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On local and global approaches in model reduction of mechanisms of chemical kinetics

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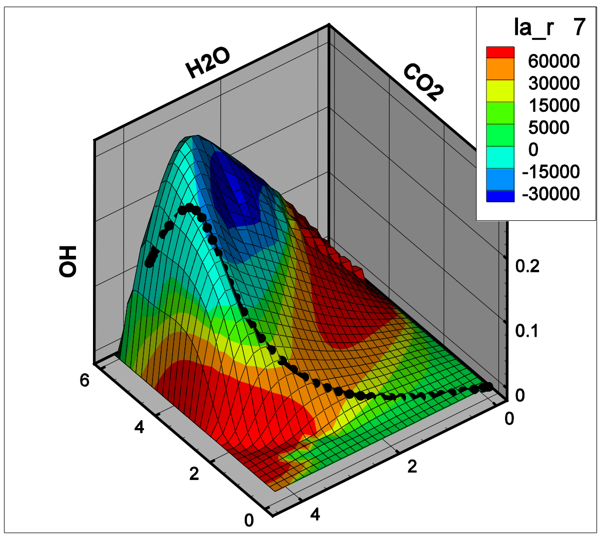
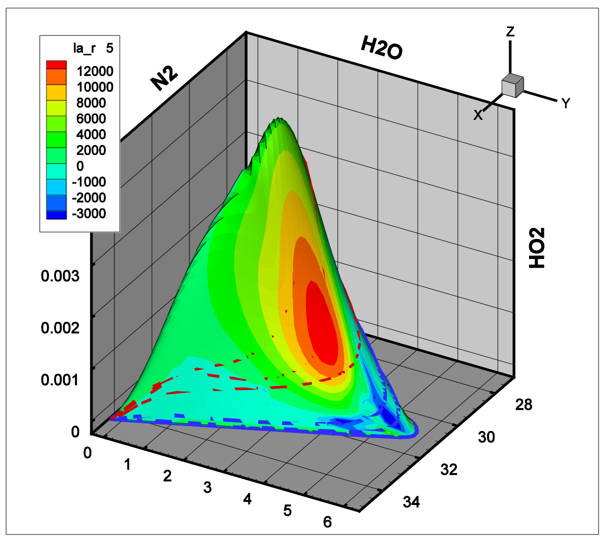
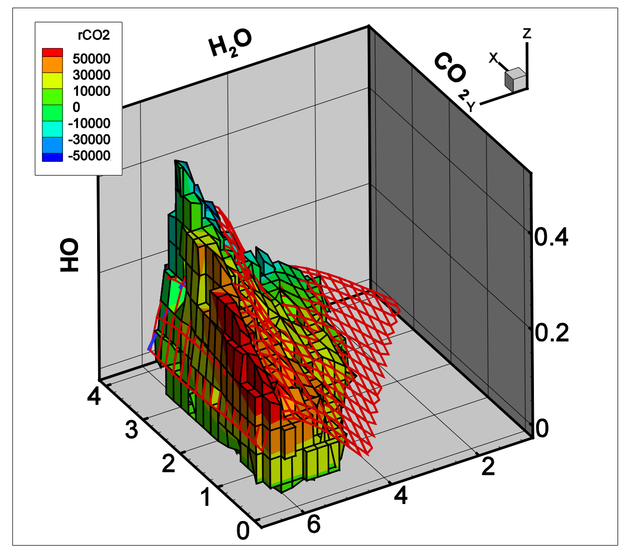
INSTITUT FÜR TECHNISCHE THERMODYNAMIK







Some questions of model reduction

- Why one would reduce the model?
  - High dimensionality, non-linearity + multiple-scales = complexity + stiffness
- Is it possible to reduce the system dimension?
  - Which properties of the system under consideration allow reduction?
- How can these special properties be used to formulate the reduced model?

- "Scientists discover the world that exists; engineers create the world that never was.“

THEODORE VON KARMAN

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

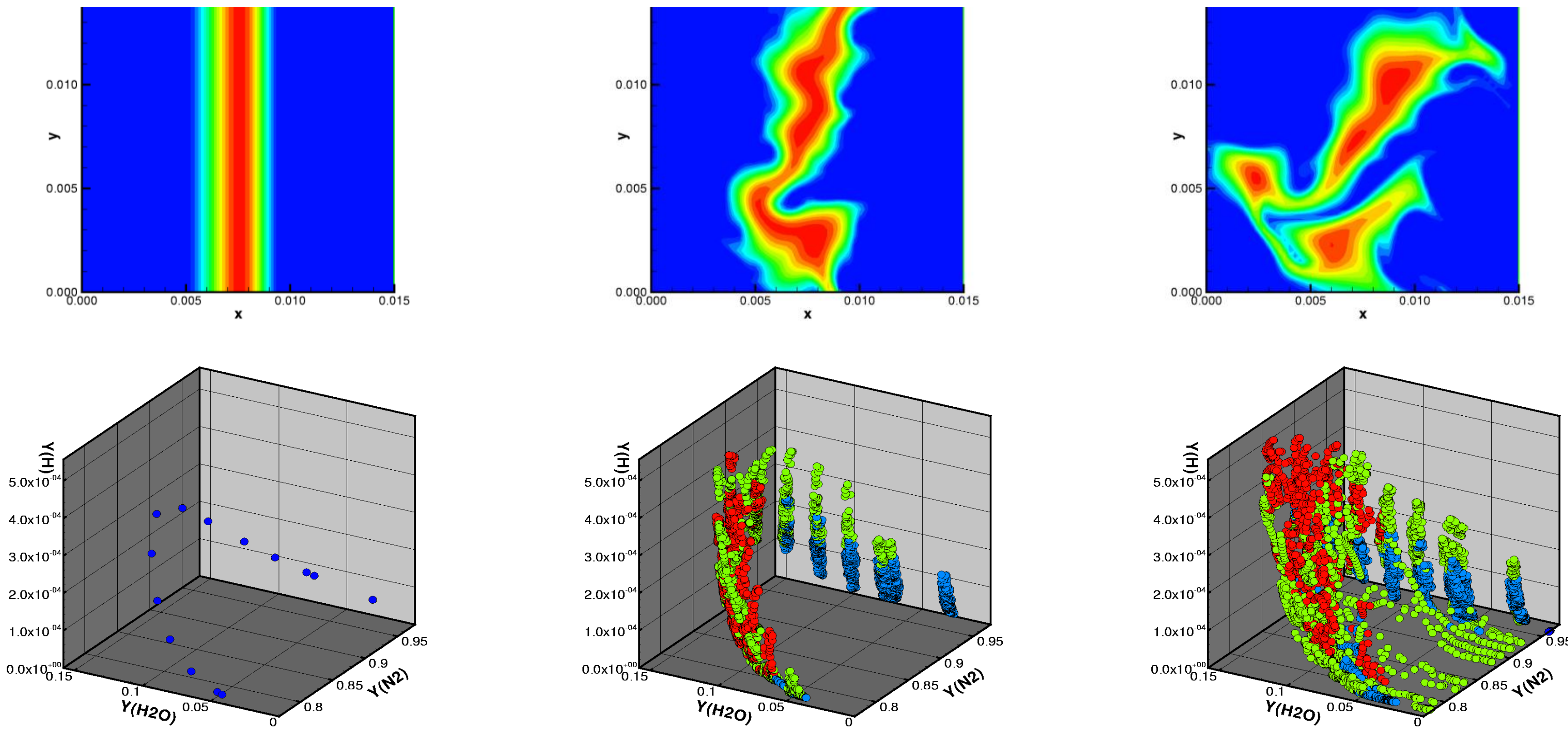
see e.g.: Warnatz, Maas, Dibble:
Combustion, Springer 2004

