Automatic Compact Modelling for MEMS: Applications, Methods and Tools

Lecture 4:
Advanced Topics in Model Reduction

Evgenii B. Rudnyi, Jan G. Korvink

http://www.imtek.uni-freiburg.de/simulation/mor4ansys/

IMTEK

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Outline

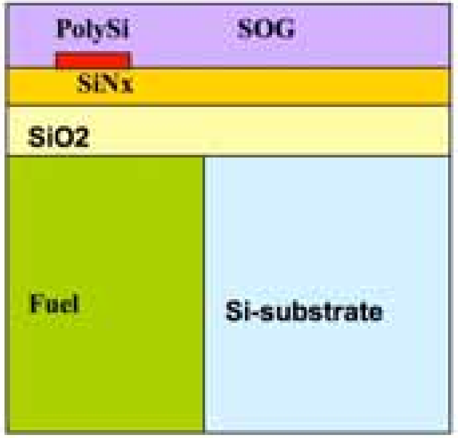
- Parametric model reduction
- Coupling reduced models with each other
- SVD-Krylov
- Nonlinear model reduction

ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

Boundary Condition Independent

$$q_{\perp} = h(T - T_{bulk})$$

- Film coefficients are not known in advanced:
  - ✓Mixed boundary conditions.



$$E\dot{\mathbf{T}}(t) + (K + \sum_i h_i K_{m,i})\mathbf{T}(t) = \mathbf{f}u(t)$$

- 2004, Dr Feng, postdoc
- Award of Krupp's foundation to research in Germany.

ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

Formal Problem Statement

- **Given:**
  - ✓A system of ODEs.
  - ✓System matrices contain parameters.
  - ✓May include a second-order derivative.

$$E\dot{\mathbf{x}} + K\mathbf{x} = F\mathbf{u}$$

$$E = E_0 + \sum_i q_i E_i$$

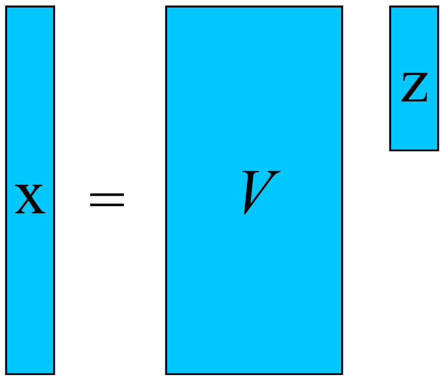
$$K = K_0 + \sum_i p_i K_i$$

- **Find:**
  - ✓Low-dimensional approximation (projection subspace).
  - ✓Preserve parameters in the symbolic form.

$$\mathbf{x} = V\mathbf{z} + \varepsilon$$

Projection is Working

$$\mathbf{x} = V\mathbf{z} + \varepsilon$$



$$V^T E V \dot{\mathbf{z}} + V^T K V \mathbf{z} = V^T F \mathbf{u}$$

$$V^T E V = V^T E_0 V + \sum_i q_i V^T E_i V$$

$$V^T K V = V^T K_0 V + \sum_i p_i V^T K_i V$$

- **Projection should not depend on parameters.**
- **Parameters are preserved.**

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Multivariate Expansion

- Moment matching for both *s* and parameters

- Weile (Illinois, 1999, 2001)
  - ✓Two parameters.
- Daniel (MIT, 2004)
  - ✓Generalization to many parameters.
- Gunupudi (Carleton, 2002)
  - ✓Independent discovery.

$$E\dot{\mathbf{x}} + K\mathbf{x} = \mathbf{f}\mathbf{u}$$

$$H(s) = \{sE + K\}^{-1}\mathbf{f}$$

$$H(s) = \sum_{0}^{\infty} m_i (s - s_0)^i$$

$$m_i = m_{i,red}, \quad i = 0, \ldots, r$$

$$H(s, p_i) = \{sE + K_0 + \sum_i p_i K_i\}^{-1}\mathbf{f}$$

$$H(s, p_i) = \sum_{0}^{\infty} m_{ij\ldots} (s - s_0)^i (p_1 - p_{1,0})^j \ldots$$

Theory, Daniel 2004

$$
\begin{aligned}
x &= \left[I - (\tilde{s}_1 M_1 + \cdots + \tilde{s}_p M_p)\right]^{-1} B_M u = \sum_{m=0}^{\infty} \left[\tilde{s}_1 M_1 + \cdots + \tilde{s}_p M_p\right]^m B_M u \\
&= \sum_{m=0}^{\infty} \sum_{k_2=0}^{m-(k_3+\cdots+k_p)} \cdots \sum_{k_{p-1}=0}^{m-k_p} \sum_{k_p=0}^{m} \left[F^m_{k_2,\ldots,k_p}(M_1,\ldots,M_p) B_M u\right] \tilde{s}_1^{m-(k_2+\cdots+k_p)} \tilde{s}_2^{k_2} \cdots \tilde{s}_p^{k_p}
\end{aligned}
\tag{23}
$$

$$
F^m_{k_2,\ldots,k_p}(M_1,\ldots,M_p) = \begin{cases} 0, & \text{if } k_i \notin \{0,1,\ldots,m\} i = 2,\ldots,p \\ 0, & \text{if } k_2 + \cdots + k_p \notin \{0,1,\ldots,m\} \\ I, & \text{if } m = 0 \\ M_1 F^{m-1}_{k_2,\ldots,k_p}(M_1,\ldots,M_p) + M_2 F^{m-1}_{k_2-1,\ldots,k_p}(M_1,\ldots,M_p) + \cdots & \\ \quad \cdots + M_p F^{m-1}_{k_2,\ldots,k_p-1}(M_1,\ldots,M_p) & \end{cases}
\tag{24}
$$

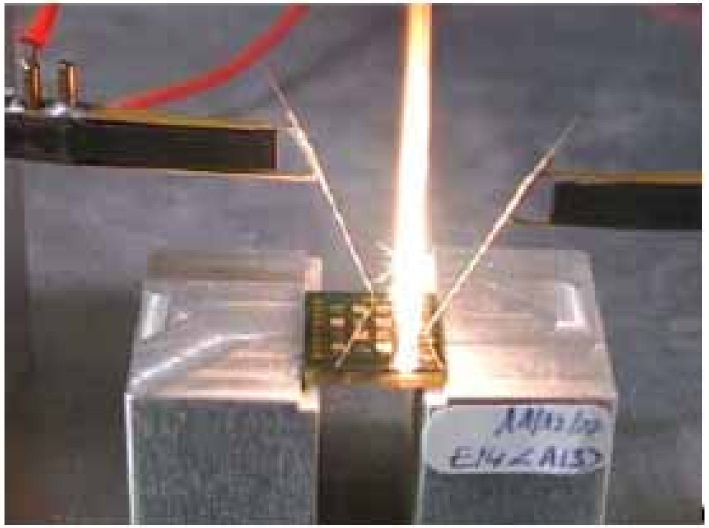
$$
\begin{aligned}
\operatorname{colspan}(V) &= \operatorname{span}\left\{b_M, M_1 b_M, M_2 b_M, \ldots, M_p b_M, M_1^2 b_M, (M_1 M_2 + M_2 M_1) b_M, \ldots,\right. \\
&\qquad \left.(M_1 M_p + M_p M_1) b_M, M_2^2 b_M, (M_2 M_3 + M_2 M_3) b_M, \ldots\right\}, \qquad (25) \\
&= \operatorname{span}\left\{ \bigcup_{m=0}^{m_q} \bigcup_{k_2=0}^{m-(k_p+\cdots+k_3)} \cdots \bigcup_{k_{p-1}=0}^{m-k_p} \bigcup_{k_p=0}^{m} F^m_{k_2,\ldots,k_p}(M_1,\ldots,M_p) b_M \right\}. \qquad (26)
\end{aligned}
$$

$$
\begin{aligned}
&\hat{F}^m_{k_2,\ldots,k_p}\left[-\left(V^T \hat{E}_0 V\right)^{-1} V^T \hat{E}_1 V, \ldots, -\left(V^T \hat{E}_0 V\right)^{-1} V^T \hat{E}_p V\right] \left(V^T \hat{E}_0 V\right)^{-1} V^T b \\
&= V^T F^m_{k_2,\ldots,k_p}\left[-\hat{E}_0^{-1} \hat{E}_1, \ldots, -\hat{E}_0^{-1} \hat{E}_p\right] \hat{E}_0^{-1} b.
\end{aligned}
\tag{27}
$$

- **It is necessary to modify the algorithm:**
Direct use of moments is numerically unstable.

