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LAV

MODEL REDUCTION by using INVARIANT GRIDS

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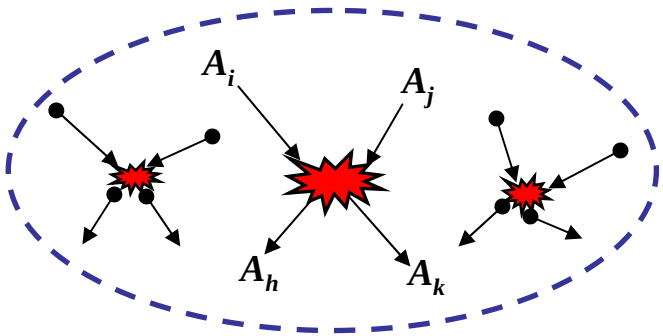
OUTLINE

1. *SOME FUNDAMENTALS AND NOTATIONS*
2. *INVARIANT MANIFOLDS AND INVARIANCE EQUATION*
3. *FEATURES OF THERMODYNAMIC PROJECTOR*
4. *THE METHOD OF INVARIANT GRIDS*
5. *QUASI-EQUILIBRIUM MANIFOLDS*
6. *QUASI-EQUILIBRIUM GRID APPROXIMATION*
7. *GRID PARAMETERIZATION AND TIME INTEGRATION*
8. *INITIAL CONDITION ISSUE*
9. *CONCLUSIONS*

MODELING COMPLEXITY: notations…

***EXAMPLE*: N SPECIES $(A_1,\ldots,A_N)$ AND L ELEMENTS $(E_1,\ldots,E_L)$ IN A CLOSED SYSTEM.**



THE EQUATIONS FOR MODELING:

$$\begin{cases} \dot{\vec{c}} = \vec{f} = \sum_{i=1}^{r} \left(\vec{\beta}_s - \vec{\alpha}_s\right)\left[k_s^+ \prod_{j=1}^{N} c_j^{\alpha_j} - k_s^- \prod_{j=1}^{N} c_j^{\beta_j}\right] \\ \left(\vec{d}_i, \vec{c}\right) = const, \quad i = 1,\ldots,L \\ \vec{\alpha}_s = [\alpha_{s1},\ldots,\alpha_{sN}], \quad \vec{\beta}_s = [\beta_{s1},\ldots,\beta_{sN}] \end{cases}$$

REPRESENTATION BY MEANS OF THE STOICHIOMETRIC MECHANISM (r STEPS):

$$\alpha_{s1}A_1 + \ldots + \alpha_{sN}A_N \Leftrightarrow \beta_{s1}A_1 + \ldots + \beta_{sN}A_N, \quad s = 1,\ldots,r$$

NUMBER OF MOLECULES (SPECIES A_i, VOLUME V): n_{A_i}

CONCENTRATION OF SPECIES A_i: $c_i = n_{A_i}/V$

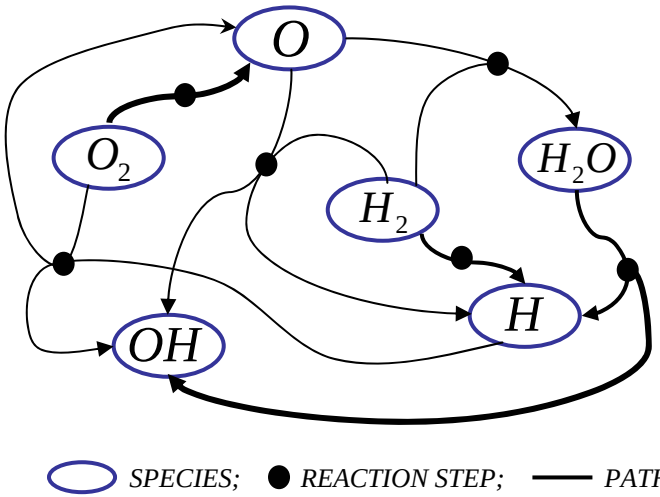
CONCENTRATION VECTOR: $\vec{c} = [c_1,\ldots,c_N]$

IN SOME RELEVANT CASES :

- DIFFERENT ORDER OF MAGNITUDE FOR $k_s^{\pm}$ (*STIFF SYSTEMS!!!*)
- N IS A BIG NUMBER (*COMPLEXITY!!!*)

THE PHASE-SPACE GEOMETRY…for stiff systems

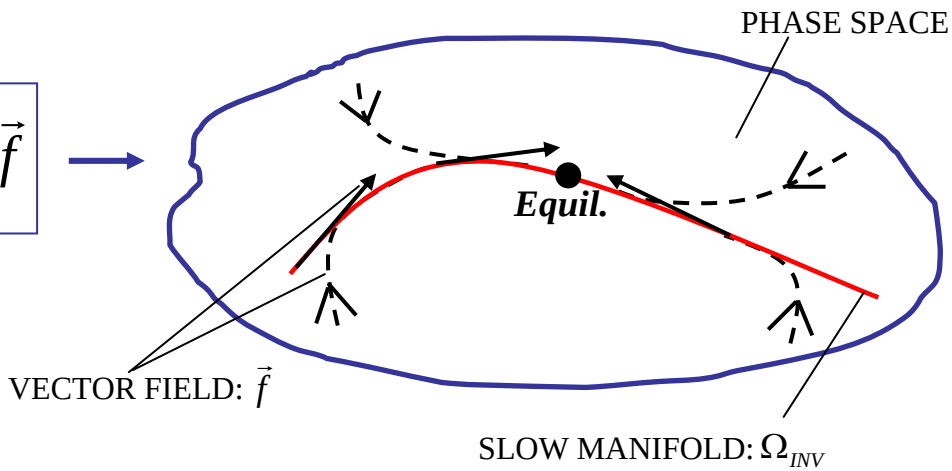
REACTION NETWORK:



MODELING:

$$\frac{d\vec{c}}{dt} = \vec{f}$$

PHASE-SPACE GEOMETRY:



FEATURES OF SLOW MANIFOLDS:

- **INVARIANCE**: THE DYNAMICS TAKES PLACE ON Ω_{INV}
- **SLOWNESS**: EXHAUSTED FAST MOTIONS
- **LOW DIMENSIONALITY**: $M < N$

THE FIST GOAL OF THE REDUCED DESCRIPTION FOR SUCH A SYSTEM IS TO "FILTER" THE SLOW MANIFOLD OUT OF THE INDIVIDUAL TRAJECTORIES!!!

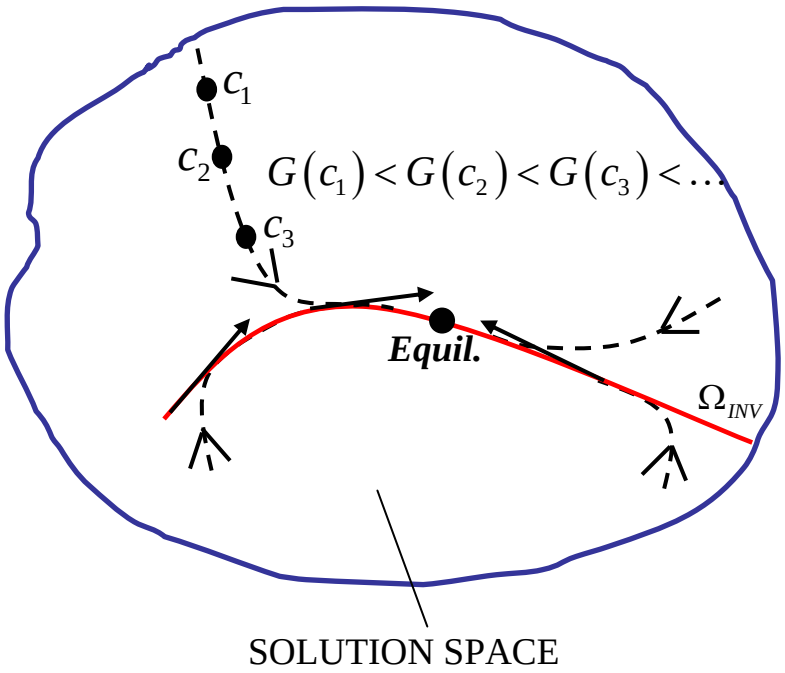
SYSTEM FEATURES

• CLOSED SYSTEM;

• ONE EQUILIBRIUM POINT;

• PURE DISSIPATIVE SYSTEM: A CONVEX *LYAPUNOV FUNCTION* "*G*" SUPPORTS THE SYSTEM.

$$\frac{d\vec{c}}{dt} = \vec{f}, \quad \dot{G} = \left(\nabla G, \vec{f}\right) \le 0$$



NEW SCALAR PRODUCT AND METRICS:

$$H = \frac{\partial^2 G}{\partial c_i \partial c_j}, \quad \left\langle \vec{x}, \vec{y} \right\rangle = \left(\vec{x}, H\vec{y}\right), \quad \left\|\vec{x}\right\| = \left\langle \vec{x}, \vec{x} \right\rangle$$

EXAMPLE: (*V* AND *T* CONSTANT):

BOLTZMANN ENTROPY

$$G = \sum_{i=1}^{N} c_i \left[\ln\left(\frac{c_i}{c_i^{eq}}\right) - 1 \right]$$

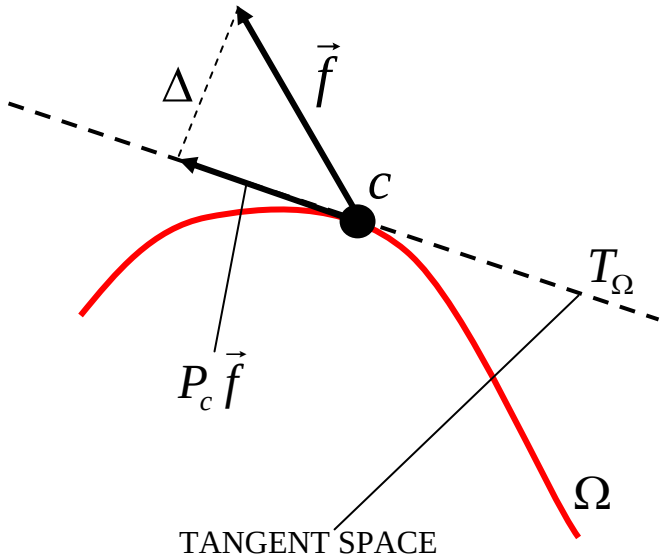
THE INVARIANCE EQUATION

THE INVARIANCE REQUIREMENT FOR THE MANIFOLD Ω

$$\vec{c}\left(t_0\right) \in \Omega \Rightarrow \vec{c}\left(t\right) \in \Omega, \quad \forall t \geq t_0$$

INTRODUCE A *PROJECTOR* OPERATOR ONTO THE *TANGENT SPACE* OF THE MANIFOLD P_c

$$P_c\left(P_c \vec{f}\right) = P_c \vec{f}$$



AN INVARIANT MANIFOLD FULFILLS THE *INVARIANCE EQUATION*: NO *INVARIANCE DEFECT* IN ANY POINT.

