POD for Coupled Nonlinear PDE Systems

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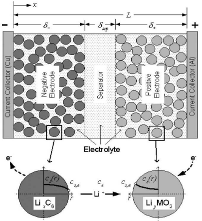
Motivation and Outline



$$\|\bar{u}_\delta - \bar{u}_\delta^\ell\| \le C\,\|\zeta_\delta^\ell\|$$

$$\|\bar{u} - \bar{u}^\ell\| \le C\,\|\zeta^\ell\|$$

- Multi component systems (battery equations)
  - PDEs with different types
  - nonlinear coupling

  → **What is a good POD model?**
- Optimization and model reduction
  - inexact second-order methods
  - inexactness by model reduction

  → **Can we ensure convergence (rate)?**
- Nonlinear model reduction
  - nonlinear optimal control
  - solve of reduced-order model

  → **Can we apply error estimates?**

POD-(D)EIM for coupled systems

[Lass/V.'11]

Fine model (well-posedness see [Wu/Xu/Zou'06])

- Elliptic-parabolic systems: $T = 1$, $\Omega = (a, b)$

$$\begin{aligned} y_t - \nabla \cdot (c_1 \nabla y) - \mathcal{N}(y, p, q; \mu) &= 0 && \text{in } Q = (0, T) \times \Omega \\ -\nabla \cdot (c_2 \nabla p) - \mathcal{N}(y, p, q; \mu) &= 0 && \text{in } Q \\ -\nabla \cdot (c_3 \nabla q) + \mathcal{N}(y, p, q; \mu) &= 0 && \text{in } Q \end{aligned}$$

- Parameter-dependent nonlinearity: $\mu = (\mu_1, \mu_2) \geq 0$

$$\mathcal{N}(y, p, q; \mu) = \mu_2 \sqrt{y} \sinh(\mu_1(q - p - \ln y))$$

- Boundary conditions: $y_x(t, a) = y_x(t, b) = p(t, a) = p_x(t, b) = 0$, $q_x(t, a) = q(t, b) = 0$
- Discretization: FE (2nd order) and implicit Euler method
- Numerical solution method: (damped) Newton algorithm

Reduced-Order Model (ROM)

- Fine model:

$$\text{(FM)}\qquad \begin{aligned} y_t - \nabla\cdot(c_1\nabla y) - \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q\\ -\nabla\cdot(c_2\nabla p) - \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q\\ -\nabla\cdot(c_3\nabla q) + \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q \end{aligned}$$

- Idea of ROM: Replace (FM) by ROM, which is reliable (i.e., sufficiently accurate), but fast to evaluate
- Procedure: Galerkin projection of (FM) with appropriate ansatz function containing characteristics of (FM)
- Methods: Reduced-Basis, **P**roper **O**rthogonal **D**ecompostion,...
- Efficiency: decouple computation in off- and online phase, where the online phase is independent of discretization of (FM)

POD basis computation

- POD criterium: $\ell \leq \dim(\operatorname{span}\{y(t) \mid t \in [0, T]\})$

$$\min \int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle \, \psi_i \Big\|^2 \mathrm{d}t \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij}$$

- Inner product: $L^2(\Omega)$ or $H^1(\Omega)$ (+b.c.)
- Solution to optimization problem:
    - $\mathcal{R}\psi_i = \int_0^T \langle y(t), \psi_i \rangle \, y(t) \, \mathrm{d}t = \lambda_i \psi_i$, $i = 1, \ldots, \ell$
    - $(\mathcal{K} v_i)(t) = \int_0^T \langle y(t), y(\cdot) \rangle \, v_i \, \mathrm{d}s = \lambda_i v_i(t)$, $i = 1, \ldots, \ell$
    - Relation via SVD: $\psi_i = \int_0^T v_i(t) y(t) \, \mathrm{d}t / \sqrt{\lambda_i}$
- Discrete variant: $\alpha_j = \mathcal{O}(\Delta t)$

$$\min \sum_{j=1}^{N_t} \alpha_j \, \Big\| y(t_j) - \sum_{i=1}^{\ell} \langle y(t_j), \psi_i \rangle \, \psi_i \Big\|^2 \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle = \delta_{ij}$$