Case Study: Film Coefficient

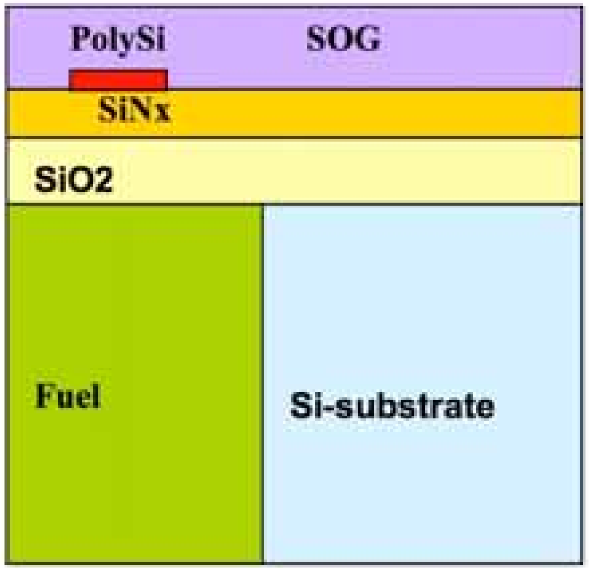
- EU FP 5 FET Project: Microthruster array.



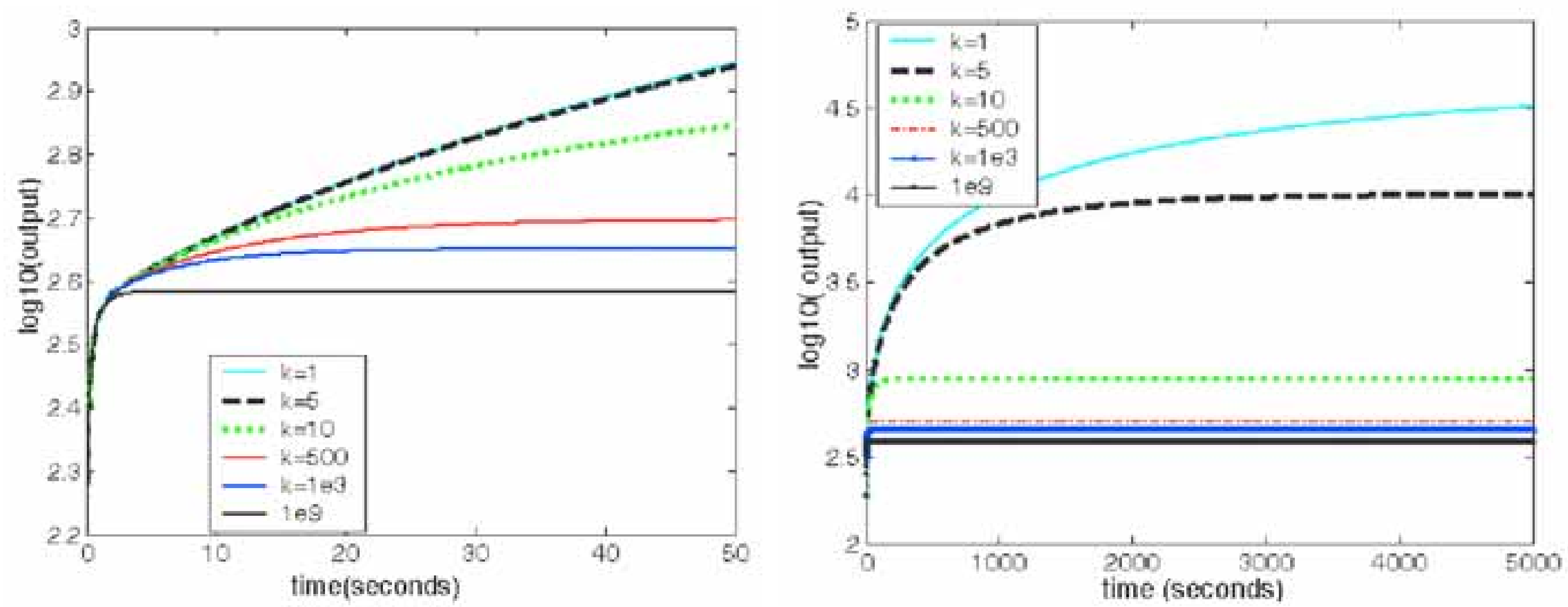
- Goal is different with IC.
- Mathematics is similar.

$$E\dot{\mathbf{T}}(t) + (K + hK_m)\mathbf{T}(t) = \mathbf{f}u(t)$$

- 2D-axisymmetrical model, 4257 equations.
- Film coefficient to change from 1 to 10^9.



Heater Temperature for Full Model



log$_{10}$(T) vs. time, left is the enlarged part of the right figure.

- **Error norm for a reduced model:**

$$error = \left\{ \sum_{i=1}^{n} (T_i - \hat{T}_i)^2 / \sum_{i=1}^{n} T_i^2 \right\}^{1/2}$$

Conventional Projection

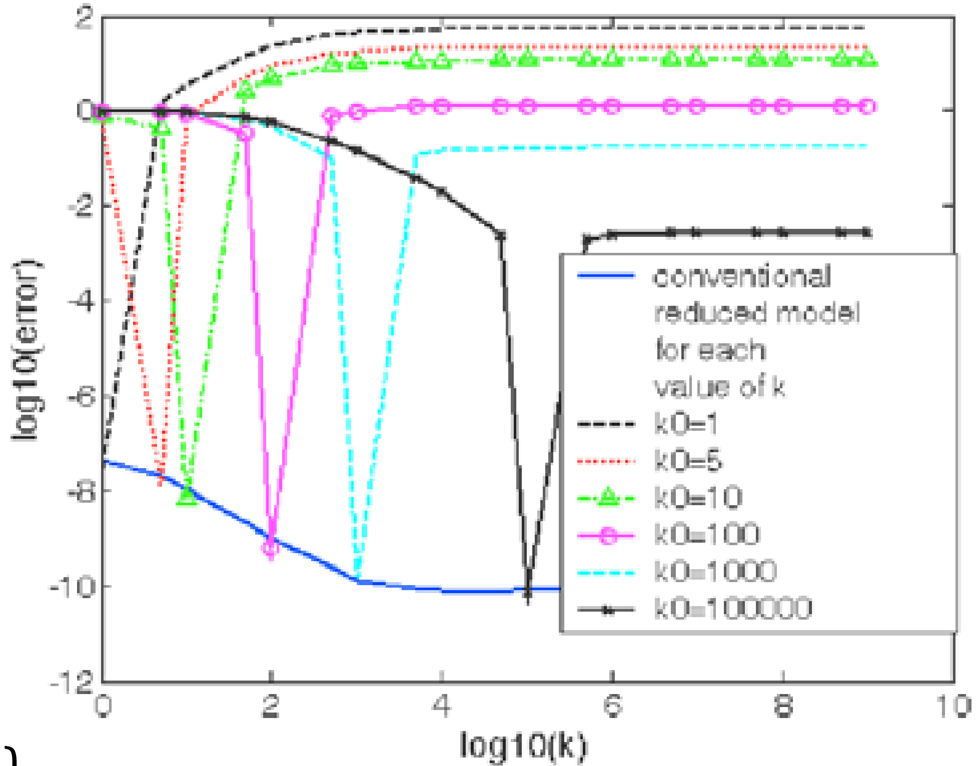
- Moment matching for the transfer function

$$H(s) = \{sE + K + hK_m\}^{-1}\mathbf{f}$$

- Projection is the basis of the Krylov subspace

$$\Im\left\{(K + hK_m)^{-1}E, (K + hK_m)^{-1}\mathbf{f}\right\}$$

must be constant



full - 4257, reduced - 20

$$error = \left\{\sum_{i=1}^{n}(T_i - \hat{T}_i)^2 / \sum_{i=1}^{n} T_i^2\right\}^{1/2}$$

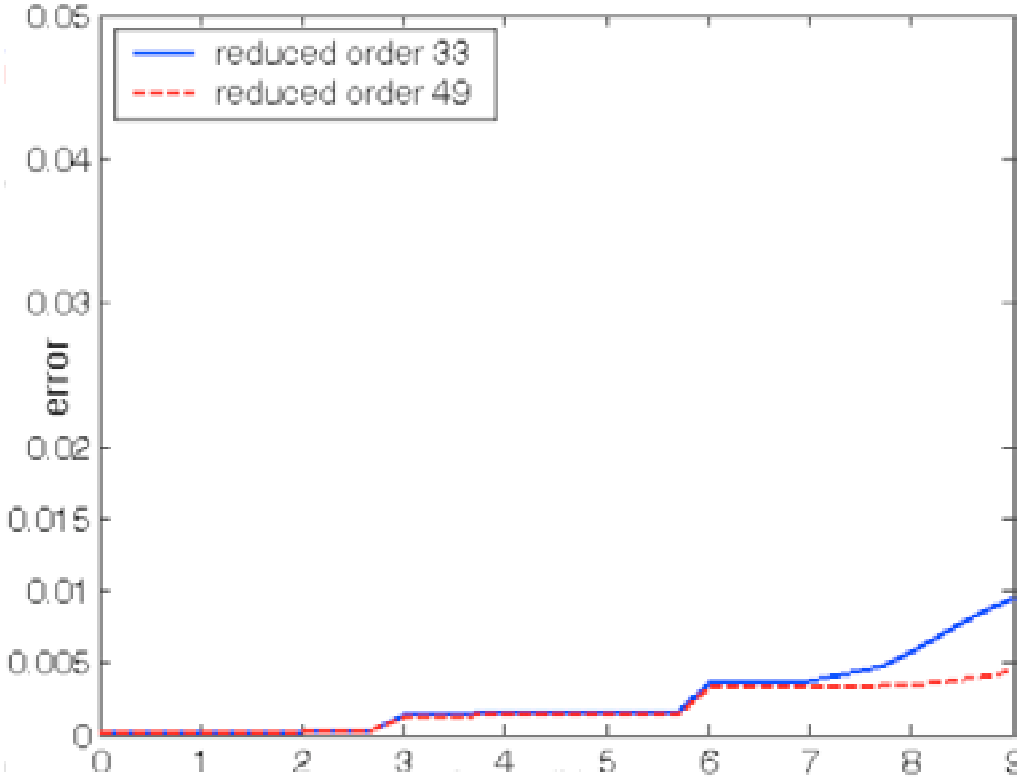
ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Multivariate Expansion

