Modelling of reacting flows: chemical reaction mechanisms and model reduction

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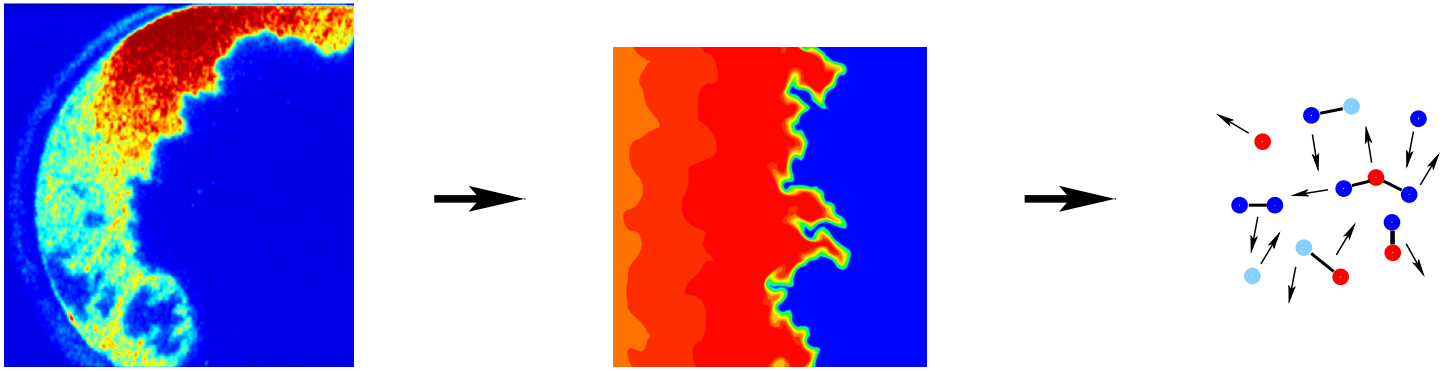


Modeling of reacting flows

- A phenomenon of a reacting flow is characterized by strong coupling in time and in space of
  - Species composition fields
  - Thermodynamic fields
  - Hydrodynamic field
- Problem of modeling of a reacting system concerns
  - Adequate description of interrelations between the fields
  - A lack of rigorous validation methodologies

System of governing equations

- Composition or state space:

$$\psi = \left(h, p, \frac{w_1}{M_1}, ..., \frac{w_{n_s}}{M_{n_s}} \right)^T, \; n = n_s + 2, \; \psi_i = \psi_i(t, x)$$

- System in vector notation (scalar variables only):

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

Detailed chemical kinetics

H_2 / O_2 Mechanism

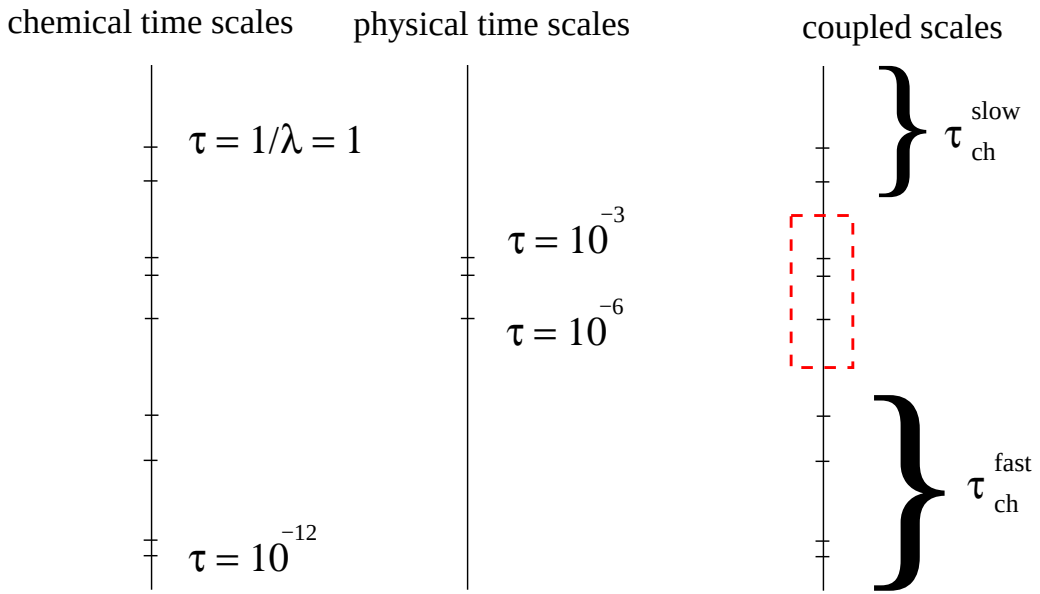
O_2	+	H		=	OH	+ O
H_2	+	O		=	OH	+ H
H_2	+	OH		=	H_2O	+ H
OH	+	OH		=	H_2O	+ O
H	+	H	+ M	=	H_2	+ M
H	+	OH	+ M	=	H_2O	+ M
O	+	O	+ M	=	O_2	+ M
H	+	O_2	+ M	=	HO_2	+ M
HO_2	+	H		=	OH	+ OH
HO_2	+	H		=	H_2	+ O_2
HO_2	+	H		=	H_2O	+ O
HO_2	+	O		=	OH	+ O_2
HO_2	+	OH		=	H_2O	+ O_2
HO_2	+	HO_2		=	H_2O_2	+ O_2
OH	+	OH	+ M	=	H_2O_2	+ M
H_2O_2	+	H		=	H_2	+ HO_2
H_2O_2	+	H		=	H_2O	+ OH
H_2O_2	+	O		=	OH	+ HO_2
H_2O_2	+	OH		=	H_2O	+ HO_2

see e.g.: Warnatz, Maas, Dibble:
Combustion, Springer 1996

- Problems of detailed chemical kinetics:
  - several hundred chemical species
  - several thousand elementary reactions
  - stiffness of the governing equation system
- Computational problems:

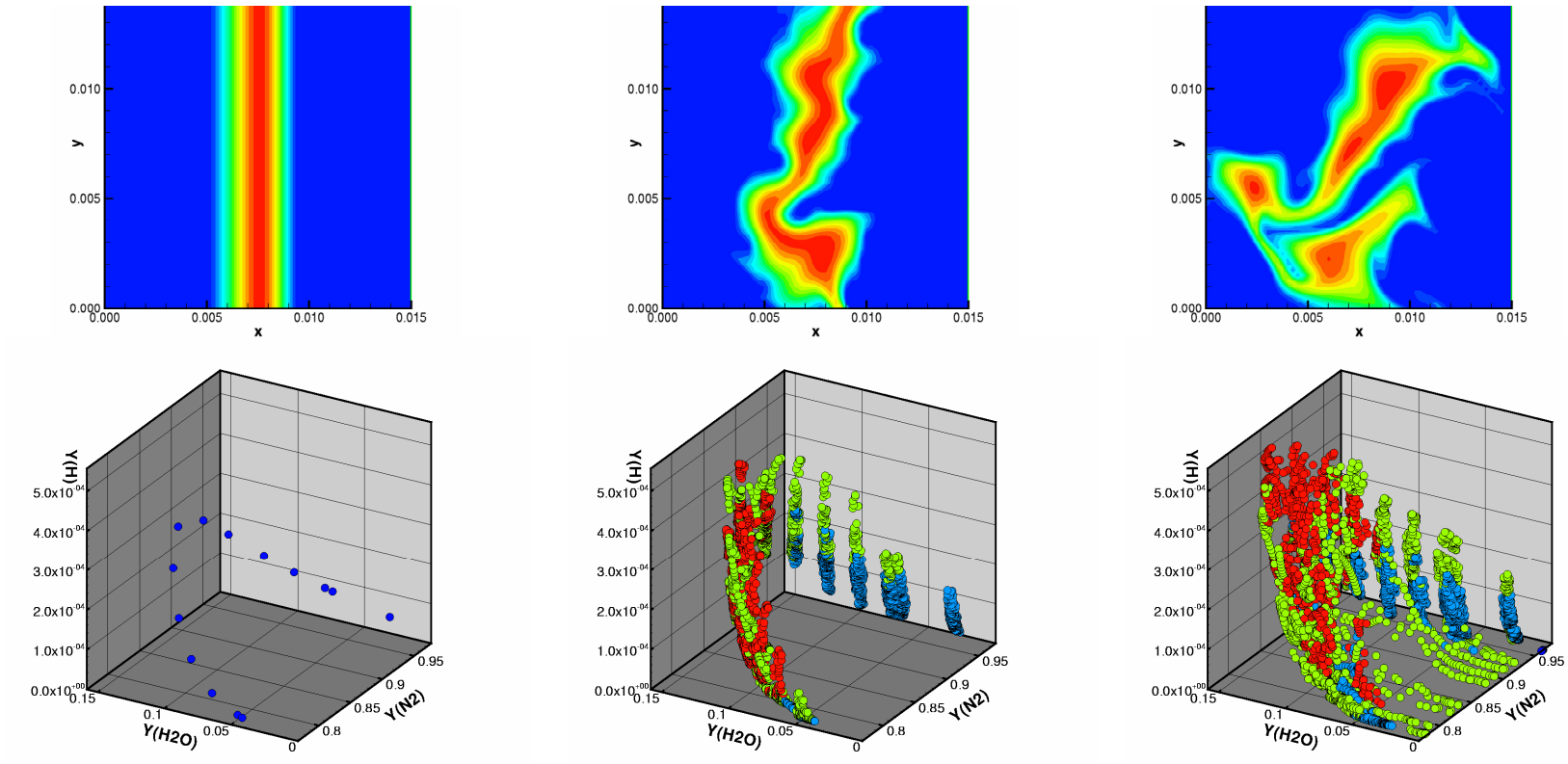
  - Scaling problems in space
  - Scaling problems in time
  - Large number of equations

Multi-scales



- But: only few reactions are rate limiting! Is it possible to decouple the fast chemical processes and to handle the slow ones?!
- This would
  - reduce the number of governing equations
  - remove part of the scaling problems in space and in time
  - simplify the system analysis

Multi-scales phenomena: DNS



Maas & Thévenin 1998

- DNS of a turbulent non-premixed hydrogen flame
- Only a small subspace is actually accessed
- In addition the accessed space is confined to low-dimensional manifolds
- Chemistry and transport cause the existence of low-dimensional attractors

Multi-scales structure

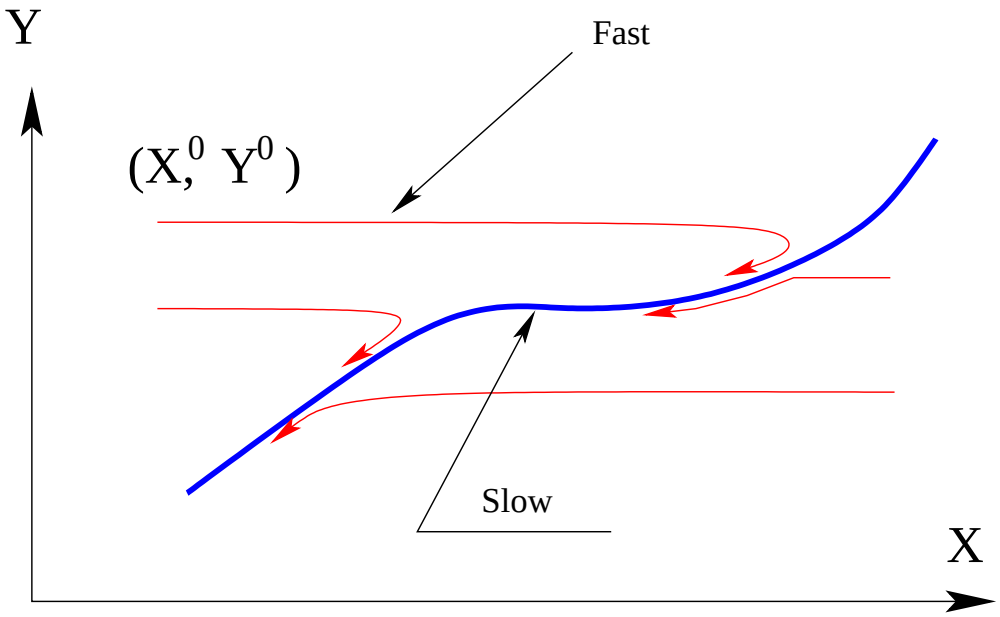
consider a system that exhibits multi-scale phenomena: $\psi' = F(\psi)$

Mathematical model is SPS!