- Solution: $YY^\top \psi_i = \lambda_i \psi_i$, $Y^\top Y v_i = \lambda_i v_i$, $Y v_i = \sqrt{\lambda_i} \psi_i$

ROM: different POD bases for y, p, and q

- Fine model:

$$
\text{(FM)}\qquad
\begin{aligned}
y_t - \operatorname{div}(c_1\nabla y) - \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q\\
-\operatorname{div}(c_2\nabla p) - \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q\\
-\operatorname{div}(c_3\nabla q) + \mathcal{N}(y,p,q;\mu) &= 0 \quad \text{in } Q
\end{aligned}
$$

- FE model for (FM): $y^h(t) = \sum_{i=1}^{N_{FE}} \bar y_i(t)\varphi_i$ etc.

$$
\begin{aligned}
M\bar y_t(t) + S_{c_1}\bar y(t) - \bar{\mathcal{N}}(\bar y(t),\bar p(t),\bar q(t);\mu) &= 0\\
S_{c_2}\bar p(t) - \bar{\mathcal{N}}(\bar y(t),\bar p(t),\bar q(t);\mu) &= 0\\
S_{c_3}\bar q(t) + \bar{\mathcal{N}}(\bar y(t),\bar p(t),\bar q(t);\mu) &= 0
\end{aligned}
$$

- ROM for (FM): $y^\ell(t) = \sum_{i=1}^{\ell^y} \hat y_i(t)\psi_i^y$ etc. [Off-/Online]

$$
\begin{aligned}
\Psi_y^\top M\Psi_y\hat y_t(t) + \Psi_y^\top S_{c_1}\Psi_y\hat y(t) - \Psi_y^\top\bar{\mathcal{N}}(y^\ell(t),p^\ell(t),q^\ell(t);\mu) &= 0\\
\Psi_p^\top S_{c_2}\Psi_p\hat p(t) - \Psi_p^\top\bar{\mathcal{N}}(y^\ell(t),p^\ell(t),q^\ell(t);\mu) &= 0\\
\Psi_q^\top S_{c_3}\Psi_q\hat q(t) + \Psi_q^\top\bar{\mathcal{N}}(y^\ell(t),p^\ell(t),q^\ell(t);\mu) &= 0
\end{aligned}
$$

Problems for the ROM

- ROM for (FM): $y^\ell(t)=\sum_{i=1}^{\ell^y}\hat y_i(t)\psi_i^y$ etc.

$$M^{\ell^y}\hat y_t(t)+S_{c_1}^{\ell^y}\hat y(t)-\Psi_y^\top\bar{\mathcal N}(y^\ell(t),p^\ell(t),q^\ell(t);\mu)=0$$
$$S_{c_2}^{\ell^p}\Psi_p\hat p(t)-\Psi_p^\top\bar{\mathcal N}(y^\ell(t),p^\ell(t),q^\ell(t);\mu)=0$$
$$S_{c_3}^{\ell^q}\hat q(t)+\Psi_q^\top\bar{\mathcal N}(y^\ell(t),p^\ell(t),q^\ell(t);\mu)=0$$

- Problem 1: Imply the reconstruction error

$$\int_0^T\Big\|y(t)-\sum_{i=1}^{\ell}\langle y(t),\psi_i\rangle\,\psi_i\Big\|^2\,\mathrm{d}t=\sum_{i>\ell}\lambda_i$$

the error relation

$$\|y-y^\ell\|^2+\|p-p^\ell\|^2+\|q-q^\ell\|^2=\mathcal O\big(\textstyle\sum_{i>\ell}\lambda_i\big)$$

