

POD Model Order Reduction for Coupled Systems of Integrated Circuits

Application of Discrete Empirical Interpolation

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joint work with Michael Hinze* and Ulrich Matthes*

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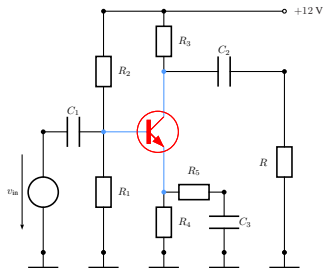
SCEE 2010, Toulouse



Overview

Goal:

Efficient simulation of circuits containing semiconductors.



Our approach:

- ▶ Describe the semiconductors by PDEs (drift-diffusion equations).
- ▶ Discretize PDEs in space by FEM, obtain a high dimensional DAE for the circuit. → “method of lines”.
- ▶ Integrate DAE for a set of inputs and take snapshots.
- ▶ Perform a POD on the snapshot trajectories, obtain a reduced state-space approximation.
- ▶ Again discretize in space; but: singular vectors as ansatz functions.

Outline

Coupled model and FEM discretization

Construction of the reduced model

Application of Discrete Empirical Interpolation

Residual based parameter adaptivity

Outlook

Coupled circuit and semiconductor models [M. Günther '01, C. Tischendorf '03]

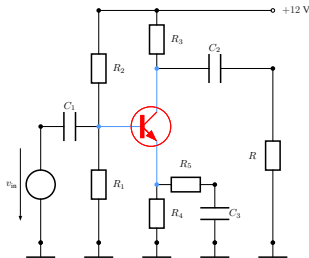
Kirchhoff's' laws (no semiconductors) read

$$A_j = 0, \quad v = A^T e$$

A: (reduced) incidence matrix.

Voltage-current relations of components:

$$j_C = \frac{dq_C}{dt}(v_C, t), \quad j_R = g(v_R, t), \quad v_L = \frac{d\phi_L}{dt}(j_L, t)$$



Modified Nodal Analysis: join all equations to DAE system

$$A_C \frac{dq_C}{dt} \left(A_C^T e(t), t \right) + A_{Rg} \left(A_R^T e(t), t \right) + A_L j_L(t) + A_V j_V(t) = -A_I i_s(t),$$

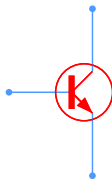
$$\frac{d\phi_L}{dt} (j_L(t), t) - A_L^T e(t) = 0,$$

$$A_V^T e(t) = v_s(t).$$

Coupled circuit and semiconductor models [M. Günther '01, C. Tischendorf '03]

PDE-model (drift-diffusion equations) for semiconductors

$$\begin{aligned}
 \operatorname{div}(\varepsilon \nabla \psi) &= q(n - p - C), \\
 -q \partial_t n + \operatorname{div} J_n &= qR(n, p), \\
 q \partial_t p + \operatorname{div} J_p &= -qR(n, p), \\
 J_n &= \mu_n q (-U_T \nabla n - n \nabla \psi), \\
 J_p &= \mu_p q (-U_T \nabla p - p \nabla \psi),
 \end{aligned}$$



on $\Omega \times [0, T]$ with $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$).

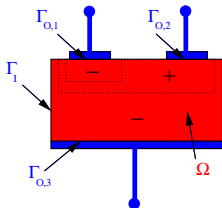
Dirichlet boundary constraints at $\Gamma_{O,k}$:

$$\psi(t, x), \quad n(t, x) = \tilde{n}(x), \quad p(t, x) = \tilde{p}(x)$$

and Neumann boundary constraints at Γ_I :

$$\nabla \psi(t, x) \cdot \nu(x) = J_n \cdot \nu(x) = J_p(t, x) \cdot \nu(x) = 0$$

or mixed boundary conditions at MI contacts (MOSFETs).