- **Moment matching for both *s* and *h***

$$H(s) = \{sE + K + hK_m\}^{-1}\mathbf{f}$$

- **Numerically stable method from Ms Feng.**



1838 IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, VOL. 24, NO. 12, DECEMBER 2005

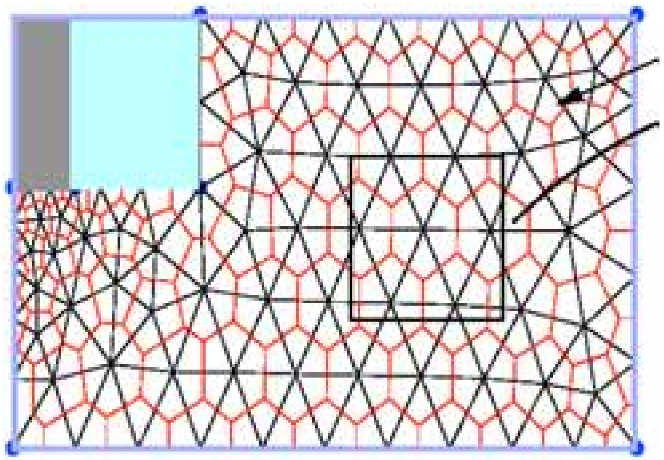
Preserving the Film Coefficient as a Parameter in the Compact Thermal Model for Fast Electrothermal Simulation

Lihong H. Feng, *Associate Member, IEEE*, Evgenii B. Rudnyi, and Jan G. Korvink

Case Study: Electrochemistry

$$E\dot{c}(t) + [K + \sum_i s_i(U(t))K_i]c(t) = \mathbf{f}$$

- **Scanning Electrochemical Microscopy:**
  - ✓high resolution imaging of chemical reactivity;
  - ✓topography of various interfaces;
  - ✓emphasis on biological systems;
  - ✓nano-patterning.
- **Convection can be neglected.**
- **Diffusion equation.**
- **Buttler-Volmer equation:**
  - ✓Mixed boundary conditions.



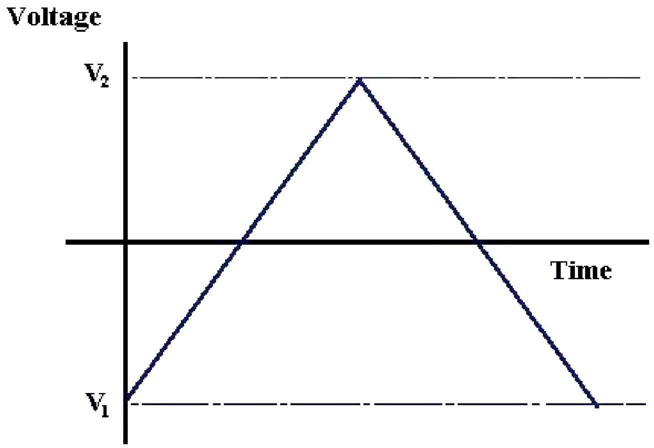
$$Ox + e^- \underset{k_b}{\overset{k_f}{\Leftrightarrow}} Red \qquad dc_1/dt = D_1 \cdot \nabla^2 c_1$$

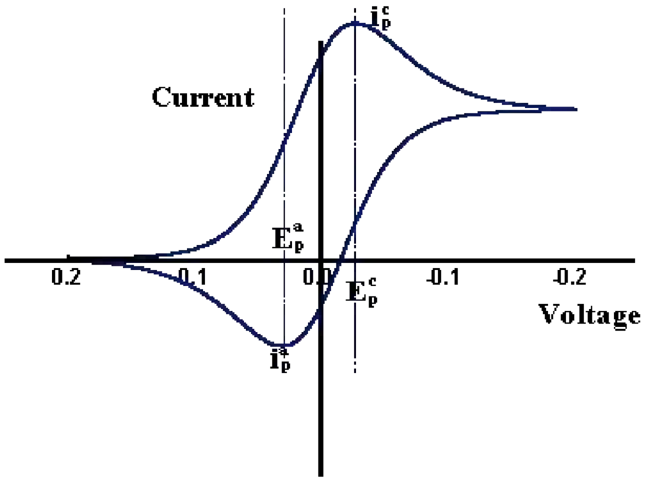
$$j = k_{Ox} \cdot c_{Ox} - k_{\mathrm{Re}d} \cdot c_{\mathrm{Re}d}$$

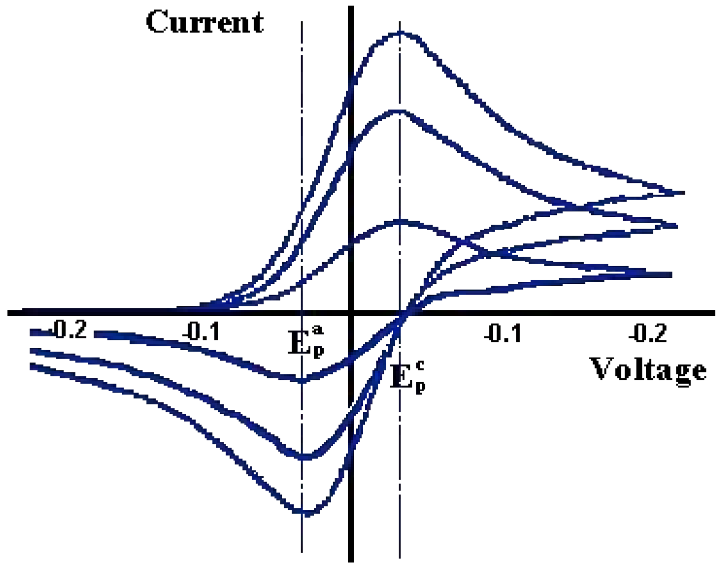
$$k_{Ox} = k^0 e^{\left(\frac{\alpha z F U}{RT}\right)}$$

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Cyclic Voltammetry: Voltammogram