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

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

$$m_f + m_s = n, \quad 0 < \varepsilon << 1$$



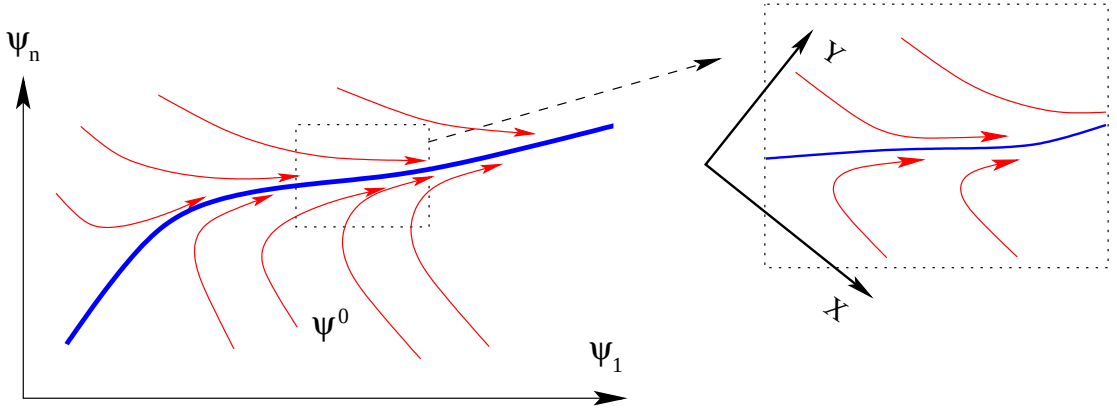
Questions:

- How can this special representation be found?
- What the system small parameter is?

Source term local analysis - ILDM

- Homogenous system of ODEs

$$\frac{d\psi}{dt} = F(\psi)$$



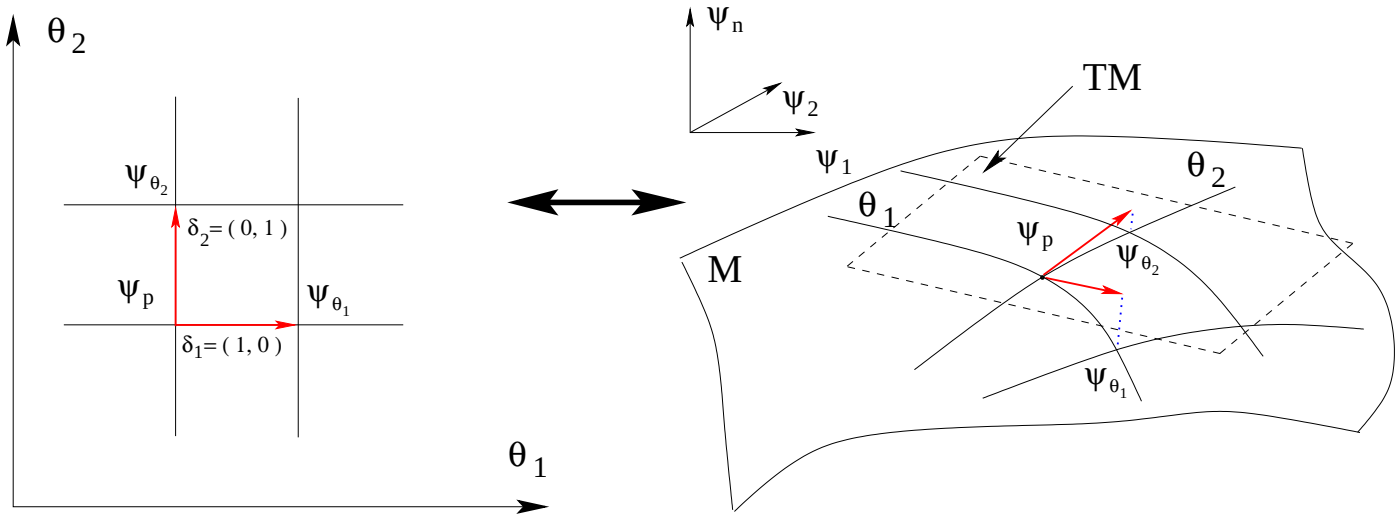
$$F_\psi = (Z_s(\psi)\, Z_f(\psi)) \begin{pmatrix} N_s & 0 \\ 0 & N_f \end{pmatrix} \begin{pmatrix} \tilde{Z}_s(\psi) \\ \tilde{Z}_f(\psi) \end{pmatrix} \Rightarrow \begin{pmatrix} Y \\ X \end{pmatrix} \sim \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix} \psi$$

$$M_s = \left\{ \psi(\theta) : R^m \to R^n, \tilde{Z}_f(\psi(\theta)) F(\psi(\theta)) = 0 \right\}$$

- The manifold that annihilates the fast subspace!

Technical tool - tabulation

- Generalized coordinates:



$$\frac{d\psi}{dt} = F(\psi)$$

$$M = \left\{\psi(\theta) : \tilde{Z}_f(\psi(\theta))F(\psi(\theta)) = 0\right\}$$

- In this way an explicit representation of the reduced space/manifold is found!