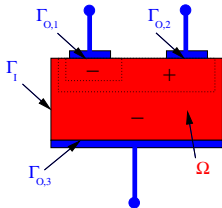
Coupled circuit and semiconductor models [M. Günther '01, C. Tischendorf '03]

Coupling conditions:

$$j_{S,k}(t) = \int_{\Gamma_{O,k}} (J_n + J_p - \varepsilon \partial_t \nabla \psi) \cdot \nu \, d\sigma,$$

$$\psi(t, x) = \psi_{bi}(x) + (A_S^\top e(t))_k$$

for $(t, x) \in [0, T] \times \Gamma_{O,k}$,



and add current j_S to Kirchhoff's current law:

$$A_C \frac{dq_C}{dt} (A_C^\top e, t) + A_{RG} (A_R^\top e, t) + A_L j_L + A_V j_V + A_S j_S = -A_I i_S,$$

$$\frac{d\phi_L}{dt} (j_L, t) - A_L^\top e = 0,$$

$$A_V^\top e = v_s.$$

Add DD-equations + coupling conditions for each semiconductor.

Mixed formulation

$E = -\nabla\psi$ plays dominant role in DD-equations.

Mixed formulation

[Brezzi et al. '05]

Provide additional variable g_ψ and equation

$$g_\psi = \nabla\psi.$$

Scaled DD equations then read:

$$\begin{aligned}\lambda \operatorname{div} g_\psi &= n - p - C, \\ -\partial_t n + \nu_n \operatorname{div} J_n &= R(n, p), \\ \partial_t p + \nu_p \operatorname{div} J_p &= -R(n, p), \\ g_\psi &= \nabla\psi, \\ J_n &= \nabla n - n g_\psi, \\ J_p &= -\nabla p - p g_\psi.\end{aligned}$$

Finite Element approximation

Finite elements

- ▶ piecewise constant ansatz functions for ψ , n and p .
 Basis functions: φ_i , $i = 1, \dots, N$, $N = |\mathcal{T}|$.
- ▶ Raviart-Thomas elements for g_ψ , J_n and J_p .
 Basis functions: ϕ_j , $i = 1, \dots, M$, $M = |\mathcal{E}| - |\mathcal{E}_N|$.

$$RT_0 := \{y : \Omega \rightarrow \mathbb{R}^d : y|_T(x) = a_T + b_T x, a_T \in \mathbb{R}^d, b_T \in \mathbb{R}, [y]_E \cdot \nu_E = 0, \text{ for all inner edges } E\}.$$

Galerkin formulation:

$$\psi^h(t, x) = \sum_{i=1}^N \psi_i(t) \varphi_i(x), \quad g_\psi^h(t, x) = \sum_{j=1}^M g_{\psi,j}(t) \phi_j(x),$$

and analogously for n , p , J_n , and J_p .

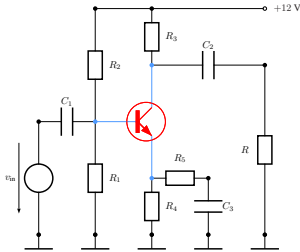
Finite Element approximation

FEM yields a high-dimensional DAE for each semiconductor (method of lines)

$$\begin{pmatrix} 0 \\ -M_L \dot{n}(t) \\ M_L \dot{p}(t) \\ 0 \\ 0 \\ 0 \end{pmatrix} + \underbrace{\begin{pmatrix} -M_L & M_L & \lambda D & & & \\ & & & \nu_n D & & \\ & & & & \nu_p D & \\ D^T & & & M_H & & \\ & D^T & & & M_H & \\ & & -D^T & & & M_H \end{pmatrix}}_{A_{FEM}} \begin{pmatrix} \psi(t) \\ n(t) \\ p(t) \\ g_\psi(t) \\ J_n(t) \\ J_p(t) \end{pmatrix} + \mathcal{F}(n^h, p^h, g_\psi^h) = b(A_S^T e(t)),$$

$$\mathcal{F}(n^h, p^h, g_\psi^h) = \begin{pmatrix} 0 \\ -\int_{\Omega} R(n^h, p^h) \varphi \\ \int_{\Omega} R(n^h, p^h) \varphi \\ 0 \\ \int_{\Omega} n^h g_\psi^h \cdot \phi \\ \int_{\Omega} p^h g_\psi^h \cdot \phi \end{pmatrix}, \quad b = \begin{pmatrix} -\int_{\Omega} C \varphi \\ 0 \\ 0 \\ \int_{\Gamma} \psi^h(A_S^T e(t)) \phi \cdot \nu \\ \int_{\Gamma} n^h \phi \cdot \nu \\ -\int_{\Gamma} p^h \phi \cdot \nu \end{pmatrix}.$$