- 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

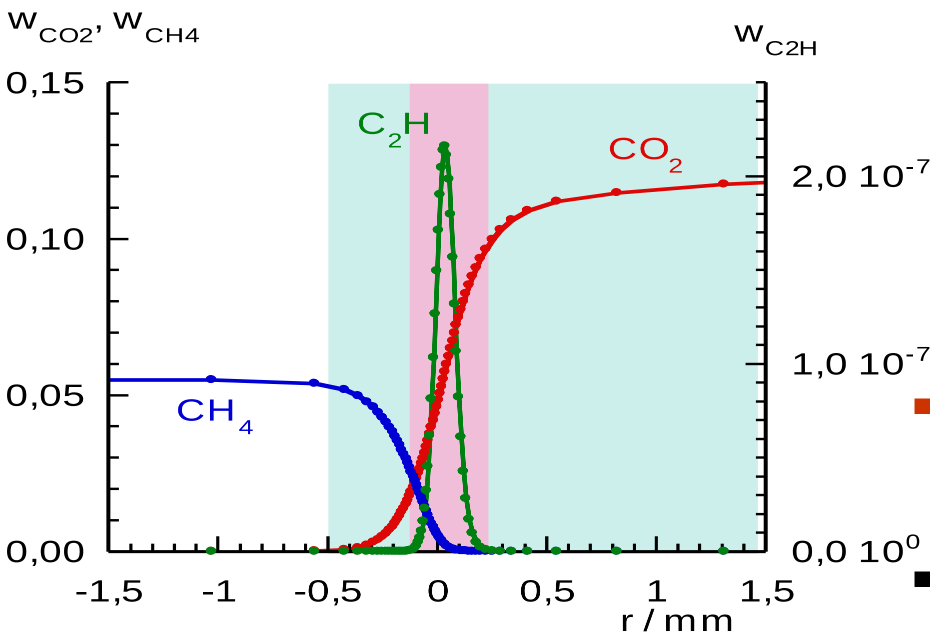
Multiple-scale phenomena



Maas & Thévenin 1998

- DNS of a turbulent non-premixed hydrogen flame
- Stiff chemical kinetics as well as molecular transport processes cause the existence of attractors in composition space!

Detailed chemical kinetics



1-dimensional cut through a CH_4-air flame

The question: What is a source of high complexity?

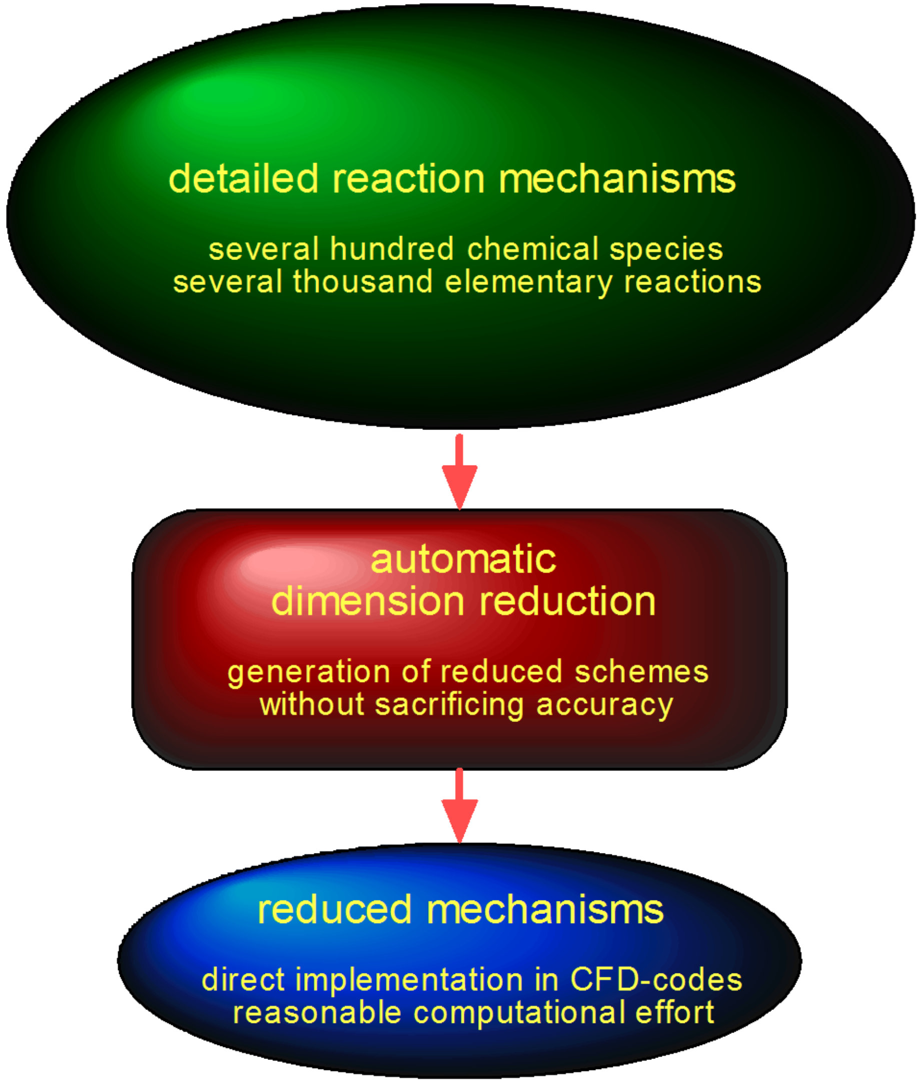
- Problems:
  - extremely high dimension of the system!
  - non-linear chemical source terms
  - stiffness of the governing equation system
  - different chemical time scales do not only introduce stiffness, but also cause the existence of very small length scales
- Is it possible to decouple the fast chemical processes?
- This would
  - reduce the number of governing equations
  - remove part of the scaling problems in space!

Concept: dimension reduction

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

- But: only few reactions are rate limiting!

- Fundamental concepts to be used:
  - Multiple-scales
  - Decomposition of motions
  - Existence of invariant manifolds of fast and slow motions in the system state space



Motivation – QSSA and PEA empirics

- Original coordinate system is suitable for the decomposition in terms of the species or elementary reactions:

$$\psi = \left(h,\ p,\ \frac{w_1}{M_1},\ldots,\frac{w_{n_s}}{M_{n_s}} \right)^T$$

$$a_{1,i}S_1 + \ldots + a_{n_s,i}S_{n_s} \Leftrightarrow \tilde{a}_{1,i}S_1 + \ldots + \tilde{a}_{n_s,i}S_{n_s}$$

$$F_i = \sum_{k=1}^{n_r} \left(\tilde{a}_{i,k} - a_{i,k} \right) R_k,\ s_{i,k} = \left(\tilde{a}_{i,k} - a_{i,k} \right) \ \Rightarrow$$

$$R_k = A_k T^{\beta_k} \exp\left(-E_{a,k} / RT \right) \prod_{i=1}^{n_s} c_i^{a_{i,k}}$$

$$\psi' = F(\psi) = \begin{pmatrix} s_{1,1} & s_{1,2} & \ldots & s_{1,n_r} \\ \ldots & \ldots & \ldots & \ldots \\ s_{n_s,1} & s_{n_s,2} & \ldots & s_{n_s,n_r} \end{pmatrix} \cdot \begin{pmatrix} R_1(\psi) \\ R_2(\psi) \\ \ldots \\ R_{n_r}(\psi) \end{pmatrix} = \begin{pmatrix} F_1(\psi) \\ F_2(\psi) \\ \ldots \\ F_n(\psi) \end{pmatrix}$$

$$M_{QSSA}^{0} = \left\{ F_{j_1}(\psi) = 0, \ldots, F_{j_{n_f}}(\psi) = 0 \right\}$$

$$M_{QSSA}^{0,\,fast} = \left\{ \psi_{j_1} = const, \ldots, \psi_{j_1} = const \right\}$$

$$M_{PEA}^{0} = \left\{ R_{i_1}(\psi) = 0, \ldots, R_{i_{n_f}}(\psi) = 0 \right\} \quad m = n - n_f$$

$$M_{PEA}^{0,\,fast} = ???$$

- QSSA assumes several species at quasi-steady states, while PEA some elementary reactions at partial equilibrium!
- Which and why?