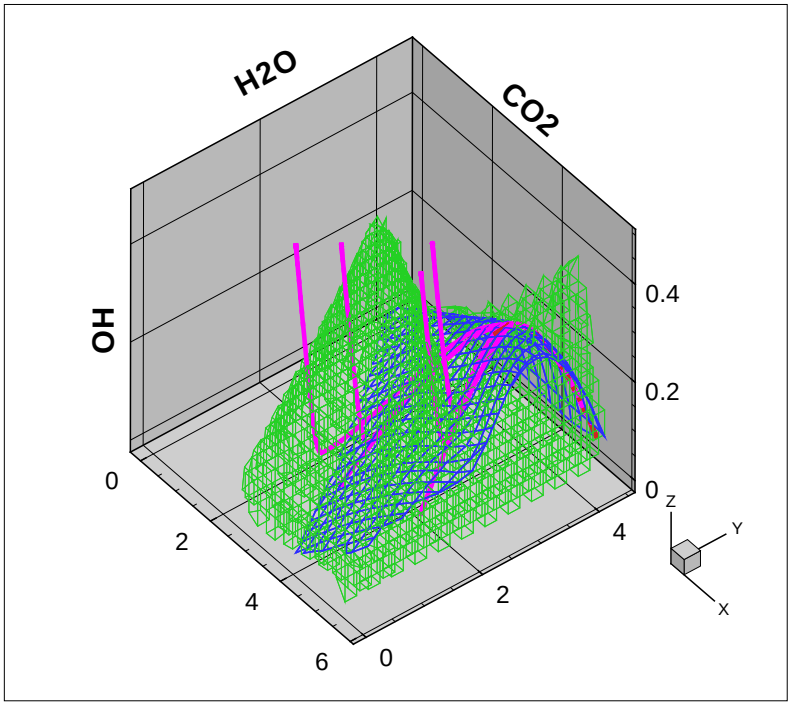
Reduced spaces - manifolds

- Homogenous system of ODEs

$$\frac{d\psi}{dt} = F(\psi) \quad \overset{???}{\Rightarrow} \quad \frac{d\theta}{dt} = \tilde{F}(\theta)$$

$$M: \ \psi(\theta_0), \quad \psi_\theta(\theta_0)$$

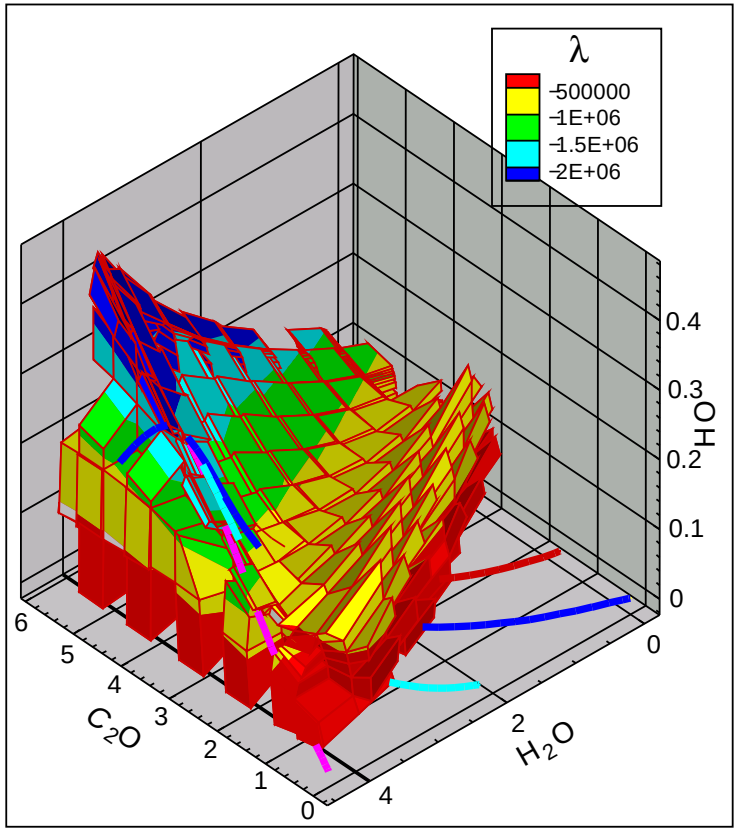
$$\frac{\partial\theta}{\partial t} = \tilde{F}(\theta): \quad \tilde{F}(\theta) = \psi_\theta^+(\theta)F(\theta)$$

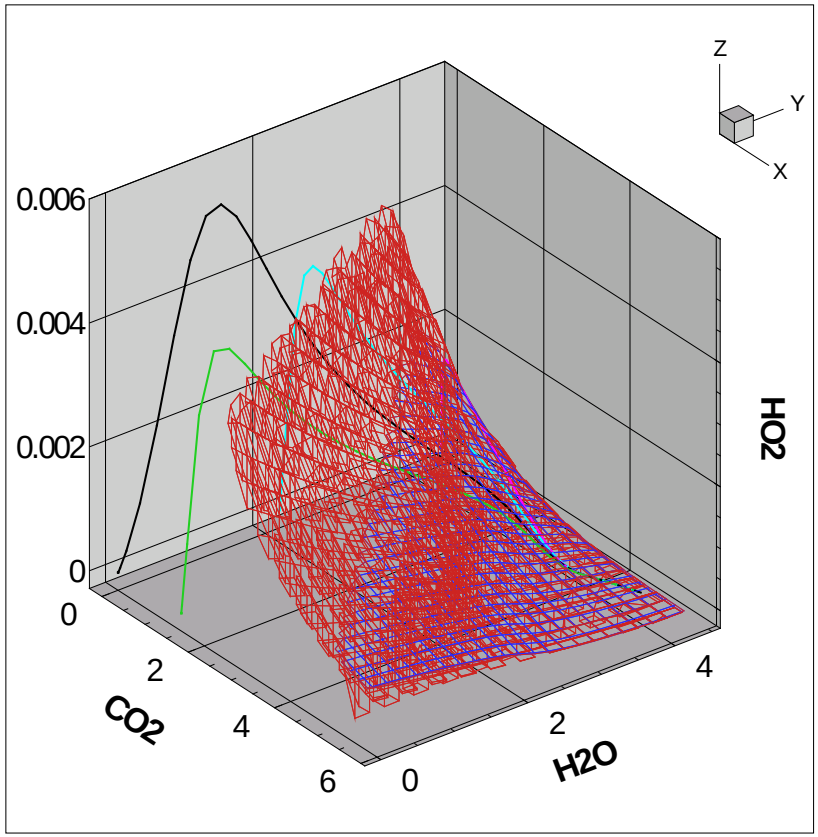


$CO-H_2-O_2$ homogeneous system, magenta – system trajectories, blue is 2D ILDM, green represents 3D ILDM

- Any reduced model defines a low dimensional manifold in the state or composition space!

