MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

1998
2023

CSC

COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

A Posteriori Error Estimation for Model Order Reduction of Parametric Systems

Peter Benner

Joint work with:
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Collaborators:
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6th International Workshop on Model Reduction Techniques (MORTech23)
November 22 – 24, 2023
Paris, France

Talk outline

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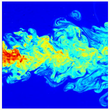
Motivation



Truth

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} + \nabla\mathbf{p} = \nu\Delta\mathbf{v}, \qquad \nabla.\mathbf{v} = \mathbf{0}$$

Model

$$\mathcal{E}\frac{d\mathbf{x}}{dt} = \mathcal{A}\mathbf{x} + \mathbf{f}(\mathbf{x}) + \mathbf{B}\mathbf{u}, \qquad \mathbf{y} = \mathbf{C}\mathbf{x}$$

Discrete

$$\widehat{\mathcal{E}}\frac{d\widehat{\mathbf{x}}}{dt} = \widehat{\mathcal{A}}\widehat{\mathbf{x}} + \widehat{\mathbf{f}}(\mathbf{x}) + \widehat{\mathbf{B}}\mathbf{u}, \qquad \widehat{\mathbf{y}} = \widehat{\mathbf{C}}\widehat{\mathbf{x}}$$

Reduced

- **Goal:** modelling physical phenomena,

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- **Reduced** models are key to enable real-time/multi-query computations.

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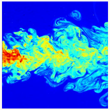

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Truth → **Model** → **Discrete** → **Reduced**

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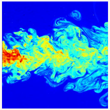
The Accuracy Chain

Model error
↓
Discretization error
↓
Reduction error



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→ **Crucial to quantify reduction error in applications like digital twins.**

→ **Error estimation key to drive adaptive model reduction.**

Talk outline

Mathematical setting

Full-order model (FOM)

$$\begin{aligned}\mathbf{E}(\boldsymbol{\mu})\dot{\mathbf{x}}(t,\boldsymbol{\mu}) &= \mathbf{A}(\boldsymbol{\mu})\mathbf{x}(t,\boldsymbol{\mu}) + \mathbf{f}(\mathbf{x},\boldsymbol{\mu}) + \mathbf{B}\mathbf{u}(t),\\ \mathbf{x}(0,\boldsymbol{\mu}) &= \mathbf{x}_0(\boldsymbol{\mu}),\\ \mathbf{y}(t,\boldsymbol{\mu}) &= \mathbf{C}(\boldsymbol{\mu})\mathbf{x}(t,\boldsymbol{\mu}).\end{aligned}$$

- $\mathbf{x}(t,\boldsymbol{\mu}), \mathbf{f}(\mathbf{x},\boldsymbol{\mu}) \in \mathbb{R}^N$
- $\mathbf{E}(\boldsymbol{\mu}), \mathbf{A}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times N}$
- $\mathbf{B}(\boldsymbol{\mu}) \in \mathbb{R}^{N\times N_I}$, $\mathbf{u}(t) \in \mathbb{R}^{N_I}$
- $\mathbf{C}(\boldsymbol{\mu}) \in \mathbb{R}^{N_O} \times N$, $\mathbf{y}(t,\boldsymbol{\mu}) \in \mathbb{R}^{N_O}$
- $t \in [0,\, T]$, $\boldsymbol{\mu} \in \mathcal{P} \subset \mathbb{R}^p$

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- $\widehat{\mathbf{x}}(t,\boldsymbol{\mu}), \widehat{\mathbf{f}}(\mathbf{x},\boldsymbol{\mu}) \in \mathbb{R}^n$
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- $\mathbf{V} \in \mathbb{R}^{N\times n}$, $n \ll N$

Mathematical setting

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Model order reduction:

- Need $\boldsymbol{\mu}$-independent projection matrix $\mathbf{V}$
- Approaches: Reduced Basis Method (RBM), Moment-matching (MM), ...

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Certifying accuracy:

- State error: $\|\mathbf{x}(t,\boldsymbol{\mu}) - \widetilde{\mathbf{x}}(t,\boldsymbol{\mu})\| \leq \Delta_{\mathbf{x}}(t,\boldsymbol{\mu})$
- Output error: $\|\mathbf{y}(t,\boldsymbol{\mu}) - \widehat{\mathbf{y}}(t,\boldsymbol{\mu})\| \leq \Delta_{\mathbf{y}}(t,\boldsymbol{\mu})$

A posteriori error estimation

Prior work:

- a posteriori state/output error bounds/estimators in RBM literature

  [Veroy et al. '02, Rovas '03, Grepl '05], [Haasdonk/Ohlberger '08, Drohmann et al. '12, Wirtz et al. '14], [Urban/Patera '14, Hain et al. '19] and many more...

- a posteriori state/output error bounds/estimators in moment-matching literature

  [Grimme '97, Bechtold et al. '04, Hetmanuik et al. '14, Bodendiek/Bollhöfer '14, Feng et al. '17] and many more...

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  and many more...

Some shortcomings:

- For time-dependent systems, involves summation of residuals over time
  $\rightsquigarrow$ overestimation of error.
- Precludes use of ODE solvers as residual expression needs to be known.
- Cost of computing coercivity/inf-sup constant; overestimation for nearly unstable problems.
- Need knowledge of weak-form/discretization.

⋮

Linear systems:

- L. Feng and P. Benner.
  On error estimation for reduced-order modeling of linear non-parametric and parametric systems.
  ESAIM: Math. Model. Numer. Anal., 55(2):561–594, 2021
- S. Chellappa, L. Feng, V. de la Rubia, and P. Benner.
  Adaptive interpolatory MOR by learning the error estimator in the parameter domain.
  In *Model Reduction of Complex Dynamical Systems*, volume 171 of *International Series of Numerical Mathematics*, pages 97–117. Birkhäuser, Cham, 2021
- S. Chellappa, L. Feng, V. de la Rubia, and P. Benner.
  Inf-sup-constant-free state error estimator for model order reduction of parametric systems in electromagnetics.
  IEEE Trans. Microw. Theory Techn., 71(11):4762–4777, 2023
- L. Feng, L. Lombardi, G. Antonini, and P. Benner.
  Multi-fidelity error estimation accelerates greedy model reduction of complex dynamical systems.
  Int. J. Numer. Methods. Engrg., 124(23):5312–5333, 2023

Nonlinear systems:

- S. Chellappa, L. Feng, and P. Benner.
  Adaptive basis construction and improved error estimation for parametric nonlinear dynamical systems.
  Int. J. Numer. Methods. Engrg., 121(23):5320–5349, 2020
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Review paper:

L. Feng, S. Chellappa, P. Benner, A Posteriori Error Estimation for Model Order Reduction of Parametric Systems, 2023. `10.21203/rs.3.rs-3410762/v1`