INVARIANCE EQUATION

$$\vec{f} - P_c \vec{f} = 0, \quad \forall c \in \Omega$$

INVARIANCE DEFECT

$$\Delta = \vec{f} - P_c \vec{f}$$

THERMODYNAMIC PROJECTOR

THE INVARIANCE EQUATION IS VALID FOR DIFFERENT CHOICES OF "P_c" (Only one requirement: *im(P_c)=tangent space*.), but…

FOR DISSIPATIVE CLOSED SYSTEMS, THE THERMODYNAMIC CONSISTENCY REQUIRES THAT ENTROPY (-G) GROWS MONOTONICALLY FROM THE INITIAL CONDITION TO EQUILIBRIUM:

$$\left(\nabla G, PJ(c)\right) \le 0, \quad \forall c \in \Omega$$

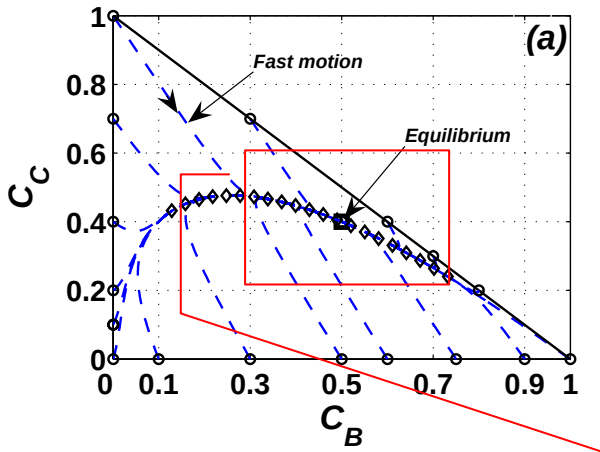
Ref.: A.N. Gorban, I.V.Karlin, *Invariant Manifolds for Physical and Chemical Kinetics, Lect. Notes Phys. 660 (Springer Berlin Heidelberg 2005)*

$$\begin{cases} P_c\vec{x} = P_0\vec{x} + \left(\nabla G, \vec{x}\right)\vec{e}, \quad \vec{e} \in T_\Omega \\ T_{0\Omega} = T_\Omega \cap \ker \nabla G, \quad \left\langle \vec{e}, \vec{y} \right\rangle = 0, \quad \forall \vec{y} \in T_{0\Omega} \\ \left(\nabla G, \vec{e}\right) = 1, \quad P_0 \ orth. \ proj. \ to \ T_{0\Omega} \end{cases}$$

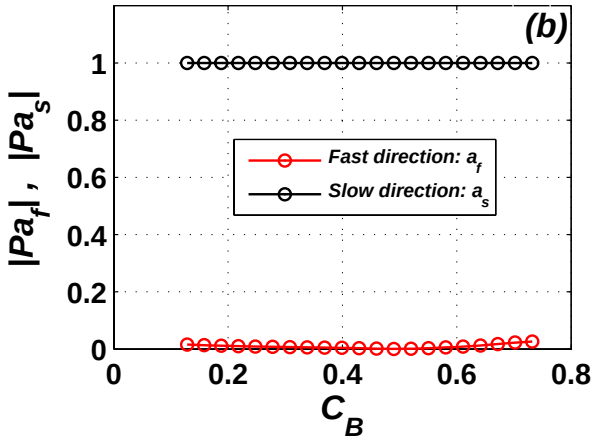
WHY THE THERMODYNAMIC PROJECTOR?

EXAMPLE: THREE-SPECIES FOUR-STEP MECHANISM

Phase space geometry



Jacobian eigenvectors projection



Mechanism

(d)

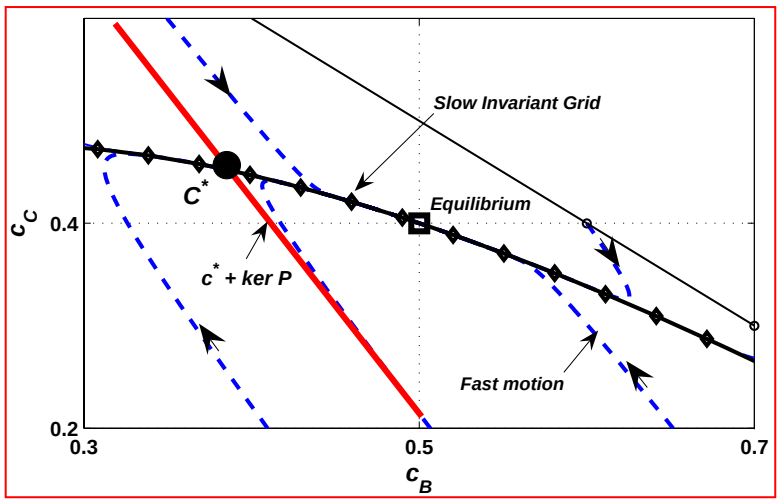
1) $A \Leftrightarrow B$, $k_1^+=1$,

2) $B \Leftrightarrow C$, $k_2^+=1$,

3) $C \Leftrightarrow A$, $k_3^+=1$,

4) $A + B \Leftrightarrow 2C$ $k_4^+=50.$

$C_A + C_B + C_C = const = 1.$



THE THERMODYNAMIC PROJECTOR FOR A 1D MANIFOLD:

$$\begin{cases} P_c\vec{x} = \left(\nabla G, \vec{x}\right)\vec{e} \\ \left(\nabla G, \vec{e}\right) = 1, \quad \vec{e} \in T_\Omega \end{cases}$$

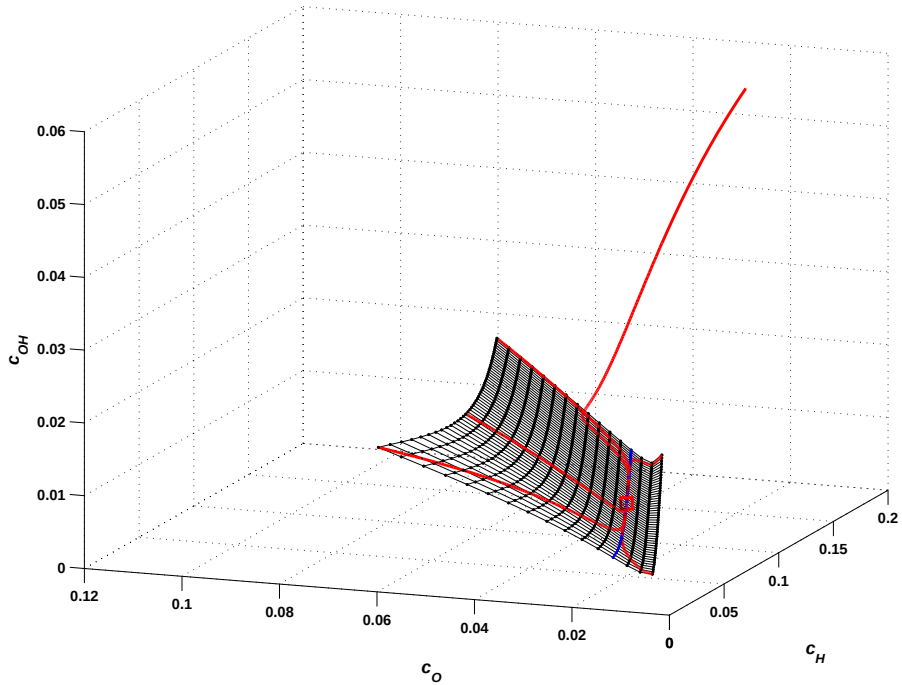
CONSIDER THE TWO EIGENDIRECTION (FAST, SLOW) AT THE SLOW MANIFOLD POINTS:

$$\vec{a}_f\,,\ \vec{a}_s \qquad \left|\vec{a}_f\right| = \left|\vec{a}_s\right| = 1$$

PROPERTIES

$$\begin{cases} 1.\ \vec{a}_f \in \ker\left(P_c\right) \\ 2.\left\langle \mathrm{im}\left(P_c\right), \ker\left(P_c\right)\right\rangle \cong 0 \end{cases}$$

WHY THE THERMODYNAMIC PROJECTOR?