Multiple-scales

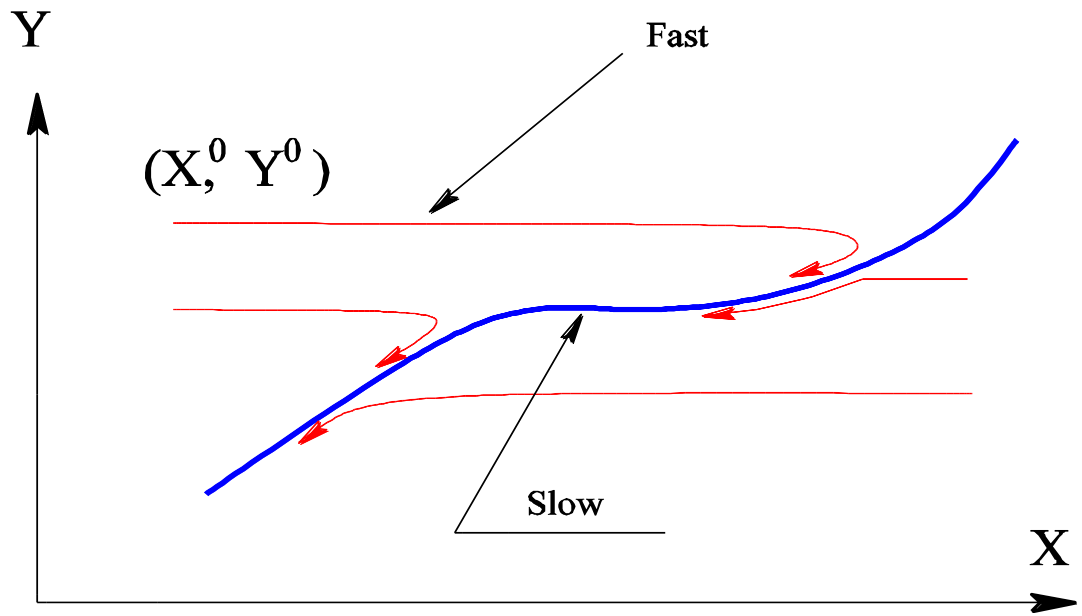
consider a system that exhibits multi-scale phenomena: $\frac{d\psi}{dt} = F(\psi) = S \circ R(\psi)$

Mathematical model is the SPS!

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

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

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



Questions:

- How can this special representation be found?

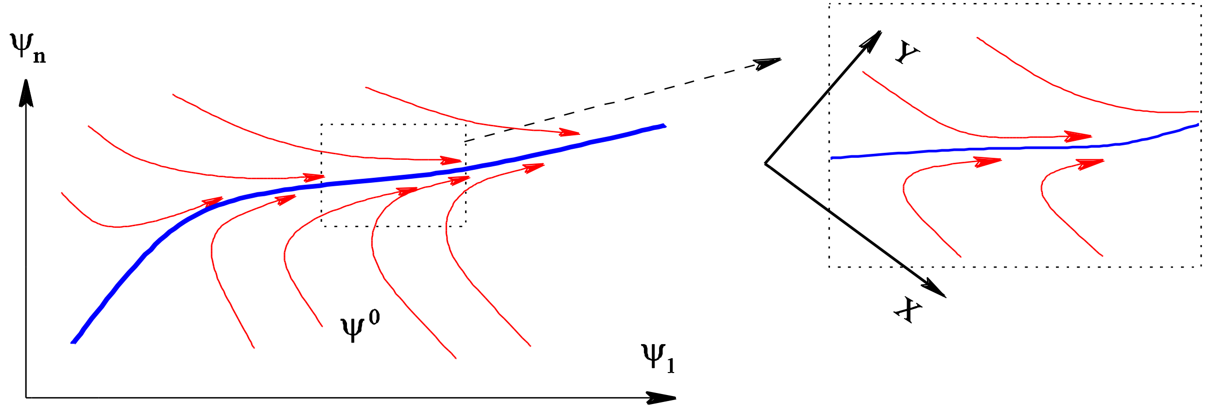
- What the system small parameter is?

Explicit decomposition

- Homogenous system of ODEs

$$\begin{pmatrix} Y \\ X \end{pmatrix} \sim \begin{pmatrix} \tilde{Z}_s(\psi) \\ \tilde{Z}_f(\psi) \end{pmatrix} \Rightarrow \begin{cases} \dfrac{dY}{dt} = F_s(X,Y) \\ \dfrac{dX}{dt} = F_f(X,Y) \end{cases}$$

$$F_f(X,Y) >> F_s(X,Y)$$



- The manifold of stationary states of the fast subsystem and the manifold of conserved slow variables!

$$\psi = Z\begin{pmatrix} Y \\ X \end{pmatrix}$$

$$M_s^0 = \{\psi : F_f(X(\psi), Y(\psi)) = 0\}$$
$$M_f^0(\psi_0) = \{\psi : Y(\psi) = Y(\psi_0)\}$$

Singularly Perturbed Vector Field (SPVF)

- informal definition: parametric family of vector fields $\frac{d\psi}{dt} = F(\psi, \varepsilon)$
- is a singular perturbed one, if for any fixed ψ the limiting vector field belongs to a priory fixed linear subspace of smaller dimension:

$$F(\psi,0) \in L_f(\psi), \quad \dim\left(L_f(\psi)\right) = n_f < n$$

- Moreover, the dimension does not depend on the point. Then, a fast manifold M_f associated with ψ satisfies $F(\psi,0) \in TM_f$
- and a slow manifold given by

$$M_s = \{\psi : F(\psi,0) = 0\}$$

• Reference: Bykov et. al. J. Phys.: Conf. Ser., 55 (2006), Bykov et. al. CTM, 12(2) (2008)

It is obvious that this construction is almost useless in applications if there is no efficient algorithm to identify the fast manifold!

Example 1: SPS

- informal definition: parametric family of vector fields

$$\frac{dX}{dt} = \frac{1}{\varepsilon} F_f(X,Y), \quad X \in R^{n_f}$$
$$\frac{dY}{dt} = F_s(X,Y), \quad Y \in R^{n_s}$$
$$n_f + n_s = n, \quad 0 < \varepsilon << 1$$

$$\frac{d\psi}{dt} = F(\psi,\varepsilon), \quad \psi = (X,Y)^T$$
$$dt \to d\tau$$
$$F(X,Y;\varepsilon) = \begin{pmatrix} F_f(X,Y) \\ 0 \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ F_s(X,Y) \end{pmatrix}$$

$$F(\psi,0) \in L_f(\psi) = \{\psi = (X,Y) \mid Y = const\}, \quad \dim(L_f) = n_f < n$$

$$F(\psi,0) \in TM_f = L_f$$

$$M_s = \{\psi : F(\psi,0) = 0\} \Leftrightarrow \{\psi = (X,Y) : F_f(X,Y) = 0\}$$

Since vector field decomposition is trivial the limit of the small system parameter tends to zero coincides with the SPS, e.g. for slow manifold!

Example 2: Van der Pol Oscillator

- Original model

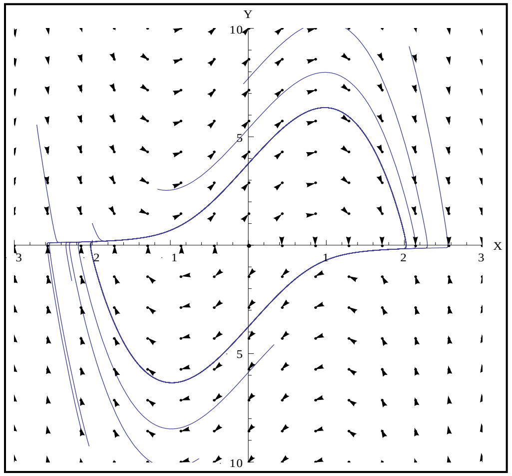
$$\ddot{x} - \mu\left(1 - x^2\right)\dot{x} + x = 0$$

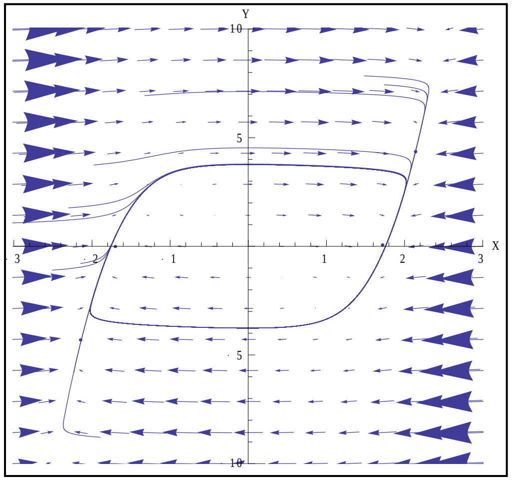
- Vector form, μ = 4

$$\begin{cases} \dfrac{dx}{d\tau} = y \\ \dfrac{dy}{d\tau} = -x + \mu\left(1 - x^2\right)y \end{cases}$$

- Liénard form, μ = 4

$$\begin{cases} \dfrac{dx'}{d\tau} = y' + \mu\left(1 - \dfrac{1}{3}x'^2\right)x' \\ \dfrac{dy'}{d\tau} = -x' \end{cases}$$





19-22 August 2014
Model reduction across disciplines
University of Leicester, UK
Viatcheslav Bykov