- Problem 2: evaluation of the nonlinear terms

$$\Psi_y^\top\bar{\mathcal N}(y^\ell(t),p^\ell(t),q^\ell(t);\mu)\text{ etc.}$$

is of complexity $N_{FE}\gg\ell$

Problem 1: A-priori error estimation

- Problem 1: Imply the reconstruction error

$$\int_0^T \Big\| y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i \rangle \, \psi_i \Big\|^2 \, \mathrm{d}t = \sum_{i>\ell} \lambda_i$$

the error relation

$$\|y - y^\ell\|^2 + \|p - p^\ell\|^2 + \|q - q^\ell\|^2 = \mathcal{O}\big(\textstyle\sum_{i>\ell} \lambda_i\big)$$

- Theorem: There is a constant $C > 0$ such that

$$\int_0^T \|y(t) - y^\ell(t)\|^2 + \|p(t) - p^\ell(t)\|^2 + \|q(t) - q^\ell(t)\|^2 \, \mathrm{d}t$$
$$\leq C \big(\|\mathcal{P}^{\ell^y} y_\circ - y^\ell(0)\|^2 + \|\mathcal{P}^{\ell^y} y_t - y_t\|^2 \big)$$
$$+ \, C \Big(\sum_{i>\ell^y} \lambda_i^y + \sum_{i>\ell^p} \lambda_i^p + \sum_{i>\ell^q} \lambda_i^q \Big)$$

Problem 2: evaluation of $\Psi_y^\top \bar{\mathcal{N}}(y^\ell(t), p^\ell(t), q^\ell(t); \mu)$

- Replacement:
  $F(t) = \bar{\mathcal{N}}(y^\ell(t), p^\ell(t), q^\ell(t); \mu) \approx \sum_{i=1}^m c_i(t) u_i \in \mathbb{R}^{N_{FE}}$.
- Interpolation condition for $1 \le k \le m \ll N_{FE}$:

$$\big(F(t)\big)_{\mathrm{p}_k} = \Big(\sum_{i=1}^m c(t) u_i\Big)_{\mathrm{p}_k} = \sum_{i=1}^m c_i(t) \big(u_i\big)_{\mathrm{p}_k}, \quad \mathrm{p}_k \in \{1, \ldots, N_{FE}\}$$

- Computation of $c(t)$: $\underbrace{(P^T U)}_{m \times m} c(t) = P^T F(t) \in \mathbb{R}^m$
- Complexity reduction: $P^T F(t) = \bar{\mathcal{N}}(P^T y^\ell(t), P^T p^\ell(t), P^T q^\ell(t); \mu)$
- Choice for U (DEIM): POD basis for $\mathrm{span}\,\{F(t_j)\}_{j=0}^{N_t}$.
- Theorem: error estimate for POD-DEIM [compare Chaturantabut/Sorensen]
- Alternative: EIM [Maday, Patera et al.]

Run 1: accuracy (a-priori analysis) for fixed parameter μ

- "Truth" solution: $N_x = 1000$, $N_t = 100$, 2^{nd} order elements
- POD and EIM: $\ell_y = 12$, $\ell_p = 10$, $\ell_q = 10$, $\ell_{DEIM} = \ell_{EIM} = 25$
- Average relative L^2 error (FEM and POD):

	ROM	ROM-EIM	ROM-DEIM
y	1.6765×10^{-7}	1.6763×10^{-7}	1.6762×10^{-7}
p	2.8723×10^{-7}	2.7560×10^{-7}	2.7467×10^{-7}
q	9.7545×10^{-8}	9.4332×10^{-8}	9.1929×10^{-8}

- CPU time:

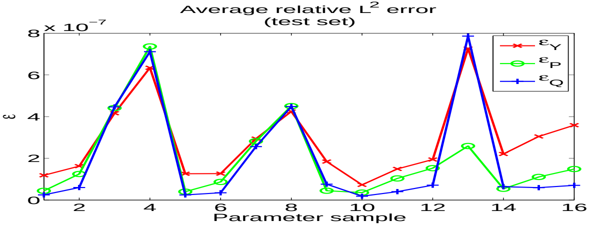
FEM	POD	EIM	DEIM	ROM	ROM-EIM	ROM-DEIM
18.20	0.20	0.19	0.03	6.03	**0.24** ($\approx 1/75$)	**0.48**