Higher dimensions





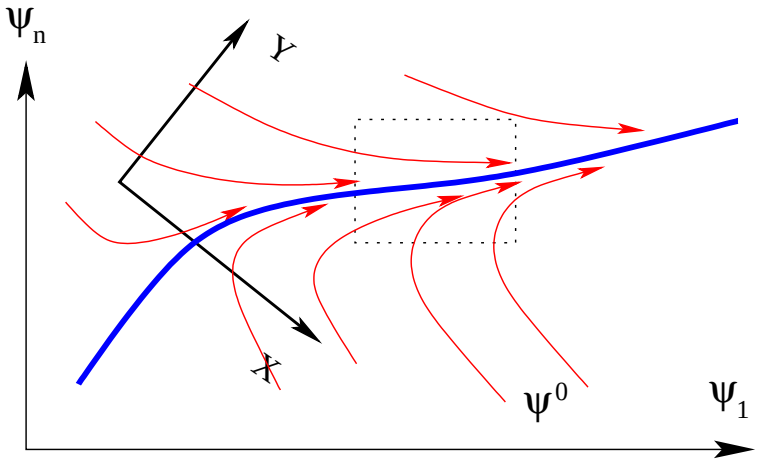
Projection of the state space of the CO-H_2-O_2 system
(n = 15)

Source term global analysis - GQL

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

$$T : \psi_i \mapsto F(\psi_i) \quad \Rightarrow$$

$$T = (Z_s \; Z_f) \begin{pmatrix} \Lambda_s & 0 \\ 0 & \Lambda_f \end{pmatrix} \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix}$$



- If there is a gap between eignevalues of the GQL

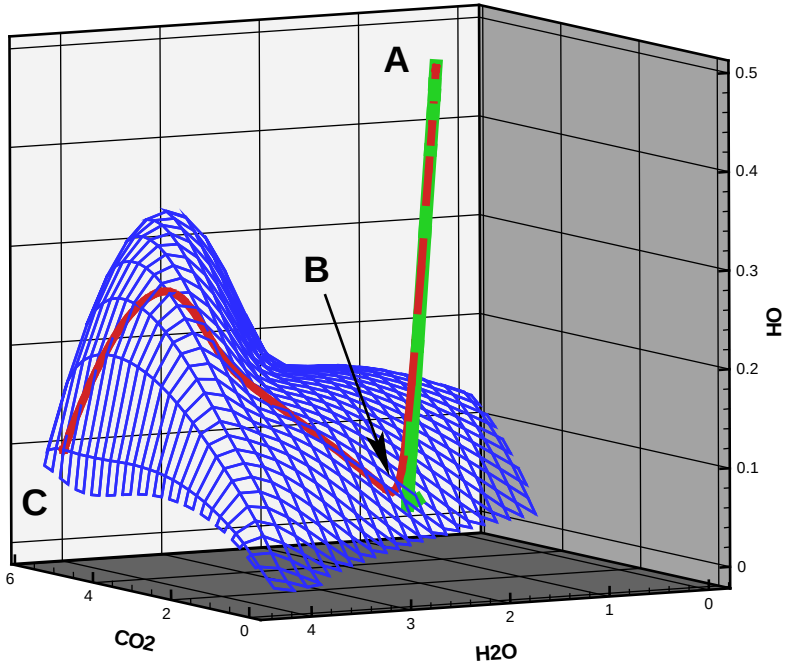
$$\Lambda_s = \begin{pmatrix} \lambda_1(T) & * & * \\ 0 & \ldots & * \\ 0 & 0 & \lambda_{m_s}(T) \end{pmatrix} \quad \Lambda_f = \begin{pmatrix} \lambda_{m_s+1}(T) & * & * \\ 0 & \ldots & * \\ 0 & 0 & \lambda_n(T) \end{pmatrix} \quad \Rightarrow \quad \varepsilon = \left(\frac{|\lambda_{m_s+1}(T)|}{|\lambda_{m_s}(T)|} \right)^{-1}$$

…then the system small parameter is estimated by the gap!

System projection and decomposition

$$P_{TM_f} = Z_f \tilde{Z}_f$$

$$\begin{cases} \dfrac{d\psi}{dt} = Z_f \tilde{Z}_f F(\psi) \\ \tilde{Z}_s \psi = \tilde{Z}_s \psi_0 \end{cases}$$



$$P_{TM_s} = Z_s \tilde{Z}_s$$

$$\begin{cases} \dfrac{d\psi}{dt} = Z_s \tilde{Z}_s F(\psi) \\ \tilde{Z}_f F(\psi) = 0 \end{cases}$$

- Original coordinates can be used by the method due to available projections operators!

- Reference: Bykov, Gol'dshtein, Maas, CTM, 12 (2), 389 – 405 (2008)
- Original Idea: Bykov, Goldfarb, Gol'dshtein, Sazhin, Sazhina, Computer&Fluids 36, 601–610 (2007)

Hierarchy system analysis

The suggested methods allow at the same time

- **Check the system hierarchy!**
- **Estimate the reduced dimension!**
- **Approximate the reduced manifolds!**
- **Decompose the system!**

Application to the auto-ignition problem

- An original model for cyclohexane/air combustion mechanism consists of 50 species, plus two thermodynamic quantities – temperature and pressure

$$\psi = \left(T, p, c_1, ..., c_{n_s}\right)^T, \; n = n_s + 2, \; \psi_i = \psi_i(t)$$

- The stoichiometric fuel oxygen mixture is considered within an interval of 700 K – 900 K for initial temperature and of 7.5×10^5 - 10^6 Pa initial pressures typical for rapid compression machine experiments.