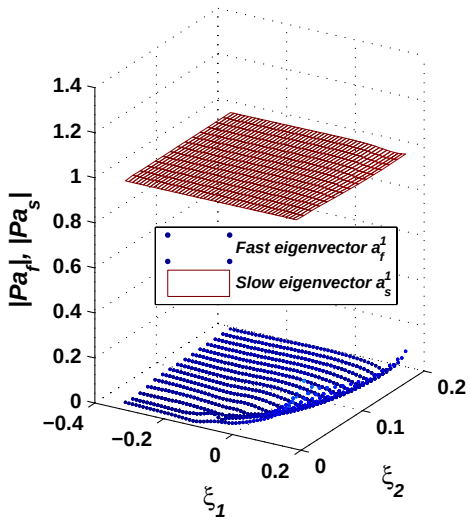


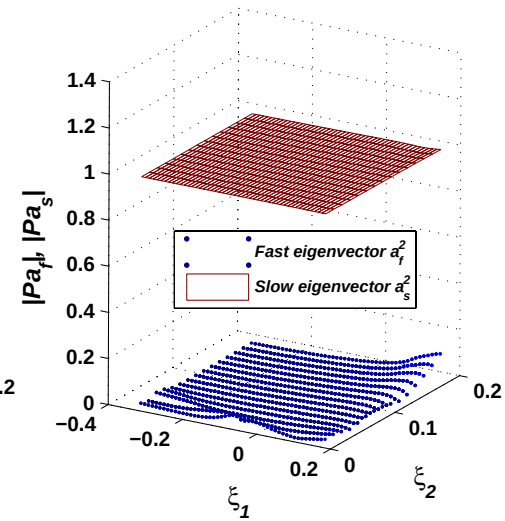
EXAMPLE: HYDROGEN OXIDATION

$$\begin{cases} 1.H_2 \leftrightarrow 2H, \quad k_1^+ = 2, \\ 2.O_2 \leftrightarrow 2O, \quad k_2^+ = 1, \\ 3.H_2O \leftrightarrow H + OH, \quad k_3^+ = 1, \\ 4.H_2 + O \leftrightarrow H + OH, \quad k_4^+ = 10^3, \\ 5.O_2 + H \leftrightarrow O + OH, \quad k_5^+ = 10^3, \\ 6.H_2 + O \leftrightarrow H_2O, \quad k_6^+ = 10^2. \end{cases}$$

$$\begin{cases} \dfrac{d\vec{c}}{dt} = \vec{f} \\ J = \left[\dfrac{\partial f_i}{\partial c_j} \right] \\ G = \sum_{i=1}^{6} c_i \left[\ln\left(\dfrac{c_i}{c_i^{eq}} \right) - 1 \right] \end{cases}$$

$$\begin{cases} P_c \vec{x} = \left\langle \vec{k}, \vec{x} \right\rangle \vec{k} + (\nabla G, \vec{x}) \vec{e}, \\ \vec{k} = T_\Omega \cap \ker \nabla G, \quad \left\| \vec{k} \right\| = 1, \quad \left\langle \vec{k}, \vec{e} \right\rangle = 0, \\ \vec{e} \in T_\Omega, \quad (\nabla G, \vec{e}) = 1. \end{cases}$$

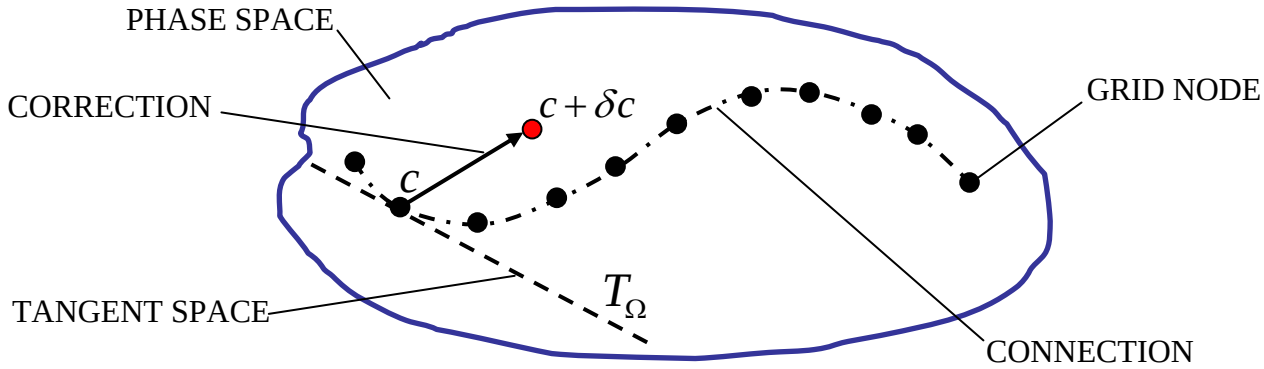




THE METHOD of INVARIANT GRID (MIG)

1) INTRODUCE A NEW OBJECT: ***THE INITIAL GRID***

GRID: SET OF POINTS IN THE PHASE-SPACE + CONNECTION



2) EVALUATE THE DEFECT OF INVARIANCE IN ANY GRID NODE. IN GENERAL $\Delta = \vec{f} - P_c \vec{f} \neq 0$

3) CORRECT THE PREVIOUS GRID SO THAT: $\Delta(c+\delta c) < \Delta(c)$

CORRECTIONS CAN BE FOUND BY SOLVING THE
(INCOMPLETE) LINEARIZED INVARIANCE EQUATION
+
EXTRA CONDITION

$$\begin{cases} [1-P_c]\left[\vec{f} + J(c)\delta c\right] = 0, \quad J = \left[\dfrac{\partial f_i}{\partial c_j}\right] \\ P_c \delta c = 0 \quad \textit{HYPOTHETIC FAST DIRECTION!} \end{cases}$$

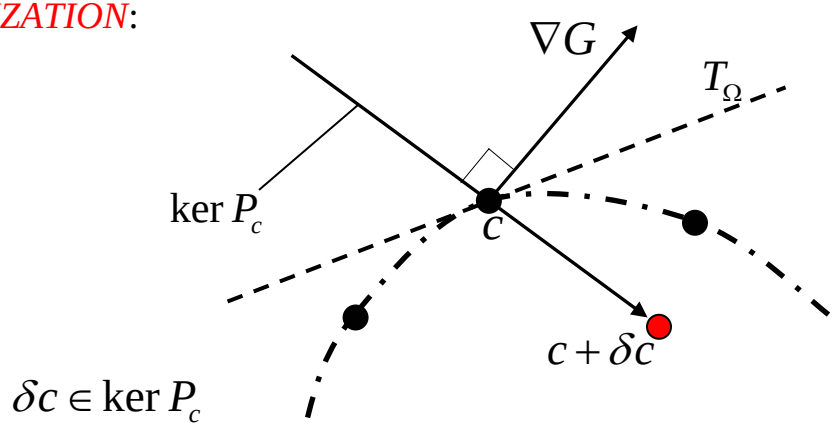
THE METHOD of INVARIANT GRID (MIG)

TWO POSSIBLE PROCEDURES TO FIND CORRECTIONS

1) THE *NEWTON METHOD WITH INCOMPLETE LINEARIZATION*:

$$\begin{cases} [1-P_c]\left[\vec{f} + J(c)\delta c\right] = 0, \quad J = \left[\dfrac{\partial f_i}{\partial c_j}\right] \\ P_c \delta c = 0 \end{cases}$$

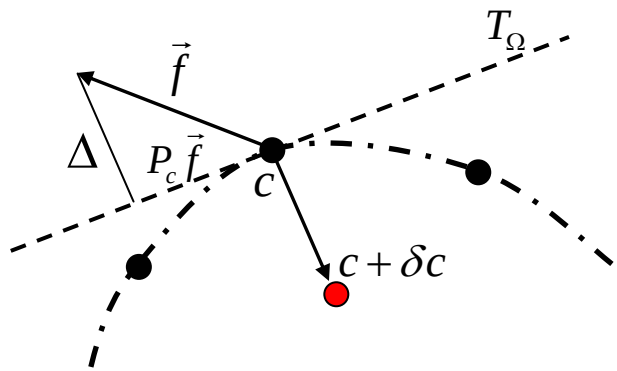
HYPOTHETIC FAST DIRECTION!



$\delta c \in \ker P_c$

2) THE *RELAXATION METHOD*:

$$\delta c = \tau \cdot \Delta, \quad \tau = -\frac{\langle \Delta, \Delta \rangle}{\langle \Delta, J\Delta \rangle}$$



$\delta c \,//\, \Delta$

Ref.: A.N. Gorban, I.V.Karlin, A. Y. Zinovyev, *Invariant grids for reaction kinetics, Physica A 333 106-154 (2004).*

MIG INITIALIZATION

A REASONABLE SLOW MANIFOLD APPROXIMATION IS GIVEN BY THE *Quasi Equilibrium Manifold (QEM)*

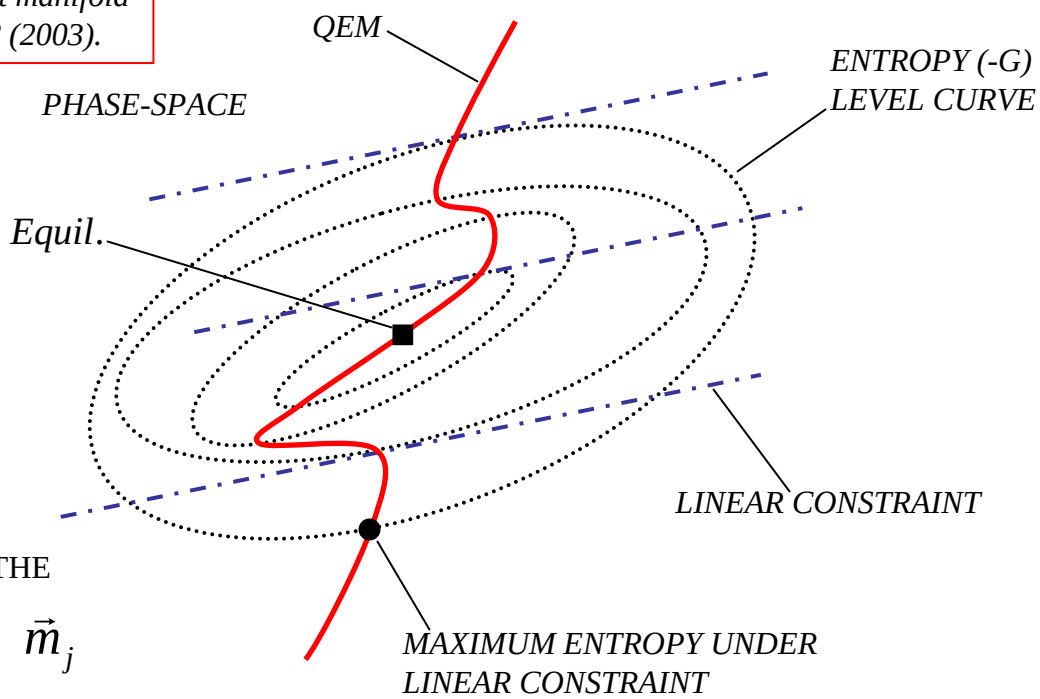
Ref.: A.N. Gorban, I.V.Karlin, *Method of invariant manifold for chemical kinetics, Chem. Eng. Sci. 58 4751-4768 (2003).*

