Error estimates for POD Galerkin schemes

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Outline of the talk

- Continuous POD
- Numerical example: heat equation
- Snapshot POD
- Numerical example: Laser surface hardening of steel

Abstract linear evolution problem

- H, V Hilbert spaces, $V \hookrightarrow H = H' \hookrightarrow V'$ (e.g., $H = L^2$, $V = H^1$)
- Symmetric bilinear form $a(\varphi, \psi) = \langle \varphi, \psi \rangle_V$ for $\varphi, \psi \in V$
- Evolution problem:

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle y(t), \varphi \rangle_H + a(y(t), \varphi) = \langle f(t), \varphi \rangle_H \quad \text{for } t \in [0, T], \ \varphi \in V$$
$$\langle y(0), \varphi \rangle_H = \langle y_\circ, \varphi \rangle_H \quad \text{for } \varphi \in V$$

  with $y_\circ \in H$ and $f \in L^2(0, T; H)$
- Unique solution y with $\|y\| \leq C\big(\|y_\circ\| + \|f\|\big)$

Continuous POD

- Topology: $X = H$ or $X = V$
- Snapshot ensemble: $\mathcal{V} = \{y(t) \,|\, t \in [0, T]\} \subset X$, $d = \dim \mathcal{V} \le \infty$
- EVD for linear and symmetric $\mathcal{R}$ in X:

$$\mathcal{R}u_i = \int_0^T \langle u_i, y(t)\rangle_X y(t)\,\mathrm{d}t = \sigma_i^2 u_i \qquad (YY^T u_i = \sigma_i^2 u_i)$$

  and set $\lambda_i^\infty = \sigma_i^2$, $\psi_i^\infty = u_i$, $1 \le i \le \ell$

- Error formula for the POD basis of rank ℓ:

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

POD Galerkin scheme for the state equation

- POD ansatz space: $V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\} \subset V$
- POD Galerkin scheme:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle y^\ell(t), \psi\rangle_H + a(y^\ell(t), \psi) = \langle f(t), \psi\rangle_H \quad \text{for } t \in [0, T],\ \psi \in V^\ell$$
$$\langle y^\ell(0), \psi\rangle_H = \langle y_\circ, \psi\rangle_H \quad \text{for } \psi \in V^\ell$$

- Unique solution y^ℓ with $\|y^\ell\| \leq C\big(\|y_\circ\| + \|f\|\big)$
- Goal: Estimation of

$$\sup_{t\in[0,T]} \|y^\ell(t) - y(t)\|_H + \int_0^T \|y^\ell(t) - y(t)\|_V^2\,\mathrm{d}t$$

in terms of $\sum_{i=\ell+1}^{\infty} \lambda_i^\infty$

Estimation of POD error (Part 1)

- Orthogonal projection: $\mathcal{P}^\ell\varphi = \sum_{i=1}^{\ell} \langle \varphi, \psi_i^\infty \rangle_V \psi_i^\infty$ for $\varphi \in V$

  $\Rightarrow a(\mathcal{P}^\ell\varphi, \psi) = a(\varphi, \psi)$ for $\varphi \in V$, $\psi \in V^\ell$ (Ritz projector)

  $\Rightarrow y(t) - \sum_{i=1}^{\ell} \langle y(t), \psi_i^\infty \rangle_V \psi_i^\infty = y(t) - \mathcal{P}^\ell y(t)$ for $t \in [0, T]$

  $\Rightarrow \int_0^T \|y(t) - \mathcal{P}^\ell y(t)\|_V^2 \, \mathrm{d}t = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$

- Set $\vartheta(t) = \mathcal{P}^\ell y(t) - y^\ell(t) \in V^\ell$, $\varrho(t) = y(t) - \mathcal{P}^\ell y(t) \in (V^\ell)^\perp$

$$y(t) - y^\ell(t) = y(t) - \mathcal{P}^\ell y(t) + \mathcal{P}^\ell y(t) - y^\ell(t) = \varrho(t) + \vartheta(t)$$

