Universität Hamburg

SyreNe

Parametric model order reduction of semiconductors in electrical networks

IFIP 2011 : MS 34; Reduced Basis and Proper Orthogonal Decomposition: Analysis, Simulation and Optimal Control

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September 12, 2011

Outline

PDAE-model

2D/3D - Finite Element Method

Simulation results

Construction of the reduced model

Combined reduction using PABTEC and POD

Residual based parameter sampling

Further aspects of the reduction method

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

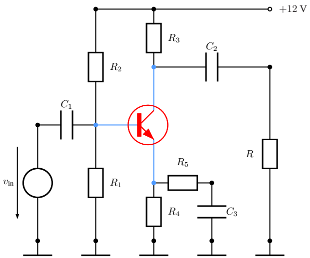
Kirchhoff's' laws (no semiconductors) read

$$Aj = 0, \quad v = A^\top e$$

A: (reduced) incidence matrix.

Voltage-current relations of components:

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



Modified Nodal Analysis: join all equations to DAE system

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

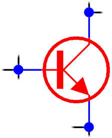
$$\frac{d\phi_L}{dt}(j_L(t), t) - A_L^\top e(t) = 0,$$

$$A_V^\top e(t) = v_s(t).$$

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

How can semiconductors be introduced?

- replace semiconductor by a (possibly nonlinear) electrical network,
- stamp semiconductor network into surrounding network,
- apply Modified Nodal Analysis.

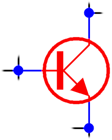


Here: use PDE model for semiconductors

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

on $\Omega \times [0, T]$.
Dirichlet boundary conditions for ψ, n, p (Ohmic contacts)
or Neumann boundary constraints for grad ψ, J_n, J_p (insolation).

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



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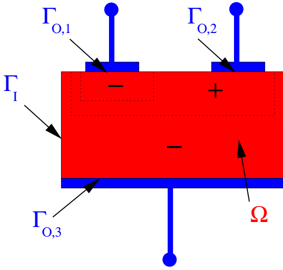

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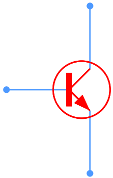
Coupled circuit and semiconductor models [M. Günther '01, C. Tischendorf '03]

PDE-model (drift-diffusion equations) for semiconductors

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



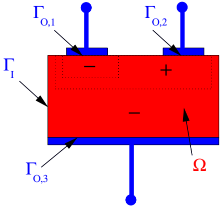
on $\Omega \times [0, T]$ with $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$.
Dirichlet boundary constraints at $\Gamma_{O,k}$:

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

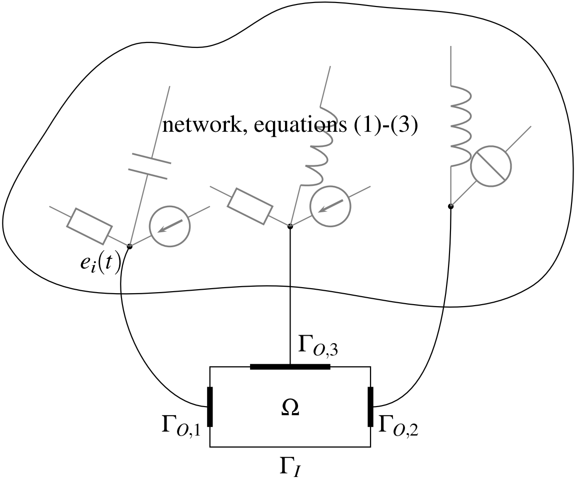
and Neumann boundary constraints at Γ_I:

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

or mixed boundary conditions at MI contacts (MOSFETs).

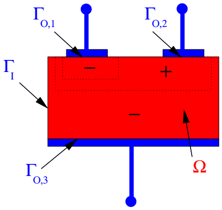


Coupled circuit and semiconductor models [M. Günther ’01, C. Tischendorf ’03]



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

Coupling conditions:



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

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

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

and add current j_S to Kirchhoff's current law:

$$A_C \frac{\mathrm{d}q_C}{\mathrm{d}t}\left(A_C^\top e, t\right) + A_R g\left(A_R^\top e, t\right) + A_L j_L + A_V j_V + A_S j_S = -A_I i_s,$$

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

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

Add DD-equations + coupling conditions for each semiconductor.