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Time-discrete FOM

$$\mathbf{E}\mathbf{x}^k = \mathbf{A}\mathbf{x}^{k-1} + \delta t\left(\mathbf{f}(\mathbf{x}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1}\right),$$
$$\mathbf{x}^0 = \mathbf{x}_0,$$
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Time-discrete ROM

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Hyperreduced Time-discrete ROM

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Dual system:

$$\mathbf{E}^\mathsf{T}\mathbf{x}_{\mathsf{du}} = \mathbf{C}^\mathsf{T}.$$

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Reduced dual system:

$$\widehat{\mathbf{E}}^\mathsf{T}\widehat{\mathbf{x}}_{\mathsf{du}} = \widehat{\mathbf{C}}^\mathsf{T}.$$

Theorem (simplified) [Zhang/Feng/B. '15]

The output error $\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\|$ can be bounded as

$$\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\| \leq \tilde{\rho}\,\Phi^k \left\|\mathbf{r}_{\mathsf{pr}}^k\right\| =: \Delta_{\mathbf{y},\mathsf{out1}}.$$

- $\tilde{\rho} := \dfrac{\left\|\check{\mathbf{r}}_{\mathsf{pr}}^k\right\|}{\left\|\mathbf{r}_{\mathsf{pr}}^k\right\|}$ and $\Phi^k := \left\|\mathbf{E}^{-1}\right\| \left\|\mathbf{r}_{\mathsf{du}}\right\| + \left\|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\right\|$.

- Error contributions from RB and (D)EIM approximations:

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$$\mathbf{r}_{\mathsf{pr}}^k = \underbrace{\mathbf{A}\widetilde{\mathbf{x}}^{k-1} + \widehat{\mathbf{f}}(\widetilde{\mathbf{x}}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1} - \mathbf{E}\widetilde{\mathbf{x}}^k}_{\mathbf{r}_{\mathsf{pr,RB}}^k} + \underbrace{\mathbf{f}(\mathbf{V}\widehat{\mathbf{x}}^{k-1}) - \mathcal{I}[\mathbf{f}(\mathbf{V}\widehat{\mathbf{x}}^{k-1})]}_{\mathbf{e}_{\mathsf{EI}}^k}.$$

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- Auxiliary residual $\check{\mathbf{r}}_{\text{pr}}^k := \mathbf{A}\mathbf{x}^{k-1} + \mathcal{I}[\mathbf{f}(\mathbf{x}^{k-1})] + \mathbf{B}\mathbf{u}^{k-1} - \mathbf{E}\widetilde{\mathbf{x}}^k$
  $\rightsquigarrow$ needs true solution!

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- Error indicator:

$$\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\| \lessapprox \bar{\rho}(\boldsymbol{\mu}^*)\,\Phi^k \,\|\mathbf{r}_{\mathsf{pr}}^k\| =: \tilde{\Delta}_{\mathbf{y},\mathsf{out1}}.$$

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- Error contributions from RB and (D)EIM approximations:

$$\mathbf{r}_{\mathsf{pr}}^k = \underbrace{\mathbf{A}\widetilde{\mathbf{x}}^{k-1} + \widehat{\mathbf{f}}(\widetilde{\mathbf{x}}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1} - \mathbf{E}\widetilde{\mathbf{x}}^k}_{\mathbf{r}_{\mathsf{pr,RB}}^k} + \underbrace{\mathbf{f}(\mathbf{V}\widehat{\mathbf{x}}^{k-1}) - \mathcal{I}[\mathbf{f}(\mathbf{V}\widehat{\mathbf{x}}^{k-1})]}_{\mathbf{e}_{\mathsf{EI}}^k}.$$

- Auxiliary residual $\check{\mathbf{r}}_{\mathsf{pr}}^k := \mathbf{A}\mathbf{x}^{k-1} + \mathcal{I}[\mathbf{f}(\mathbf{x}^{k-1})] + \mathbf{B}\mathbf{u}^{k-1} - \mathbf{E}\widetilde{\mathbf{x}}^k$
  $\rightsquigarrow$ needs true solution!

- Error indicator:

$$\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\| \lessapprox \bar{\rho}(\boldsymbol{\mu}^*)\,\Phi^k\,\|\mathbf{r}_{\mathsf{pr}}^k\| =: \tilde{\Delta}_{\mathbf{y},\mathrm{out1}}.$$

- No quadratic convergence of the error!

Theorem (simplified) [Chellappa/Feng/B. '19]

For the modified output $\bar{\mathbf{y}}^k := \widehat{\mathbf{y}}^k + (\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}^k_{\mathsf{du}})^\mathsf{T}\mathbf{r}^k_{\mathsf{pr}}$, the output error $\left\|\mathbf{y}^k - \bar{\mathbf{y}}^k\right\|$ can be bounded as

$$\left\|\mathbf{y}^k - \bar{\mathbf{y}}^k\right\| \leq \tilde{\rho}\|\mathbf{E}^{-1}\|\,\|\mathbf{r}^k_{\mathsf{du}}\|\,\|\mathbf{r}^k_{\mathsf{pr}}\| + \|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}^k_{\mathsf{du}}\|\|\mathbf{r}^k_{\mathsf{pr}} - \check{\mathbf{r}}^k_{\mathsf{pr}}\| =: \Delta_{\mathbf{y},\mathsf{out2}}.$$

- Error indicator:

$$\left\|\mathbf{y}^k - \bar{\mathbf{y}}^k\right\| \lessapprox \left(\bar{\rho}(\boldsymbol{\mu}^*)\|\mathbf{E}^{-1}\|\,\|\mathbf{r}^k_{\mathsf{du}}\| + |1 - \bar{\rho}(\boldsymbol{\mu}^*)|\|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\|\right)\|\mathbf{r}^k_{\mathsf{pr}}\| =: \tilde{\Delta}_{\mathbf{y},\mathsf{out2}}.$$

Theorem (simplified) [Chellappa/Feng/B. '19]

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$$\left\|\mathbf{y}^k - \bar{\mathbf{y}}^k\right\| \leq \tilde{\rho}\|\mathbf{E}^{-1}\| \, \|\mathbf{r}^k_{\mathsf{du}}\| \, \|\mathbf{r}^k_{\mathsf{pr}}\| + \|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}^k_{\mathsf{du}}\| \|\mathbf{r}^k_{\mathsf{pr}} - \check{\mathbf{r}}^k_{\mathsf{pr}}\| =: \Delta_{\mathbf{y},\mathsf{out2}}.$$

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- $\bar{\rho}(\boldsymbol{\mu}^*) \to 1.$

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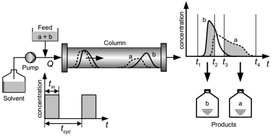
$$\left\|\mathbf{y}^k - \bar{\mathbf{y}}^k\right\| \lessapprox \left(\bar{\rho}(\boldsymbol{\mu}^*)\|\mathbf{E}^{-1}\| \, \|\mathbf{r}^k_{\text{du}}\| + |1 - \bar{\rho}(\boldsymbol{\mu}^*)| \|\mathbf{V}_{\text{du}}\widehat{\mathbf{x}}_{\text{du}}\|\right) \|\mathbf{r}^k_{\text{pr}}\| =: \tilde{\Delta}_{\mathbf{y},\text{out2}}.$$

- $\bar{\rho}(\boldsymbol{\mu}^*) \to 1.$
- Still no quadratic convergence, but close $\rightsquigarrow$ tighter estimate!
- Shortcoming: Applicable to IMEX discretizations only!

