Towards parametric model order reduction for nonlinear PDE systems in networks

MoRePas II 2012

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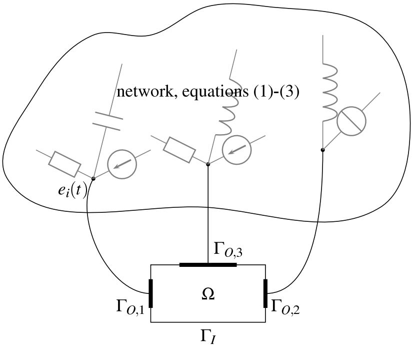
Outline

Motivation: Coupled circuit and semiconductor models



Aim

- Accurate reduced order models for semiconductors in networks
- Validity over relevant parameter range
- Accurate *physical* reduced order model of the coupled system

Outline

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

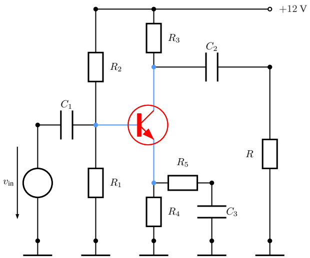
Kirchhoff's' laws (no semiconductors) read

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

A: incidence matrix.

Voltage-current relations of components:

$$j_C = \frac{\mathrm{d}q_C}{\mathrm{d}t}(v_C, t),\ j_R = g(v_R, t),\ v_L = \frac{\mathrm{d}\phi_L}{\mathrm{d}t}(j_L, t)$$



Modified Nodal Analysis: join all equations to DAE system

$$\begin{aligned} A_C \frac{\mathrm{d}q_C}{\mathrm{d}t}\left(A_C^\top e(t), t\right) + A_R g\left(A_R^\top e(t), t\right) + A_L j_L(t) + A_V j_V(t) &= -A_I i_s(t), \\ \frac{\mathrm{d}\phi_L}{\mathrm{d}t}\left(j_L(t), t\right) - A_L^\top e(t) &= 0, \\ A_V^\top e(t) &= v_s(t). \end{aligned}$$

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

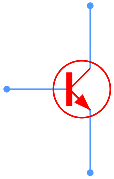
How can semiconductors be introduced?

- replace semiconductor by a (possibly nonlinear) electrical network,
- stamp semiconductor network into surrounding network,
- apply Modified Nodal Analysis.
- Here: use PDE model for semiconductors $\rightarrow$ DD equations.

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

PDE-model (drift-diffusion equations) for semiconductors

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



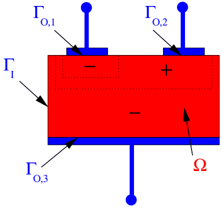
on $\Omega \times [0,T]$ with $\Omega \subset \mathbb{R}^d$ ($d = 1,2,3$).
Dirichlet boundary constraints at $\Gamma_{O,k}$:

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

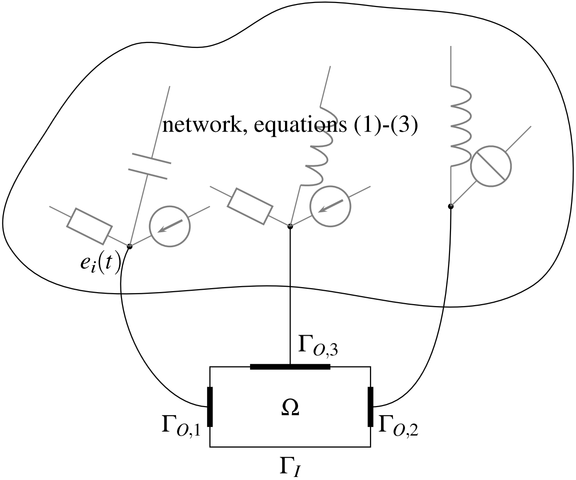
and Neumann boundary constraints at Γ_I:

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

or mixed boundary conditions at MI contacts (MOSFETs).