Example 2: Van der Pol Oscillator

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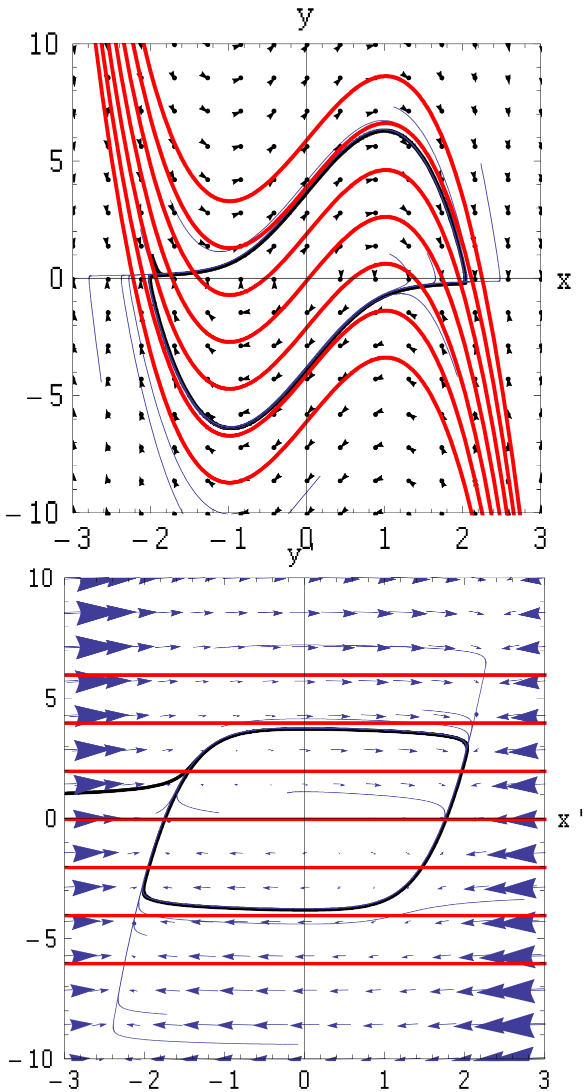
- Vector form, μ = 4

$$\begin{cases} \dfrac{dx}{d\tau} = y \\ \dfrac{dy}{d\tau} = -x + \mu(1-x^2)y \end{cases} \Leftrightarrow \begin{cases} \dfrac{dx'}{d\tau} = y' + \mu\left(1-\dfrac{1}{3}x'^2\right)x' \\ \dfrac{dy'}{d\tau} = -x' \end{cases}$$

- Liénard variables

$$\begin{cases} x' = x \\ y' = y - \mu\left(1-\dfrac{1}{3}x^2\right)x \end{cases}$$

- The suggested framework allows reconcile the most suitable coordinate frame for the analysis



• Reference: Bykov, J. Phys.: Conf. Ser. 268, 012003, 2011

Linearly decomposed SPVFs

- definition: parametric family of vector fields

$$\frac{d\psi}{dt} = F(\psi, \varepsilon) \qquad F(\psi,\varepsilon) = \begin{pmatrix} s_{1,1} & s_{1,2} & \dots & s_{1,n_r} \\ \dots & \dots & \dots & \dots \\ s_{n_s,1} & s_{n_s,2} & \dots & s_{n_s,n_r} \end{pmatrix} \cdot \begin{pmatrix} R_1(\psi) \\ R_2(\psi) \\ \dots \\ R_{n_r}(\psi) \end{pmatrix} = \begin{pmatrix} F_1(\psi) \\ F_2(\psi) \\ \dots \\ F_n(\psi) \end{pmatrix}$$

- is a linearly decomposed singular perturbed vector field, iff

$$M_f(\psi) = \{\psi\} + L_f$$

- It means there exists constant matrix Z such that

$$\begin{pmatrix} X \\ Y \end{pmatrix} = Z\,\psi : \qquad \frac{d}{dt}\begin{pmatrix} X \\ Y \end{pmatrix} = \begin{pmatrix} \frac{1}{\varepsilon} F_f \\ F_s \end{pmatrix}$$

Purpose: Develop an algorithm, which allows to identify fast manifolds and/or approximate linear subspace of fast motions!

Global Quasi-Linearization - (GQL)

$$\psi' = F(\psi) = S \circ R(\psi)$$

Answers the questions:

1. How can we check if a given system defines a linearly decomposed singularly perturbed vector field?
2. How to estimate the system small parameter – difference in time scales?
3. How the vector field can be decomposed?

GQL&ILDM – global versus local approach

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

$$T:\psi_i \mapsto F(\psi_i) \quad \Rightarrow \quad F^* = \begin{bmatrix} F(\psi_1)\ldots & F(\psi_n) \\ \ldots \quad \ldots & \ldots \\ | & | \end{bmatrix}, \Psi = \begin{bmatrix} \psi_1\ldots & \psi_n \\ \ldots \quad \ldots & \ldots \\ | & | \end{bmatrix} \quad \Rightarrow \quad \boxed{T = F^* \Psi^{-1}}$$

- If there is a gap between eignevalues of the GQL or of Jacobi matrix

$$F_\psi(\psi) = \left(Z_s(\psi)\, Z_f(\psi)\right) \begin{pmatrix} \Lambda_s(\psi) & * \\ 0 & \Lambda_f(\psi) \end{pmatrix} \begin{pmatrix} \tilde{Z}_s(\psi) \\ \tilde{Z}_f(\psi) \end{pmatrix} \qquad T = \left(Z_s\, Z_f\right) \begin{pmatrix} \Lambda_s & 0 \\ 0 & \Lambda_f \end{pmatrix} \begin{pmatrix} \tilde{Z}_s \\ \tilde{Z}_f \end{pmatrix}$$

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

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

- Reference: Bykov et. al. J. Phys.: Conf. Ser., 55 (2006), Bykov et. al. CTM, 12(2) (2008)

Suggested approach – explicit form of the manifold

- The states of the system are confined to a low dimensional manifold imbedded into the system state space

$$M = \{\psi = \psi(\theta), \dim\theta << \dim\psi\}$$

- Algebraic definition – ILDM

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

- Algebraic definition – GQL

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

• Reference: Maas and Pope, Combust. Flame, 1992
• Reference: Bykov et al, 2008, 2009

Multiple-scales analysis

The suggested combination of local and global methods allows at the same time

- Check globally the existence of multiple characteristic time scales!
- Estimate the dimension of the decomposition!
- Approximate slow manifolds and fast manifolds!
- Explicitly decompose the system!
- Implement the reduced model as evolution of the system on the manifold!

Coordinate free singular perturbations, local and global analysis provide with

- Manifolds equation
- Intrinsic properties of the manifold
  - Stable, unstable, turning manifolds
  - Boundary of the manifold
  - Suitable parameterization (accounts for the fast transient behaviour)
- Improving the manifold
  - using invariance property
  - optimal choice of global coordinates