- The main aim of the next part is to show the implementation stages of the developed model reduction strategy!

Sample of trajectories

- Pressure profiles:

…there are two and even three stages of the ignition….

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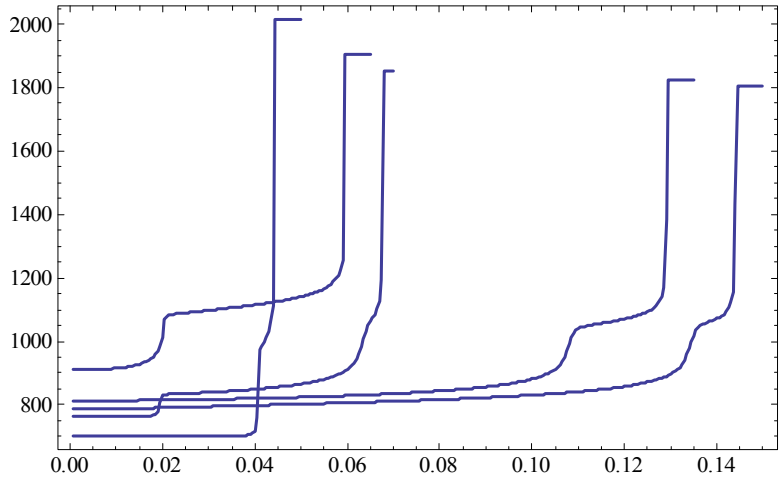

- Hydrogen peroxide profiles:

…several elementary reaction nets are getting activated within each stage…

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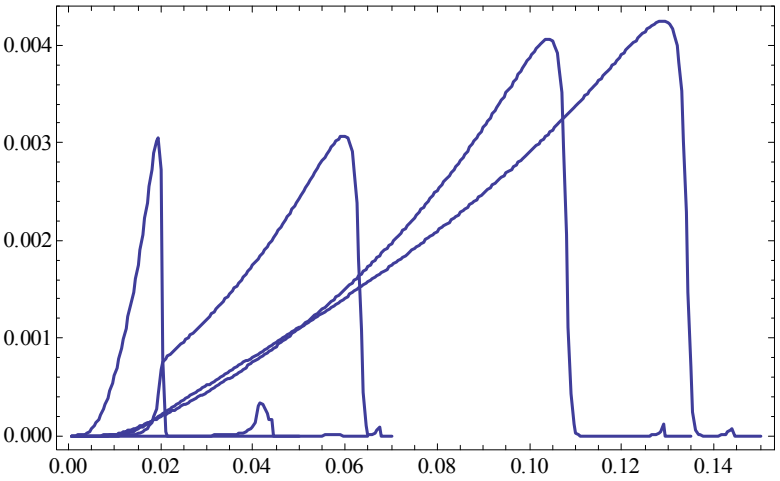
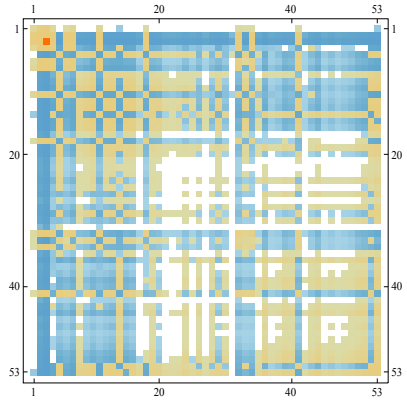
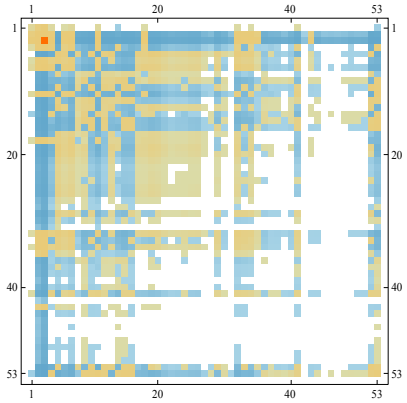


Eigenvalues of GQL

- Preliminary result of the system hierarchy analysis:



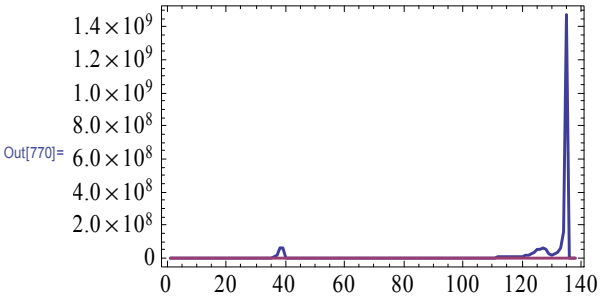


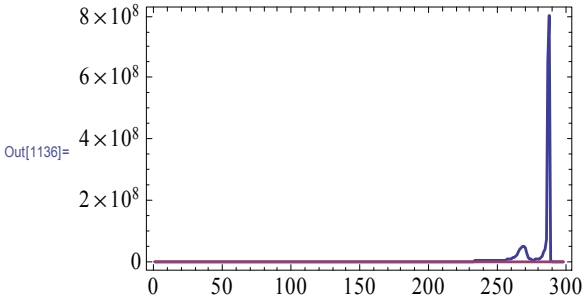
Eigenvalues =

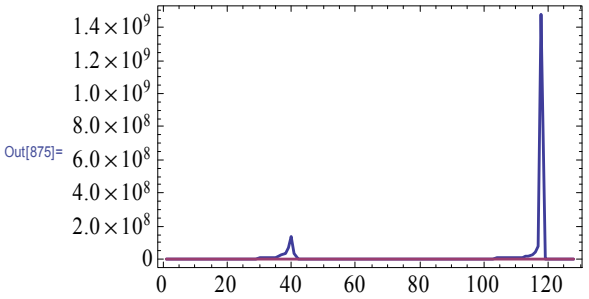
1.71798×10^{16}	1.59894×10^{16}	3.60913×10^{15}	4.40609×10^{15}	1.71798×10^{16}
827 954.	1.04993×10^{6}	5.38796×10^{6}	3.82993×10^{6}	827 954.
2.05601	1.93785	0.506787	0.562119	2.05601
1.14728	0.254002	0.477561	0.514244	1.14728
0.761098	0.250541	0.13167	0.183512	0.761098
0.00842871	0.0317744	0.023226	0.043341	0.00842871
0.00445612	0.0263073	0.0092604	0.00702355	0.00445612
0.0021204	0.0147793	0.00178438	0.00169965	0.0021204
0.00123496	0.00644845	0.000367062	0.000979047	0.00123496
0.000488444	0.00365177	0.000107895	0.000277567	0.000488444
0.000351803	0.000489559	0.000082597	0.000114728	0.000351803
0.0000347786	0.0000440986	0.0000434897	0.0000383994	0.0000347786
0.0000277699	0.0000361705	0.0000185039	0.0000102595	0.0000277699
0.0000157843	0.0000314396	9.77676×10^{-6}	5.72456×10^{-6}	0.0000157843
0.0000152799	0.000029792	9.23832×10^{-6}	4.5337×10^{-6}	0.0000152799
5.97512×10^{-7}	0.0000238645	7.58866×10^{-6}	3.68798×10^{-6}	5.97512×10^{-7}
6.76227×10^{-8}	0.0000110737	2.82686×10^{-6}	2.86213×10^{-7}	6.76227×10^{-8}
1.52473×10^{-8}	2.98129×10^{-6}	1.16334×10^{-7}	1.76654×10^{-7}	1.52473×10^{-8}
1.35622×10^{-8}	2.52948×10^{-6}	5.90024×10^{-8}	1.42194×10^{-7}	1.35622×10^{-8}
1.49527×10^{-9}	5.18466×10^{-7}	3.29344×10^{-8}	2.28431×10^{-8}	1.49527×10^{-9}
1.30024×10^{-9}	8.24196×10^{-8}	3.01287×10^{-8}	2.24362×10^{-8}	1.30024×10^{-9}
2.03025×10^{-10}	4.83098×10^{-8}	5.24078×10^{-9}	9.05694×10^{-9}	2.03025×10^{-10}
1.40606×10^{-10}	2.73729×10^{-8}	9.45246×10^{-10}	4.36175×10^{-10}	1.40606×10^{-10}
2.51997×10^{-11}	2.39035×10^{-9}	4.61409×10^{-10}	2.25274×10^{-10}	2.51997×10^{-11}
2.5935×10^{-12}	1.16251×10^{-9}	8.55196×10^{-12}	3.52484×10^{-11}	2.5935×10^{-12}
4.00118×10^{-13}	7.53226×10^{-10}	8.03268×10^{-12}	8.5522×10^{-12}	4.00118×10^{-13}
3.61781×10^{-13}	4.31238×10^{-11}	2.15683×10^{-12}	6.3178×10^{-13}	3.61781×10^{-13}
1.39146×10^{-13}	2.74705×10^{-11}	2.15214×10^{-12}	3.30179×10^{-13}	1.39146×10^{-13}
2.60308×10^{-14}	2.68516×10^{-12}	1.70578×10^{-13}	8.17799×10^{-14}	2.60308×10^{-14}
2.04056×10^{-14}	2.36227×10^{-12}	1.53349×10^{-13}	8.11337×10^{-14}	2.04056×10^{-14}
9.1832×10^{-15}	2.181×10^{-12}	1.38658×10^{-13}	7.47828×10^{-14}	9.1832×10^{-15}
7.27014×10^{-15}	6.71933×10^{-14}	1.04115×10^{-14}	3.3164×10^{-14}	7.27014×10^{-15}
5.52824×10^{-15}	4.5745×10^{-14}	4.7606×10^{-15}	1.66639×10^{-14}	5.52824×10^{-15}
3.11551×10^{-16}	1.27685×10^{-14}	2.36986×10^{-15}	2.49272×10^{-15}	3.11551×10^{-16}
3.00235×10^{-16}	7.57727×10^{-15}	8.90727×10^{-16}	2.99107×10^{-16}	3.00235×10^{-16}
2.03925×10^{-16}	1.15803×10^{-15}	1.08277×10^{-16}	1.00602×10^{-16}	2.03925×10^{-16}
3.1086×10^{-18}	4.87333×10^{-16}	3.72176×10^{-17}	4.7375×10^{-17}	3.1086×10^{-18}
1.80792×10^{-18}	5.94925×10^{-17}	2.76564×10^{-17}	1.10864×10^{-17}	1.80792×10^{-18}
1.06721×10^{-18}	5.39091×10^{-17}	2.38354×10^{-17}	8.8745×10^{-18}	1.06721×10^{-18}
8.04548×10^{-19}	3.46437×10^{-17}	5.4596×10^{-18}	4.70496×10^{-18}	8.04548×10^{-19}
5.57279×10^{-19}	1.55851×10^{-17}	3.14954×10^{-18}	4.07573×10^{-18}	5.57279×10^{-19}
2.47092×10^{-19}	5.94552×10^{-18}	1.50505×10^{-18}	3.47153×10^{-18}	2.47092×10^{-19}
1.6085×10^{-19}	4.91253×10^{-18}	1.13561×10^{-18}	3.31441×10^{-19}	1.6085×10^{-19}
4.78442×10^{-20}	3.41682×10^{-18}	8.52541×10^{-19}	1.41238×10^{-19}	4.78442×10^{-20}
3.97665×10^{-20}	1.85069×10^{-18}	8.14104×10^{-19}	1.31575×10^{-19}	3.97665×10^{-20}
8.59874×10^{-21}	1.47449×10^{-19}	5.86524×10^{-19}	5.34711×10^{-20}	8.59874×10^{-21}
7.97667×10^{-21}	2.95901×10^{-20}	3.26992×10^{-20}	5.17313×10^{-20}	7.97667×10^{-21}
5.05762×10^{-22}	1.4528×10^{-20}	2.76553×10^{-20}	1.50408×10^{-20}	5.05762×10^{-22}
3.03379×10^{-22}	4.41014×10^{-21}	1.77849×10^{-20}	6.76606×10^{-21}	3.03379×10^{-22}
3.83288×10^{-24}	3.79268×10^{-21}	5.58503×10^{-21}	3.51769×10^{-21}	3.83288×10^{-24}
2.13348×10^{-24}	7.47579×10^{-22}	1.62155×10^{-21}	5.8549×10^{-23}	2.13348×10^{-24}
2.47318×10^{-25}	3.19593×10^{-23}	1.19778×10^{-22}	8.55162×10^{-24}	2.47318×10^{-25}
9.56695×10^{-26}	6.9062×10^{-25}	4.66176×10^{-26}	5.76307×10^{-26}	9.56695×10^{-26}