- Error formula:

$$\int_0^T \|\varrho(t)\|_X^2 \, \mathrm{d}t = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

- Topology: $X = V$, at least

Estimation of POD error (Part 2)

- $\vartheta(t) = \mathcal{P}^\ell y(t) - y^\ell(t)$ and $a(\mathcal{P}^\ell\varphi,\psi) = a(\varphi,\psi)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\vartheta^\ell(t),\psi\rangle_H + a(\vartheta^\ell(t),\psi) = \langle y_t(t) - \mathcal{P}^\ell y_t(t),\psi\rangle_H \quad \text{for } \psi\in V^\ell$$

- $\psi = \vartheta(t)\in V^\ell$ and $a(\varphi,\varphi) = \|\varphi\|_V^2$ for $\varphi\in V$

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\vartheta(t)\|_H^2 + \|\vartheta(t)\|_V^2 \le C\,\|y_t(t) - \mathcal{P}^\ell y_t(t)\|_H^2$$

- Integrating over $(0,t)$, $t\in[0,T]$

$$\|\vartheta(t)\|_H^2 + \int_0^t \|\vartheta(s)\|_V^2\,\mathrm{d}s \le \|\vartheta(0)\|_H^2 + \int_0^T \|\underbrace{y_t(s) - \mathcal{P}^\ell y_t(s)}_{=\varrho(s)}\|_H^2\,\mathrm{d}s$$

- Recall: $y(t) - y^\ell(t) = \varrho(t) + \vartheta(t)$

Estimation of POD error (Part 3)

- New ansatz for POD: $X = V$, $\mathcal{P}^\ell\varphi = \sum_{i=1}^{\ell} \langle \varphi, \psi_i^\infty \rangle_V \psi_i^\infty$

$$\min \int_0^T \|y(t) - \mathcal{P}^\ell y(t)\|_V^2 + \|y_t(t) - \mathcal{P}^\ell y_t(t)\|_V^2 \,\mathrm{d}t \quad \text{s.t.} \quad \langle \psi_i, \psi_j \rangle_V = \delta_{ij}$$

- Error formula: $\varrho(t) = y(t) - \mathcal{P}^\ell y(t)$

$$\int_0^T \|\varrho(t)\|_V^2 + \|\varrho_t(t)\|_V^2 \,\mathrm{d}t = \|\varrho(t)\|_{H^1(0,T;V)}^2 = \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

- Consequences: $\vartheta(t) = \mathcal{P}^\ell y(t) - y^\ell(t)$

$$\sup_{t\in[0,T]} \|\varrho(t)\|_H^2 + \int_0^T \|\varrho(t)\|_V^2 \,\mathrm{d}t \le C \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

$$\sup_{t\in[0,T]} \|\vartheta(t)\|_H^2 + \int_0^T \|\vartheta(t)\|_V^2 \,\mathrm{d}t \le \|\vartheta(0)\|_H^2 + C \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

Estimation of POD error (Part 4)

- Recall $y(t) - y^\ell(t) = \varrho(t) + \vartheta(t)$ and triangle inequality

$$\sup_{t\in[0,T]} \|y^\ell(t) - y(t)\|_H^2 + \int_0^T \|y^\ell(t) - y(t)\|_V^2 \,\mathrm{d}t$$

$$\leq \underbrace{\|y^\ell(0) - \mathcal{P}^\ell y_\circ\|_H^2}_{\text{error in initial data}} + \underbrace{C \sum_{i=\ell+1}^{\infty} \lambda_i^\infty}_{\text{error in POD}}$$

- Assumptions: POD with topology $X = V$ and time derivatives
- FE: estimates for function classes, e.g., $V = H^1(\Omega)$ $\Rightarrow \|y_t(t) - R^h y_t(t)\| \sim h^p$ for any $y_t(t) \in V$, $t \in [0, T]$
- POD: estimates only for included snapshots

Empirical order of decay (EOD) [Hinze/V.]