Dynamical system of apoptosis signaling network

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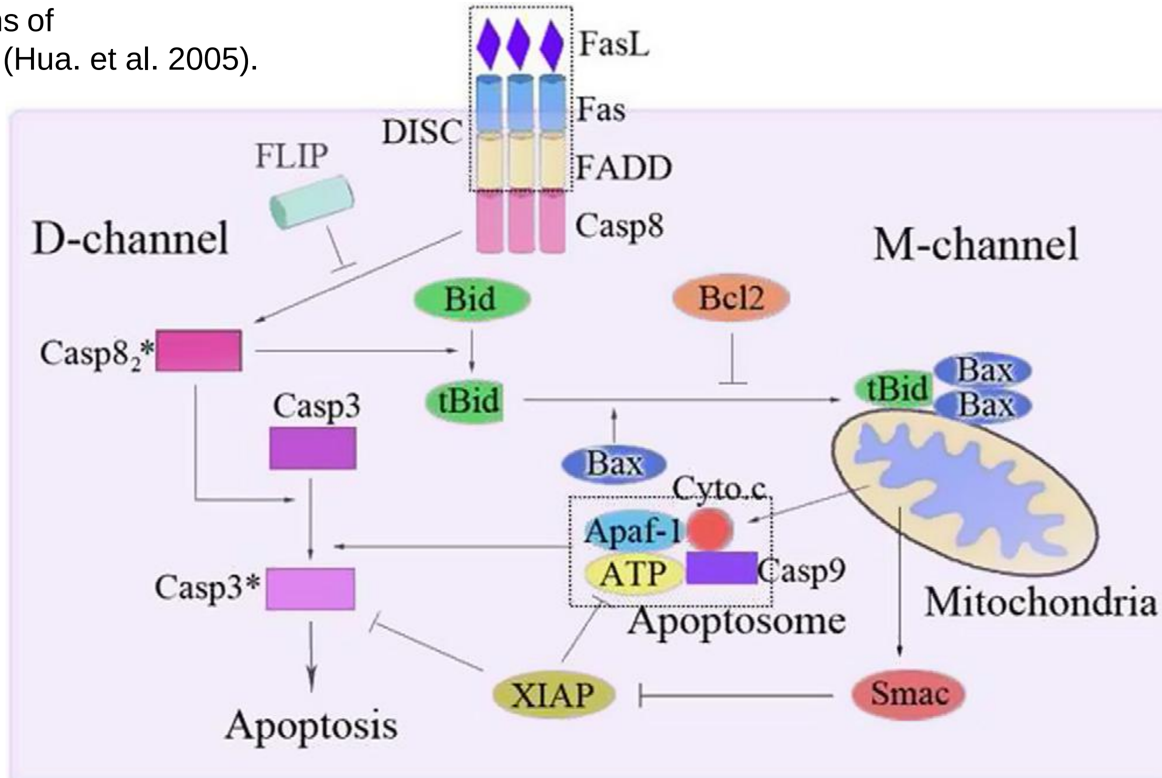
- The system comprises 28 species and 20 elementary reactions
  - Rank of the stoichiometry matrix is 19

{Casp82},
{Casp82Casp3},
{Casp82Bid},
{Bid},
{tBid},
{tBidBax},
{tBidBax2},
{Bcl2tBid},
{Bax},
{Bcl2Bax},
{Bcl2},
{Citoc},
{CitocStar},
{CitocStarApafATP},
{CitocStarApafATPCasp9},
{CitocStarApafATPCasp92},
{Apaf},
{Casp9Star},
{Casp9},
{Casp3},
{Casp9StarCasp3},
{Casp3Star},
{Smac},
{SmacStar},
{XIAP},
{SmacStarXIAP},
{Casp9XIAP},
{Casp3StarXIAP}

Non-zero initial concentrations of
the species in the ISS model (Hua. et al. 2005).

Species Initial concentration:

Casp3	200.00
Bid	25.00
Bcl2	75.00
Bax	83.33
Cyto.c	100.00
Smac	100.00
XIAP	30.00
Casp9	20.00
ATP	10000.00
Apaf	100.00



• Reference: Y.-J. Huang, W.-A. Yong, Mathematical Biosciences 246 (2013)

Apoptosis system – time scale analysis

- Jacobi matrix and GQL spectrum and a gap condition
  - There are three groups of eigenvalues representing three characteristic time scales:

Eigenvalues J[t=0]= {
4.86099,0.85228,0.809632,0.33666,0.233497,0.21221,0.186891,0.158503,
0.0765,0.0755176,0.0473823,0.00905915,0.0063,8.93154×10^{-7},8.92706×10^{-7},8.92706×10^{-7},8.82398×10^{-7},8.82398×10^{-7},
1.38644×10^{-16},1.86341×10^{-17},1.86341×10^{-17},1.04569×10^{-18},1.04569×10^{-18},1.01981×10^{-18},7.86392×10^{-19},0.,0.,0.}

Eigenvalues J[t=t_{f}]= {
4.8585,0.842225,0.801438,0.160749,0.131953,0.106937,
0.0998059,0.0878569,0.0539073,0.0340042,0.0279269,0.0152488,0.00266029,0.0010145,0.000860528,0.000860528,0.000539256,0.000346436,
3.67416×10^{-17},2.82355×10^{-17},1.54948×10^{-17},1.54948×10^{-17},5.59547×10^{-18},2.94488×10^{-18},2.94488×10^{-18},1.95688×10^{-18},1.03917×10^{-18},7.57263×10^{-19}}

Eigenvalues T = {
1277.21,1099.43,1099.43,27.7404,
3.01862,1.348,0.8092,0.218932,0.101026,0.101026,0.00684151,0.00684151,0.00451876,0.00345011,0.00345011,0.00101978,0.00101978,
1.55738×10^{-7},1.55738×10^{-7},2.63276×10^{-10},2.63276×10^{-10},2.02073×10^{-10},1.25947×10^{-11},5.15767×10^{-12},4.37962×10^{-12},3.09182×10^{-12},3.09182×10^{-12},5.87537×10^{-17}}

Apoptosis system – analysis

- Invariant subspace of GQL $M = \left\{ \psi(\theta) : \tilde{Z}_f \cdot F\left(\psi(\theta)\right) = 0 \right\} \Rightarrow \boxed{\tilde{Z}_f \cdot S \cdot R(\psi) = 0}$
  - Transfer to the elementary reactions space

$$n = 28,\ n_f = 4:\ \tilde{Z}_f - (n_f \times n),\ \tilde{Z}_f \cdot S - (n_f \times n_r)$$

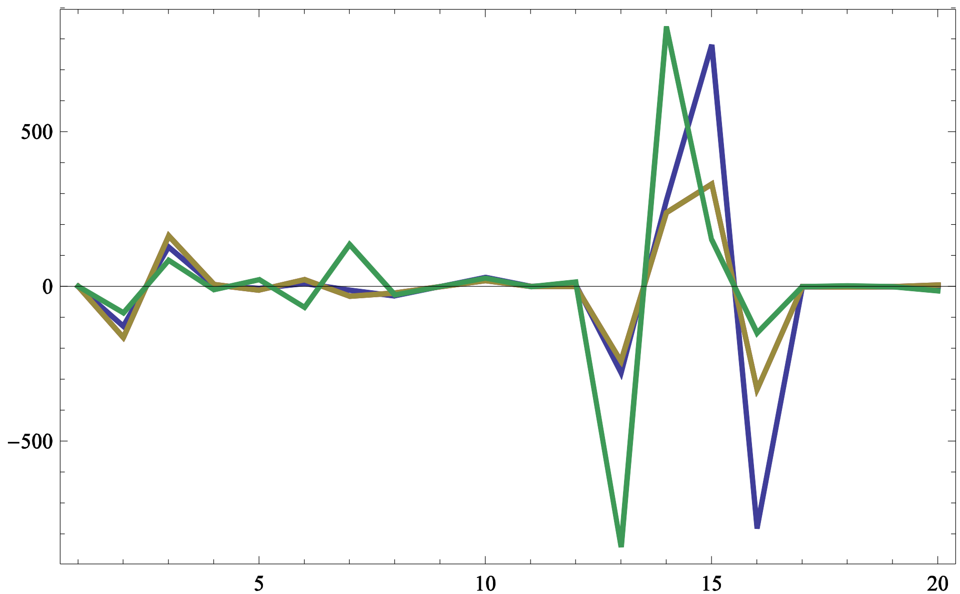
$$\mathrm{Re}\left(\tilde{Z}_f \cdot S\right)$$

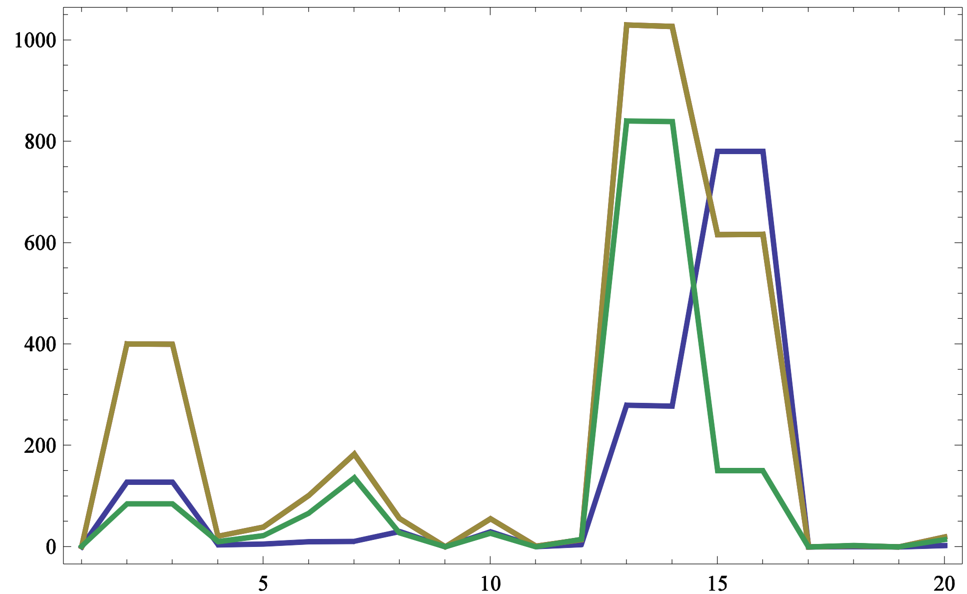
$$\mathrm{Abs}\left(\tilde{Z}_f \cdot S\right)$$