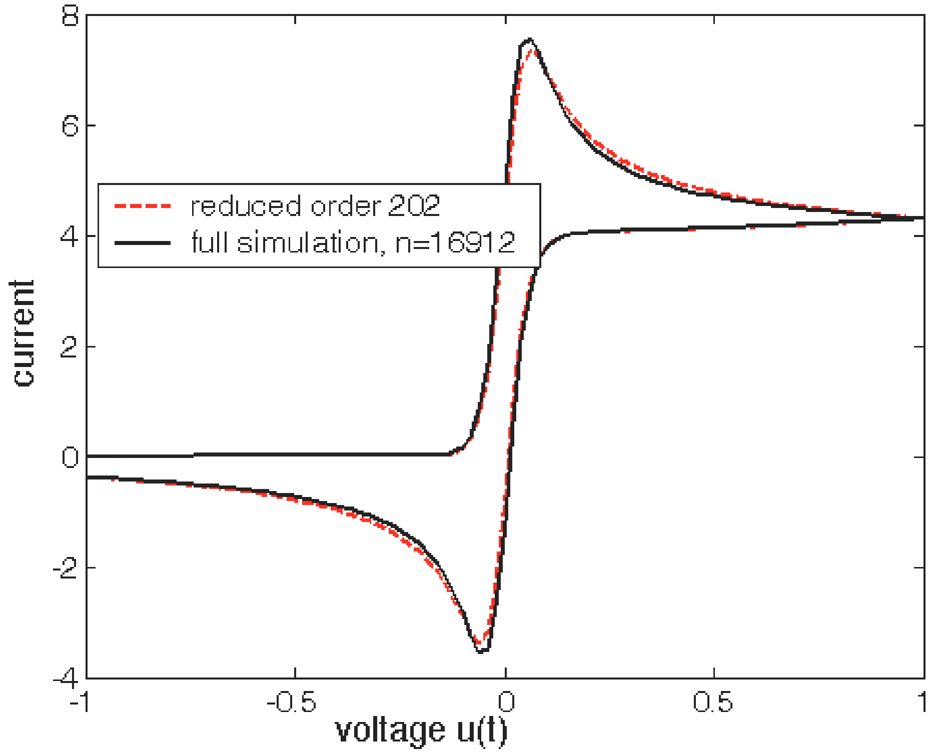




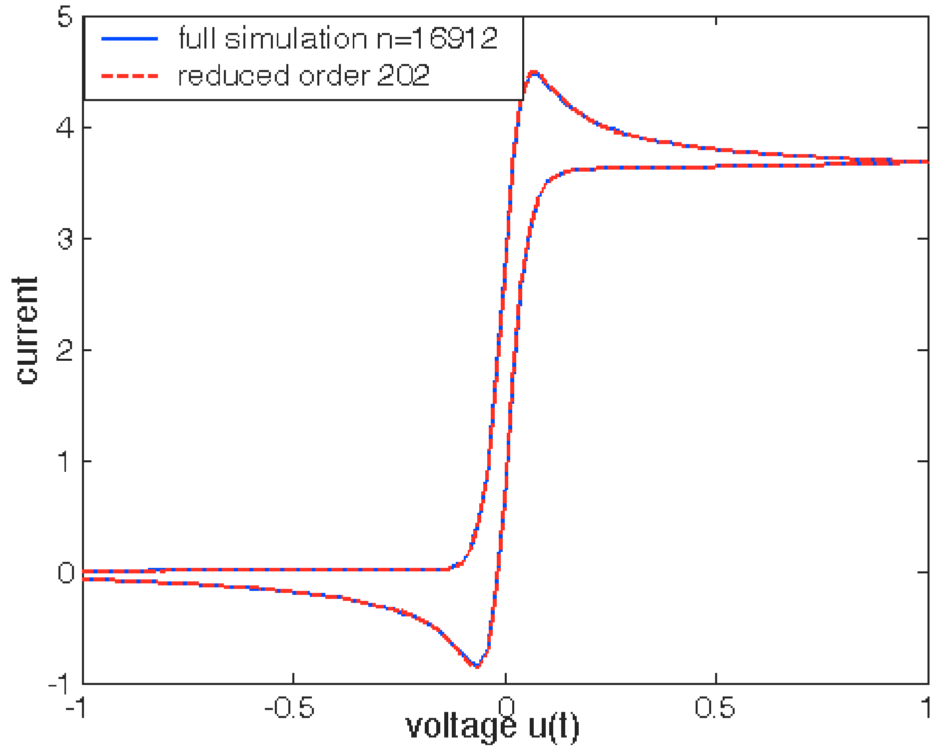


•http://www.cartage.org.lb/en/themes/Sciences/Chemistry/Electrochemis/Electrochemical/CyclicVoltammetry/CyclicVoltammetry.htm

Results I

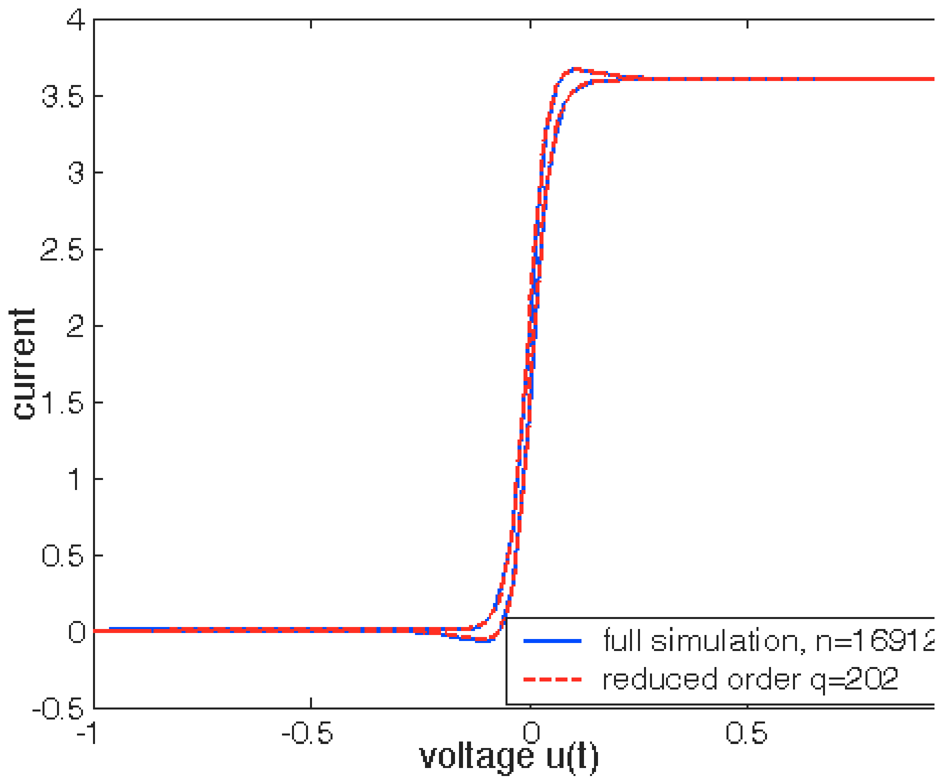


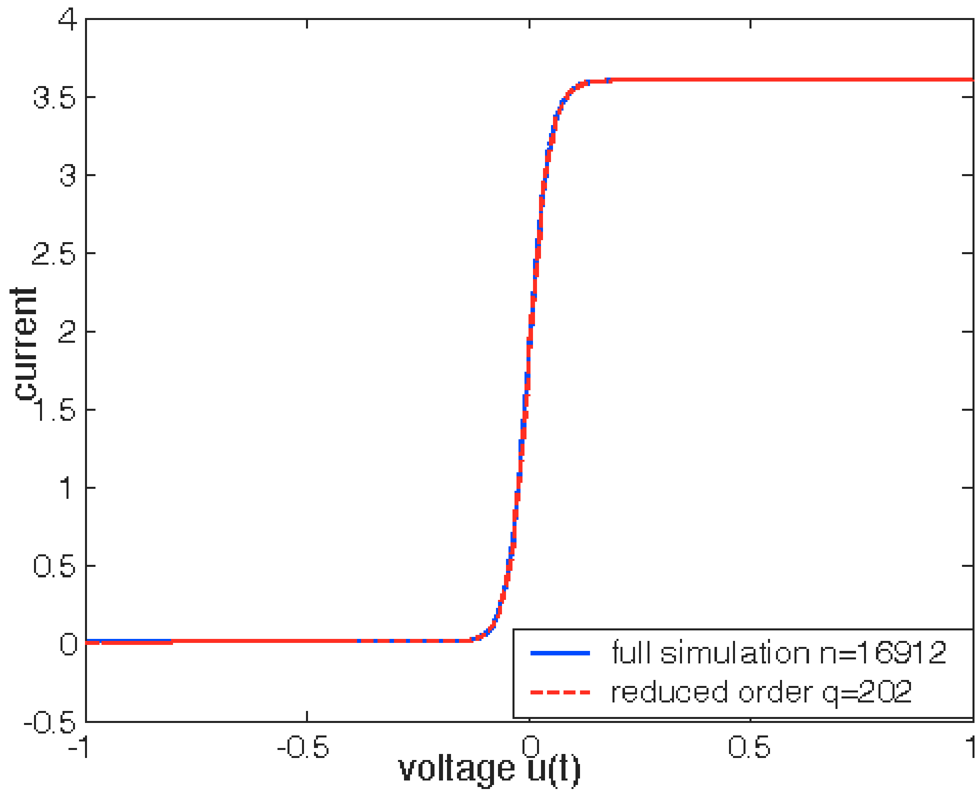
$$du/dt = \pm 0.5$$



$$du/dt = \pm 0.05$$

Results II





$du/dt = \pm 0.005$

$du/dt = \pm 0.0005$

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Problems to Solve

- **Main practical problem is the explosion of the number of mixed moments:**
  - ✓Choosing the maximum order of derivatives and generate all moments does not work.
- **Do we need the same number of moments for time and parameters?**
- **How to choose the number and type of moments automatically?**

- **Preserve four parameters:**
  - ✓Five parameters in the Laplace domain.
- **All first derivatives:**
  - ✓6 moments.
- **All second derivatives:**
  - ✓21 moments.
- **All third derivatives:**
  - ✓56 moments.
- **All forth derivatives:**
  - ✓126 moments.