MINIMIZATION PROBLEM:

$$\begin{cases} G = \sum_{i=1}^{N} c_i \left[\ln\left(\frac{c_i}{c_i^{eq}} \right) - 1 \right] \rightarrow \min \\ \left(\vec{d}_j, c \right) = const_j \quad \textit{ATOM BALANCES} \\ \left(\vec{m}_j, c \right) = \xi_j \quad \textit{SLOW VARIABLES} \end{cases}$$

THE QEM IS DEPENDENT ON THE

PARAMETERIZATION VECTORS $\vec{m}_j$



SOLUTION:

LAGRANGE MULTIPLIERS METHOD!!!

SPECIAL CHOICE:

$\vec{m}_j$ SLOW LEFT EIGENVECTORS AT EQUILIBRIUM

↓

SPECTRAL QUASI EQUILIBRIUM MANIFOLD (SQEM)

Ref.: E. Chiavazzo, A. N. Gorban, I. V. Karlin, *Comparison of invariant manifolds for model reduction in chemical kinetics, Comm. In Comput. Physics Vol. 2, No. 5, p. 964-992 (2007).*

QUASI EQUILIBRIUM GRID ALGORITHM

THE SQEM ANALITICAL CONSTRUCTION MAY GET MASSIVE FOR BIG SYSTEMS!!!

EXAMPLE: TWO-STEP FOUR COMPONENT REACTION

$$\begin{cases} A_1 + A_2 \overset{k_1^+=1}{\Leftrightarrow} A_3 \overset{k_2^+=0.4}{\Leftrightarrow} A_2 + A_4 \\ c_{A_1}^{eq} = 0.5;\ c_{A_2}^{eq} = 0.1;\ c_{A_3}^{eq} = 0.1;\ c_{A_4}^{eq} = 0.4 \end{cases}$$

↓ *WRITE MINIMIZATION PROBLEM*

$$\begin{cases} G = \sum_{i=1}^{4} c_{Ai}\left[\ln\left(\frac{c_{Ai}}{c_{Ai}^{eq}}\right) - 1\right] \rightarrow \min \\ c_{A_1} + c_{A_3} + c_{A_4} = 1 \\ c_{A_2} + c_{A_3} = 0.2 \\ c_{A_1} - 1.25 c_{A_4} = \xi \end{cases}$$

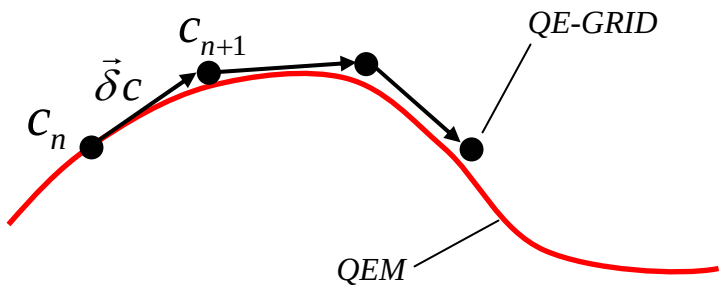
↓ *APPLY LAGRANGE MULTIPLIERS METHOD*

$$\left(\frac{\xi + 1.25 c_{A_4}}{c_{A_1}^{eq}}\right)^{1.25} \left(\frac{c_{A_3}^{eq}\xi + 2.25 c_{A_4} - 0.8}{c_{A_2}^{eq} - \xi - 2.25 c_{A_4} + 1}\right)^{2.25} \frac{c_{A_4}}{c_{A_4}^{eq}} - 1 = 0$$

↓

SOLVE AND GET THE SQEM!!!

ALTERNATIVELY: CONSTRUCT A DISCRETE ANALOG

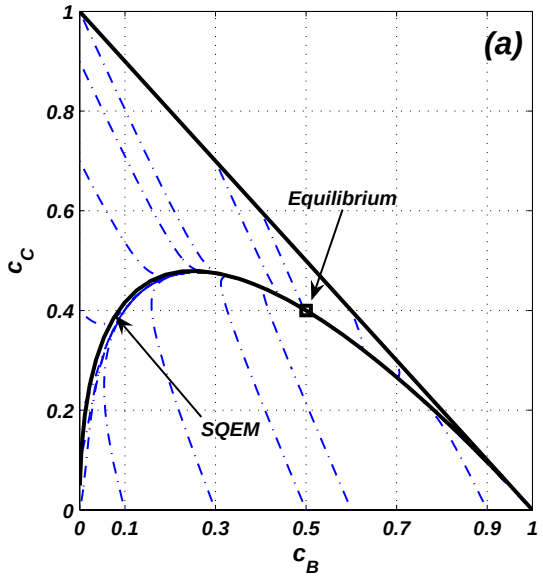


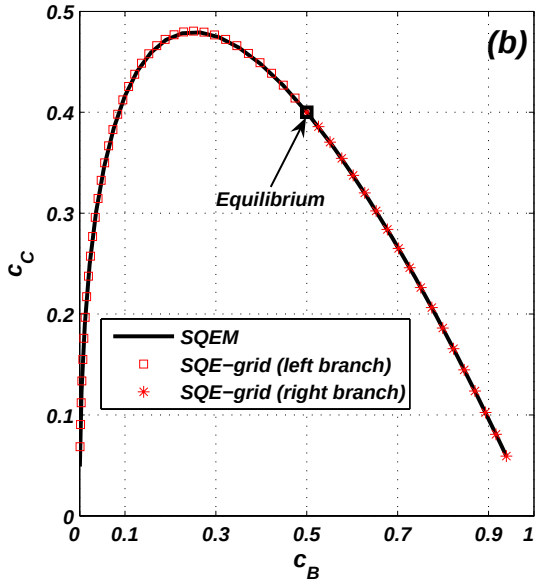
THE *QUASI-EQUILIBRIUM ALGORITHM* IS AN *AUTOMATIC PROCEDURE* THAT PROVIDES A SET OF NODES CLOSE TO THE QEM.

THE QE-GRID IS CHARACTERIZED BY THE PARAMETER:

$$\varepsilon = \left|c_{n+1} - c_n\right| = \left|\vec{\delta}c\right|$$

QE-MANIFOLD VS QE-GRID





THE ANALITICAL PROCEDURE DELIVERS:

$$\left(\frac{0.3072+0.7867\xi-0.518\phi}{0.1}\right)^{-0.518}\left(\frac{0.6928-0.7867\xi-0.482\phi}{0.5}\right)^{-0.482}\left(\frac{\phi}{0.4}\right)-1=0$$

THE QE-ALGORITHM:

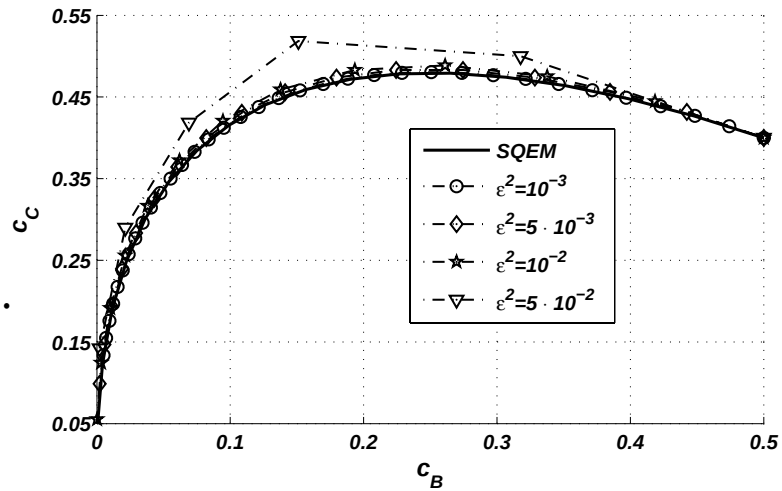
$$\begin{cases}\langle \vec{t},\vec{\rho}_1\rangle \mu_1+\langle \vec{t},\vec{\rho}_2\rangle \mu_2=0\\ \mu_1^2+\mu_2^2=\varepsilon^2\end{cases}$$

WITH SOME FIXED VECTORS: $\vec{t}$, $\vec{\rho}_1$, $\vec{\rho}_2$

EXAMPLE: FOUR-STEP THREE-COMPONENT REACTION. CLOSED SYSTEM (V,T=*const*) AND:

$$G=\sum_{i=1}^{3} c_i\left[\ln\left(\frac{c_i}{c_i^{eq}}\right)-1\right]$$

$$\begin{cases}1.A\leftrightarrow B, & k_1^+=1,\\ 2.B\leftrightarrow C, & k_2^+=1,\\ 3.C\leftrightarrow A, & k_3^+=1,\\ 4.A+B\leftrightarrow 2C, & k_4^+=50.\end{cases}$$