Full model



$$\begin{aligned}
 A_C \frac{dq_C}{dt} (A_C^T e(t), t) + A_{RG} (A_R^T e(t), t) \\
 + A_L j_L(t) + A_V j_V(t) + A_S j_S(t) = -A_I j_S(t), \\
 \frac{d\phi_L}{dt} (j_L(t), t) - A_L^T e(t) = 0, \\
 A_V^T e(t) = v_S(t),
 \end{aligned}$$

$$j_S(t) - C_1 j_n(t) - C_2 j_p(t) - C_3 \dot{g}_\psi(t) = 0,$$

$$\begin{pmatrix} 0 \\ -M_L \dot{n}(t) \\ M_L \dot{p}(t) \\ 0 \\ 0 \\ 0 \end{pmatrix} + A_{FEM} \begin{pmatrix} \psi(t) \\ n(t) \\ p(t) \\ g_\psi(t) \\ j_n(t) \\ j_p(t) \end{pmatrix} + \mathcal{F}(n^h, p^h, g_\psi^h) - b(A_S^T e(t)) = 0.$$

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Snapshot-POD (Proper Orthogonal Decomposition) [L. Sirovich '87]

Full simulation yields snapshots (here: $y = \psi, n, p, \dots$)

$$\{y(t_i, \cdot)\}_{i=1, \dots, m} \subset \text{span}\{\varphi_j\}_{j=1, \dots, N}, \quad \text{with} \quad y(t_i, x) = \sum_{j=1}^N \vec{y}_j(t_i) \varphi_j(x).$$

Gather coefficients in matrix

$$Y := (\vec{y}(t_1), \dots, \vec{y}(t_m)) \in \mathbb{R}^{N \times m}.$$

POD in Hilbert space X as eigenvalue problem:

$$Kv^k = \sigma_k^2 v^k, \quad \text{with} \quad K_{ij} := \langle y(t_i, \cdot), y(t_j, \cdot) \rangle_X.$$

Note that $K = Y^T M Y$ with $M_{ij} = \langle \varphi_i, \varphi_j \rangle_X$. Write POD in terms of SVD:

$$\tilde{U} \Sigma \tilde{V}^T = L^T Y, \quad \text{with} \quad LL^T := M.$$

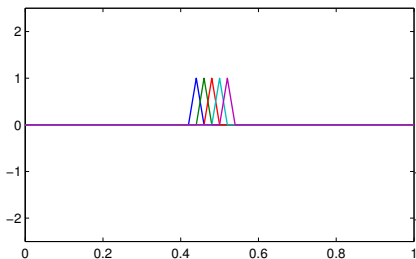
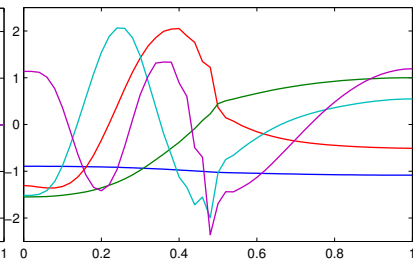
Then, the s -dimensional POD basis is

$$\left\{ u^i := \sum_{j=1}^N \tilde{u}_j^i \varphi_j(\cdot) \right\}_{i=1, \dots, s}, \quad U := (\vec{u}^1, \dots, \vec{u}^s) := L^{-T} \tilde{U}_{(:, 1:s)}.$$