A Way to Proceed

- **Simplest solution:**
  - ✓Ignore the mixed moments.
  - ✓First used by Nakhla's group.
- **Then a number of subspaces to generate = 1 + number of parameters.**
- **Local Error Control to choose the number of moments along each variable.**

$$E\dot{\mathbf{x}} + \left(K_0 + \sum_i p_i K_i\right)\mathbf{x} = \mathbf{f}\mathbf{u}$$

$$H(s, p_i) = \{sE + K_0 + \sum_i p_i K_i\}^{-1}\mathbf{f}$$

$$\partial^k H / \partial s^k$$

$$s\,(time): \quad V_s = \Im(K_0^{-1}C_0, K_0^{-1}F)$$

$$\partial^k H / \partial p_i^k$$

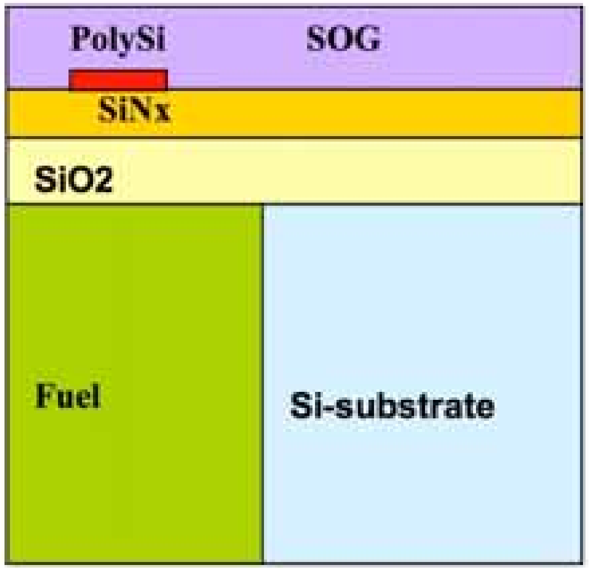
$$p_i: \quad V_{p_i} = \Im(K_0^{-1}K_i, K_0^{-1}F)$$

$$V = span(V_s, V_{p_i})$$

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Case Study: Film Coefficients

- Now three film coefficients as independent parameters:
  - ✓Top,
  - ✓Side,
  - ✓Bottom.
- 2D-axisymmetrical model, 4257 equations.
- Film coefficients to change from 1 to 10^6.



$$E\dot{\mathbf{T}}(t) + (K + h_t K_t + h_s K_s + h_b K_b)\mathbf{T}(t) = \mathbf{f}u(t)$$

- See tutorial on the MOR for ANSYS site.

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Local Error Control: Idea

- Specify parameter range

$$s_{\min} < s < s_{\max}$$
$$h_{i,\min} < h_i < h_{i,\max}$$

- Choose an expansion point

$$s = 0, \quad h_i = h_0$$

- Use the difference between the original and reduced system to choose the number of moments.

- Evaluation of the transfer function of the original transfer function is expensive:
  - ✓The number of evaluations should be minimal.
  - ✓We target the number of evaluations equation to p + 1.
  - ✓In the future - error indicators.

$$\left\| H(s_{\max}, h_i) - H_{reduced}(s_{\max}, h_i) \right\| < \varepsilon$$

Local Error Control: Example

- Laplace variable, control at

$$H[s_{\max}, h_{t,0}, h_{s,0}, h_{b,0}]$$

- First parameter, control at

$$H[s_{\max}, h_{t,\max}, h_{s,0}, h_{b,0}]$$

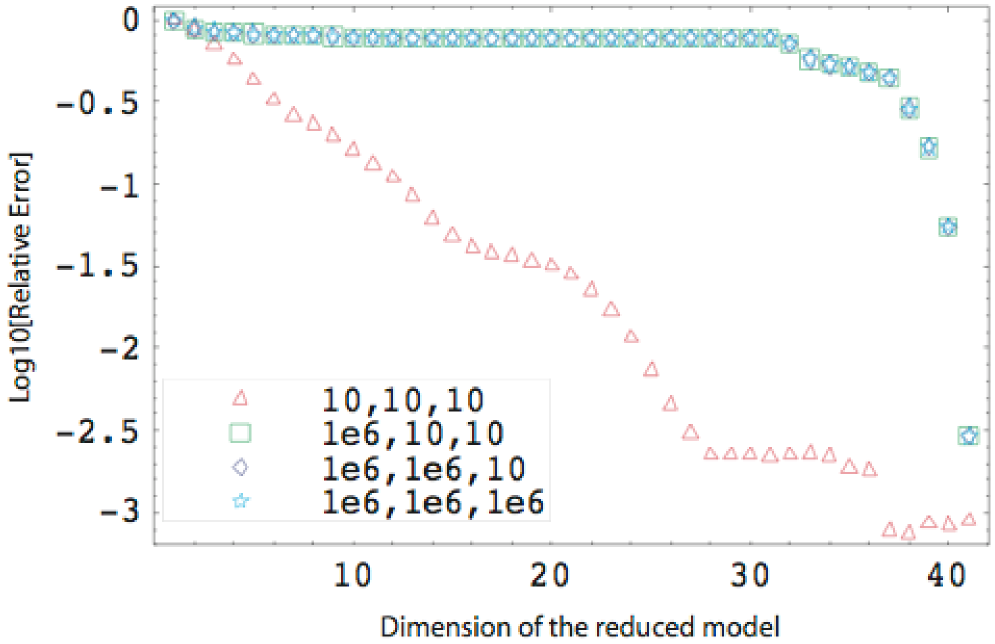
- 2nd parameter, control at

$$H[s_{\max}, h_{t,\max}, h_{s,\max}, h_{b,0}]$$

- 3rd parameter, control at

$$H[s_{\max}, h_{t,\max}, h_{s,\max}, h_{b,\max}]$$

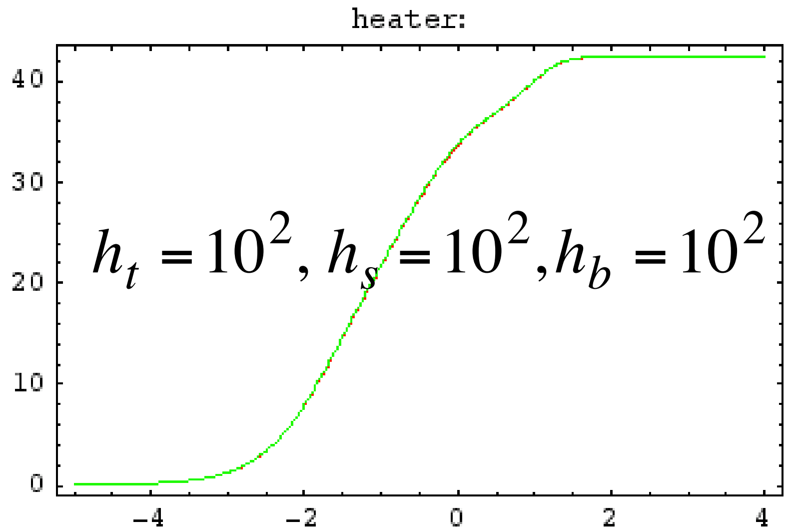
- Happens to work in our case.

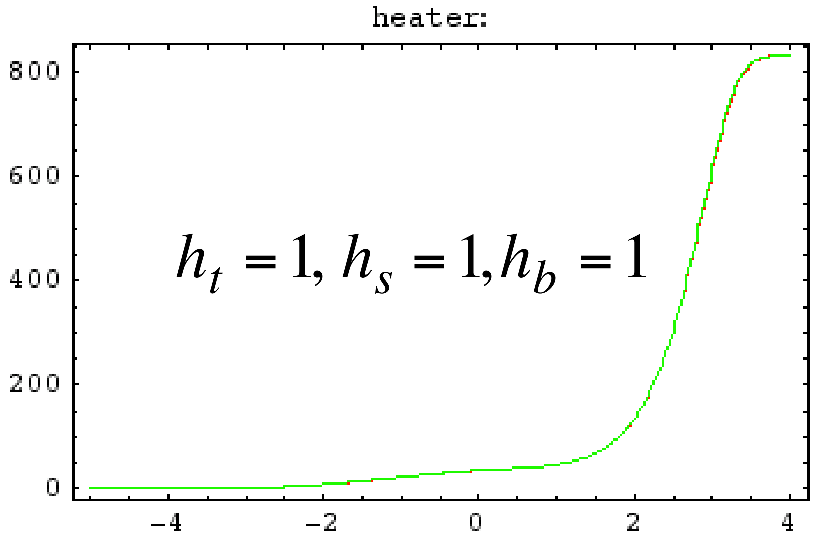


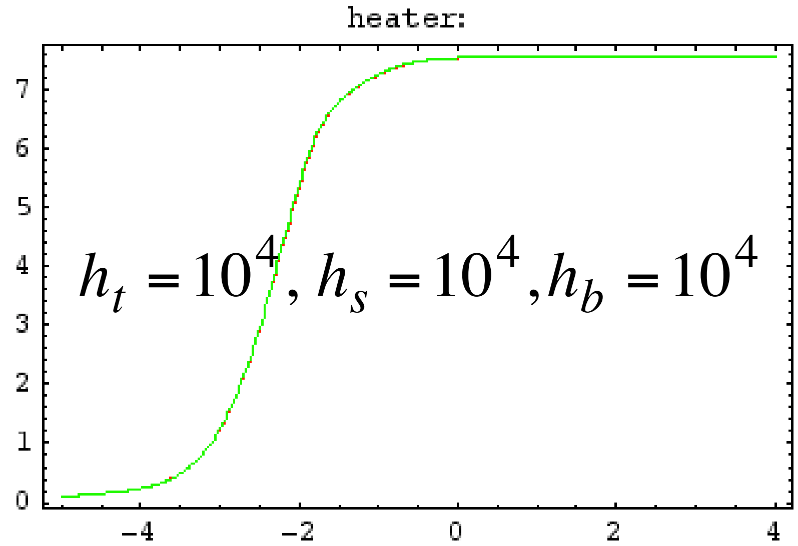
- 28 vectors to reach convergence for s, and then 13 vectors for the 1st parameter.