- POD error: $y_\circ = 0$

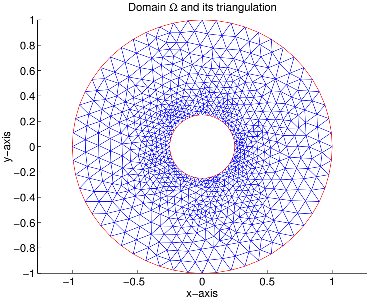
$$\sup_{t\in[0,T]} \|y^\ell(t) - y(t)\|_H^2 + \int_0^T \|y^\ell(t) - y(t)\|_V^2 \,\mathrm{d}t \sim \sum_{i=\ell+1}^{\infty} \lambda_i^\infty$$

- Ansatz for the eigenvalues: $\lambda_i^\infty = \lambda_1^\infty e^{-\alpha(i-1)}$ for $i \geq 1$
- Goal: estimation of α based on the POD error
- $\frac{\|y^\ell - y\|^2}{\|y^{\ell+1} - y\|^2} \sim \frac{\sum_{i=\ell+1}^{\infty} \lambda_i}{\sum_{i=\ell+2}^{\infty} \lambda_i} = \frac{\sum_{i=\ell+1}^{\infty} e^{-\alpha(i-1)}}{\sum_{i=\ell+2}^{\infty} e^{-\alpha(i-1)}} = \frac{\sum_{i=0}^{\infty} \left(e^{-\alpha}\right)^i}{\sum_{i=0}^{\infty} \left(e^{-\alpha}\right)^i - 1} = e^\alpha$
- Set: $Q(\ell) = \ln \frac{\|y^\ell - y\|^2}{\|y^{\ell+1} - y\|^2} \sim \alpha$
- $EOD = \frac{1}{\ell_{\max}} \sum_{\ell=1}^{\ell_{\max}} Q(\ell)$ so that $EOD \approx \alpha$

Numerical example (Part 1)

$$\begin{aligned} y_t - \Delta y &= 0 && \text{in } Q = (0,1)\times\Omega \\ \frac{\partial y}{\partial n} &= 0 && \text{on } \Sigma_1 = (0,1)\times\Gamma_1 \\ \frac{\partial y}{\partial n} &= q && \text{on } \Sigma_2 = (0,1)\times\Gamma_2 \\ y(0) &= 0 && \text{on } \Omega\subset\mathbb{R}^2 \end{aligned}$$

- $\Gamma_1 = \{\mathrm{x}=(x,y)\in\partial\Omega \,|\, \|\mathrm{x}\| = 1\}$, $\Gamma_2 = \partial\Omega\setminus\Gamma_1$
- $q(t,\mathrm{x}) = e^{-(x-0.7\cos(2\pi t))^2-(y-0.7\sin(2\pi t))^2}$
- $m = 868$ finite elements, $\delta t = 1/499$
- y^m FE solution, $\overline{\partial}_t y^m(t_j) = (y^m(t_j) - y^m(t_{j-1}))/\delta t$



- Snapshot ensemble: $\mathcal{V} = \mathrm{span}\left\{\{y^m(t_j)\}_{j=1}^n, \{\overline{\partial}_t y^m(t_j)\}_{j=2}^n\right\}$
- EVD for linear and symmetric $\mathcal{R}^n$ in X:

$$\mathcal{R}^n u_i = \sum_{j=1}^n \alpha_j \langle u_i, y^m(t_j)\rangle_X y^m(t_j) + \sum_{j=2}^n \alpha_j \langle u_i, \overline{\partial}_t y^m(t_j)\rangle_X \overline{\partial}_t y^m(t_j) = \sigma_i^2 u_i$$

and set $\lambda_i = \sigma_i^2$, $\psi_i = u_i$

Numerical example (Part 2)