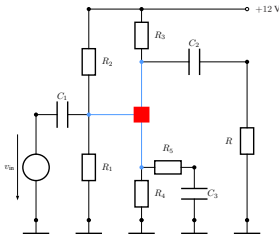
Model Order Reduction

- ▶ Simulate the complete network at one or more reference parameters.
- ▶ Take snapshots of the state of each semiconductor at time points t_i .
- ▶ Perform POD **component wise** on ψ , n , p , g_ψ , J_n and J_p .
- ▶ Use the POD basis functions as (non local) FEM ansatz/test functions:

$$\psi^{POD}(t, x) = \sum_{i=1}^S \gamma_{\psi,i}(t) u_{\psi}^i(x)$$

1D-FEM ansatz functions for J_n first 5 POD basis functions for J_n 

Reduced model



$$\begin{aligned}
 A_C \frac{dq_C}{dt} (A_C^T e(t), t) + A_{Rg} (A_R^T e(t), t) \\
 + A_L j_L(t) + A_V j_V(t) + A_S j_S(t) = -A_I i_S(t), \\
 \frac{d\phi_L}{dt} (j_L(t), t) - A_L^T e(t) = 0, \\
 A_V^T e(t) = v_S(t),
 \end{aligned}$$

$$j_S(t) - C_1 U_{J_n} \gamma_{J_n}(t) - C_2 U_{J_p} \gamma_{J_p}(t) - C_3 U_{g_\psi} \dot{\gamma}_{g_\psi}(t) = 0,$$

$$\begin{pmatrix} 0 \\ -\dot{\gamma}_n(t) \\ \dot{\gamma}_p(t) \\ 0 \\ 0 \\ 0 \end{pmatrix} + A_{POD} \begin{pmatrix} \gamma_\psi(t) \\ \gamma_n(t) \\ \gamma_p(t) \\ \gamma_{g_\psi}(t) \\ \gamma_{J_n}(t) \\ \gamma_{J_p}(t) \end{pmatrix} + U^T \mathcal{F}(n^{POD}, p^{POD}, g_\psi^{POD}) - U^T b(A_S^T e(t)) = 0.$$

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Computational complexity

For the sake of presentation we only consider the recombination term:

$$F_n(n(t), p(t)) = \begin{pmatrix} \int_{\Omega} R \left(\sum_{i=1}^N n_i(t) \varphi_i(x), \sum_{i=1}^N p_i(t) \varphi_i(x) \right) \varphi_1(x) dx \\ \vdots \\ \int_{\Omega} R \left(\sum_{i=1}^N n_i(t) \varphi_i(x), \sum_{i=1}^N p_i(t) \varphi_i(x) \right) \varphi_N(x) dx \end{pmatrix}.$$

In the reduced model we compute

$$\underbrace{U_n^T}_{\text{size } s_n \times N} \underbrace{F_n}_{N \text{ evaluations}} \left(\underbrace{U_n}_{\text{size } N \times s_n} \gamma_n(t), \underbrace{U_p}_{\text{size } N \times s_p} \gamma_p(t) \right),$$

and for example the derivative with respect to γ_p :

$$\underbrace{U_n^T}_{\text{size } s_n \times N} \underbrace{\frac{\partial F_n}{\partial p}(U_n \gamma_n(t), U_p \gamma_p(t))}_{\text{size } N \times N, \text{ sparse}} \underbrace{U_p}_{\text{size } N \times s_p}.$$

Computational complexity of the POD-ROM is still $O(N)$.

Discrete Empirical Interpolation Md. (DEIM) [S. Chaturantabut, D. Sorensen '09]

DEIM

- ▶ Collect snapshots $\{F_n(n(t_k), p(t_k))\}$ of the nonlinearity.
- ▶ Do POD on snapshots $\{F_n(n(t_k), p(t_k))\}$, obtain basis $V_n \in \mathbb{R}^{N \times \tau_n}$.
- ▶ Ansatz:

$$F_n(U_n \gamma_n(t), U_p \gamma_p(t)) \approx V_n c(t)$$

is overdetermined.

- ▶ Select τ_n “useful” rows:

$$P_n^T F_n(\dots) \approx P_n^T V_n c(t).$$

- ▶ If $P_n^T V_n$ is regular:

$$F_n(\dots) \approx V_n c(t) = V_n (P_n^T V_n)^{-1} P_n^T F_n(\dots)$$

The regularity of $P_n^T V_n$ can be guaranteed and the growth of a global error bound is limited, see [CS09].