Comparison

- T vs. log10[time]
- red - original (4257)
- green - reduced (41)







ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

Parametric MOR Summary

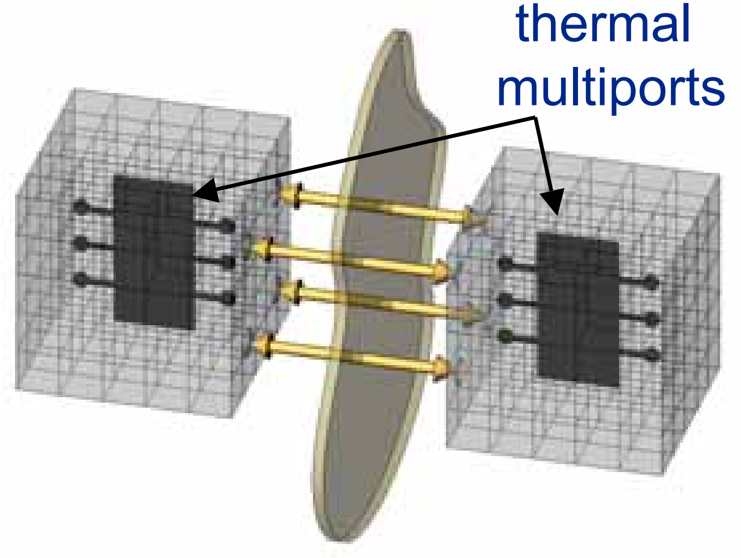
- Parametric model reduction is very important in many engineering applications.

- Multivariate expansion seems to be the right way to solve the problem.

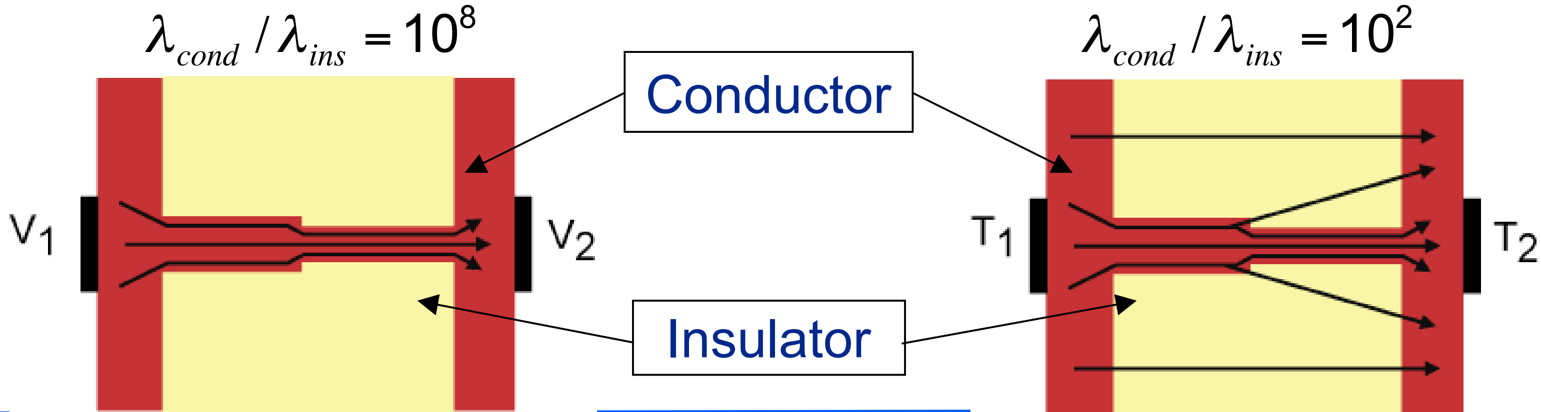
- In our experience one can neglect mixed moments.

- Error estimates are missing.

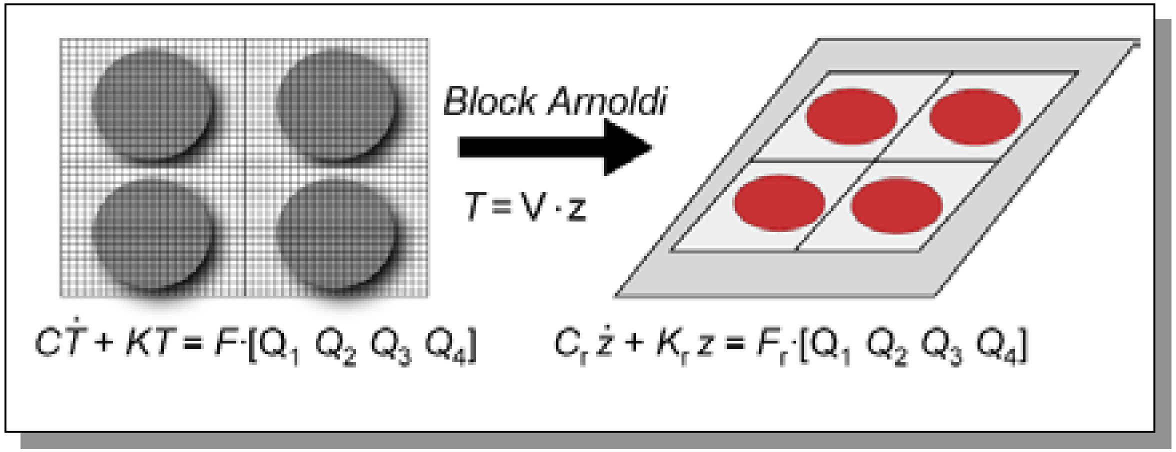
Coupling of Reduced Models



- Tamara Bechtold
- How to find a thermal multiport representation?
- How to reduce the number of shared FE nodes?