Ref.: E. Chiavazzo, I. V. Karlin, *Quasi Equilibrium Grid Algorithm: geometric construction for model reduction, arXiv: 0704.2317, (2007).*

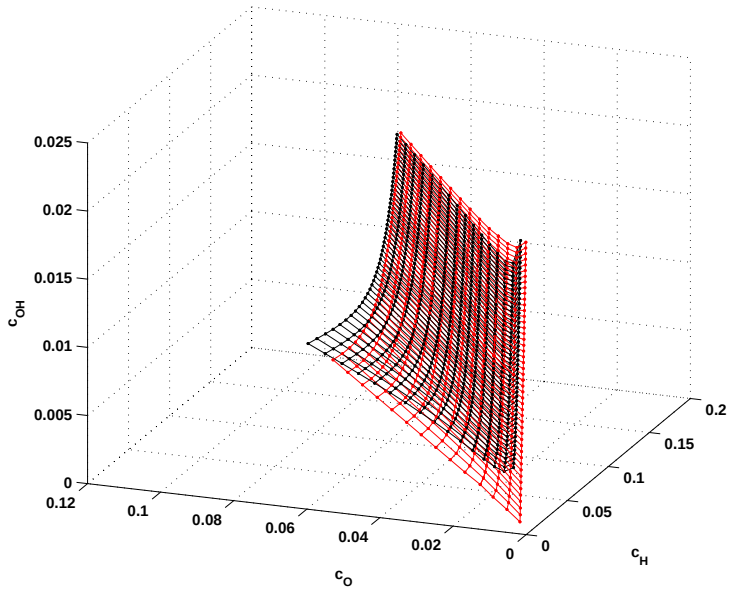
QEG-ALGORITHM: some more examples

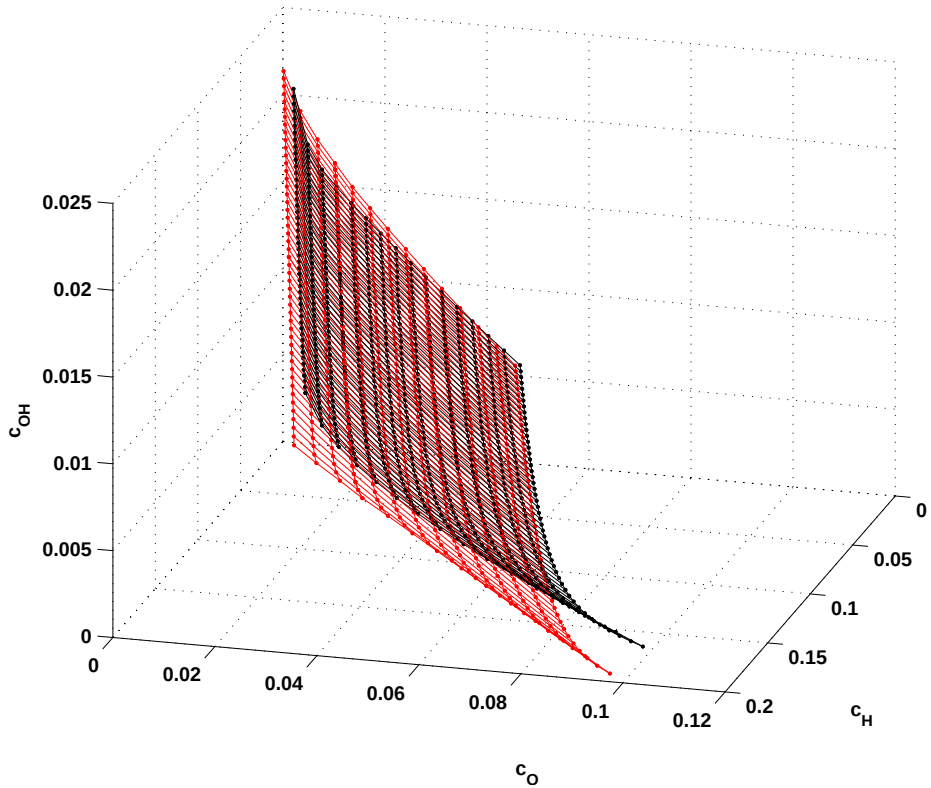
HYDROGEN OXIDATION: SIX-STEP SIX-COMPONENT REACTION. CLOSED SYSTEM (V,T=*const*)

$$\begin{cases} 1.H_2 \leftrightarrow 2H, \quad k_1^+ = 2, \\ 2.O_2 \leftrightarrow 2O, \quad k_2^+ = 1, \\ 3.H_2O \leftrightarrow H + OH, \quad k_3^+ = 1, \\ 4.H_2 + O \leftrightarrow H + OH, \quad k_4^+ = 10^3, \\ 5.O_2 + H \leftrightarrow O + OH, \quad k_5^+ = 10^3, \\ 6.H_2 + O \leftrightarrow H_2O, \quad k_6^+ = 10^2. \end{cases}$$

$$\begin{cases} \dfrac{d\vec{c}}{dt} = \vec{f} \\ J = \left[\dfrac{\partial f_i}{\partial c_j} \right] \\ G = \sum_{i=1}^{6} c_i \left[\ln\left(\dfrac{c_i}{c_i^{eq}} \right) - 1 \right] \end{cases}$$

COMPARISON BETWEEN THE *INVARIANT GRID* (BLACK DOTS) AND THE *SQEG* (RED DOTS)





LI, ZHAO, KAZAKOV, DRYER MECHANISM

1. $H + O_2 \leftrightarrow O + OH$
2. $O + H_2 \leftrightarrow H + OH$
3. $H_2 + OH \leftrightarrow H_2O + H$
4. $O + H_2O \leftrightarrow OH + OH$
5. $H_2 + N_2 \leftrightarrow H + H + N_2$
6. $O + O + N_2 \leftrightarrow O_2 + N_2$
7. $O + H + N_2 \leftrightarrow OH + N_2$
8. $H + OH + N_2 \leftrightarrow H_2O + N_2$
9. $H + O_2 \left(+N_2\right) \leftrightarrow HO_2 \left(+N_2\right)$
10. $HO_2 + H \leftrightarrow H_2 + O_2$
11. $HO_2 + H \leftrightarrow OH + OH$
12. $HO_2 + O \leftrightarrow O_2 + OH$
13. $HO_2 + OH \leftrightarrow H_2O + O_2$
14. $HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2$
15. $HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2$
16. $H_2O_2 \left(+N_2\right) \leftrightarrow OH + OH \left(+N_2\right)$
17. $H_2O_2 + H \leftrightarrow H_2O + OH$
18. $H_2O_2 + H \leftrightarrow HO_2 + H_2$
19. $H_2O_2 + O \leftrightarrow OH + HO_2$
20. $H_2O_2 + OH \leftrightarrow HO_2 + H_2O$
21. $H_2O_2 + OH \leftrightarrow HO_2 + H_2O$

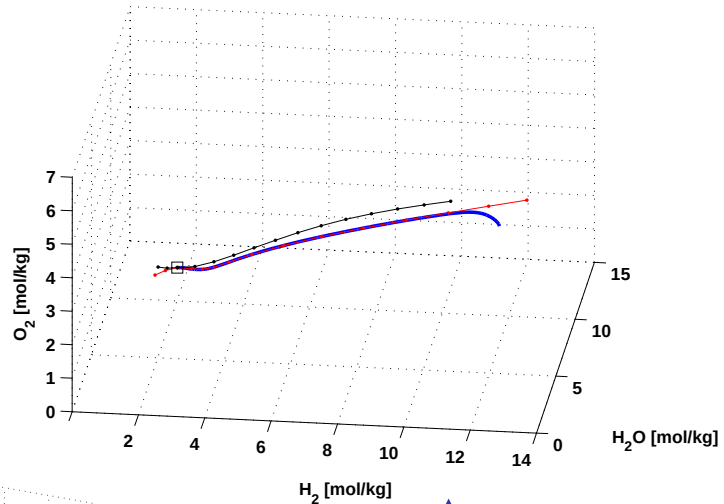
Ref.: J. Li, Z. Zhao, A. Kazakov, F. L. Dryer: *International Journal of Chemical Kinetics, Vol. 36, p. 566-575, 2004.*

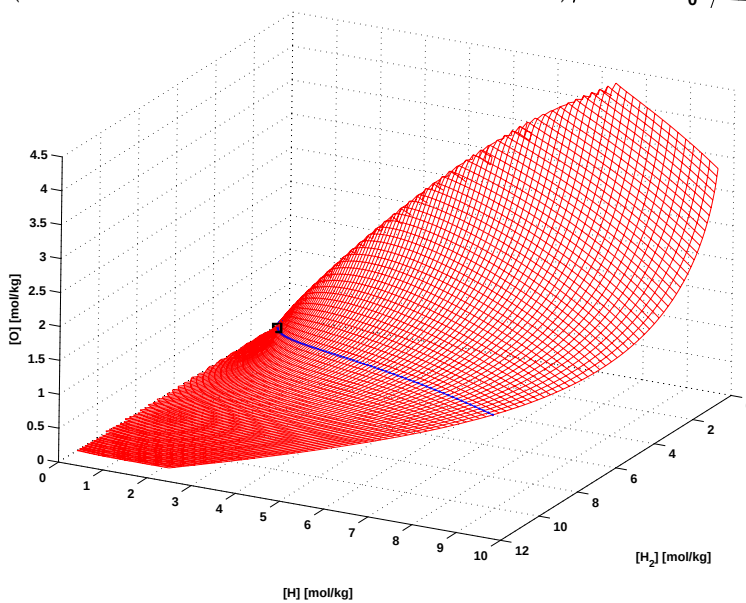
SETUP: CLOSED SYSTEM UNDER CONSTANT DENSITY AND ENERGY.