Run 2: multiple parameters

- Sample set: $\mu_{sample} \in \{1,2\} \times \{1,2\}$
- Test set: $\mu_{test} \in \{0.5, 1.5, 2.5, 3\} \times \{0.5, 1.5, 2.5, 3\}$
- POD and EIM: $\ell_y = 20$, $\ell_p = 18$, $\ell_q = 18$, $\ell_{EIM} = \ell_{DEIM} = 40$
- CPU time:

FEM	POD	EIM	DEIM	ROM	ROM-EIM	ROM-DEIM
$\sim$ **18**	0.54	0.74	0.09	$\sim$ 7.50	$\sim$ **0.30**	$\sim$ **0.60**

- Average relative L^2 error:



ROM based inexact/multilevel SQP

[Kahlbacher/V.'11]

SQP framework

- Infinite dimensional optimization:

$$(\mathbf{P}) \qquad \min J(x) \quad \text{s.t.} \quad e(x) = 0$$

- Lagrange functional for (**P**): $\mathcal{L}(x,p) = J(x) + \langle e(x), p\rangle$
- (Local) SQP method: at $z_k = (x_k, p_k)$ solve

$$(\mathbf{QP}^k) \qquad \begin{cases} \min\limits_{x_\delta} \mathcal{L}_x(z_k)x_\delta + \frac{1}{2}\mathcal{L}_{xx}(z_k)(x_\delta, x_\delta) \\ \text{s.t. } e(x_k) + e'(x_k)x_\delta = 0 \end{cases}$$

- KKT system: solution $\bar{x}_\delta$ to $(\mathbf{QP}^k)$ is characterized by

$$\underbrace{\begin{pmatrix} \mathcal{L}_{xx}(z_k) & e'(x_k)^* \\ e'(x_k) & 0 \end{pmatrix}}_{A_k} \cdot \underbrace{\begin{pmatrix} \bar{x}_\delta \\ \bar{p}_\delta \end{pmatrix}}_{\bar{z}_\delta} = \underbrace{-\begin{pmatrix} \mathcal{L}_x(z_k) \\ e(x_k) \end{pmatrix}}_{b_k}$$

Inexact SQP by using POD or RB

- KKT system: inexact solve of $A_k \bar{z}_\delta = b_k$ by discretization
- Discretization: (POD or RB or BT or...) model reduction

$$A_k^\ell \bar{z}_\delta^\ell = b_k^\ell \in \mathbb{R}^n, \quad n = n(\ell)$$

- Convergence of (local) SQP method: $\bar{z}_\delta^\ell$ reduced-order solution

$$\|A_k \mathcal{P} \bar{z}_\delta^\ell - b_k\| = \mathcal{O}\big(\|\mathcal{L}'(z_k)\|^q\big), \quad q \in [1,2],$$

  with prolongation $\mathcal{P}$

- Rate of convergence: superlinear ($1 < q < 2$), quadratic ($q = 2$)
- Control of reduced-order approach:

$$\|A_k \mathcal{P} \bar{z}_\delta^\ell - b_k\| \simeq \|\bar{z}_\delta - \mathcal{P} \bar{z}_\delta^\ell\| \simeq \|\mathcal{L}'(z_k)\|^q$$