Couple semiconductor to circuit [M. Günther '01, C. Tischendorf '03]

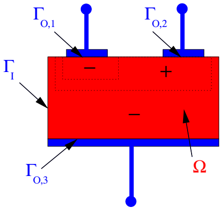


Couple semiconductor to circuit [M. Günther ’01, C. Tischendorf ’03]

Coupling conditions:

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

$$\psi(t,x) = \psi_{bi}(x) + (A_S^\top e(t))_k \quad \text{for } (t,x) \in [0,T] \times \Gamma_{O,k},$$



and add current j_S to Kirchhoff’s current law:

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

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

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

Add DD-equations + coupling conditions for each semiconductor.

Outline

Mixed formulation

The electric field $E = -\boldsymbol{\nabla}\psi$ plays dominant role in DD-equations.

Mixed formulation [Brezzi et al. '05]

Provide additional variable g_ψ and equation

$$g_\psi = \boldsymbol{\nabla}\psi.$$

Scaled DD equations then read:

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

Finite Element approximation

Finite elements

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

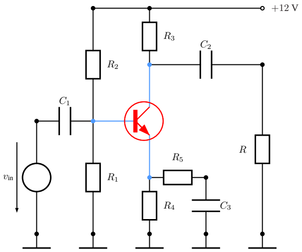
$$RT_0 := \{y : \Omega \to \mathbb{R}^d : \; y|_T(x) = a_T + b_T x, \; a_T \in \mathbb{R}^d, \; b_T \in \mathbb{R}, \\ [y]_E \cdot \boldsymbol{\nu}_E = 0, \; \text{for all inner edges } E\}.$$

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

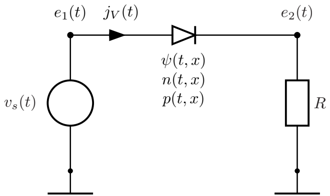


$$
\begin{aligned}
A_C \frac{\mathrm{d}q_C}{\mathrm{d}t}\left(A_C^\top e(t), t\right) + A_R g\left(A_R^\top e(t), t\right) & \\
+ A_L j_L(t) + A_V j_V(t) + A_S j_S(t) &= -A_I i_s(t), \\
\frac{\mathrm{d}\phi_L}{\mathrm{d}t}(j_L(t), t) - A_L^\top e(t) &= 0, \\
A_V^\top e(t) &= v_s(t), \\
j_S(t) - C_1 J_n(t) - C_2 J_p(t) - C_3 \dot{g}_\psi(t) &= 0,
\end{aligned}
$$

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

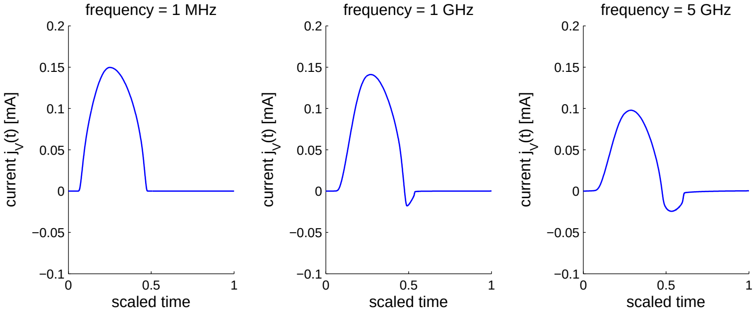
Outline

Basic test circuit, simulation results



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

similar results obtained by MECS [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 $K = Y^\top MY$ with $M_{ij} = \langle\varphi_i,\varphi_j\rangle_X$. Write POD in terms of SVD:

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

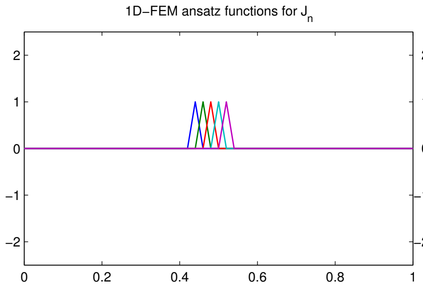
Then, the s-dimensional POD basis is

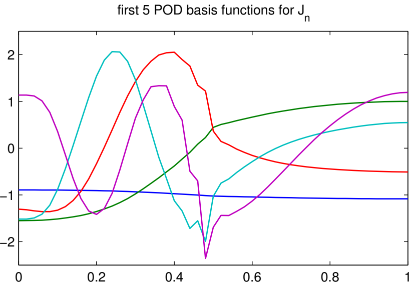
$$\left\{u^i := \sum_{j=1}^{N} \vec{u}^i_j \varphi_j(\cdot)\right\}_{i=1,\ldots,s}, \qquad U := (\vec{u}^1,\ldots,\vec{u}^s) := L^{-\top}\tilde{U}_{(:,1:s)}.$$

Model Order Reduction

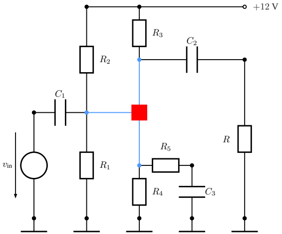
- Simulate the complete network at one or more reference parameters.
- Take snapshots of the state of each semiconductor at time points t_i.
- Perform POD component wise on ψ, n, p, g_ψ, J_n and J_p.
- Use the POD basis functions as (non local) FEM ansatz functions:

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





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:

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

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

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

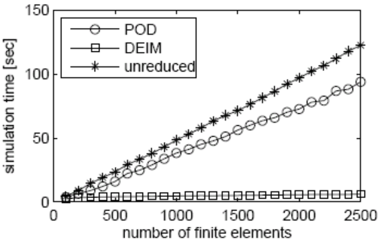
with DEIM:

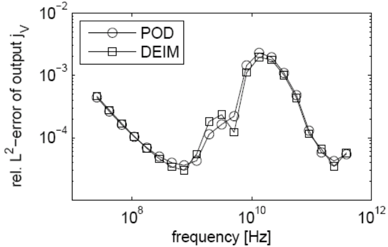
$$\underbrace{(U^\top W(P^\top W)^{-1})}_{n_{POD}\times n_{DEIM},\text{ block-dense}} \quad \underbrace{P^\top}_{n_{DEIM}} F(\underbrace{U_n\gamma_n}_{n_{FEM}}, U_p\gamma_p, U_{g_\psi}\gamma_{g_\psi})$$

Results for 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		$\approx n_{FEM}^{1.18}$		$\approx n_{FEM}^{1.10}$		$\approx n_{FEM}^{0.578}$

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

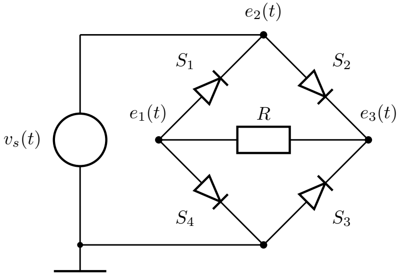


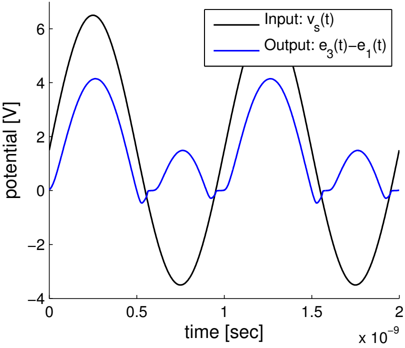


Outline

Reduced model depends on position of diode in network

Bridge rectifier with 4 diodes:





Reduced model depends on position of diode in network

The distance between the spaces U^1 and U^2 which are spanned, e.g., by the POD-functions U^1_ψ of the diode S_1 and U^2_ψ of the diode S_2 respectively, is measured by

$$d(U^1, U^2) := \max_{\substack{u \in U^1 \\ \|u\|_2 = 1}} \min_{\substack{v \in U^2 \\ \|v\|_2 = 1}} \|u - v\|_2 = \sqrt{2 - 2\sqrt{\boldsymbol{\lambda}}},$$