$$\begin{cases} \rho = 4.58\ kg/m^3 \\ e = 1.28\ MJ/kg \end{cases}$$

CHEMKIN COLLECTION 3.7.1

$$G = \left(\sum_{i=1}^{9} \left(S_i^0(T) - R \ln X_i - R \ln \left(P / P_{atm} \right) \right) X_i \right) \Big/ \bar{W}$$





1D SQEG (BLACK), 1D INVARIANT GRID (RED), SOLUTION TRAJECTORY (BLU)

2D SQEG

QEG-ALGORITHM WITHOUT ENTROPY

CHAIN BRANCHING MODEL:

$$\begin{cases} R \to C, k_i \\ C + R \to P + \alpha C, k_p \\ C \to P, k_t \end{cases}$$

$$\begin{cases} x = \dfrac{c_R}{c_R^0} \\ y = c_C \dfrac{k_p}{k_i} \\ \varepsilon = c_R^0 \dfrac{k_i}{k_p} \\ \gamma = c_R^0 \dfrac{k_t}{k_p} \end{cases}$$

$\Longleftrightarrow$

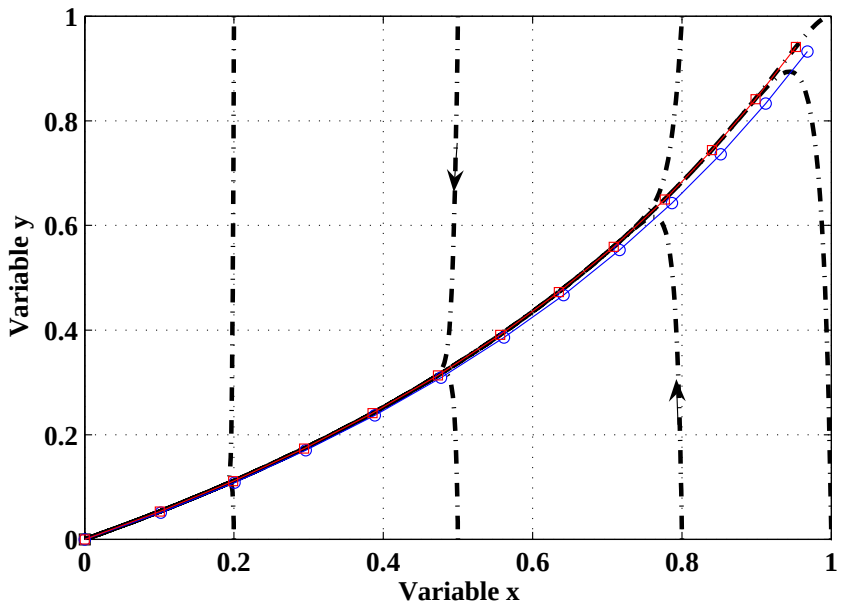
$$\begin{cases} \dot{x} = -x - xy = f_x \\ \dot{y} = \dfrac{1}{\varepsilon}\left[x + (\alpha - 1) xy - \gamma y \right] = f_y \end{cases}$$

Ref.: **F.A.Williams**, *Combustion Theory, (1985), 2nd ed., App. B. 2.5.3, page 520.*

$$\vec{f} = \left[f_x, f_y \right], \vec{z} = [x, y] \Rightarrow E = \left(\vec{f}, \vec{f} \right)$$

SOLUTION TRAJECTORIES (BLACK), THE MANIFOLD OF MINIMA OF E (BLUE), ONE RELAXATION ITERATION (RED).

$\Longleftrightarrow$



$$\begin{cases} E = \left(\vec{f}, \vec{f} \right) \to \min \\ \left(\vec{m}, \vec{z} \right) = \xi \end{cases}$$

$\vec{m}$

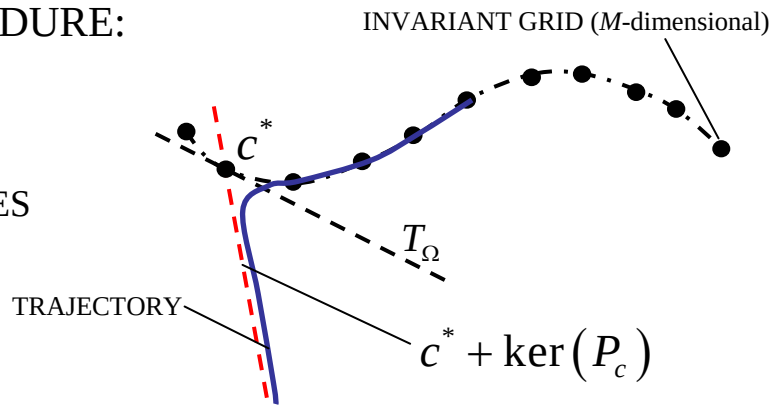
Left slow eigenvector of the Jacobian at the equilibrium

***THE IDEA**: THE MAGNITUDE OF THE VECTOR FIELD DECAYS ALONG THE FAST MOTIONS…*

A POSTERIORI PARAMETERIZATION

AVAILABLE INFO AFTER THE REFINEMENT PROCEDURE:

1) A SET OF NODES IN THE PHASE-SPACE
2) APPROXIMATE TANGENT SPACE AT THE GRID NODES
3) THERMODYNAMIC PROJECTOR P_c



FULL SYSTEM:

$$\begin{cases} \dfrac{d\vec{c}}{dt} = \vec{f} \\ \vec{c}(t_0) = \vec{c}_0 \end{cases} \longleftrightarrow \begin{cases} \begin{bmatrix} \dot{c}_1 \\ \vdots \\ \dot{c}_N \end{bmatrix} = \begin{bmatrix} f_1 \\ \vdots \\ f_N \end{bmatrix} \\ \vec{c}(t_0) = \vec{c}_0 \end{cases}$$

CHOOSE M SLOW VECTORS: $\vec{m}^i = \left[m_1^i, \ldots, m_N^i \right]$

INTRODUCE M NEW VARIABLES:

$$\xi^i = \sum_{j=1}^{N} m_j^i c_j, \quad \forall i = 1, \ldots, M$$

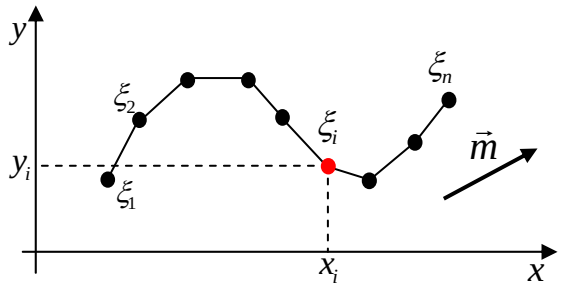
REDUCED SYSTEM:

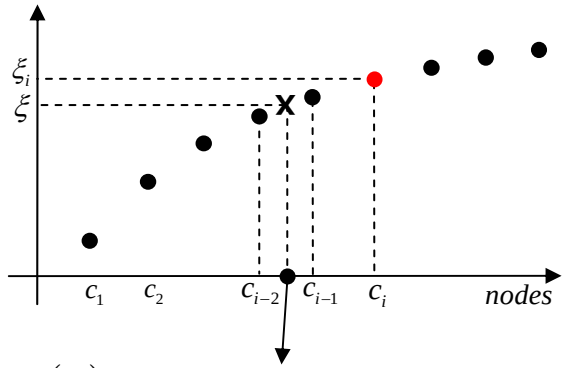
$$\begin{bmatrix} \dot{\xi}^1 \\ \vdots \\ \dot{\xi}^M \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{N} m_j^1 \left(P_c \vec{f} \right)_j \\ \vdots \\ \sum_{j=1}^{N} m_j^M \left(P_c \vec{f} \right)_j \end{bmatrix} = RHS(c_1, \ldots, c_N) \longrightarrow \begin{bmatrix} c_1 \\ \vdots \\ c_N \end{bmatrix} \Leftrightarrow L.U.T. \Leftrightarrow \begin{bmatrix} \xi^1 \\ \vdots \\ \xi^M \end{bmatrix}$$

A LINK BETWEEN REDUCED VARIABLES AND PRIMITIVE ONES CAN BE ESTABLISHED VIA *L.U.T.*.

WHEN DOES IT WORK?

$$\begin{bmatrix} c_1 \\ \vdots \\ c_N \end{bmatrix} \Rightarrow \begin{bmatrix} \xi^1 \\ \vdots \\ \xi^M \end{bmatrix}$$





$$\begin{cases} c_i = [x_i, y_i] & \textit{PRIMITIVE VARIABLES} \\ \xi_i = (c_i, \vec{m}) & \textit{REDUCED VARIABLE} \end{cases}$$

I.E. USE SOME LAGRANGIAN WEIGHTS: $c(\xi) = w_{i-2}c_{i-2} + w_{i-1}c_{i-1} + w_i c_i$