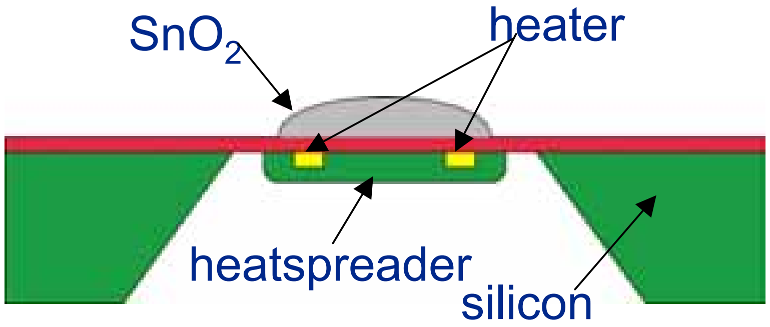


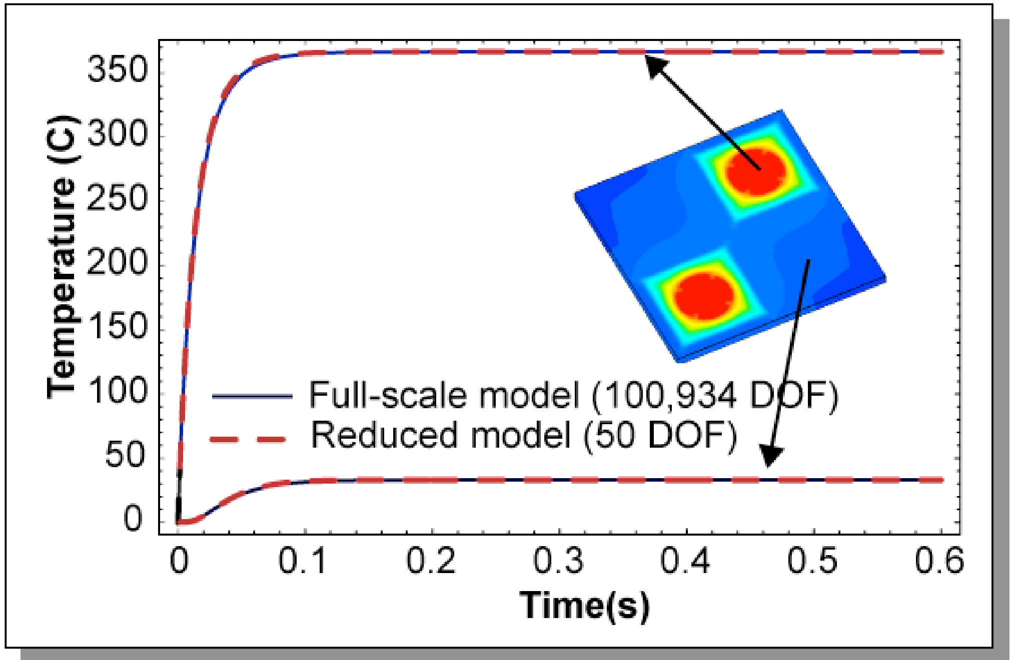
Block Arnoldi



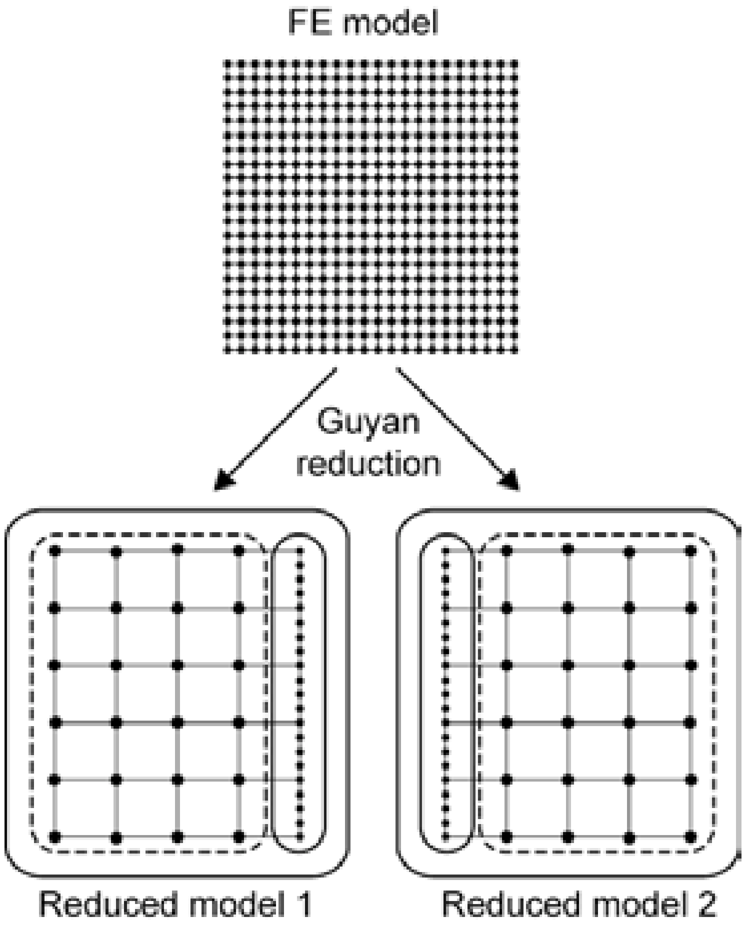
- brute force method for MIMO systems
- without decoupling
- does not scale well

gas sensor (ETH Zurich)

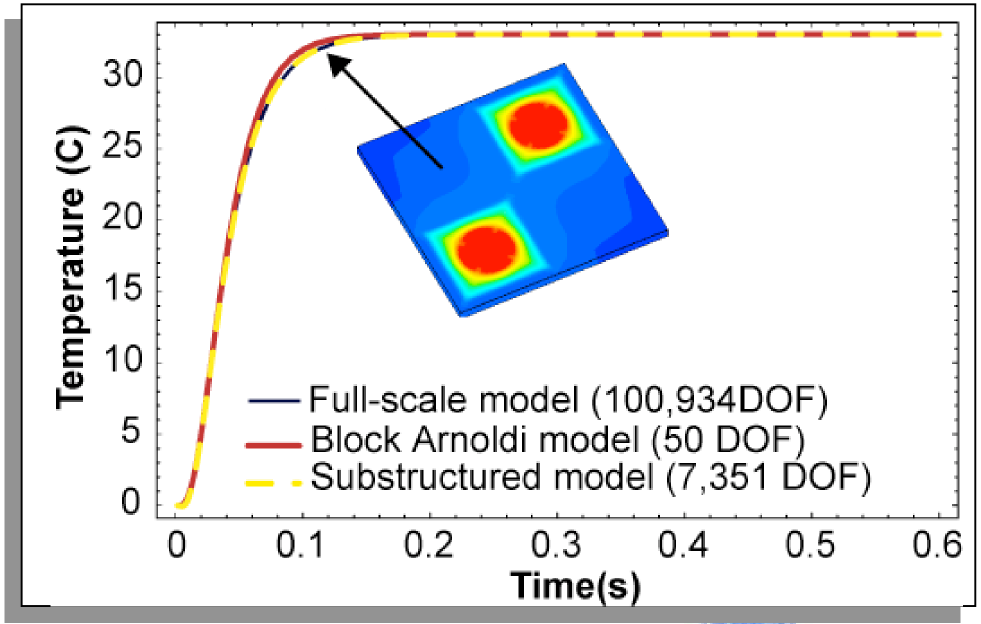




Guyan-Based Substructuring

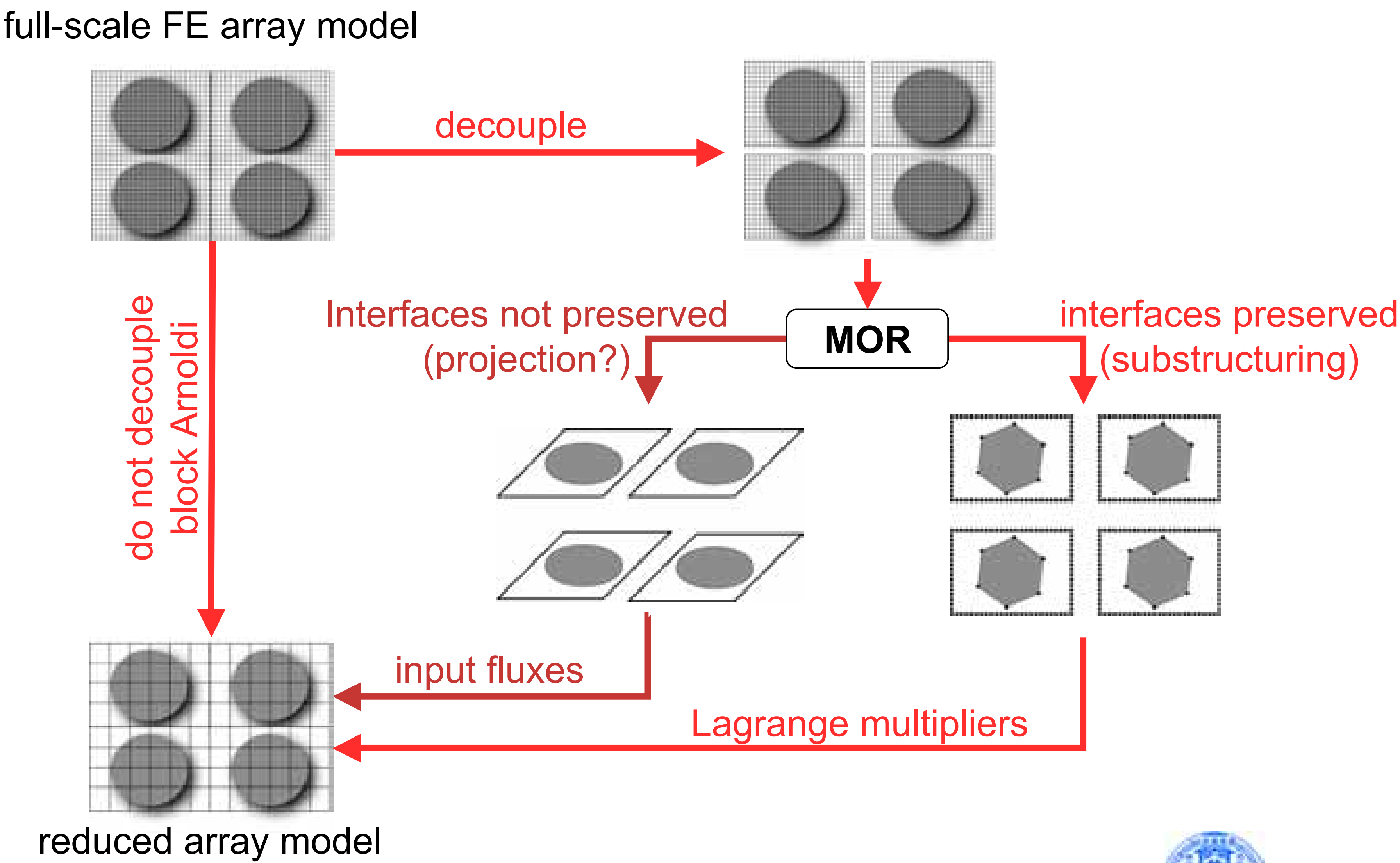


- available in ANSYS
- minimum order defined by the number of interface nodes
- results in unnecessary large reduced model size



ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

MOR of Interconnected Systems



ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

SVD-Krylov

- Solution of large-scale Lyapunov equations
- Iterative methods
- Low-rank Gramian
- Connection to moment matching
- Cross-Gramian
- Software

Solving Lyapunov Equations by Iterative Methods

- **Lyapunov equations can be expressed as a normal linear system of order N^2.**
- **One can apply iterative methods by making use of a special form for such a system.**
- **See a chapter in B. N. Datta, "Numerical Methods for Linear Control systems", Elsevier, 2004.**

$$AX + XB = C$$

$$Gx = c$$

$$G = A \otimes I + I \otimes B^T$$

Low-rank Gramian approximation

- **Penzl; Lee and White; Gugercin, Sorensen and Antoulas.**
- **Express Grammian as** $P = XX^T$
- **Substitute into the Lyapunov equations and find an iterative method.**
- **Software LYAPACK, www.netlib.org/lyapack/**
- **Problems:**
  - there are two Lyapunov equations to solve
  - model reduction theory for symmetric systems
  - may not preserve stability

$$AP + PA^T = -BB^T \qquad A^T Q + QA = -C^T C$$

Connection to Moment Matching

- Theorem from Jing-Rebecca Li for symmetric systems.
- Low-rank Grammian approximation is equivalent to multi-point expansion.
- Gives us some approximate theory how to choose expansion points.
- Input: maximum and minimum eigenvalues of the system matrix and tolerance.
- Computing elliptic integrals.
- Output: number and values of expansion points.