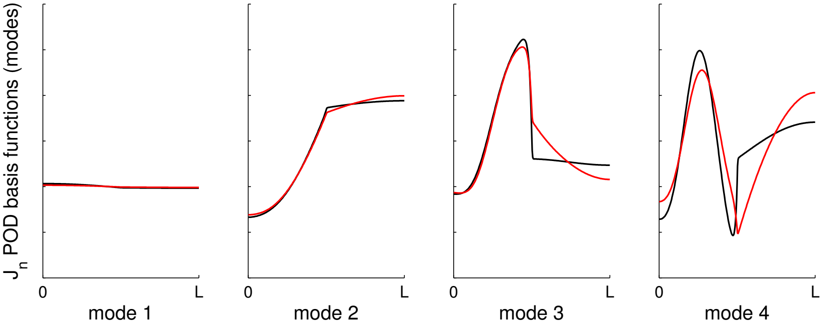
where $\boldsymbol{\lambda}$ is the smallest eigenvalue of the positive definite matrix $SS^\top$ with $S_{ij} = \langle u^1_{\psi,i}, u^2_{\psi,j} \rangle_2$.

Δ	$d(U^1, U^2)$	$d(U^1, U^3)$
10^{-4}	0.61288	$5.373 \cdot 10^{-8}$
10^{-5}	0.50766	$4.712 \cdot 10^{-8}$
10^{-6}	0.45492	$2.767 \cdot 10^{-7}$
10^{-7}	0.54834	$1.211 \cdot 10^{-6}$

Table: Distances between reduced models in the rectifier network.

Modes

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

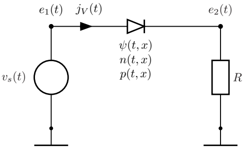


Outline

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.

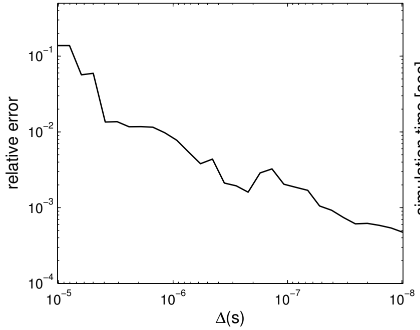


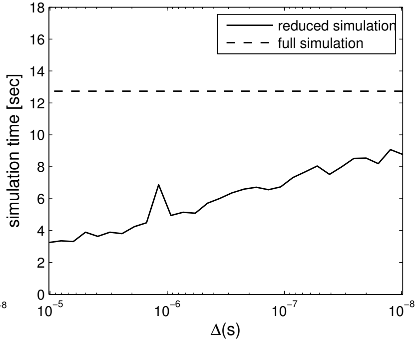
Lack of information

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.

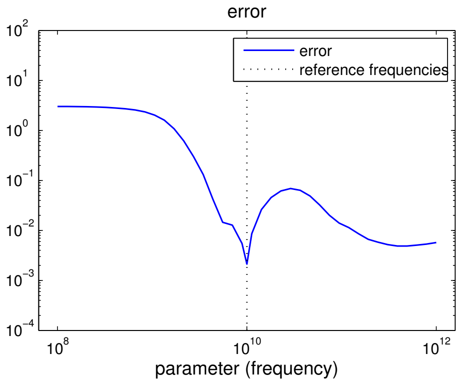




Reduced model over parameter space

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

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

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

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

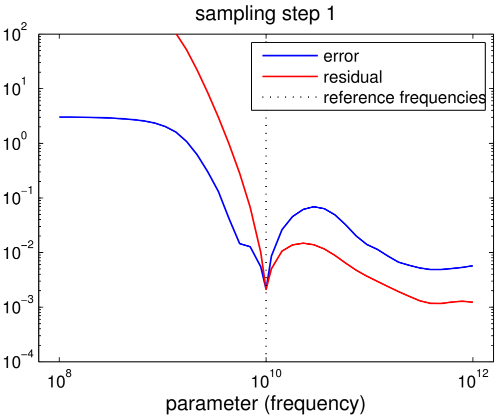
Residual based sampling

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, ..., f_k.
8. Set $P_{k+1} := P_k \cup \{f_{k+1}\}$, $k := k + 1$ and goto 3.