Batch chromatography:[1]

$$\frac{\partial c_z}{\partial t} + \frac{1-\epsilon}{\epsilon}\frac{\partial q_z}{\partial t} = -\frac{\partial c_z}{\partial v} + \frac{1}{Pe}\frac{\partial^2 c_z}{\partial v^2},$$
$$\frac{\partial q_z}{\partial t} = \frac{L}{Q/\epsilon A_c}\kappa_z(q_z^{\mathsf{Eq}} - q_z).$$



parameter space $(Q, t_{in}) \in [0.0667, 0.1667] \times [0.5, 2.0]$, $N = 4 \times 800$.

Adaptive POD-Greedy:

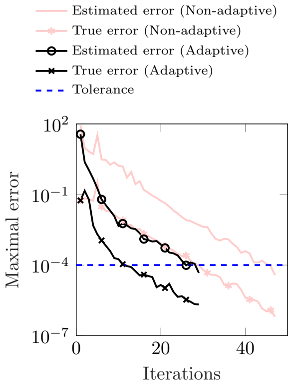
- adaptive basis update:
  $\rightarrow$ update projection basis based on estimated error, e.g.

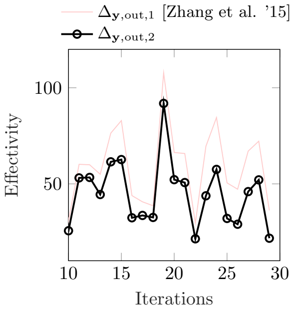
$$\delta n_{\mathsf{RB}} := \left\lfloor \log_{10}\left(\frac{\Delta_{\mathbf{y}}(\boldsymbol{\mu}^*)}{\mathtt{tol}}\right)\right\rfloor.$$

- adaptive training set sampling:
  $\rightarrow$ update training set Ξ iteratively, using radial basis interpolation.

[1] S. Chellappa, L. Feng, and P. Benner. Adaptive basis construction and improved error estimation for parametric nonlinear dynamical systems. *Int. J. Numer. Methods. Engrg.*, 121(23):5320–5349, 2020

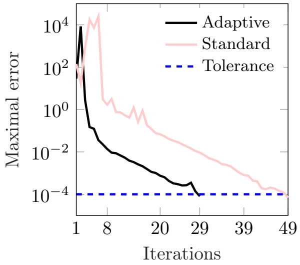
Adaptive basis updates:



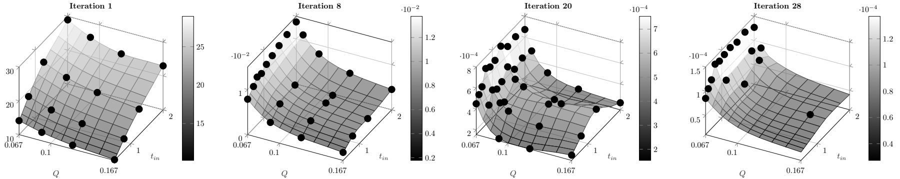


	Standard	Adaptive
ROM Size (n, n_{EI})	$(47, 109)$	$(46, 50)$
Offline time (s)	11260	**7140**
Iterations	47	**29**

Adaptive parameter sampling:

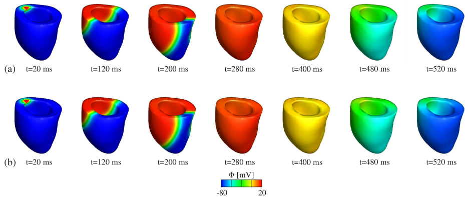


	Standard	Adaptive
ROM Size (n, n_{EI})	$(49, 99)$	$(48, 49)$
Offline time (s)	2421	**1436**
Iterations	49	**29**



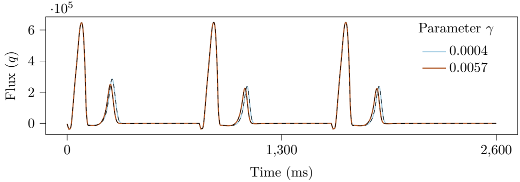
Left ventricle of the human heart:[2]

- FEM model of the left ventricle with $N = 2 \times 4129$.
- POD-Greedy with adaptive basis updates + adaptive parameter sampling.
- ROM: $n, n_{\mathsf{EI}} = (76, 187) \to$ Speedup: 49-x.



Transmembrane potential from FOM (top) and ROM (bottom).

ECG at two test parameters.



[2] S. Chellappa, B. Cansiz, L. Feng, P. Benner, and M. Kaliske. Fast and reliable reduced-order models for cardiac electrophysiology. e-prints 2311.06164, arXiv, 2023

- Previous error estimators (e.g., $\Delta_{\mathbf{y},\text{out1}}$, $\Delta_{\mathbf{y},\text{out2}}$) are **residual-based** and need knowledge of the time discretization scheme used.
- In many applications, adaptive order, adaptive time-stepping ODE solvers may be preferred, e.g., **stiff systems**.
- Most scientific computing software implement efficient ODE solvers e.g., MATLAB®, Python, PETSc, Julia, ...
- We use **closure modelling** to derive an error estimator independent of the time discretization scheme used.[3]

[3] S. Chellappa, L. Feng, and P. Benner. Accurate error estimation for model reduction of nonlinear dynamical systems via data-enhanced error closure.
e-prints 2307.11138, arXiv, 2023

- Consider the following time continuous FOM solved with an ODE solver:

$$\mathcal{E}\frac{d}{dt}\mathbf{x}(t) = \mathcal{A}\mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t)) + \mathbf{B}\mathbf{u}(t). \tag{1}$$

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- Impose a chosen implicit-explicit (IMEX) time discretization scheme on (1), resulting in

$$\mathbf{E}_{\text{ie}}\mathbf{x}_{\text{ie}}^{k} = \mathbf{A}_{\text{ie}}\mathbf{x}_{\text{ie}}^{k-1} + \delta t\left(\mathbf{f}(\mathbf{x}_{\text{ie}}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1}\right). \tag{2}$$