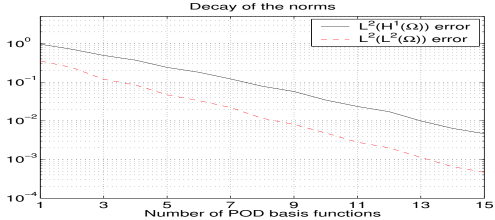
- CPU times: 2GHz desktop PC (Linux)

Computing the FE mesh and matrices	18.0 seconds
FE solve	5.0 seconds
Computing 15 POD basis functions	36.9 seconds
Computing the reduced-order model, $\ell = 15$	$<$ 0.1 seconds
POD solve, $\ell = 15$	$<$ 0.1 seconds

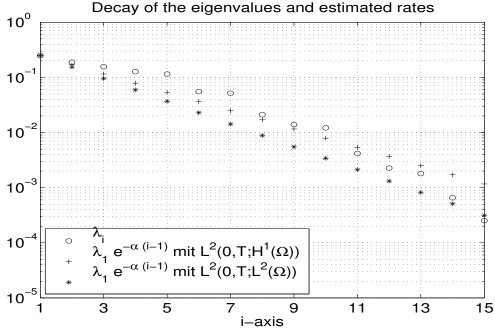
- Error: $\|\varphi\|_{L^2(0,T;X)} = \sqrt{\int_0^T \|\varphi(t)\|_X^2 \mathrm{d}t}$

X	ensemble	$\|y^h - y^\ell\|_{L^2(0,T;H^1(\Omega))}$	$\|y^h - y^\ell\|_{L^2(0,T;L^2(\Omega))}$
L^2	no DQ	0.0104	0.0012
H^1	no DQ	0.0064	0.0007
L^2	DQ	0.0064	0.0007
H^1	DQ	0.0060	0.0006

Numerical example (Part 3)



POD error with $X = H^1(\Omega)$ and included difference quotients



$$EOD = \frac{1}{\ell_{\max}} \sum_{\ell=1}^{\ell_{\max}} Q(\ell) \quad \text{with}$$

$$Q(\ell) = \ln \frac{\|y^\ell - y\|^2}{\|y^{\ell+1} - y\|^2}$$

Snapshot POD for dynamical systems

- Dynamical system (e.g., Navier Stokes) in a Hilbert space H:

$$\dot{y}(t) + Ay(t) + B(y(t)) = f(t) \text{ for } t \in (0, T) \quad \text{and} \quad y(0) = y_\circ$$

- $V \subset H$ Hilbert space with $V \hookrightarrow H = H' \hookrightarrow V'$, $X = H$ or $X = V$
- Time grid: $0 \le t_1 < t_2 < \dots t_n \le T$, $\delta t_j = t_j - t_{j-1}$ for $2 \le j \le n$
- Snapshots: $y_j = y(t_j)$, $1 \le j \le n$ and $\overline{\partial}_t y_j = \frac{y_j - y_{j-1}}{\delta t_j}$, $2 \le j \le n$
- Snapshot ensemble: $\mathcal{V} = \mathrm{span}\,\{y_1, \dots, y_n, \overline{\partial}_t y_2, \dots, \overline{\partial}_t y_n\}$, $d = \dim \mathcal{V}$
- Orthogonal decomposition in X: $\mathcal{P}^\ell \varphi = \sum_{i=1}^{\ell} \langle \varphi, \psi_i \rangle_X \psi_i$ for $\varphi \in X$
- POD basis of rank $\ell < d$: with weights $\alpha_j \ge 0$

$$\min \sum_{j=1}^{n} \alpha_j \big\| y_j - \mathcal{P}^\ell y_j \big\|_X^2 + \sum_{j=2}^{n} \alpha_j \big\| \overline{\partial}_t y_j - \mathcal{P}^\ell \overline{\partial}_t y_j \big\|_X^2 \text{ s.t. } \langle \psi_i, \psi_j \rangle_X = \delta_{ij}$$