Outline

Mixed formulation

The electric field $E = -\nabla\psi$ 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:

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

Finite Element approximation

Finite elements

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

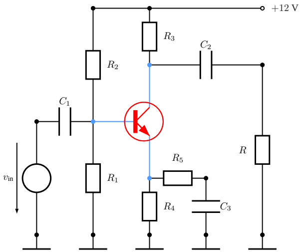
$$RT_0 := \{y : \Omega \to \mathbb{R}^d : \ y|_T(x) = a_T + b_T x, \ a_T \in \mathbb{R}^d, \ b_T \in \mathbb{R}, \\ [y]_E \cdot \boldsymbol{\nu}_E = 0, \ \text{for all inner edges } E\}.$$

Galerkin ansatz:

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

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

Full model



$$A_C \frac{\mathrm{d}q_C}{\mathrm{d}t}\left(A_C^\top e(t), t\right) + A_R g\left(A_R^\top e(t), t\right) + A_L j_L(t) + A_V j_V(t) + A_S j_S(t) = -A_I i_s(t),$$

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

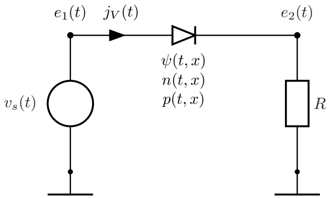
$$A_V^\top e(t) = v_s(t),$$

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

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

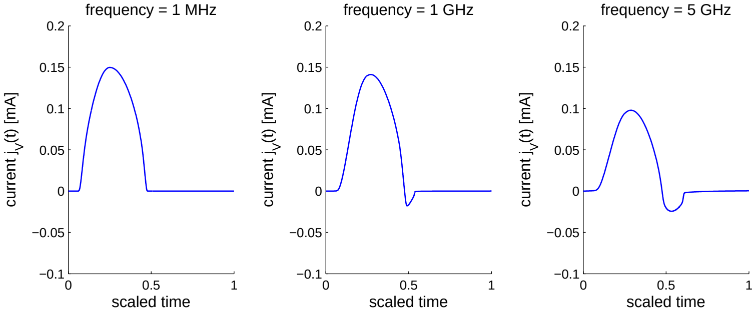
Outline

Basic test circuit, simulation results



input voltage: $v_s(t) = 5[V] \cdot \sin(2\pi f \cdot t)$

similar results obtained by MECS [M. Selva Soto]



Outline

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

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

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

Gather coefficients in matrix

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

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

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

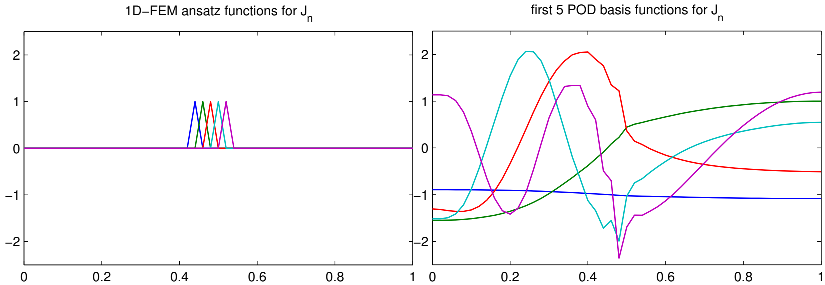
Then, the s-dimensional POD basis is

$$\left\{u^i := \sum_{j=1}^{N} \vec{u}^i_j \varphi_j(\cdot)\right\}_{i=1,\ldots,s}, \qquad U := (\vec{u}^1,\ldots,\vec{u}^s) := L^{-\top}\tilde{U}_{(:,1:s)}.$$

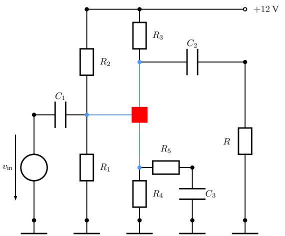
Model Order Reduction

- 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 functions:

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



Reduced model



$$A_C \frac{\mathrm{d}q_C}{\mathrm{d}t}\left(A_C^\top e(t), t\right) + A_R g\left(A_R^\top e(t), t\right)$$

$$+A_L j_L(t) + A_V j_V(t) + A_S j_S(t) = -A_I i_s(t),$$

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

$$A_V^\top e(t) = v_s(t),$$

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

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

Computational complexity

Computational complexity of reduced model still depends on n_{FEM}:

$$U^\top \mathcal{F}(n^{POD}, p^{POD}, g_\psi^{POD}) = \underbrace{U^\top}_{n_{POD} \times n_{FEM}} \underbrace{F}_{n_{FEM}}(\underbrace{U_n}_{n_{FEM} \times n_{POD}} \gamma_n, U_p \gamma_p, U_{g_\psi} \gamma_{g_\psi}).$$

With matrix-matrix multiplications in Jacobian computation:

$$\underbrace{U^\top}_{n_{POD} \times n_{FEM},\ \text{block-dense}} \quad \underbrace{F'(\ldots)}_{n_{FEM} \times n_{FEM},\ \text{sparse}} \quad \underbrace{U}_{n_{FEM} \times n_{POD},\ \text{block-dense}} .$$

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

DEIM

- Do POD on snapshots $\{F(n(t_i), p(t_i), g_\psi(t_i))\}$, obtain basis $W \in \mathbb{R}^{n_{FEM} \times n_{DEIM}}$ (block diagonal matrix).
- Ansatz
$$F(U_n\gamma_n(t), U_p\gamma_p(t), U_{g_\psi}\gamma_{g_\psi}(t)) \approx Wc(t)$$
is overdetermined.
- Select n_{DEIM} "useful" rows:
$$P^\top F(\ldots) \approx P^\top Wc(t).$$
- If $P^\top W$ is regular:
$$F(\ldots) \approx Wc(t) = W(P^\top W)^{-1}P^\top F(\ldots)$$

The regularity of $P^\top W$ can be guaranteed, see [CS09].
Again we apply the method component-wise.

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

Reduced model

$$U^\top F(U_n\gamma_n, U_p\gamma_p, U_{g_\psi}\gamma_{g_\psi})$$

with DEIM:

$$\underbrace{(U^\top W(P^\top W)^{-1})}_{n_{POD}\times n_{DEIM}\text{, block-dense}} \quad \underbrace{P^\top}_{n_{DEIM}} F(\underbrace{U_n\gamma_n}_{n_{FEM}}, U_p\gamma_p, U_{g_\psi}\gamma_{g_\psi})$$

First results with 1D-diode:

	n_{FEM}	FEM	n_{POD}	ROM	n_{DEIM}	ROM + DEIM
	3003	3.15 sec.	220	3.52 sec.	187	1.93 sec.
	15009	23.5 sec.	229	19.9 sec.	198	4.04 sec.
	48015	82.3 sec.	229	74.2 sec.	199	9.87 sec.
order		$\approx n_{FEM}^{1.18}$		$\approx n_{FEM}^{1.10}$		$\approx n_{FEM}^{0.578}$

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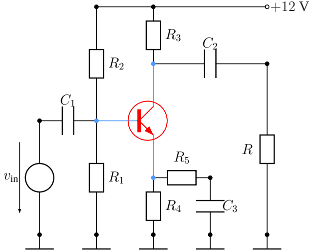
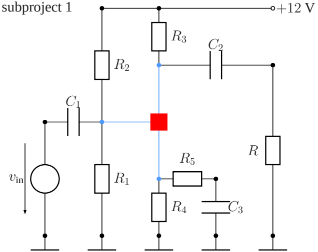
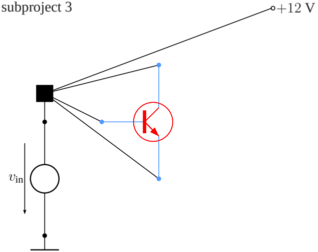
Combination of PABTEC and POD; joint work with [A. Steinbrecher, T. Stykel]