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- Insert ODE solver solution $\mathbf{x}^k$ in (2) to define the defect/closure term as:

$$\mathbf{d}^{k} := \mathbf{E}_{\mathsf{ie}}\mathbf{x}^{k} - \mathbf{A}_{\mathsf{ie}}\mathbf{x}^{k-1} - \delta t\left(\mathbf{f}(\mathbf{x}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1}\right). \tag{3}$$

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- The corrected FOM (C-FOM) is:

$$\mathbf{E}_{\text{ie}}\mathbf{x}_{\text{ie,c}}^{k} = \mathbf{A}_{\text{ie}}\mathbf{x}_{\text{ie,c}}^{k-1} + \delta t\left(\mathbf{f}(\mathbf{x}_{\text{ie,c}}^{k-1}) + \mathbf{B}\mathbf{u}^{k-1}\right) + \mathbf{d}^{k}. \tag{4}$$

- Consider the following time continuous FOM solved with an ODE solver:

$$\mathcal{E}\frac{d}{dt}\mathbf{x}(t) = \mathcal{A}\mathbf{x}(t) + \mathbf{f}(\mathbf{x}(t)) + \mathbf{B}\mathbf{u}(t). \tag{1}$$

- Impose a chosen implicit-explicit (IMEX) time discretization scheme on (1), resulting in

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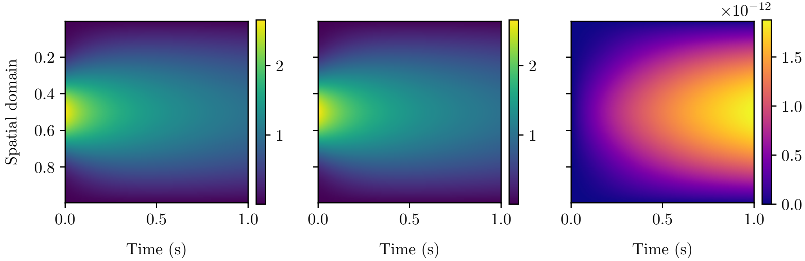
$\rightarrow$ **If $d^k(\boldsymbol{\mu})$ is accurate, $\mathbf{x}_{\text{ie,c}}^k(\boldsymbol{\mu})$ recovers the ODE solver solution $\mathbf{x}^k(\boldsymbol{\mu})$.**

Heat equation:

$$\frac{\partial}{\partial t}v(z,t;\mu) - \mu\frac{\partial^2}{\partial z^2}v(z,t;\mu) = 0.$$



Solution to the heat equation;
Left: ODE solver; **Middle:** C-FOM; **Right:** pointwise errors.

C-FOM:

$$\mathbf{E}_{\mathsf{ie}}\mathbf{x}^k_{\mathsf{ie,c}} = \mathbf{A}_{\mathsf{ie}}\mathbf{x}^{k-1}_{\mathsf{ie,c}} + \delta t\big(\mathbf{f}(\mathbf{x}^{k-1}_{\mathsf{ie,c}}) + \mathbf{B}\mathbf{u}^k\big) + \mathbf{d}^k,$$
$$\mathbf{y}^k_{\mathsf{ie1,c}} = \mathbf{C}\mathbf{x}^k_{\mathsf{ie1,c}}.$$

C-ROM:

$$\widehat{\mathbf{E}}_{\mathsf{ie}}\widehat{\mathbf{x}}^k_{\mathsf{ie,c}} = \widehat{\mathbf{A}}_{\mathsf{ie}}\widehat{\mathbf{x}}^{k-1}_{\mathsf{ie,c}} + \delta t\big(\widehat{\mathbf{f}}(\widehat{\mathbf{x}}^{k-1}_{\mathsf{ie,c}}) + \widehat{\mathbf{B}}\mathbf{u}^k\big) + \widehat{\mathbf{d}}^k,$$
$$\widehat{\mathbf{y}}^k_{\mathsf{ie,c}} = \widehat{\mathbf{C}}\widehat{\mathbf{x}}^k_{\mathsf{ie,c}}.$$

C-FOM:

$$\mathbf{E}_{\text{ie}}\mathbf{x}_{\text{ie,c}}^{k} = \mathbf{A}_{\text{ie}}\mathbf{x}_{\text{ie,c}}^{k-1} + \delta t\big(\mathbf{f}(\mathbf{x}_{\text{ie,c}}^{k-1}) + \mathbf{B}\mathbf{u}^{k}\big) + \mathbf{d}^{k},$$
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C-ROM:

$$\widehat{\mathbf{E}}_{\text{ie}}\widehat{\mathbf{x}}_{\text{ie,c}}^{k} = \widehat{\mathbf{A}}_{\text{ie}}\widehat{\mathbf{x}}_{\text{ie,c}}^{k-1} + \delta t\big(\widehat{\mathbf{f}}(\widehat{\mathbf{x}}_{\text{ie,c}}^{k-1}) + \widehat{\mathbf{B}}\mathbf{u}^{k}\big) + \widehat{\mathbf{d}}^{k},$$
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Theorem (simplified) [Chellappa/Feng/B. '23]

Given the FOM, the C-FOM and the C-ROM, we have the following error bound for the modified output $\overline{\mathbf{y}}_{\text{ie,c}}^{k} := \widetilde{\mathbf{y}}_{\text{ie,c}} + \widetilde{\mathbf{x}}_{\text{du}}^{\mathsf{T}}\mathbf{r}_{\text{pr}}^{k}$:

$$\|\mathbf{y}^{k} - \overline{\mathbf{y}}_{\text{ie,c}}^{k}\| \leq \|\mathbf{E}_{\text{ie}}^{-1}\|\,\|\mathbf{r}_{\text{du}}\|\,\|\check{\mathbf{r}}_{\text{pr}}^{k}\| + \|\mathbf{V}_{\text{du}}\widehat{\mathbf{x}}_{\text{du}}\|\,\|\mathbf{r}_{\text{pr}}^{k} - \check{\mathbf{r}}_{\text{pr}}^{k}\| =: \Delta_{\mathbf{y},\text{out3}}.$$

where

- residual: $\mathbf{r}_{\text{pr}}^{k} := \mathbf{A}_{\text{ie}}\widetilde{\mathbf{x}}_{\text{ie,c}}^{k-1} + \delta t\big(\mathbf{f}(\widetilde{\mathbf{x}}_{\text{ie,c}}^{k-1}) + \mathbf{B}\mathbf{u}^{k}\big) + \mathbf{d}^{k} - \mathbf{E}_{\text{ie}}\widetilde{\mathbf{x}}_{\text{ie,c}}^{k}.$
- auxiliary residual: $\check{\mathbf{r}}_{\text{pr}}^{k} := \mathbf{A}_{\text{ie}}\mathbf{x}_{\text{ie,c}}^{k-1} + \delta t\big(\mathbf{f}(\mathbf{x}_{\text{ie,c}}^{k-1}) + \mathbf{B}\mathbf{u}^{k}\big) + \mathbf{d}^{k} - \mathbf{E}_{\text{ie}}\widetilde{\mathbf{x}}_{\text{ie,c}}^{k},$
  $= \mathbf{E}_{\text{ie}}\big(\mathbf{x}_{\text{ie,c}}^{k} - \widetilde{\mathbf{x}}_{\text{ie,c}}^{k}\big) = \mathbf{E}_{\text{ie}}\big(\mathbf{x}^{k} - \widetilde{\mathbf{x}}_{\text{ie,c}}^{k}\big).$