Computation of the POD basis

- EVD for linear and symmetric $\mathcal{R}^n$ in X:

$$\mathcal{R}^n u_i = \sum_{j=1}^{n} \alpha_j \left\langle u_i, y_j \right\rangle_X y_j + \sum_{j=2}^{n} \alpha_j \left\langle u_i, \overline{\partial}_t y_j \right\rangle_X \overline{\partial}_t y_j = \sigma_i^2 u_i$$

  and set $\lambda_i = \sigma_i^2$, $\psi_i = u_i$

- Error formula for the POD basis of rank ℓ:

$$\sum_{j=1}^{n} \alpha_j \big\| y_j - \mathcal{P}^\ell y_j \big\|_X^2 + \sum_{j=2}^{n} \alpha_j \big\| \overline{\partial}_t y_j - \mathcal{P}^\ell \overline{\partial}_t y_j \big\|_X^2 = \sum_{i=\ell+1}^{d} \lambda_i$$

- Trapezoidal weights: $\alpha_1 = \frac{\delta t_1}{2}$, $\alpha_j = \frac{\delta t_j + \delta t_{j+1}}{2}$, $1 < j < n$, $\alpha_n = \frac{\delta t_n}{2}$

  $\Rightarrow$ Convergence to $\int_0^T \|y(t) - \mathcal{P}^\ell y(t)\|_X^2 + \|y_t(t) - \mathcal{P}^\ell y_t(t)\|_X^2 \, \mathrm{d}t$

POD Galerkin scheme

- Time grid: $0 = \tau_0 < \ldots < \tau_N = T$ and $\delta\tau_j = \tau_j - \tau_{j-1}$, $1 \le j \le N$
- Assumptions: $\Delta\tau/\delta\tau$ bounded, $\Delta t = O(\delta\tau)$ and $\Delta\tau = O(\delta t)$ with $\Delta\tau = \max \delta\tau_j$, $\delta\tau = \min \delta\tau_j$, $\Delta t = \max \delta t_j$, $\delta t = \min \delta t_j$
- Goal: Find $\{Y_j\}_{j=0}^N$ in $V^\ell = \mathrm{span}\,\{\psi_1, \ldots, \psi_\ell\}$

$$\begin{aligned} \langle \overline{\partial}_\tau Y_j + AY_j + B(Y_j), \psi \rangle_H &= \langle f(\tau_j), \psi \rangle_H \quad \text{for } \psi \in V^\ell,\ j = 1, \ldots, N \\ \langle Y_0, \psi \rangle_H &= \langle y_\circ, \psi \rangle_H \quad \text{for } \psi \in V^\ell \end{aligned}$$

with $\overline{\partial}_\tau Y_j = \frac{Y_j - Y_{j-1}}{\Delta\tau_j}$
$\Rightarrow$ low dimensional system

POD error estimate for Snapshot POD

- Goal: Estimation of

$$\sum_{j=0}^{N} \beta_j \, \|Y_j - y(\tau_j)\|_H^2 \approx \int_0^T \|Y(\tau) - y(\tau)\|_H^2 \, \mathrm{d}\tau$$

with $\beta_0 = \frac{\delta\tau_1}{2}$, $\beta_j = \frac{\delta\tau_j + \delta\tau_{j+1}}{2}$, $0 < j < N$, $\beta_N = \frac{\delta t_N}{2}$