$$\begin{cases} R_2 \sim R_3 \\ R_8 \sim R_{10} \\ R_{13} \sim R_{14} \\ R_{15} \sim R_{16} \end{cases} \Rightarrow \quad M = \left\{ \psi : R_{i_k}(\psi) - R_{j_k}(\psi) = 0 \right\}$$

$$i = \{2,8,13,15\}$$

$$j = \{3,10,14,15\}$$





Apoptosis system – results of reduced model

- Reduced vs detailed model
  - Independent

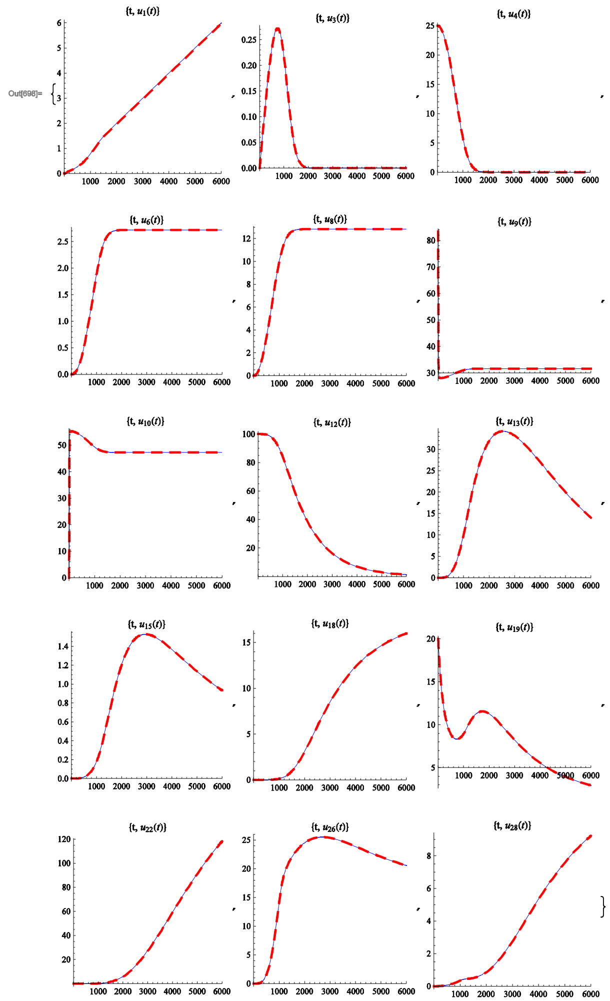
    $$m = 28 - 9 - 4 = 15$$

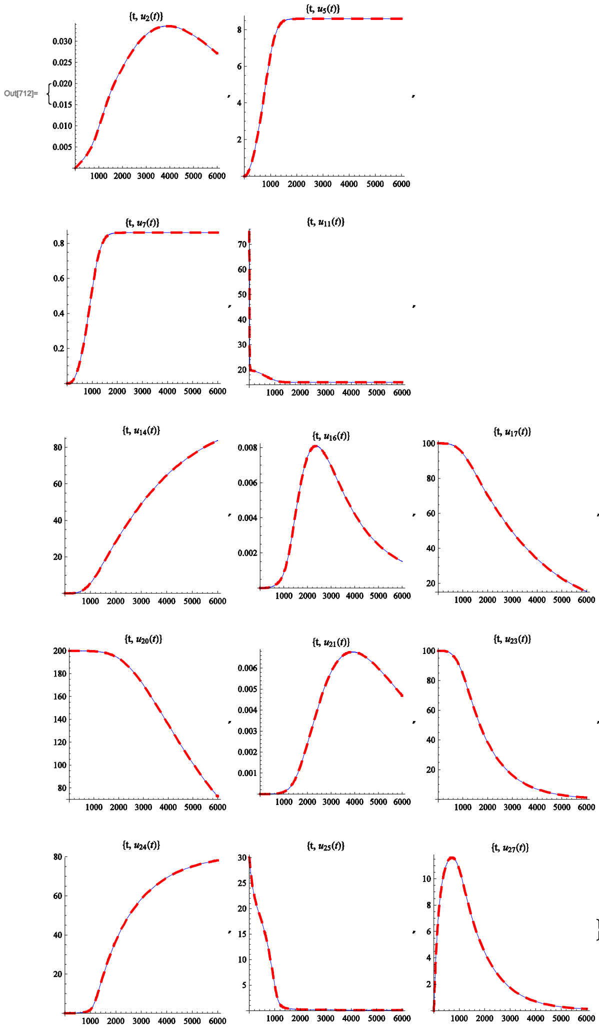
{1,3,4,6,8,9,10,12,13,15,18,19,22,26,28}

  - Dependent

    $$n - m = 28 - 15 = 13$$

{2,5,7,11,14,16,17,20,21,23,24,25,27}





Apoptosis system – results of reduced model

- Reduced vs detailed model, initial value is perturbed

  - Independent

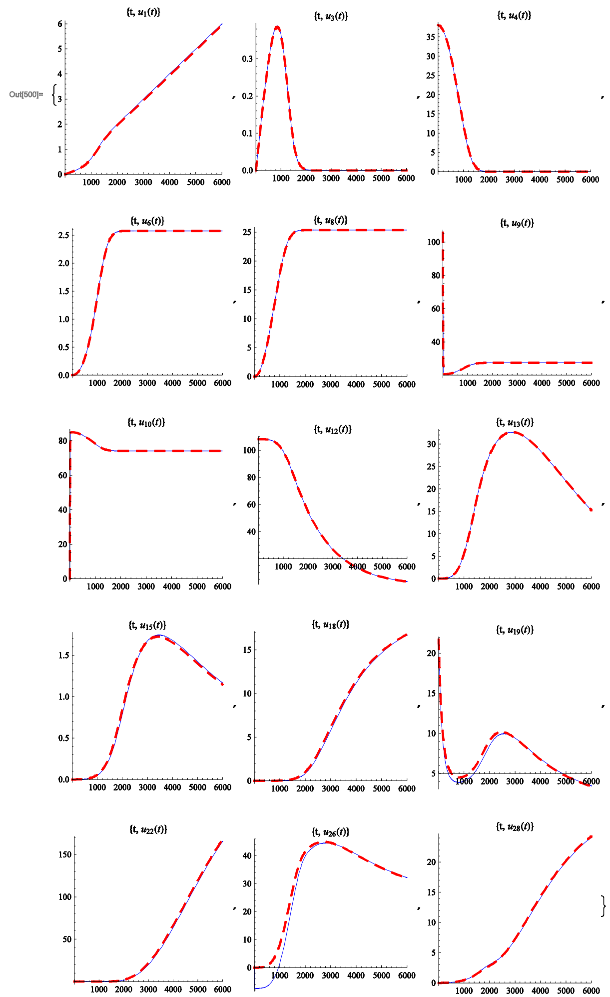
    $$m = 28 - 9 - 4 = 15$$

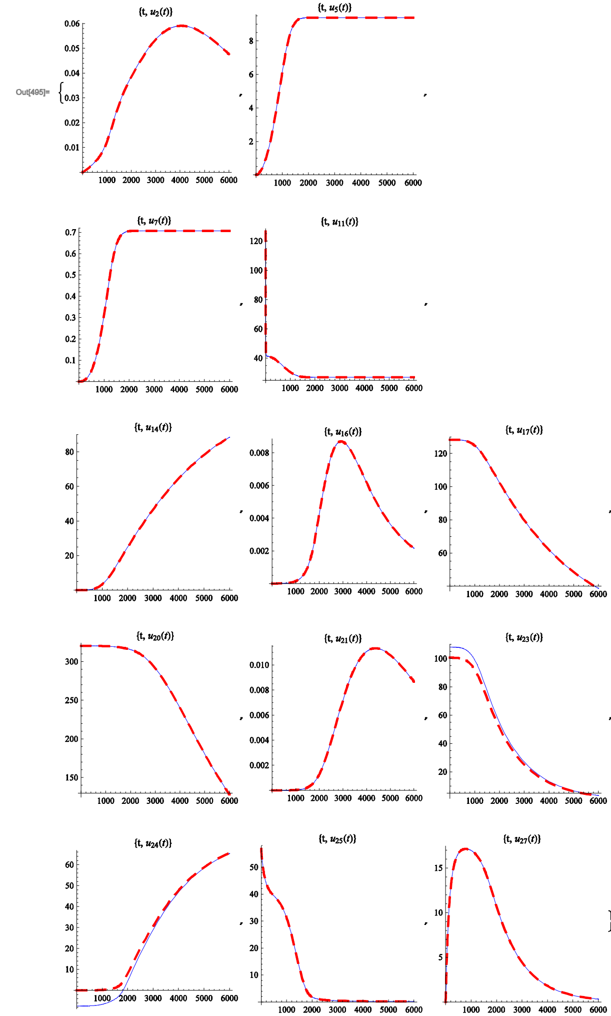
{1,3,4,6,8,9,10,12,13,15,18,19,22,26,28}