Numerical example - sampling step 1

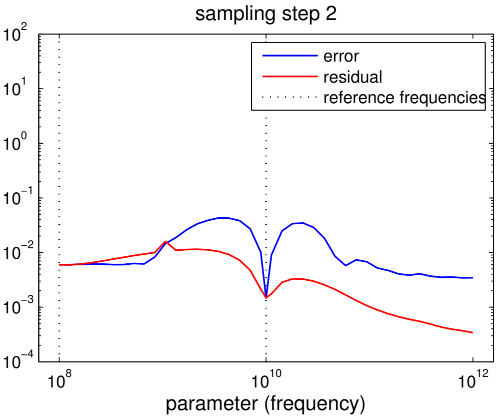
Let $f_1 := 10^{10}[Hz]$, $P_1 := \{10^{10}[Hz]\}$, $\mathcal{P} = [10^8, 10^{12}]$.



$f_2 = \arg\max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_1))\| = 10^8[Hz]$
$P_2 = \{10^8[Hz],\ 10^{10}[Hz]\}$

Numerical example - sampling step 2

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

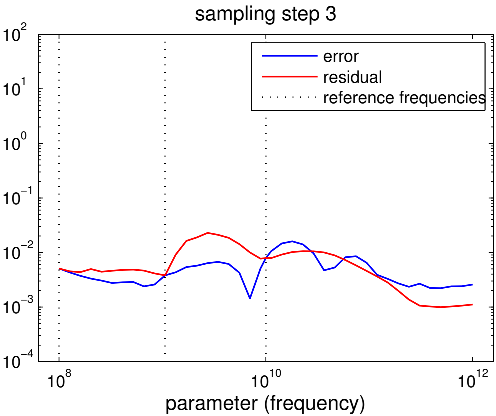


$$f_3 = \arg\max_{f \in P_{test}} \|D(f)\mathcal{R}(z^{POD}(f, P_2))\| = 1.0608 \cdot 10^9[Hz]$$

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

Numerical example - sampling step 3

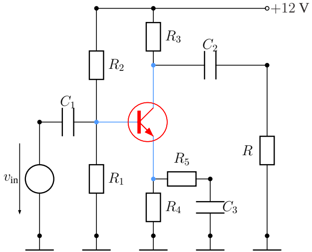
$$P_3 = \{10^8[Hz],\ 1.0608 \cdot 10^9[Hz],\ 10^{10}[Hz]\}$$



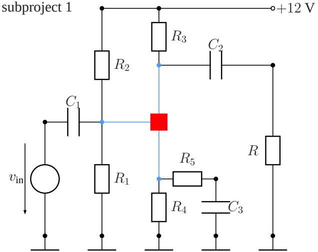
Terminate with “no progress in residual”.

Outline

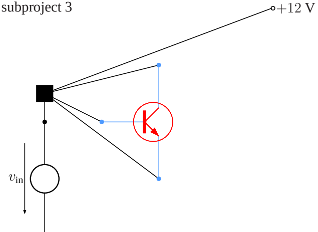
Combination of PABTEC (Reis & Stykel 2010) and POD; joint work with [A. Steinbrecher, T. Stykel]