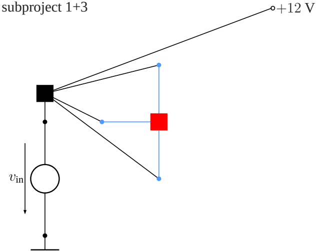
subproject 1



subproject 3



subproject 1+3



Combination of PABTEC and POD; Int. J. Numer. Model. 2011

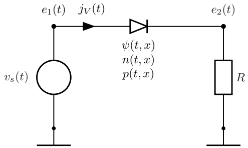
network (MNA equations)		diode (DD equations)		coupled system	simul. time	Jacobian evaluations	absolute error	relative error
type	dim.	type	dim.	dim.			$\Vert y-\hat{y}\Vert_{L_2}$	$\frac{\Vert y-\hat{y}\Vert_{L_2}}{\Vert y\Vert_{L_2}}$
unreduced	1503	unreduced	6006	7510	23.37s	20		
reduced	24	unreduced	6006	6031	16.90s	17	$2.165 \cdot 10^{-8}$	$7.335 \cdot 10^{-4}$
unreduced	1503	reduced	105	1609	1.51s	16	$2.952 \cdot 10^{-6}$	$1.000 \cdot 10^{-1}$
reduced	24	reduced	105	130	1.19s	11	$2.954 \cdot 10^{-6}$	$1.000 \cdot 10^{-1}$

Outline

Problem setting

MOR test problem

Basic circuit with frequency f of the voltage source $v_s(t) = 5[V] \cdot \sin(2\pi f \cdot t)$ as model parameter.

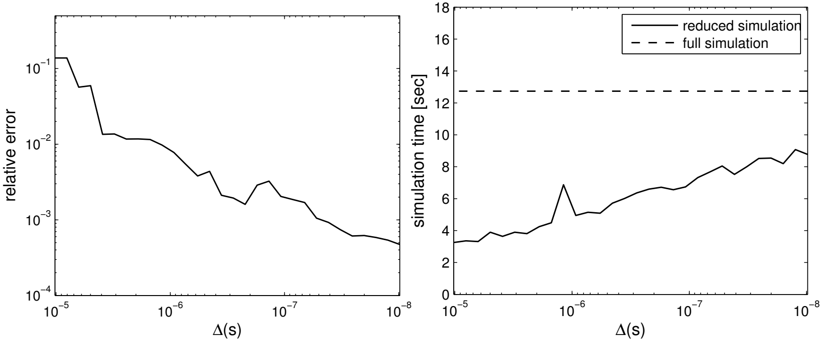


Lack of information

Select number of snapshots so that $\Delta(s) = \sqrt{\frac{\sum_{i=s+1}^{m} \sigma_i^2}{\sum_{i=1}^{m} \sigma_i^2}} \approx tol.$

Reduced model at a fixed frequency

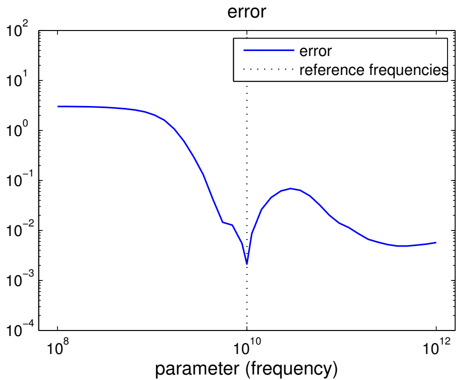
First test: Compare reduced and unreduced system at a fixed frequency.



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: $P_1 := \{f_1\} := \{10^{10}[Hz]\}$
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 admits different scales.
Scale with block diagonal matrix-valued function

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

and choose $d_\psi(f)$ according to

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

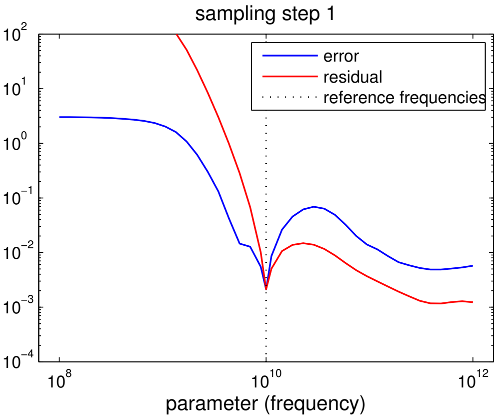
Residual based sampling

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 $d_{(.)}(f) > 0$ 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, $\ldots$, 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 $f_1 := 10^{10}[Hz]$, $P_1 := \{10^{10}[Hz]\}$, $\mathcal{P} = [10^8, 10^{12}]$.