THE MAPPING NEEDS TO BE *UNIQUE* AND HAS TO DO WITH THE PARAMETERIZATION VECTOR: $\vec{m}$

A REASONABLE WAY TO CHOOSE THAT VECTORS IS GIVEN BY THE *SQEM* PARAMETERIZATION:

$$\left\{ \vec{m}^1_{SQEG}, \ldots, \vec{m}^M_{SQEG} \right\} \longrightarrow$$

THE *M* SLOWEST LEFT EIGENVECTORS OF JACOBIAN AT THE EQUILIBRIUM POINT

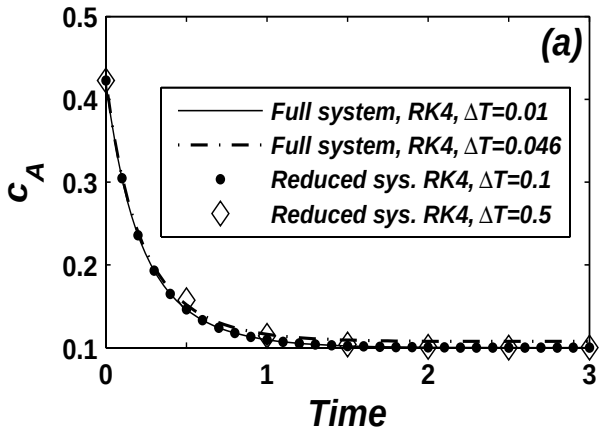
INTEGRATION ON A 1D GRID

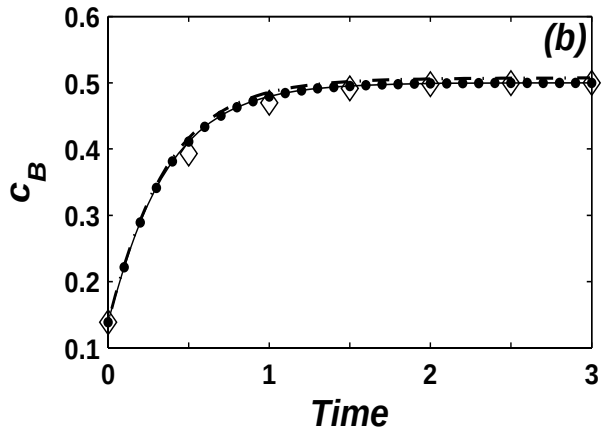
EXAMPLE: FOUR-STEP THREE-COMPONENT REACTION. CLOSED SYSTEM (V,T=*const*):

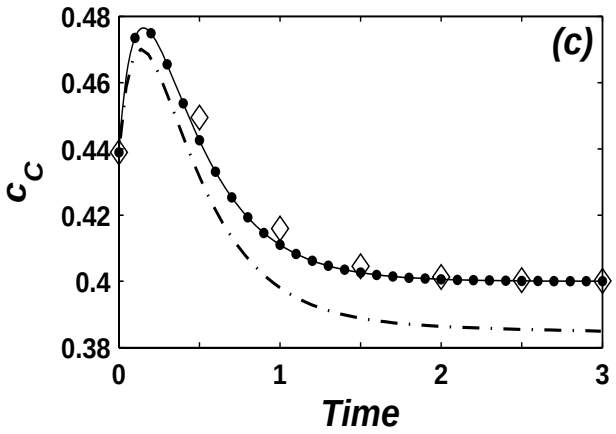
$$\begin{cases} 1.A \leftrightarrow B, \quad k_1^+ = 1, \\ 2.B \leftrightarrow C, \quad k_2^+ = 1, \\ 3.C \leftrightarrow A, \quad k_3^+ = 1, \\ 4.A + B \leftrightarrow 2C, \quad k_4^+ = 50. \end{cases}$$

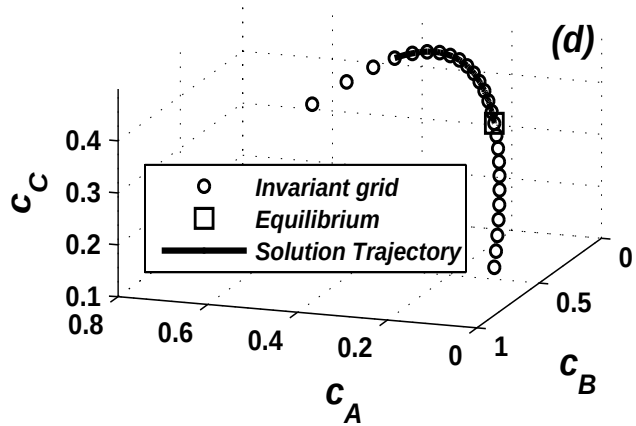
FULL SYSTEM vs REDUCED SYSTEM:

TIME INTEGRATION BY STARTING FROM AN INVARIANT GRID NODE



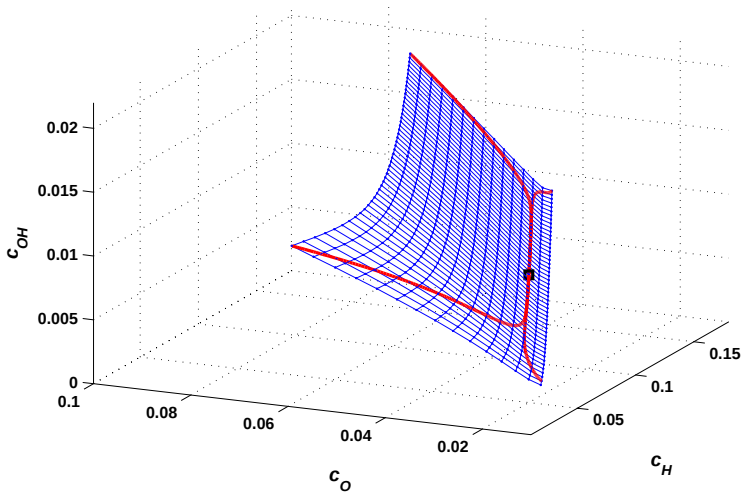




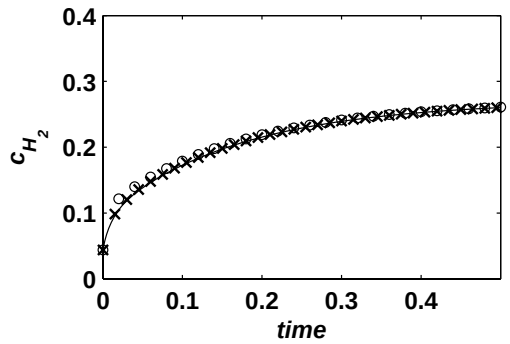


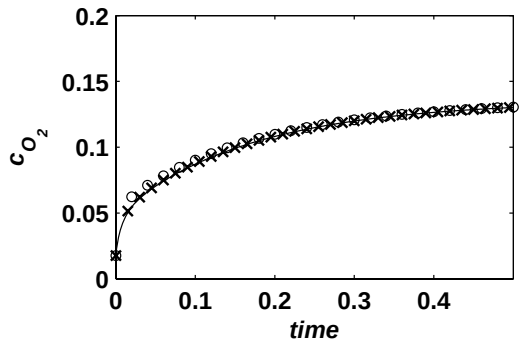
INTEGRATION ON A 2D GRID

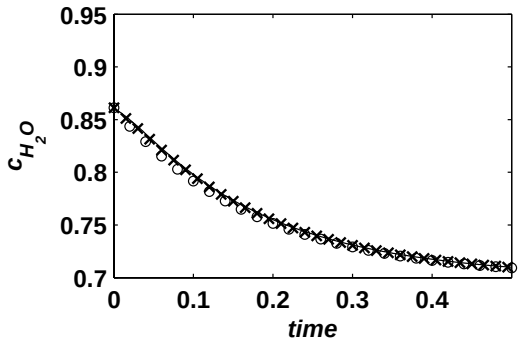
$$\begin{cases} 1.H_2 \leftrightarrow 2H, \quad k_1^+ = 2, \\ 2.O_2 \leftrightarrow 2O, \quad k_2^+ = 1, \\ 3.H_2O \leftrightarrow H + OH, \quad k_3^+ = 1, \\ 4.H_2 + O \leftrightarrow H + OH, \quad k_4^+ = 10^3, \\ 5.O_2 + H \leftrightarrow O + OH, \quad k_5^+ = 10^3, \\ 6.H_2 + O \leftrightarrow H_2O, \quad k_6^+ = 10^2. \end{cases}$$

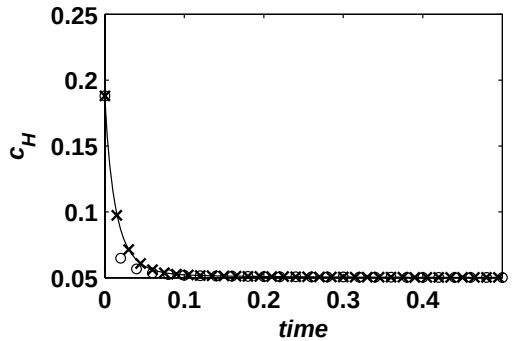


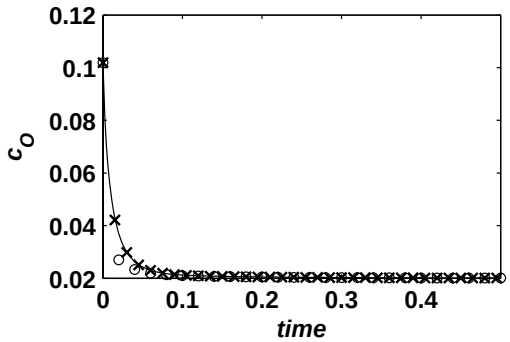
$$\begin{cases} \Delta T = 5 \cdot 10^{-4} \rightarrow \textit{full sys}, RK4(\textit{continuous line}) \\ \Delta T = 1.5 \cdot 10^{-2} \rightarrow \textit{red sys}, RK4(\textit{crosses}) \\ \Delta T = 2 \cdot 10^{-2} \rightarrow \textit{red sys}, RK4(\textit{circles}) \end{cases}$$