Discrete Empirical Interpolation Md. (DEIM) [S. Chaturantabut, D. Sorensen '09]

We obtain an approximation

$$U_n^T F_n(U_n \gamma_n(t), U_p \gamma_p(t)) \approx W_n P_n^T F_n(U_n \gamma_n(t), U_p \gamma_p(t)),$$

with

$$W_n := (U_n^T V_n (P_n^T V_n)^{-1}) \in \mathbb{R}^{s_n \times \tau_n}.$$

Discrete Empirical Interpolation Md. (DEIM) [S. Chaturantabut, D. Sorensen '09]

We obtain an approximation

$$U_n^T F_n(U_n \gamma_n(t), U_p \gamma_p(t)) \approx W_n P_n^T F_n(U_n \gamma_n(t), U_p \gamma_p(t)),$$

with

$$W_n := (U_n^T V_n (P_n^T V_n)^{-1}) \in \mathbb{R}^{s_n \times \tau_n}.$$

Require whole vector $U_n \gamma_n(t) \in \mathbb{R}^N$ for evaluation of $P_n^T F_n(\dots) \in \mathbb{R}^{\tau_n}$?
 No, here each vector component depends only on some variables:

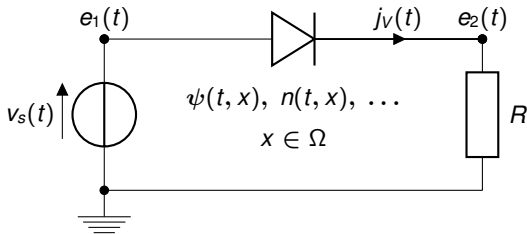
$$F_n(n(t), p(t)) = \begin{pmatrix} \int_{\Omega} R \left(\sum_{i=1}^N n_i(t) \varphi_i(x), \sum_{i=1}^N p_i(t) \varphi_i(x) \right) \varphi_1(x) dx \\ \vdots \\ \int_{\Omega} R \left(\sum_{i=1}^N n_i(t) \varphi_i(x), \sum_{i=1}^N p_i(t) \varphi_i(x) \right) \varphi_N(x) dx \end{pmatrix}.$$

Numerical results

Our C++ implementations make use of various tools:

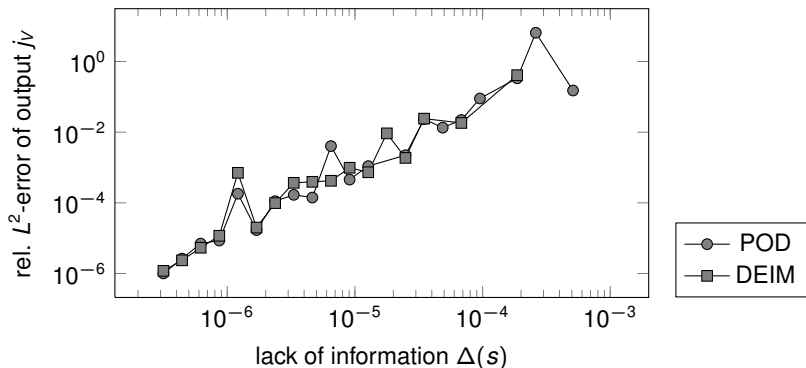
- ▶ deal.II (FEM)
- ▶ DASPK (DAE integrator, index-1 network assumed)
- ▶ ADOL-C (automatic derivatives of nonlinearities)
- ▶ SuperLU (linear solver)

Basic test circuit with one diode:



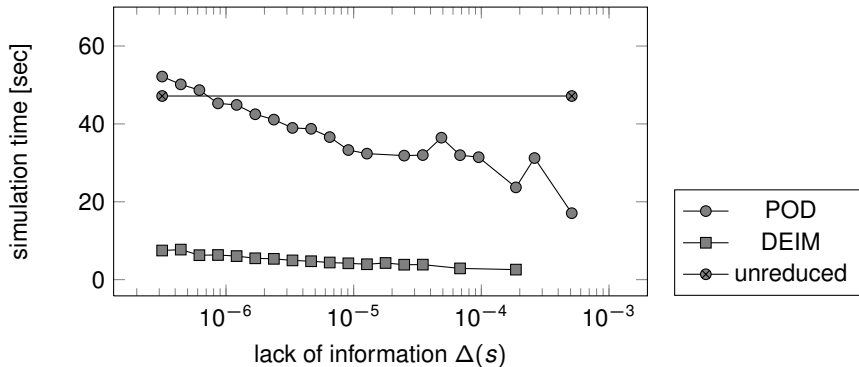
Numerical results

Relative error between reduced and unreduced problem at the fixed frequency $5 \cdot 10^9$ [Hz].



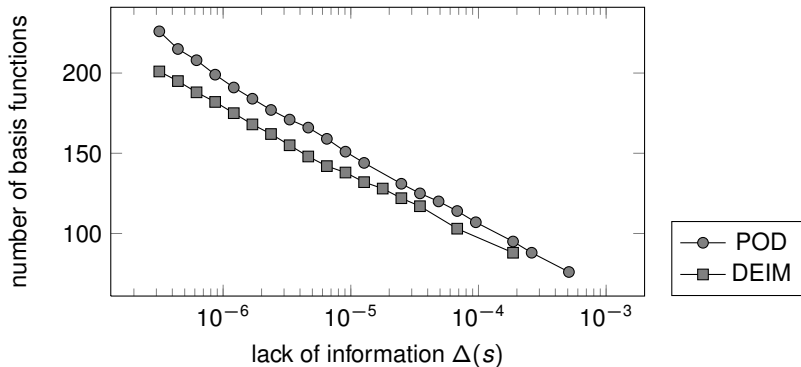
Numerical results

Time consumption for simulation runs.



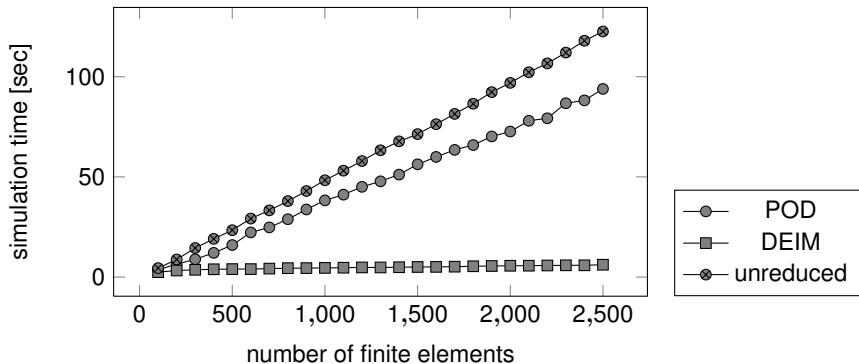
Numerical results

The number of required POD basis function and DEIM interpolation indices grows only logarithmically with the requested information content.



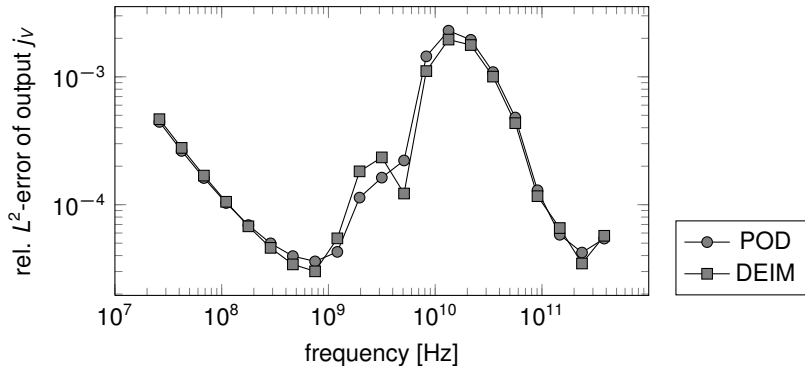
Numerical results

Computation times of the unreduced and the reduced order models plotted versus the number of finite elements. Number of variables in reduced system is ≈ 180 .