C-FOM:

$$\mathbf{E}_{\mathsf{ie}}\mathbf{x}^{k}_{\mathsf{ie,c}} = \mathbf{A}_{\mathsf{ie}}\mathbf{x}^{k-1}_{\mathsf{ie,c}} + \delta t\big(\mathbf{f}(\mathbf{x}^{k-1}_{\mathsf{ie,c}}) + \mathbf{B}\mathbf{u}^{k}\big) + \mathbf{d}^{k},$$
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C-ROM:

$$\widehat{\mathbf{E}}_{\mathsf{ie}}\widehat{\mathbf{x}}^{k}_{\mathsf{ie,c}} = \widehat{\mathbf{A}}_{\mathsf{ie}}\widehat{\mathbf{x}}^{k-1}_{\mathsf{ie,c}} + \delta t\big(\widehat{\mathbf{f}}(\widehat{\mathbf{x}}^{k-1}_{\mathsf{ie,c}}) + \widehat{\mathbf{B}}\mathbf{u}^{k}\big) + \widehat{\mathbf{d}}^{k},$$
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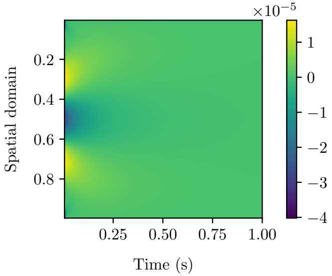
$$\|\mathbf{y}^{k} - \overline{\mathbf{y}}^{k}_{\mathsf{ie,c}}\| \leq \|\mathbf{E}^{-1}_{\mathsf{ie}}\|\,\|\mathbf{r}_{\mathsf{du}}\|\,\|\check{\mathbf{r}}^{k}_{\mathsf{pr}}\| + \|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\|\,\|\mathbf{r}^{k}_{\mathsf{pr}} - \check{\mathbf{r}}^{k}_{\mathsf{pr}}\| =: \Delta_{\mathbf{y},\mathsf{out3}}.$$

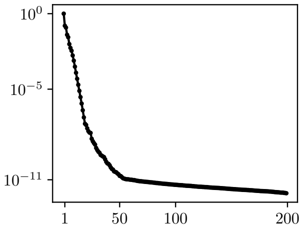
- Error indicator:

$$\|\mathbf{y}^{k} - \overline{\mathbf{y}}^{k}_{\mathsf{ie,c}}\| \lessapprox \Big(\overline{\rho}(\boldsymbol{\mu}^{*})\,\|\mathbf{E}^{-1}_{\mathsf{ie}}\|\,\|\mathbf{r}_{\mathsf{du}}\| + |1 - \overline{\rho}(\boldsymbol{\mu}^{*})|\,\|\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\|\Big)\,\|\mathbf{r}^{k}_{\mathsf{pr}}\| =: \widetilde{\Delta}_{\mathbf{y},\mathsf{out3}}.$$

- How to approximate the defect $\mathbf{d}(t, \boldsymbol{\mu})$?

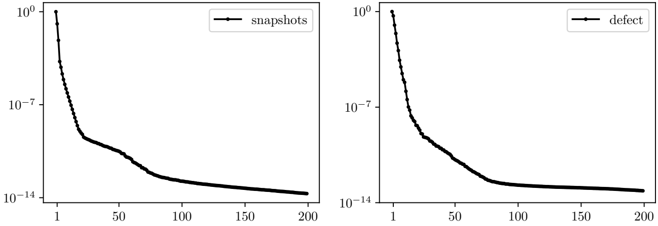
- How to approximate the defect $\mathbf{d}(t, \boldsymbol{\mu})$?
- Low-rank structure (over space) of $\mathbf{d}(t, \boldsymbol{\mu})$





Defect of the heat equation.
Left: space time variation of the defect; **Right:** singular values of the matrix $\mathbf{D} := \{\mathbf{d}^k\}_{k=0}^{K}$ at $\mu = 0.06$

- How to approximate the defect $\mathbf{d}(t, \boldsymbol{\mu})$?
- Low-rank structure (over space) of $\mathbf{d}(t, \boldsymbol{\mu})$
- Smoothness over parameter variations



Singular value decay.
Left: Solution snapshots and **Right:** Defect snapshots each at 60 different parameters $\mu \in [0.01,\ 0.1]$

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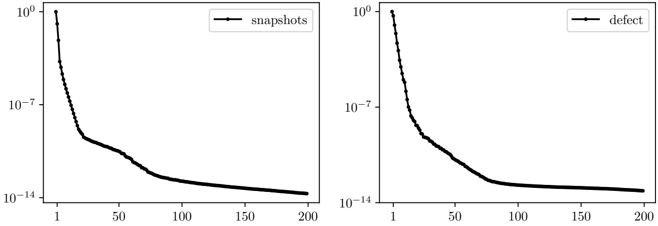


Singular value decay.
Left: Solution snapshots and **Right:** Defect snapshots each at 60 different parameters $\mu \in [0.01,\ 0.1]$

Conjecture: defect snapshots manifold inherits Kolmogorov n-width of snapshots manifold

$$\mathbf{d}(t,\boldsymbol{\mu}) \approx \widetilde{\mathbf{d}}(t,\boldsymbol{\mu}) = \sum_{i=1}^{n_d} \mathbf{v}_{d,i}\, \widehat{d}_i(t,\boldsymbol{\mu}).$$

1. Stage 1: identify basis $\mathbf{V}_d := \left[\mathbf{v}_{d,1}, \mathbf{v}_{d,2}, \ldots, \mathbf{v}_{d,n_d}\right] \in \mathbb{R}^{N \times n_d}$ via SVD.
2. Stage 2: learning the coefficient map $(t,\boldsymbol{\mu}) \mapsto \widehat{\mathbf{d}}(t,\boldsymbol{\mu}) \in \mathbb{R}^{n_d}$.

SVD-based reduction

- Collect defect snapshots $\mathbf{D}(\boldsymbol{\mu}) \in \mathbb{R}^{N \times N_t}$ and $\boldsymbol{\mu} \in \Xi_{\text{defect}}$; $|\Xi_{\text{defect}}| = d_s$.
- Obtain $\mathbf{V}_d$ through SVD; compute coefficient tensor $\widehat{\mathfrak{D}} \in \mathbb{R}^{n_d \times N_t \times d_s}$.