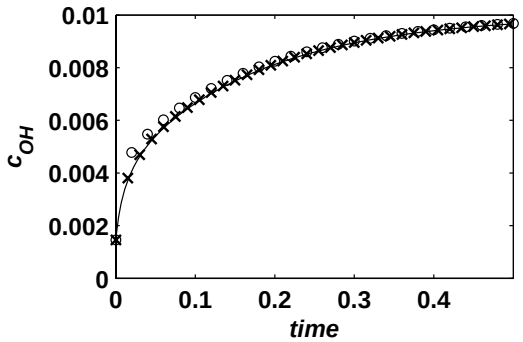






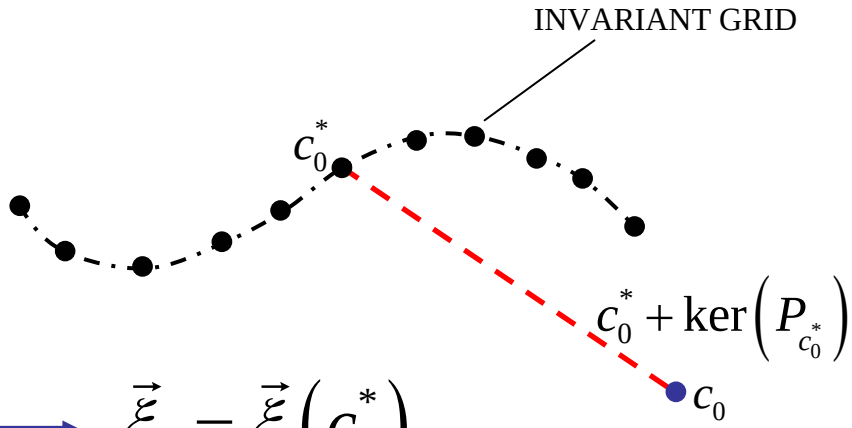






INITIAL CONDITION ISSUE

$$\begin{cases} \dfrac{d\vec{c}}{dt} = \vec{f} \\ \vec{c}\left(t_0\right) = \vec{c}_0 \end{cases} \Rightarrow \begin{cases} \dfrac{d\vec{\xi}}{dt} = \left(\vec{m}, P_c\,\vec{f}\right) \\ \vec{\xi}_0 = ? \end{cases}$$



THE INITIAL CONDITION, IN THE REDUCED SYSTEM, CAN BE FOUND BY EXPLOITING THE THERMODYNAMIC PROJECTOR:

$$\vec{\xi}_0 = \vec{\xi}\left(c_0^*\right)$$

EXAMPLE: FOUR-STEP THREE-COMPONENT REACTION. CLOSED SYSTEM (V,T=*const*):

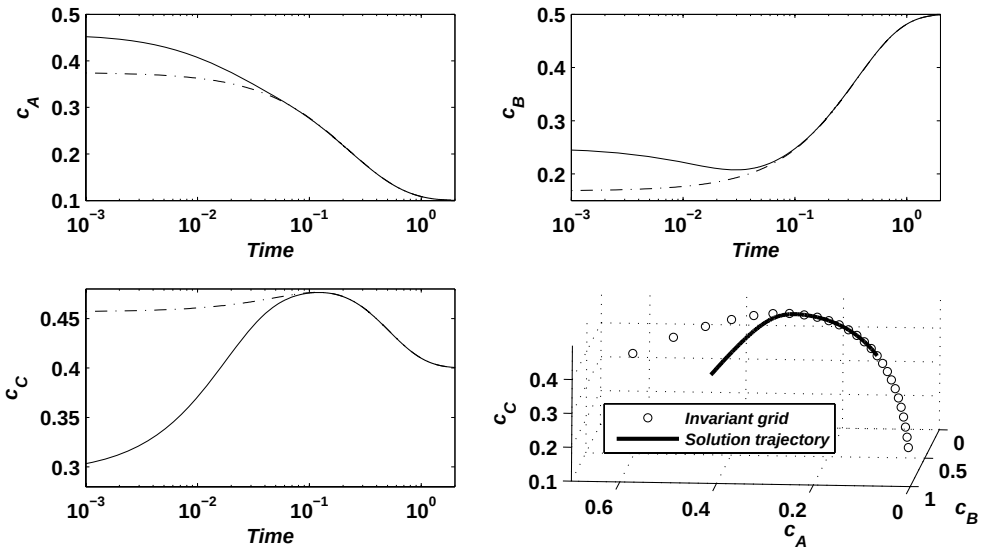
TAKE A GRID NODE:

$$c^* = \left[0.375, 0.168, 0.457\right]$$

THE FAST AFFINE SUBSPACE IS:

$$c_0 = c^* + \alpha\vec{g}_1\left(c^*\right) \quad \vec{g}_1 \equiv \ker P_c$$

$\alpha = 0, \quad \alpha = -0.2$



FINDING REDUCED INITIAL CONDITIONS

IMPLICIT EQUATION TO SOLVE:

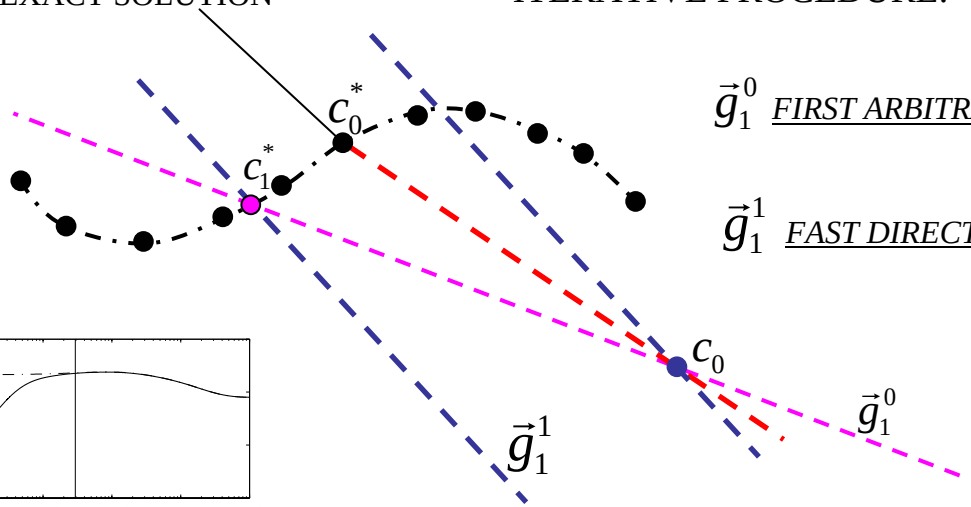
$$c_0 = c^* + \alpha \vec{g}_1\left(c^*\right)$$

UNKNOWN:

$$c^* = c^*\left(c_0\right)$$

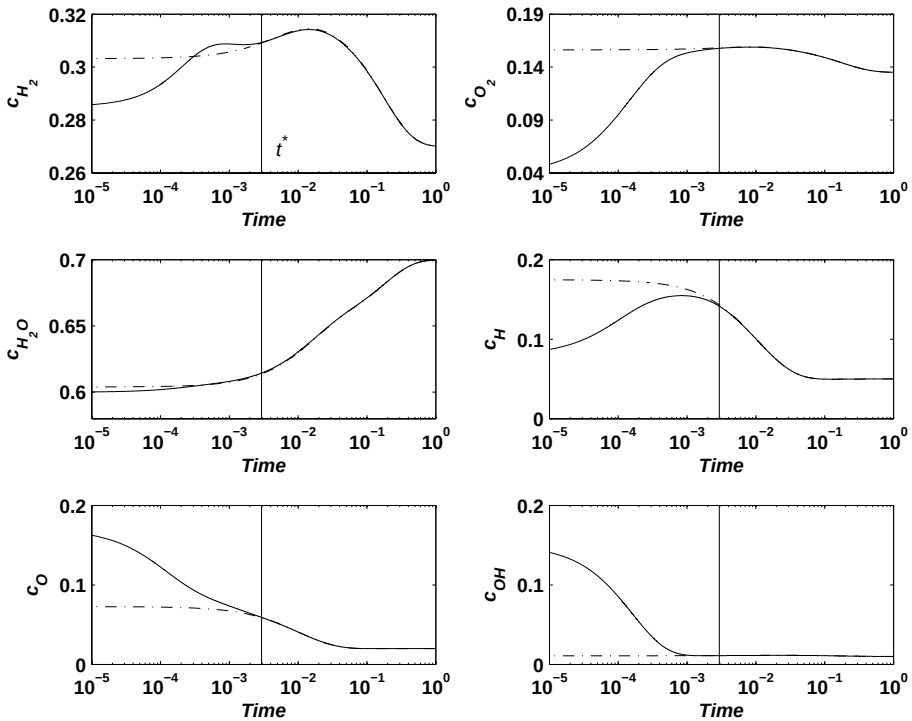
EXACT SOLUTION

ITERATIVE PROCEDURE:



$\vec{g}_1^0$ *FIRST ARBITRARY DIRECTION*

$\vec{g}_1^1$ *FAST DIRECTION IN* c_1^*



TAKE AN EXTERNAL POINT :

$$c_0 = \left[0.285, 0.04, 0.6, 0.08, 0.17, 0.15\right]$$

AFTER THREE ITERATIONS:

$$c^* = \left[0.303, 0.156, 0.604, 0.175, 0.0726, 0.0109\right]$$

Ref.: E. Chiavazzo, I. V. Karlin, *Model reduction through Invariant Grids, preprint (2007).*

CONCLUSIONS

1. *THE INVARIANT GRID APPROXIMATION WAS USED IN ORDER TO DESCRIBE THE INVARIANT MANIFOLD (SLOW SUBSPACE) FOR DISSIPATIVE SYSTEM (WITH LYAPUNOV FUNCTION).*

2. *THE FAST SUBSPACE IS CONSTRUCTED VIA THERMODYNAMIC PROJECTOR, ONCE THE REFINEMENT PROCEDURE (MIG) IS TERMINATED.*

3. *THE QUASI-EQUILIBRIUM ALGORITHM REVEALS TO BE A USEFUL TOOL IN CONSTRUCTING AN APPROXIMATE INVARIANT GRID AND INITIALIZE THE REFINEMENT PROCEDURE.*

4. *AN "A POSTERIORI" PARAMETERIZATION ALLOWS TO EXPLOIT THE INVARIANT GRID IN ORDER TO INTEGRATE THE REDUCED SYSTEM.*

5. *THE INITIAL CONDITION IN THE REDUCED SYSTEM CAN BE FOUND BY USING THE FEATURE OF THE THERMODYNAMIC PROJECTOR.*

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THANKS FOR YOUR ATTENTION!!!