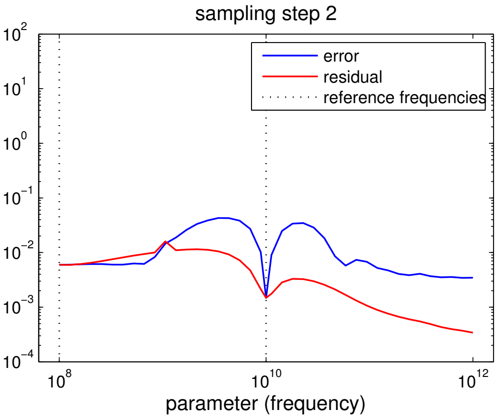


$f_2 = \arg\max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_1))\| = 10^8[Hz]$

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

Numerical example - sampling step 2

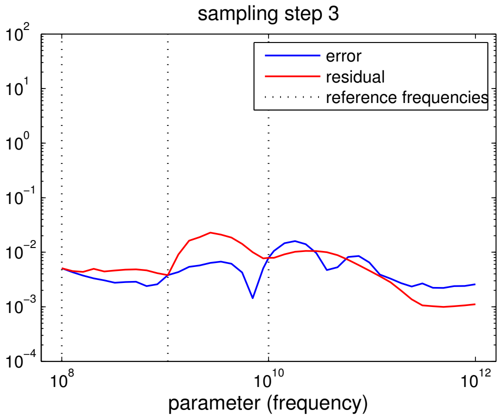
$$P_2 = \{10^8[Hz],\ 10^{10}[Hz]\}$$



$$f_3 = \arg\max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_2))\| = 1.0608 \cdot 10^9[Hz]$$
$$P_3 = \{10^8[Hz],\ 1.0608 \cdot 10^9[Hz],\ 10^{10}[Hz]\}$$

Numerical example - sampling step 3

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

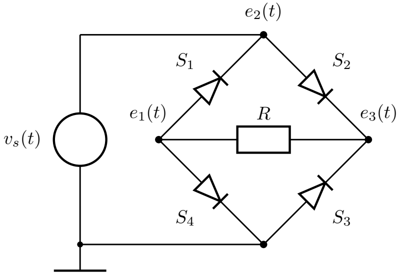


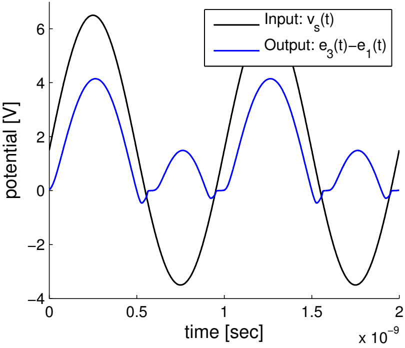
Terminate with “no progress in residual”.

Outline

Reduced model depends on position of diode in network

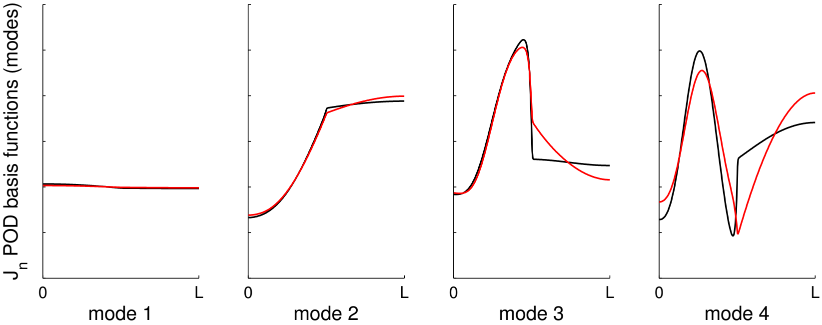
Bridge rectifier with 4 diodes:





Reduced model depends on position of diode in network

MOR yields a similar but different model for the diodes S_1 and S_2:



This can be quantified by calculating

$$\max_{\substack{u \in U^1_{J_n} \\ \|u\|_2 = 1}} \; \min_{\substack{v \in U^2_{J_n} \\ \|v\|_2 = 1}} \; \|u - v\|_2,$$

where the spaces $U^1_{J_n}$, $U^2_{J_n}$ are spanned by the J_n-POD functions of S_1, S_2.

Thank you for your attention.

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The work reported in this talk is supported by the German Federal Ministry of Education and Research (BMBF), grant no. 03HIPAE5.