Learn coefficient mapping

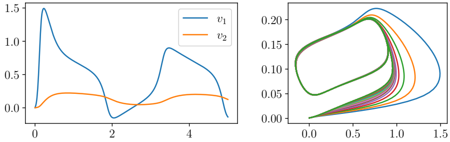
- mode-3 view of $\widehat{\mathfrak{D}}$
  $\rightsquigarrow$ RBF-based approximation
- mode-1 view of $\widehat{\mathfrak{D}}$
  $\rightsquigarrow$ NN-based approximation

FitzHugh-Nagumo equation:

$$\epsilon \frac{\partial v_1(z,t)}{\partial t} = \epsilon^2 \frac{\partial^2 v_1(z,t)}{\partial z^2} + f(v_1(z,t)) - v_2(z,t) + c,$$
$$\frac{\partial v_2(z,t)}{\partial t} = b\, v_1(z,t) - \gamma v_2(z,t) + c.$$

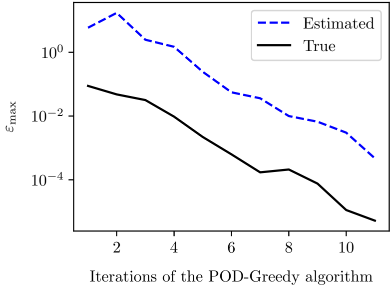
Adaptive POD-Greedy:[4]

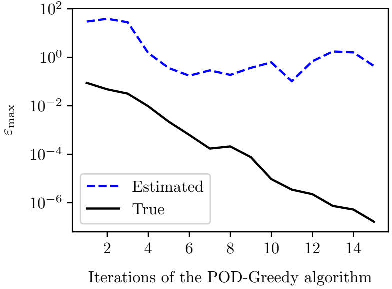
- $N = 1024$, $\texttt{tol} = 10^{-3}$,
  100 samples from $\boldsymbol{\mu} = [\epsilon, c] \in \mathcal{P} := [0.01, 0.04] \times [0.025, 0.075]$.



Output and phase portrait at $(\epsilon, c) = (0.0366, 0.0637)$

[4] S. Chellappa, L. Feng, and P. Benner. Accurate error estimation for model reduction of nonlinear dynamical systems via data-enhanced error closure. e-prints 2307.11138, arXiv, 2023



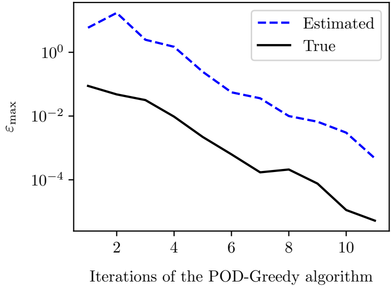


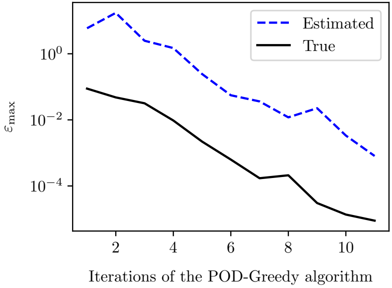
Oracle (known residual expression)

- FOM solver: `ode15s`
- ROM dim. $n = 33$

Without error closure

- FOM solver: `ode15s`
- Error estm. solver: IMEX2
- ROM dim. $n = 45$





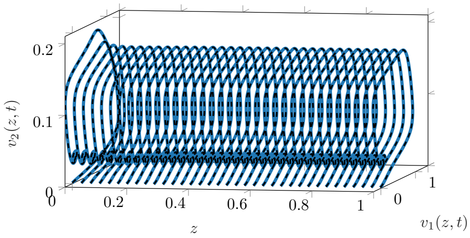
Oracle (known residual expression)

- FOM solver: `ode15s`
- ROM dim. $n = 33$

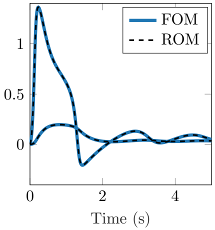
With error closure (SVD+RBF)

- FOM solver: `ode15s`
- Error estm. solver: IMEX2
- ROM dim. $n = 33$

- Data to train closure term: snapshots at 21 parameter samples (30% of training set)



(a)



(b)

FHN equation with SVD+RBF: performance at the test parameter $\boldsymbol{\mu} = (0.0267, 0.0367)$
Left: Limit cycle behaviour; **Right:** output quantities.

- A posteriori error estimators so far ($\Delta_{\mathbf{y},\text{out1}}$, $\Delta_{\mathbf{y},\text{out2}}$, $\Delta_{\mathbf{y},\text{out3}}$) require computing $\|\mathbf{E}(\boldsymbol{\mu})^{-1}\|$ (the coercivity/inf-sup-constant in the function space setting) for all parameters $\boldsymbol{\mu} \in \Xi \rightsquigarrow$ large computational effort!
- We derive inf-sup-constant-free versions of $\Delta_{\mathbf{y},\text{out1}}$, $\Delta_{\mathbf{y},\text{out2}}$, $\Delta_{\mathbf{y},\text{out3}}$.

Theorem (simplified) [Feng/Chellappa/B. '23]

The output error $\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\|$ can be bounded as

$$\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\| \leq \tilde{\rho}\, \breve{\Phi}^k \, \|\mathbf{r}_{\text{pr}}^k\| =: \Delta_{\mathbf{y},\text{iscf}}.$$

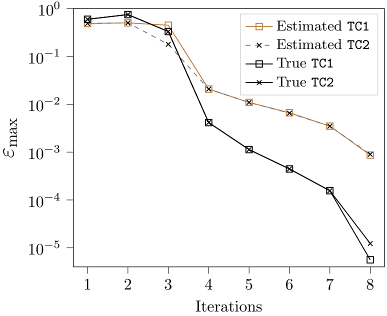
- $\tilde{\rho} := \dfrac{\|\breve{\mathbf{r}}_{\text{pr}}^k\|}{\|\mathbf{r}_{\text{pr}}^k\|}$ and $\breve{\Phi}^k := \|\mathbf{e}_{\text{du}}\| + \|\mathbf{V}_{\text{du}}\widehat{\mathbf{x}}_{\text{du}}\|$ with $\mathbf{e}_{\text{du}} := \mathbf{E}^{-1}\mathbf{r}_{\text{du}}$.

- Estimator:

$$\left\|\mathbf{y}^k - \widehat{\mathbf{y}}^k\right\| \lessapprox \bar{\rho}(\boldsymbol{\mu}^*)\, \tilde{\breve{\Phi}}^k \, \|\mathbf{r}_{\text{pr}}^k\| =: \tilde{\Delta}_{\mathbf{y},\text{iscf}}.$$

with $\tilde{\breve{\Phi}}^k := \|\widetilde{\mathbf{e}}_{\text{du}}\| + \|\mathbf{V}_{\text{du}}\widehat{\mathbf{x}}_{\text{du}}\|$ obtained with the reduced solution of the dual system.