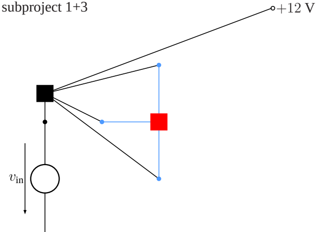
subproject 1



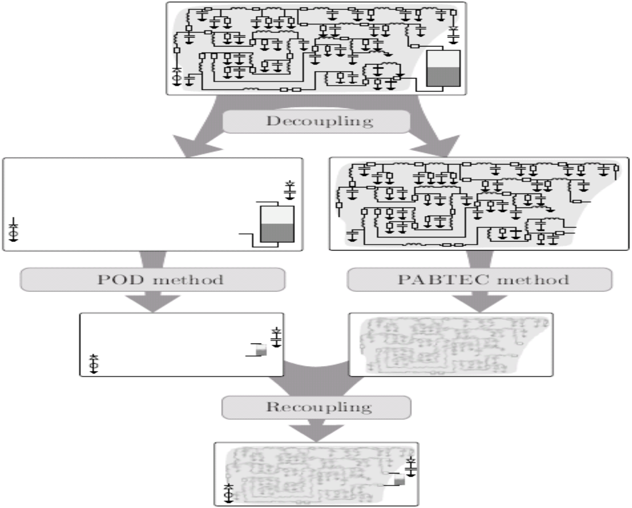
subproject 3



subproject 1+3

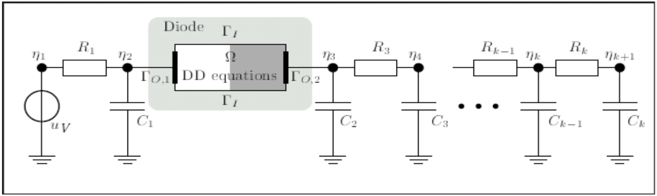


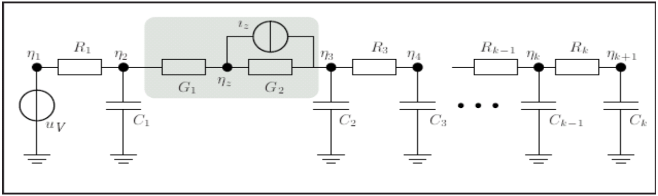
Combination of PABTEC and POD; Int. J. Numer. Model. 2012



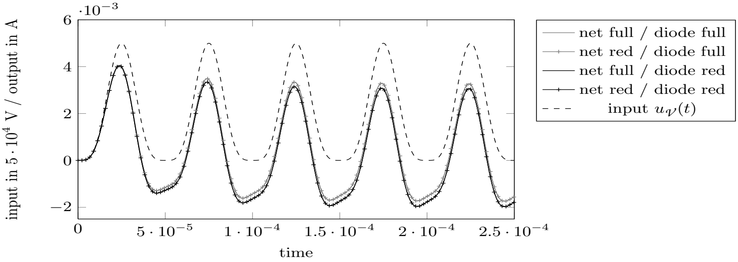
Substitution of nonlinear components for PABTEC and recoupling

A. Steinbrecher, T. Stykel (Int. J. Circuits Theory Appl., 2012):
Nonlinear inductor → current source
Nonlinear capacitor → voltage source
Nonlinear resistor → linear circuit with 2 serial resistors and one voltage source parallel to one of the resistors





Combination of PABTEC and POD; Int. J. Numer. Model. 2012



network (MNA equations) type	dim.	diode (DD equations) type	dim.	coupled system dim.	simul. time	Jacobian evaluations	absolute error $\|y-\hat{y}\|_{L_2}$	relative error $\frac{\|y-\hat{y}\|_{L_2}}{\|y\|_{L_2}}$
unreduced	1503	unreduced	6006	7510	23.37s	20		
reduced	24	unreduced	6006	6031	16.90s	17	$2.165\cdot10^{-8}$	$7.335\cdot10^{-4}$
unreduced	1503	reduced	105	1609	1.51s	16	$2.952\cdot10^{-6}$	$1.000\cdot10^{-1}$
reduced	24	reduced	105	130	1.19s	11	$2.954\cdot10^{-6}$	$1.000\cdot10^{-1}$

Next steps

- Include QDD models.
- Include EM effects.
- Generalize approach to other equation networks containing simple and complex components.

Thank you for attending!

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MoreSim_4_Nano

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