Numerical results

The reduced models are compared with the unreduced model at various input frequencies.



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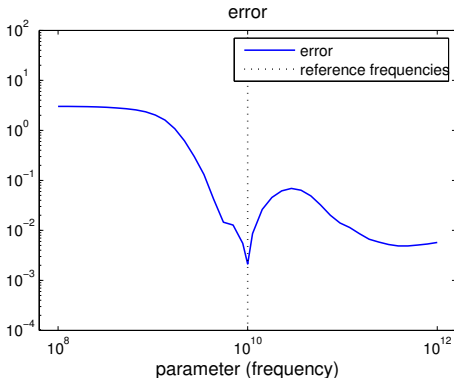
Reduced model over parameter space

Construction of reduced model requires snapshots from full simulations at reference parameters.

Is the model valid over a large parameter space?

reference parameter: $P_1 := \{f_1\} := \{10^{10}[\text{Hz}]\}$

parameter space $\mathcal{P} = [10^8, 10^{12}]$



Reduced model over parameter space - sampling

Goal

Find new sampling parameter f_{k+1} (reference frequency) without simulating the full, unreduced system. Set $P_{k+1} := P_k \cup \{f_{k+1}\}$.

- ▶ We do not consider the PDE discretization error.
- ▶ Rigorous upper bound for the error not available

$$\|\mathcal{E}(f; P_k)\| = \|y^h(f) - y^{POD}(f; P_k)\| \leq ?(s)$$

where $y^h := (\psi^h, n^h, p^h, g_\psi^h, J_n^h, J_p^h)^\top$, $y^{POD} := (\psi^{POD}, n^{POD}, \dots)^\top$.

- ▶ Rigorous RB methods, Greedy algorithm [see e.g. A. Patera, G. Rozza '07]: a-posteriori error estimates required.
- ▶ Linear ODEs [see e.g. B. Haasdonk, M. Ohlberger '09]: build difference between residual and unreduced equation to derive an ODE for the error.

Residual based sampling

Define residual $\mathcal{R}(z^{POD}(f; P_k))$: insert $z^{POD}(f; P_k)$ into unreduced equation,

$$\mathcal{R} := \begin{pmatrix} 0 \\ -M_L \dot{n}^{POD}(t) \\ M_L \dot{p}^{POD}(t) \\ 0 \\ 0 \\ 0 \end{pmatrix} + A_{FEM} \begin{pmatrix} \psi^{POD}(t) \\ n^{POD}(t) \\ p^{POD}(t) \\ g_{\psi}^{POD}(t) \\ J_n^{POD}(t) \\ J_p^{POD}(t) \end{pmatrix} + \mathcal{F}(n^{POD}, p^{POD}, g_{\psi}^{POD}) - b(e^{POD}(t)).$$

Residual is scale-variant!

Scale with block diagonal matrix-valued function

$$D(f) := \text{diag}(d_{\psi}(f)I, d_n(f)I, d_p(f)I, d_{g_{\psi}}(f)I, d_{J_n}(f)I, d_{J_p}(f)I)$$

and choose $d_{\psi}(f)$ such that it holds

$$d_{\psi}(f_j) \cdot \|\mathcal{R}_{\psi}(y^{POD}(f_j; P_k))\| = \frac{\|\psi^h(f_j) - \psi^{POD}(f_j; P_k)\|}{\|\psi^h(f_j)\|}, \quad \forall f_j \in P_k.$$