  - Dependent

    $$n - m = 28 - 15 = 13$$

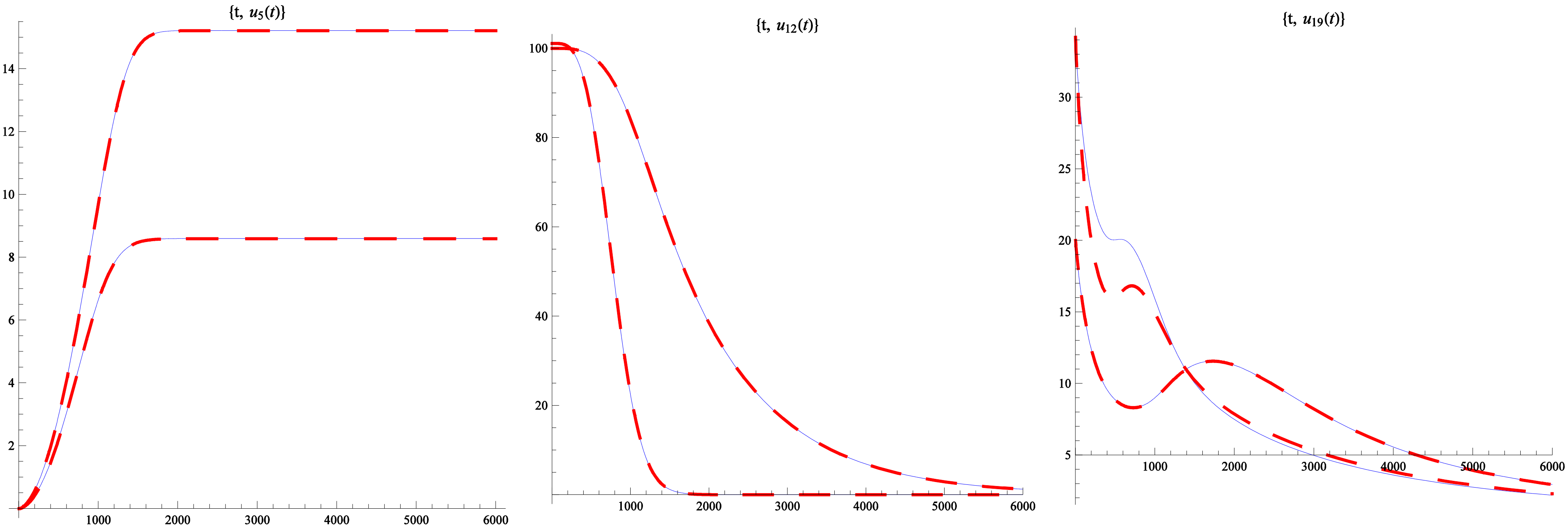
{2,5,7,11,14,16,17,20,21,23,24,25,27}





Apoptosis system – results of reduced model

- Comparison for different initial values
  - detailed – dashed red curves
  - reduced – blue curves



Conclusions

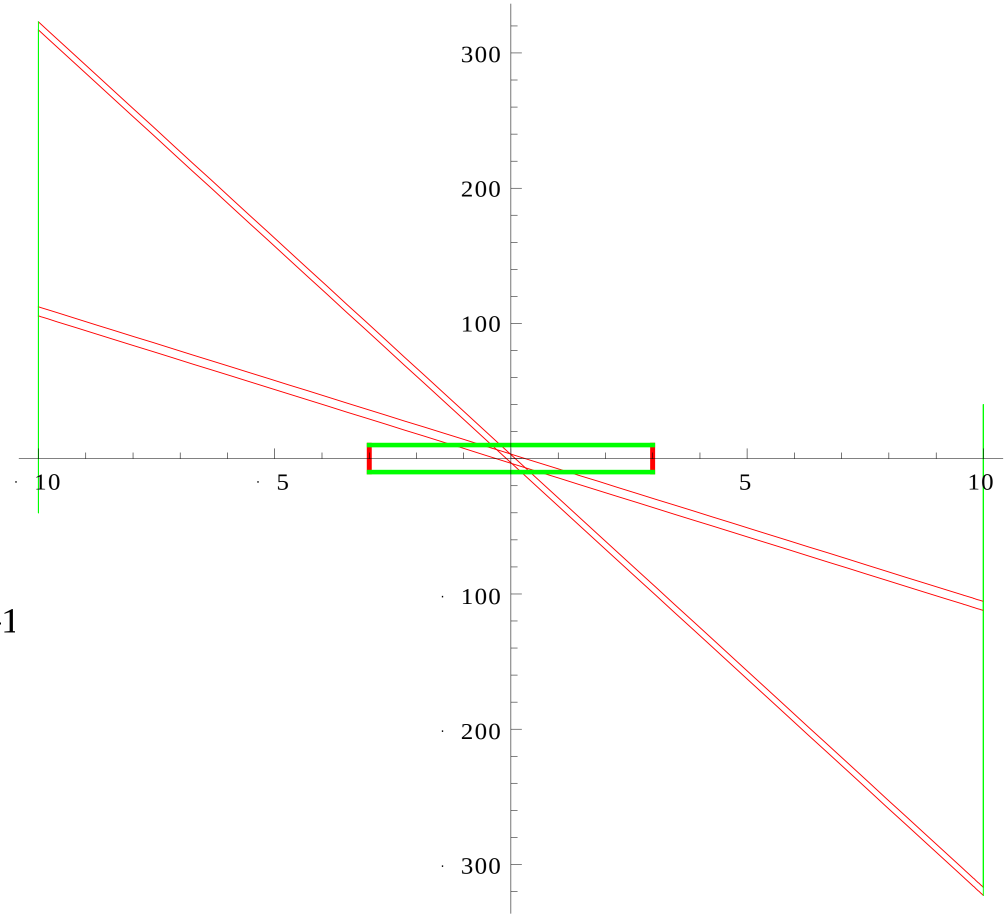
- Manifold based concept and decomposition of motions assumption to access model reduction problem were discussed
- Local (ILDM) and global (GQL) methods for kinetic mechanism reduction and its implementation to reacting flow simulation were presented
- The results of the analysis was demonstrated and illustarted by application to biochemical signaling network of the apoptosis

- Financial support by the Deutsche Forschungsgemeinschaft is gratefully acknowledged.

