rho} \| \text{grad}(\theta) \|^2 \frac{1}{m} \text{Tr}(\psi_{\theta\theta})
\]

\[
G^* \sim -\frac{d}{\rho} \psi_{\theta\theta} \circ \text{grad}(\theta) \circ \text{grad}(\theta)
\]

(a) – initial guess, (b) – after 10 iterations, (c) – 200, (d) - 700
\[
\begin{cases}
\frac{\partial \psi}{\partial t} = \left( I - \psi_0 \psi_0^+ \right) \{ F + G^* \} \\
\psi|_{t=0} = \psi_{\text{ILDM}}^\text{ex}(\theta)
\end{cases}
\]

Simple approach

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G^* = -\frac{d}{\rho} \| \text{grad}(\theta) \|^2 \frac{1}{m} \text{Tr}(\psi_{\theta\theta})
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(a) – initial guess, (b) – after 10 iterations, (c) – 200, (d) - 700
relaxation process in projection to minor and major species specific mole numbers!
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actual reduction is realized as a reformulation of the detailed system on the REDIM manifold

\[ M_{\text{REDIM}} = \{ \psi = \psi(\theta) \} \Rightarrow \psi(\theta_0), \quad \psi_\theta(\theta_0) \]

\[ \psi_\theta \frac{\partial \theta}{\partial t} = F(\theta) - \mathbf{v} \psi_\theta \cdot \text{grad}(\theta) - \frac{1}{\rho} \text{div}(D \cdot \psi_\theta \cdot \text{grad}(\theta)) \]

\[ \Xi(\theta) = D \cdot \psi_\theta \quad \tilde{F}(\theta) = \psi_\theta^+ \left( F(\theta) - \frac{1}{\rho} \text{div}(\Xi(\theta) \cdot \text{grad}(\theta)) \right) \]

\[ \frac{\partial \theta}{\partial t} = \tilde{F}(\theta) - \mathbf{v} \text{grad}(\theta) \]

The evolution of the manifold parameter is calculated and then the whole state space is recovered by the REDIM table!
suppose we have constructed a REDIM manifold, now, the question how this can be improved?

\[
\text{grad}(\theta) = \text{Const} \quad \Rightarrow \quad \text{grad}(\theta) = f(\theta)
\]

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

\[
M^{i}_{\text{REDIM}} = \left\{ \psi = \psi^{i}(\theta) \right\}
\]

\[
\frac{\partial \theta}{\partial t} = S(\theta) - \nu \text{grad}(\theta) \quad \Rightarrow \quad \theta = \theta(x) \quad \Rightarrow \quad \text{grad}(\theta) = f^{i}(\theta)
\]

\[
\theta^{*} = \theta(x^{*}) \quad \Rightarrow \quad f^{i}(\theta^{*}) = \text{grad}(\theta)|_{x=x^{*}}
\]

In this way an approximation is improved and can further be used in the relaxation REDIM procedure to yield more accurate manifold!
A REDIM from the previous relaxation process can be used as a new initial guess...

\[
\frac{\partial \psi^{i+1}}{\partial t} = \left( I - \psi^i_0 \left( \begin{array}{c} \psi^{i+1}_0 \\ \vdots \\ \psi^{i+1} \end{array} \right)^\dagger \right) \left( F(\psi^{i+1}(\theta)) - \frac{d}{\rho} (\psi^{i+1})_{\theta\theta} \circ f^i(\theta) \circ f^i(\theta) \right)
\]

\[
\psi|_{t=0} = \psi^i(\theta)
\]

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

\[
M^{i+1}_{\text{REDIM}} = \{ \psi = \psi^{i+1}(\theta) \}
\]

\[
\frac{\partial \theta}{\partial t} = S(\theta) - v \ \text{grad}(\theta) \ \Rightarrow \ \theta = \theta(x)
\]

\[
\theta_\ast = \theta(x_\ast) \ \Rightarrow \ f^{i+1}(\theta_\ast) = \text{grad}(\theta)|_{x=x_\ast} \ \Rightarrow \ \text{grad}(\theta) = f^{i+1}(\theta)
\]
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.
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.
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…