- **Theorem 1** [Kunisch/V.]: $X = V$, $\Delta\tau$ small, y sufficiently smooth

$$\sum_{j=0}^{N} \beta_j \, \|Y_j - y(\tau_j)\|_H^2 \leq C \sum_{i=\ell+1}^{d} \Big(\big|\langle \psi_i, y_\circ \rangle_V\big| + \lambda_i \Big) + O\big(\Delta\tau\Delta t + (\Delta\tau)^2\big)$$

with $\Delta\tau = \max \delta\tau_j$ and $\Delta t = \max \delta t_j$

Asymptotic error estimate

- Problem: $\lambda_i = \lambda_i^{(n)}$, $\psi_i = \psi_i^{(n)}$ depend on the snapshot grid $\{t_j\}_{j=1}^n$

$$\mathcal{R}^n = \sum_{j=1}^n \alpha_j \, \langle \bullet, y_j \rangle_X y_j + \sum_{j=2}^n \alpha_j \, \langle \bullet, \overline{\partial}_t y_j \rangle_X \overline{\partial}_t y_j$$

- Fix ℓ such that eigenvalues $\{\lambda_i^\infty\}_{i\in\mathbb{N}}$ and eigenfunctions $\{\psi_i^\infty\}_{i\in\mathbb{N}}$ of

$$\mathcal{R} = \int_0^T \langle \bullet, y(t) \rangle_V y(t) + \langle \bullet, y_t(t) \rangle_V y_t(t) \, \mathrm{d}t$$

satisfy $\lambda_\ell^\infty \neq \lambda_{\ell+1}^\infty$

- **Theorem 2** [Kunisch/V.]: $X = V$, $\Delta\tau$ small, y sufficiently smooth

$$\sum_{j=0}^N \beta_j \| Y_j - y(\tau_j) \|_H^2 \leq C \sum_{i=\ell+1}^\infty \Big(|\langle \psi_i^\infty, y_\circ \rangle_V|^2 + \lambda_i^\infty \Big) + O\big((\Delta\tau)^2\big)$$

Sketch of the proof

- Theorem 1:

$$\sum_{j=0}^{N} \beta_j \, \| Y_j - y(\tau_j) \|_H^2 \leq C \sum_{i=\ell+1}^{d} \Big(\big| \langle \psi_i, y_\circ \rangle_V \big| + \lambda_i \Big) + O\big(\Delta\tau\Delta t + (\Delta\tau)^2\big)$$

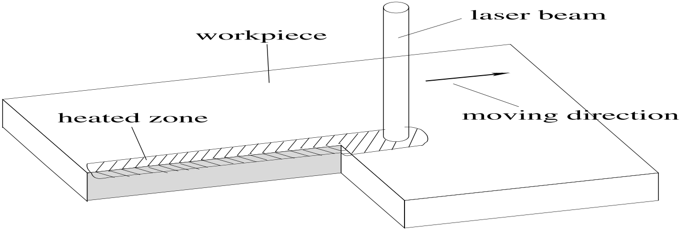
- Weights and smoothness of $y \Rightarrow \lim_{n\to\infty} \|\mathcal{R}_n - \mathcal{R}\| = 0$
- perturbation theory for eigenvalues [Kato]
- Choose $n_\circ \in \mathbb{N}$ such that for all $n \geq n_\circ$

$$\sum_{i=\ell+1}^{d(n)} \lambda_i^{(n)} \leq 2 \sum_{i=\ell+1}^{\infty} \lambda_i^{\infty}$$

$$\sum_{i=\ell+1}^{d(n)} \big| \langle \psi_i^{(n)}, y_\circ \rangle_V \big|^2 \leq 2 \sum_{i=\ell+1}^{\infty} \big| \langle \psi_i^{\infty}, y_\circ \rangle_V \big|$$

Problem formulation

- Laser surface hardening of steel [Hömberg/V.]:



- Phase transition of steel:

$$\left.\begin{array}{l}\text{ferrite}\\ \text{pearlite}\\ \text{bainite}\\ \text{martensite}\end{array}\right\} \xrightarrow{\text{heating}} \text{austenite} \xrightarrow{\text{cooling}} \left\{\begin{array}{l}\text{ferrite}\\ \text{pearlite}\\ \text{bainite}\\ \text{martensite}\end{array}\right.$$