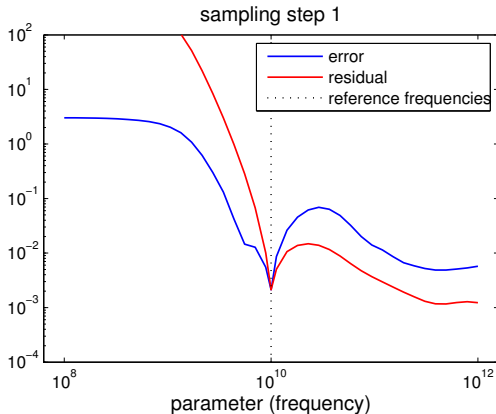
Residual based sampling

Algorithm: sampling

1. Select $f_1 \in \mathcal{P}$, $P_{test} \subset \mathcal{P}$, $tol > 0$, and set $k := 1$, $P_1 := \{f_1\}$.
2. Simulate the unreduced model at f_1 and calculate the reduced model with POD basis functions U_1 .
3. Calculate weight functions $d_{(\cdot)}(f) > 0$ for all $f \in P_k$.
4. Calculate the scaled residual $\|D(f)\mathcal{R}(z^{POD}(f, P_k))\|$ for all $f \in P_{test}$.
5. Check termination conditions, e.g.
 - ▶ $\max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_k))\| < tol$,
 - ▶ no progress in weighted residual.
6. Calculate $f_{k+1} := \arg \max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_k))\|$.
7. Simulate the unreduced model at f_{k+1} and create a new reduced model with POD basis U_{k+1} using also the already available information at f_1, \dots, f_k .
8. Set $P_{k+1} := P_k \cup \{f_{k+1}\}$, $k := k + 1$ and goto 3.

Numerical example - sampling step 1

Let $f_1 := 10^{10}[\text{Hz}]$, $P_1 := \{10^{10}[\text{Hz}]\}$, $\mathcal{P} = [10^8, 10^{12}]$.

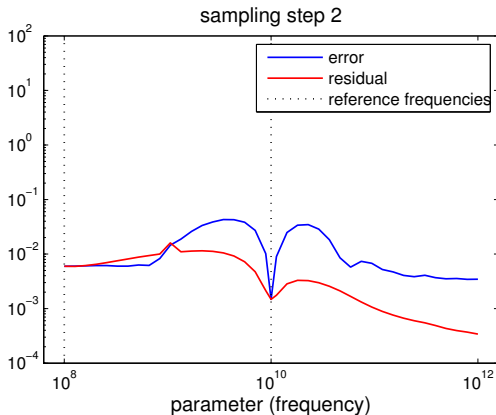


$$f_2 = \arg \max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_1))\| = 10^8[\text{Hz}]$$

$$P_2 = \{10^8[\text{Hz}], 10^{10}[\text{Hz}]\}$$

Numerical example - sampling step 2

$$P_2 = \{10^8[\text{Hz}], 10^{10}[\text{Hz}]\}$$

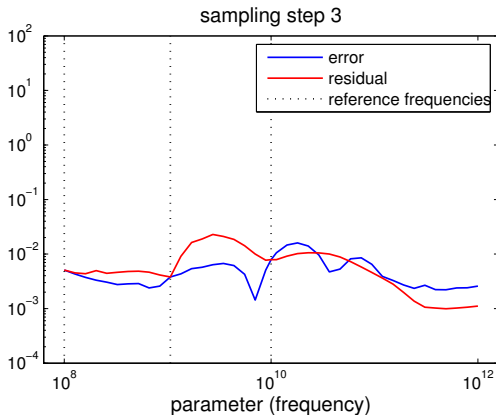


$$f_3 = \arg \max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_2))\| = 1.0608 \cdot 10^9[\text{Hz}]$$

$$P_3 = \{10^8[\text{Hz}], 1.0608 \cdot 10^9[\text{Hz}], 10^{10}[\text{Hz}]\}$$

Numerical example - sampling step 3

$$P_3 = \{10^8[\text{Hz}], 1.0608 \cdot 10^9[\text{Hz}], 10^{10}[\text{Hz}]\}$$



Terminate with “no progress in residual”.

Outlook

- ▶ Reduction of the DD-equations **and** the circuit:
first results available; joint work with subproject 3 of the SyreNe research network [A. Steinbrecher, T. Stykel]
- ▶ More realistic device models will be tackled in the BMBF research network MoreSim4Nano (Model Reduction for Fast Simulation of new Semiconductor Structures in Nano- and Microsystems-Technology)
- ▶ Final presentation of the SyreNe research network at **ModRed 2010, TU Berlin, 2-4 December 2010**

Thank you for your attention.

SyreNe

Systemreduktion für IC Design in der
Nanoelektronik

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