GQL application to original Van der Pol model

- Domain transformation, μ = 4

$$\Omega = [-3,3] \times [-10,10] \rightarrow F(\Omega)$$



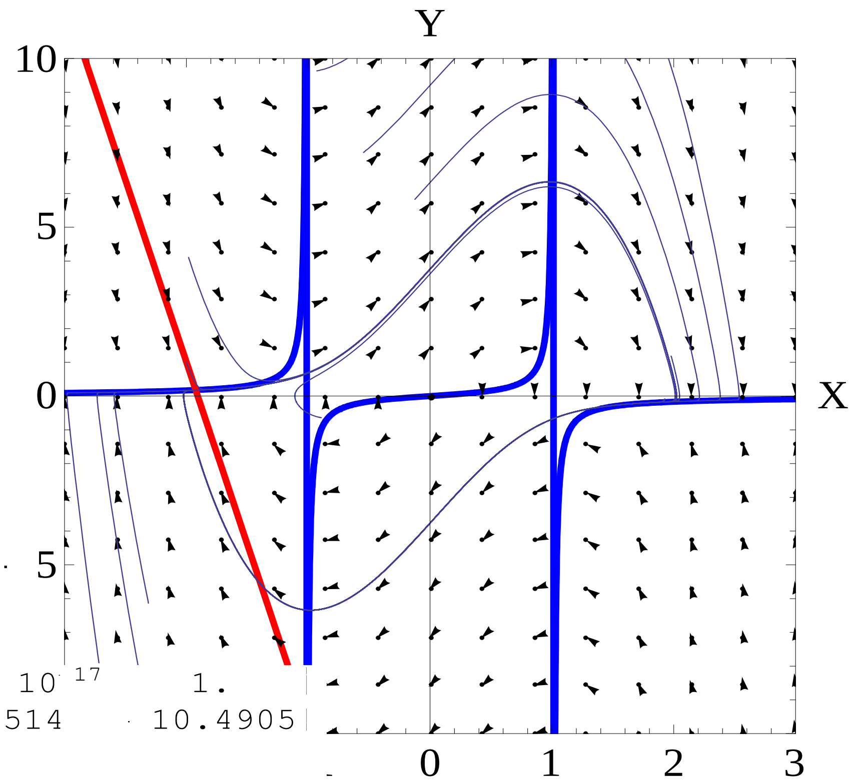
$$T_k^* = \begin{pmatrix} f(x_1, y_1) & f(x_2, y_2) \\ g(x_1, y_1) & g(x_2, y_2) \end{pmatrix} \begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix}^{-1}$$

Result of GQL: Van der Pol Oscillator

- Vector form, μ = 4

$$\begin{cases} \dfrac{dx}{d\tau} = y \\ \dfrac{dy}{d\tau} = -x + \mu\left(1 - x^2\right)y \end{cases}$$

- Result



GQL[form the set by Invariants Criteria] : $\begin{pmatrix} 5.55112\ 10^{-17} & 1. \\ -0.842514 & -10.4905 \end{pmatrix}$

Eigenvalues : $\begin{pmatrix} -10.4095 \\ -0.0809368 \end{pmatrix}$

Right basis : $\begin{pmatrix} -0.0956257 & 0.996741 \\ 0.995417 & -0.080673 \end{pmatrix}$

Left basis : $\begin{pmatrix} 0.0819466 & 1.01248 \\ 1.01113 & 0.0971353 \end{pmatrix}$

Fast Eqs : 10.2949 (0.0971353 1.01113 (2. x))

Slow Eqs : $\dfrac{1.01248\,x}{0.0819466\ 4.0499\,(1.\ 1.\,x^2)}$

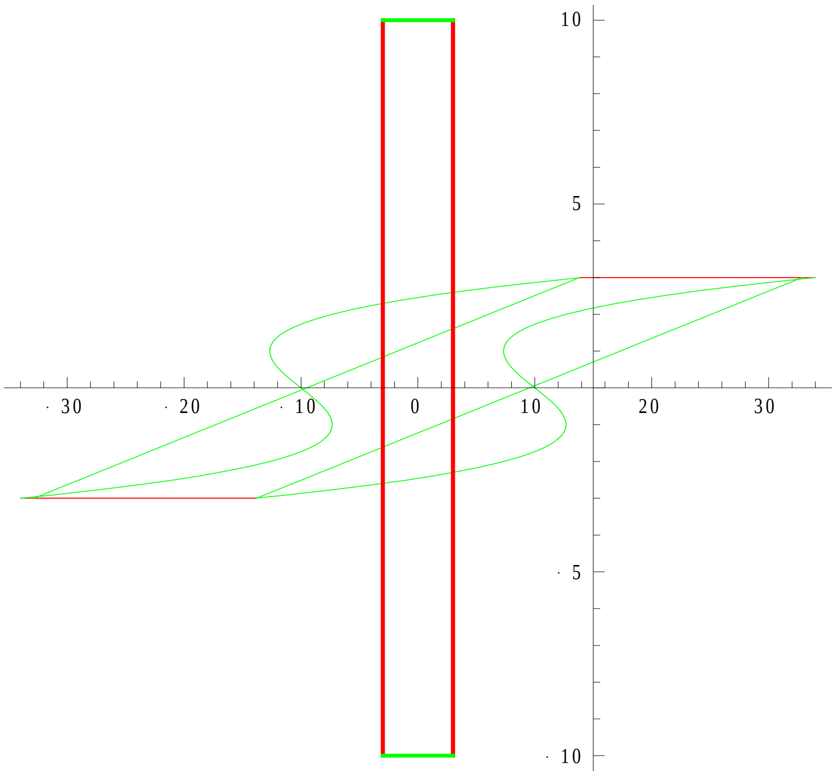
- Reference: Bykov, J. Phys.: Conf. Ser. 268, 012003, 2011

GQL application to Van der Pol model in Liénard form

- Domain transformation, μ = 4

$$\Omega = [-3,3] \times [-10,10] \rightarrow F(\Omega)$$

$$T_k^* = \begin{pmatrix} f(x_1, y_1) & f(x_2, y_2) \\ g(x_1, y_1) & g(x_2, y_2) \end{pmatrix} \begin{pmatrix} x_1 & x_2 \\ y_1 & y_2 \end{pmatrix}^{-1}$$



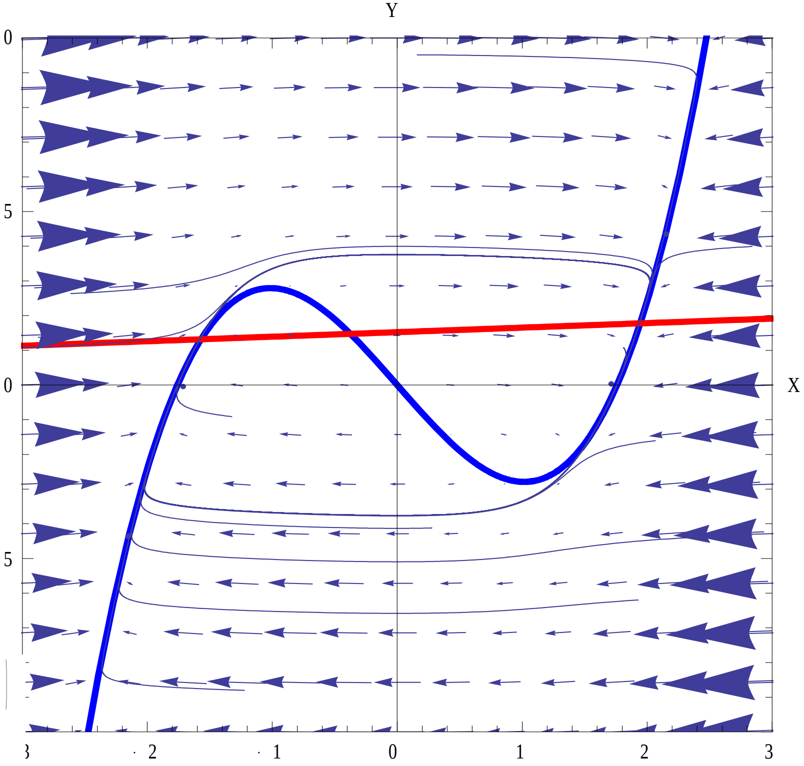
19-22 August 2014
Model reduction across disciplines
University of Leicester, UK
Viatcheslav Bykov

Result of GQL: Van der Pol Oscillator, Liénard form

- Vector form, μ = 4

$$\begin{cases} \dfrac{dx'}{d\tau} = y' + \mu\left(1 - \dfrac{1}{3}x'^2\right)x' \\ \dfrac{dy'}{d\tau} = -x' \end{cases}$$

- Original form




```
GQL ( form the set by Invariants Criteria) :  ( · 7.77553  0.95236 )
                                               (   · 1.        0.    )

Eigenvalues :  ( · 7.65106  )
               ( · 0.124474 )

Right basis :  ( · 0.991567 · 0.123521 )
               ( · 0.129599 · 0.992342 )

Left basis :  ( · 1.02518  0.127609 )
              (  0.133888 · 1.02438 )

Fast Eqs :· 0.976198( · 1.02438· 0.133888( 4.+ x))

Slow Eqs :· 0.975435( 0.127609 x+ 4.10074 x( 1.· 0.333333 x^2))
```

• Reference: Bykov, J. Phys.: Conf. Ser. 268, 012003, 2011