- **FitzHugh-Nagumo equation** - compare $\widetilde{\Delta}_{\mathbf{y},\text{out2}}$ (TC1) vs. $\widetilde{\Delta}_{\mathbf{y},\text{iscf2}}$ (TC2).
- Adaptive POD-Greedy with $\texttt{tol} = 10^{-3}$, $N = 4096$.



- TC1 $\rightarrow$ $n = 48$, offline time 467.5 seconds.
- TC2 $\rightarrow$ $n = 48$, offline time **295.6** seconds $\rightsquigarrow$ 1.6-fold speedup.

Talk outline

Error estimators for steady systems

- Obtained from elliptic PDEs or linear parametric systems obtained e.g., from frequency domain transforms of LTI systems.

FOM

$$\begin{aligned}\mathbf{M}(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}) &= \mathbf{b}(\boldsymbol{\mu}),\\ \mathbf{y}(\boldsymbol{\mu}) &= \mathbf{c}(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}).\end{aligned}$$

ROM

$$\begin{aligned}\widehat{\mathbf{M}}(\boldsymbol{\mu})\widehat{\mathbf{x}}(\boldsymbol{\mu}) &= \widehat{\mathbf{b}}(\boldsymbol{\mu}),\\ \widehat{\mathbf{y}}(\boldsymbol{\mu}) &= \widehat{\mathbf{c}}(\boldsymbol{\mu})\widehat{\mathbf{x}}(\boldsymbol{\mu}).\end{aligned}$$

Error estimators for steady systems

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$$\begin{aligned} \mathbf{M}(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}) &= \mathbf{b}(\boldsymbol{\mu}), \\ \mathbf{y}(\boldsymbol{\mu}) &= \mathbf{c}(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}). \end{aligned}$$

Dual system:

$$\mathbf{M}(\boldsymbol{\mu})^{\mathsf{T}}\mathbf{x}_{\mathsf{du}}(\boldsymbol{\mu}) = \mathbf{c}(\boldsymbol{\mu})^{\mathsf{T}}.$$

ROM

$$\begin{aligned} \widehat{\mathbf{M}}(\boldsymbol{\mu})\widehat{\mathbf{x}}(\boldsymbol{\mu}) &= \widehat{\mathbf{b}}(\boldsymbol{\mu}), \\ \widehat{\mathbf{y}}(\boldsymbol{\mu}) &= \widehat{\mathbf{c}}(\boldsymbol{\mu})\widehat{\mathbf{x}}(\boldsymbol{\mu}). \end{aligned}$$

Reduced dual system:

$$\widehat{\mathbf{M}}(\boldsymbol{\mu})^{\mathsf{T}}\widehat{\mathbf{x}}_{\mathsf{du}}(\boldsymbol{\mu}) = \widehat{\mathbf{c}}(\boldsymbol{\mu})^{\mathsf{T}}.$$

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$$\mathbf{y}(\boldsymbol{\mu}) = \mathbf{c}(\boldsymbol{\mu})\mathbf{x}(\boldsymbol{\mu}).$$

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ROM

$$\widehat{\mathbf{M}}(\boldsymbol{\mu})\widehat{\mathbf{x}}(\boldsymbol{\mu}) = \widehat{\mathbf{b}}(\boldsymbol{\mu}),$$
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Reduced dual system:

$$\widehat{\mathbf{M}}(\boldsymbol{\mu})^{\mathsf{T}}\widehat{\mathbf{x}}_{\mathsf{du}}(\boldsymbol{\mu}) = \widehat{\mathbf{c}}(\boldsymbol{\mu})^{\mathsf{T}}.$$

- Existing error estimation approaches:
  - evaluating inf-sup constant can be expensive.
  - overstimation in case of residual estimators/small inf-sup constant.
  - curse of dimensionality in case of multi-parameter systems.

FOM

$$\mathbf{M}\mathbf{x} = \mathbf{b}$$

$\xrightarrow{\mathbf{V}}$

ROM

$$\widehat{\mathbf{M}}\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$$

$\longrightarrow$

Residual

$$\mathbf{r}_{\mathrm{pr}} = \mathbf{b} - \mathbf{M}\widetilde{\mathbf{x}}$$

FOM

$$\mathbf{M}\mathbf{x} = \mathbf{b}$$

$\xrightarrow{\mathbf{V}}$

ROM

$$\widehat{\mathbf{M}}\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$$

$\longrightarrow$

Residual

$$\mathbf{r}_{\mathsf{pr}} = \mathbf{b} - \mathbf{M}\widetilde{\mathbf{x}}$$

Error-Residual FOM

$$\mathbf{M}\mathbf{e} = \mathbf{r}_{\mathsf{pr}}$$

$\xrightarrow{\mathbf{V}_e}$

Error-Residual ROM

$$\widehat{\mathbf{M}}\widehat{\mathbf{e}} = \widehat{\mathbf{r}}_{\mathsf{pr}}$$

$\longrightarrow$

Second Residual

$$\mathbf{r}_e = \mathbf{r}_{\mathsf{pr}} - \mathbf{M}\widetilde{\mathbf{e}}$$

FOM	$\xrightarrow{\mathbf{V}}$	ROM	$\longrightarrow$	Residual
$\mathbf{M}\mathbf{x} = \mathbf{b}$		$\widehat{\mathbf{M}}\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$		$\mathbf{r}_{\text{pr}} = \mathbf{b} - \mathbf{M}\widetilde{\mathbf{x}}$
Error-Residual FOM	$\xrightarrow{\mathbf{V}_e}$	Error-Residual ROM	$\longrightarrow$	Second Residual
$\mathbf{M}\mathbf{e} = \mathbf{r}_{\text{pr}}$		$\widehat{\mathbf{M}}\widehat{\mathbf{e}} = \widehat{\mathbf{r}}_{\text{pr}}$		$\mathbf{r}_e = \mathbf{r}_{\text{pr}} - \mathbf{M}\widetilde{\mathbf{e}}$

Theorem (simplified) [Chellappa/Feng/de la Rubia/B. '23]

The norm of the true error $\|\mathbf{e}(\boldsymbol{\mu})\|$ can be bounded from above and below by the proposed state error estimator $\Delta_{\mathbf{x},\text{ER}}(\boldsymbol{\mu}) := \|\widetilde{\mathbf{e}}(\boldsymbol{\mu})\|$ as follows:

$$\Delta_{\mathbf{x},\text{ER}} - \gamma \leq \|\mathbf{e}(\boldsymbol{\mu})\| \leq \Delta_{\mathbf{x},\text{ER}} + \gamma$$

where $\widetilde{\mathbf{e}}(\boldsymbol{\mu}) = \mathbf{V}_e\widehat{\mathbf{e}}(\boldsymbol{\mu})$ and $\gamma := \|\mathbf{e}(\boldsymbol{\mu}) - \widetilde{\mathbf{e}}(\boldsymbol{\mu})\| \geq 0$ is small whenever $\widetilde{\mathbf{e}}$ is a good approximation to the true error $\mathbf{e}$.