Sylvester Equation

- **Sorenson and Antoulas: model reduction based on the Sylvester equation.**
- **Valid for symmetric transfer function matrices.**
- **SISO is always appropriate.**
- **Can always be done for an arbitrary MIMO system.**

$$AP + PA^T = -BB^T$$

$$A^TQ + QA = -C^TC$$

$$AR + RA = -BC$$

cross-grammian

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Software

SpaRed: A Parallel Library for Model Reduction of Large Sparse Linear Systems

http://spine.act.uji.es/~plicmr/SpaRedW3/SpaRed.html

SpaRed:
A Parallel Library for
Model Reduction of Large Sparse Linear Systems

SpaRed

Home
Description
  Documentation
Library
  gquintan@icc.uji.es
Remote services
  Web

Brief description

SpaRed is a library of routines for model reduction of very large-scale, sparse continuous linear time invariant systems represented using the state-space model. Only one method is currently available in SpaRed: the Low Rank Square Root method. Future extensions will include soon other methods.
The library employs the serial libraries BLAS, LAPACK, and SuperLU (see http://www.netlib.org).
You can get a general idea of the possibilities of the library by examining the documentation of the library.

Obtaining the library

In order to receive the library, you need to contact us by e-mail (**gquintan@icc.uji.es**), specifying your Name and Institution.

Remote execution

You can execute the kernels in the library on our parallel cluster using our Web Service.
The jobs are executed on an Intel Pentium-II personal computer, using IEEE double precision. With this architecture, model reduction of large linear systems with sparse or banded state matrices is possible.

Nonlinear Model Reduction

- Convert to linear:
- Split a system to linear and nonlinear parts. Then reduce a linear part.
- Linearize. Small signal analysis.
- Proper Orthogonal Decomposition
- Empirical Gramians
- Trajectory piece-wise linear model reduction
- ANSYS ROM for MEMS
- Weakly nonlinear (quadratic and cubic terms)

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG

Proper Orthogonal Decomposition

- Solve the full nonlinear system:

$$\dot{x} = f(x,u)$$

- At appropriate times, take snapshots , and collect them in a matrix:

$$S = \{x_1, x_2, \ldots, x_m\}$$

- Perform Singular Value Decomposition of :

$$S = U\Sigma P^T = \sum_{i=1}^{m} \sigma_i u_i p_i^T$$

- Form the projection basis by dropping the smallest singular values:

$$\hat{S} = \sum_{i=1}^{k} \sigma_i u_i p_i^T$$

- For reduced system, form:

$$\dot{z} = V^T f(Vz,u)$$

Trajectory Piece-Wise Linear

M. Rewienski, A Trajectory Piecewise-Linear Approach to Model Order Reduction of Nonlinear Dynamical Systems, MIT, 2003.

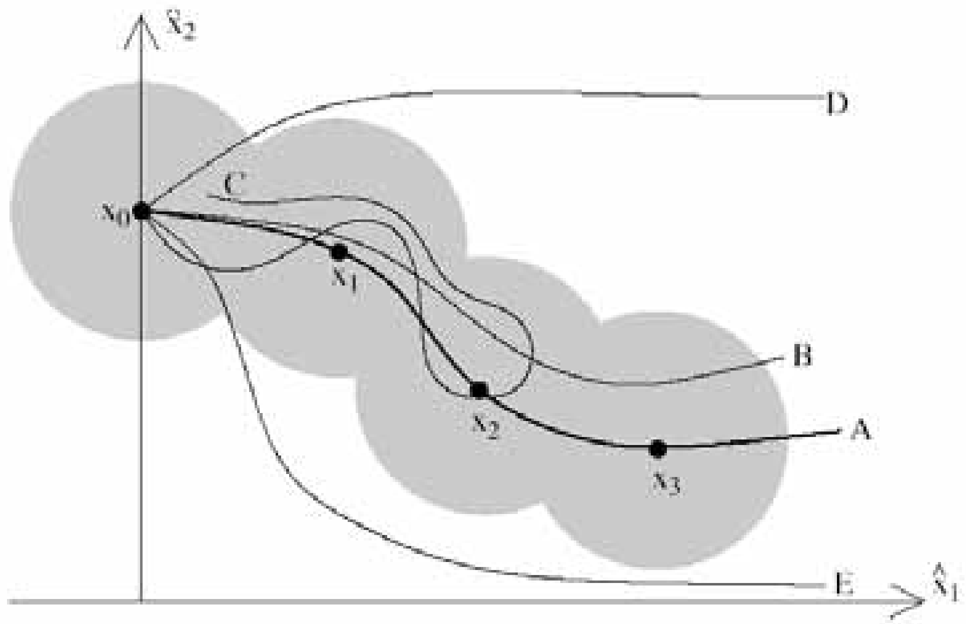


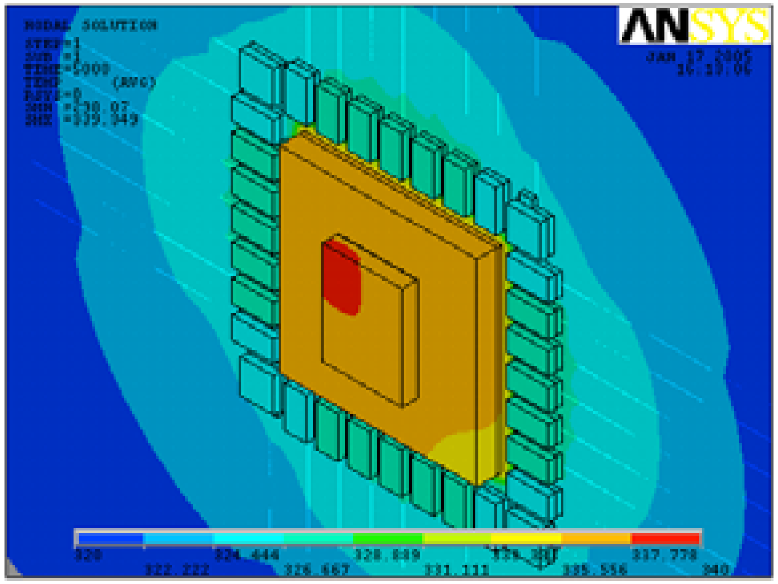
Figure 3-3: Generation of the linearized models along a trajectory of a nonlinear system in a 2D state space. Trajectory 'A' is called the 'training' trajectory.

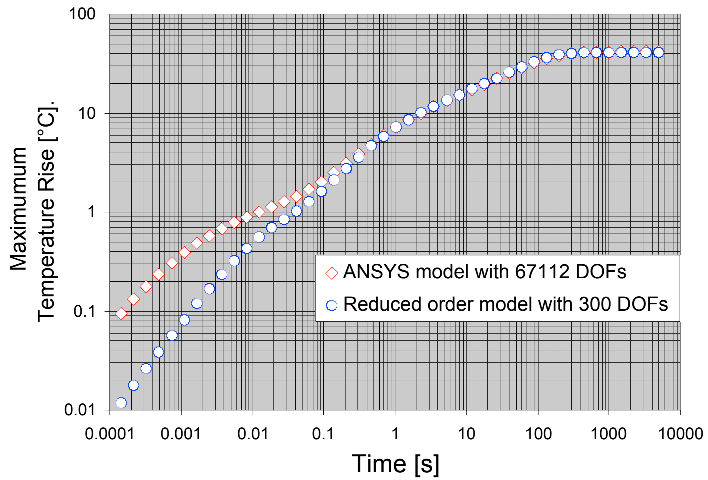
Weakly Nonlinear MOR

- Weakly nonlinear - quadratic and cubic terms:

$$Edx/dt + Kx + x^{T}Wx = bu(t)$$

- Example from Eurosime 2005: temperature-dependent film coefficient.
- Based on a projection of a nonlinear system.
- How to have nonlinear system matrices?





ALBERT-LUDWIGS-
UNIVERSITÄT FREIBURG

Summary

- Parametric model reduction
- Coupling reduced models with each other
- SVD-Krylov
- Nonlinear model reduction

ALBERT-LUDWIGS-UNIVERSITÄT FREIBURG