Multilevel approach with reduced-order models

- Convergence criterium: $\|A_k\mathcal{P}\bar{z}_\delta^\ell - b_k\| \simeq \|\bar{u}_\delta - \bar{u}_\delta^\ell\| < \mathrm{TOL}$
- A-posteriori error [Tröltzsch/V.'09]:

$$\|\bar{u}_\delta - \bar{u}_\delta^\ell\| \simeq \|\underbrace{\mathcal{L}_{uy}(z_k)\tilde{y}_\delta + \mathcal{L}_{uu}(z_k)\bar{u}_\delta^\ell + e_u(x_k)^*\tilde{p}_\delta + \mathcal{L}_u(z_k)}_{:=-\bar{\zeta}^\ell}\|$$

  with $\|\bar{\zeta}^\ell\| \to 0$ for $\ell \to \infty$ (theoretically [Studinger/V.'11])
- Convergence of $\|\bar{\zeta}^\ell\|$: no rate, basis dependent [Hinze/V.'08]
- POD basis: combination with Optimality-System POD [V.'11]
- Alternatives via nonlinear optimization: Trust-Region POD [Arian/Fahl/Sachs'00, Schu/Sachs'07]
- Combination with adaptivity: [Clever/Lang/Ulbrich/Ziems]

POD a-posteriori error estimation for nonlinear problems

[Lass/Trenz/V.'1?]

Nonlinear optimal control problem

- Optimal control problem:

$$\textbf{(P)}\quad \min J(y,\mu) = \frac{1}{2}\int_\Omega |y(T,\cdot) - y_\Omega|^2\,\mathrm{d}x + \frac{1}{200}\sum_{i=1}^{2}|\mu_i|^2$$

$$\text{s.t.}\quad \begin{cases} y_t - \Delta y + \sinh\left(y\sum_{i=1}^{2}\mu_i b_i\right) = f,\ \ \frac{\partial y}{\partial n} = 0,\ \ y(0,\cdot) = y_\circ \\ \mu \in \mathcal{D}_{ad} = \left\{\mu \in \mathbb{R}^2 \,\middle|\, 0 \le \mu\right\} \end{cases}$$

- Control-to-state mapping: $\mathcal{D}_{ad} \ni \mu \mapsto y = G(\mu)$
- Reduced cost: $\hat{J}(\mu) = J(G(\mu),\mu)$
- Reduced problem: $\min_{\mu\in\mathcal{D}_{ad}} \hat{J}'(\mu)$ with Hessian $\hat{J}''(\mu) \in \mathbb{R}^{2\times 2}$

- Reduced problem: $\min_{\mu \in \mathcal{D}_{ad}} \hat{J}'(\mu)$ with Hessian $\hat{J}''(\mu) \in \mathbb{R}^{m \times m}$
- A-posteriori estimate [Kammann/Tröltzsch'11]: $\bar{\mu}$ optimal, $\bar{\mu}^\ell$ POD

$$\|\bar{\mu} - \bar{\mu}^\ell\| \leq \frac{2}{\lambda_{\min}} \|\zeta^\ell(\bar{\mu}^\ell)\|$$

where $\lambda_{\min} = \min\{\lambda \,|\, \lambda \text{ eigenvalue of } \hat{J}''(\bar{\mu})\}$ depends on $\bar{\mu}$

- Heuristic algorithm:
  - gradient-based method with second-order information
  - estimate $\lambda_{\min}$ from BFGS matrix evaluated at $\bar{\mu}^\ell$

	POD optimization	FE optimization
$2\,\|\zeta^\ell\|/\lambda_{\min}$	$1.787 \cdot 10^{-3}$	—
$\|\bar{\mu}_h - \bar{\mu}^\ell\|$	$1.277 \cdot 10^{-3}$	—
$\lambda_{\min}$	$4.952 \cdot 10^{-2}$	$4.948 \cdot 10^{-2}$
CPU time	99 s	916 s

Conclusion and References

- efficient POD-(D)EIM for coupled system
- use of a-posteriori estimates at each level of the SQP or for the nonlinear problem (POD and Reduced Basis)

- Kahlbacher/V.: *POD a-posteriori error based inexact SQP method for bilinear elliptic optimal control problems*. To appear in M2AN
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- V.: *Optimality system POD and a-posteriori error analysis for linear-quadratic problems*. Submitted 2011