Model equations

- Energy balance and Fourier's law:

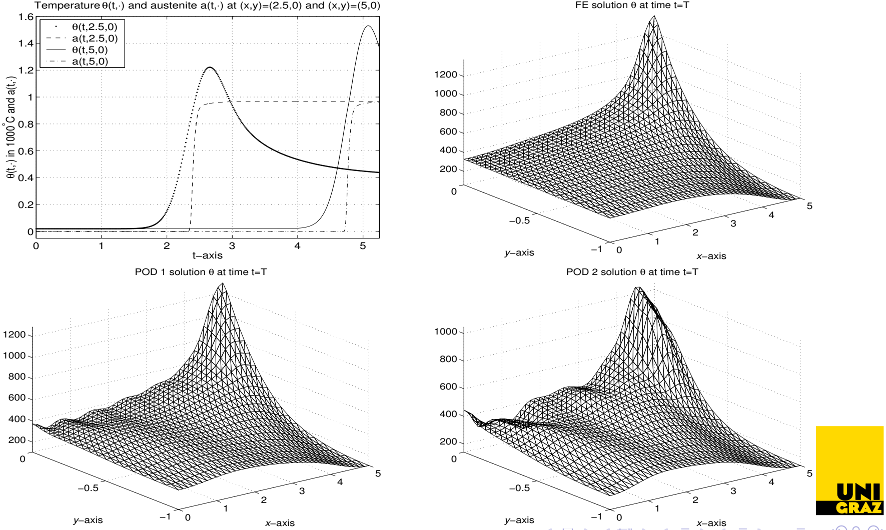
$$\begin{cases} \varrho c_p \theta_t - k\Delta\theta = \alpha u - \varrho L a_t & \text{in } Q = (0,T)\times\Omega \\ \frac{\partial\theta}{\partial n} = 0 & \text{auf } \Sigma = (0,T)\times\partial\Omega \\ \theta(0,\cdot) = \theta_\circ & \text{in } \Omega \subset \mathbb{R}^d \end{cases}$$

- Phase transition of austenite:

$$\begin{cases} a_t = f(\theta, a) & \text{in } Q \\ a(0,\cdot) = 0 & \text{in } \Omega \end{cases}$$

- Intensity of the laser: $u = u(t) \in L^2(0,T)$
- Nonlinearity: $f_+(\theta, a) = \max\left\{a_{eq}(\theta) - a, 0\right\}/\tau(\theta),\ \tau(\theta) > 0$

FE and POD temperatures at $t = T$



POD error

- Measures for the error:

$$\Psi^i = \frac{\max\limits_{0\le j\le N} \|\theta^j_\ell - \theta^j_{FE}\|_{L^\infty(\Omega)}}{\max\limits_{0\le j\le N} \|\theta^j_{FE}\|_{L^\infty(\Omega)}} \quad \text{with} \quad \begin{cases} i=1 & \text{POD with DQ} \\ i=2 & \text{POD without DQ} \end{cases}$$

	$X = L^2(\Omega)$		$X = H^1(\Omega)$	
ℓ	Ψ^1	Ψ^2	Ψ^1	Ψ^2
10	24.1%	40.6%	21.0%	40.1%
25	1.6%	26.9%	4.0%	24.6%

- Heuristic: $\mathcal{E}(\ell) = \sum_{i=1}^{\ell} \lambda_i \Big/ \sum_{i=1}^{d} \lambda_i \cdot 100\% \;\ge 94\%$

	$\ell = 10$	$\ell = 15$	$\ell = 20$	$\ell = 25$
$\mathcal{E}(\ell)$, $X = L^2(\Omega)$	94.3	98.4	99.5	99.8
$\mathcal{E}(\ell)$, $X = H^1(\Omega)$	77.7	87.4	92.5	95.7

References

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