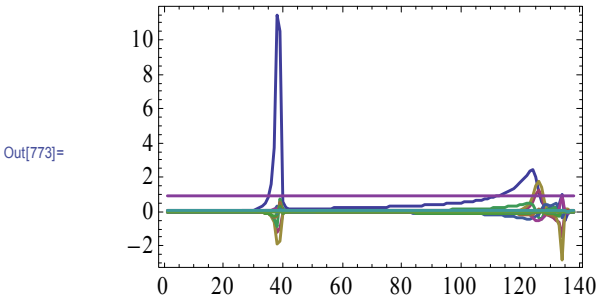
Data analysis

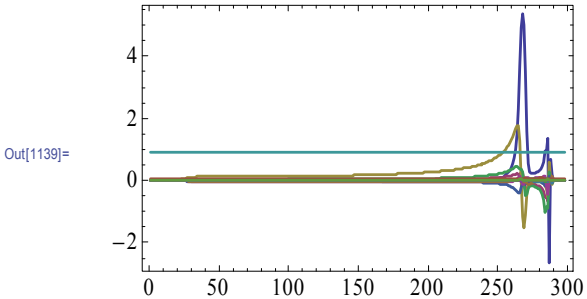
- Preliminary results of the system hierarchy analysis: $P_{TM_i} = Z_i \tilde{Z}_i, i = 1, 2, 3$

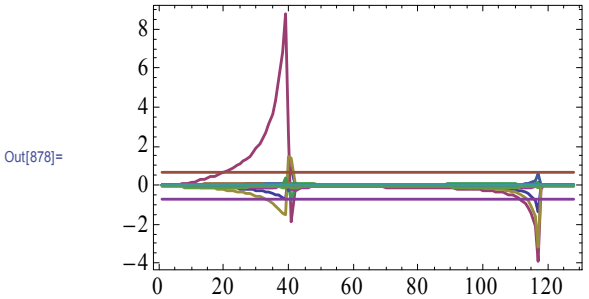


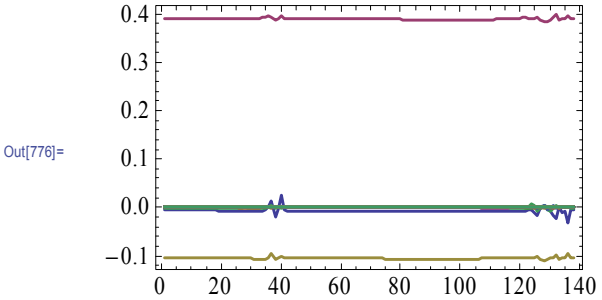


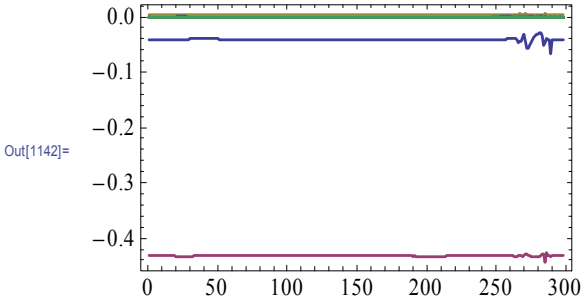


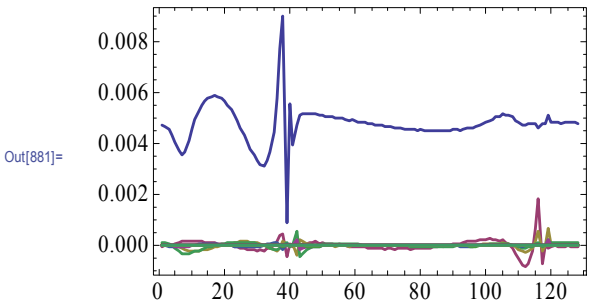












Data analysis and experiments

- The core idea is universal, e,g. linear interpolation is used to delineate main “features” of the vector function of the RHS:

$$\frac{d\psi}{dt} = F(\psi) \quad \Rightarrow \quad F : \psi = \begin{pmatrix} \psi_1 \\ \dots \\ \psi_n \end{pmatrix} \mapsto F(\psi) = \begin{pmatrix} F_1(\psi) \\ \dots \\ F_n(\psi) \end{pmatrix}$$

$$T : \psi^k \mapsto F(\psi^k), \quad \psi^k \in \Omega$$

- However, the same can be used to deal with experimental data

$$\overset{???}{f} : X \mapsto Y \qquad f : X = \begin{pmatrix} X_1 \\ \dots \\ X_M \end{pmatrix} \mapsto Y = \begin{pmatrix} Y_1(X) \\ \dots \\ Y_N(X) \end{pmatrix}$$

Many thanks for your attention!

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