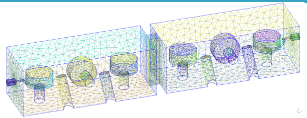
$\rightarrow$ Simultaneous greedy construction of $\mathbf{V}, \mathbf{V}_e$; 1 additional FOM solve/iteration.

Error estimators for steady systems

Inf-sup-constant-free state error estimator: Numerical example

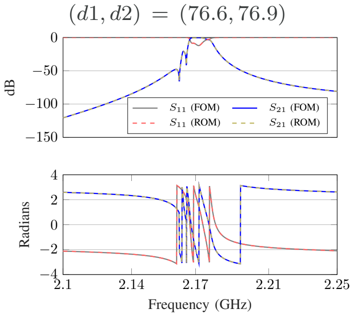
Inline dielectric filter:

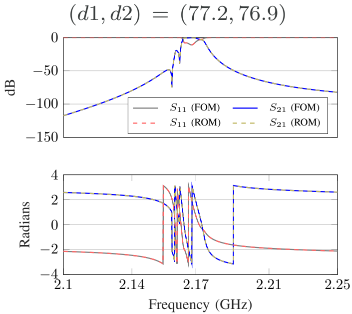
- System with multiple resonances.
- 3 parameters:
  frequency $f \in [2.1, 2.25]$ GHz,
  dielectric const. $d_1, d_2 \in [76.5, 77.5]$.



	Size	Time (s)
FOM	229,890	15
ROM	**28**	**0.015**

Test set performance:





- In [Feng/B. '21][5], a family of inf-sup-constant-free output error estimators are derived.
- Make use of **dual system** and **dual error-residual system**.

Dual FOM

$$\mathbf{M}^{\mathsf{T}}\mathbf{x}_{\mathsf{du}} = \mathbf{c}^{\mathsf{T}}$$

$\xrightarrow{\mathbf{V}_{\mathsf{du}}}$

Dual ROM

$$\widehat{\mathbf{M}}^{\mathsf{T}}\widehat{\mathbf{x}}_{\mathsf{du}} = \widehat{\mathbf{c}}^{\mathsf{T}}$$

$\longrightarrow$

Dual residual

$$\mathbf{r}_{\mathsf{du}} = \mathbf{c}^{\mathsf{T}} - \mathbf{M}^{\mathsf{T}}\widetilde{\mathbf{x}}_{\mathsf{du}}$$

[5] L. Feng and P. Benner. On error estimation for reduced-order modeling of linear non-parametric and parametric systems. *ESAIM: Math. Model. Numer. Anal.*, 55(2):561–594, 2021

- In [FENG/B. '21][5], a family of inf-sup-constant-free output error estimators are derived.
- Make use of **dual system** and **dual error-residual system**.

Dual FOM $\xrightarrow{\mathbf{V}_{\text{du}}}$ Dual ROM $\longrightarrow$ Dual residual

$$\mathbf{M}^{\mathsf{T}}\mathbf{x}_{\text{du}} = \mathbf{c}^{\mathsf{T}} \qquad \widehat{\mathbf{M}}^{\mathsf{T}}\widehat{\mathbf{x}}_{\text{du}} = \widehat{\mathbf{c}}^{\mathsf{T}} \qquad \mathbf{r}_{\text{du}} = \mathbf{c}^{\mathsf{T}} - \mathbf{M}^{\mathsf{T}}\widetilde{\mathbf{x}}_{\text{du}}$$

Dual Error-Residual FOM $\xrightarrow{\mathbf{V}_{d}}$ Dual Error-Residual ROM $\longrightarrow$ Dual Residual

$$\mathbf{M}^{\mathsf{T}}\mathbf{e}_{\text{du}} = \mathbf{r}_{\text{du}} \qquad \widehat{\mathbf{M}}^{\mathsf{T}}\widehat{\mathbf{e}}_{\text{du}} = \widehat{\mathbf{r}}_{\text{du}} \qquad \mathbf{r}_{d} = \mathbf{r}_{\text{du}} - \mathbf{M}^{\mathsf{T}}\widetilde{\mathbf{e}}_{\text{du}}$$

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Dual FOM	$\xrightarrow{\mathbf{V}_{\mathsf{du}}}$	Dual ROM	$\longrightarrow$	Dual residual
$\mathbf{M}^{\mathsf{T}}\mathbf{x}_{\mathsf{du}} = \mathbf{c}^{\mathsf{T}}$		$\widehat{\mathbf{M}}^{\mathsf{T}}\widehat{\mathbf{x}}_{\mathsf{du}} = \widehat{\mathbf{c}}^{\mathsf{T}}$		$\mathbf{r}_{\mathsf{du}} = \mathbf{c}^{\mathsf{T}} - \mathbf{M}^{\mathsf{T}}\widetilde{\mathbf{x}}_{\mathsf{du}}$
Dual Error-Residual FOM	$\xrightarrow{\mathbf{V}_{d}}$	Dual Error-Residual ROM	$\longrightarrow$	Dual Residual
$\mathbf{M}^{\mathsf{T}}\mathbf{e}_{\mathsf{du}} = \mathbf{r}_{\mathsf{du}}$		$\widehat{\mathbf{M}}^{\mathsf{T}}\widehat{\mathbf{e}}_{\mathsf{du}} = \widehat{\mathbf{r}}_{\mathsf{du}}$		$\mathbf{r}_{d} = \mathbf{r}_{\mathsf{du}} - \mathbf{M}^{\mathsf{T}}\widetilde{\mathbf{e}}_{\mathsf{du}}$

$\rightarrow$ Simultaneous greedy construction of $\mathbf{V}, \mathbf{V}_{\mathsf{du}}$ & $\mathbf{V}_{d}$; 2 additional FOM solves/iteration

[5] L. Feng and P. Benner. On error estimation for reduced-order modeling of linear non-parametric and parametric systems. *ESAIM: Math. Model. Numer. Anal.*, 55(2):561–594, 2021

Theorem (simplified) [Feng/B. '21]

The norm of the true output error $\mathbf{e}_\mathbf{y}(\boldsymbol{\mu}) = \mathbf{y}(\boldsymbol{\mu}) - \widehat{\mathbf{y}}(\boldsymbol{\mu})$ can be bounded as follows:

$$\Delta_{\mathbf{y},\mathsf{ER},1} - \gamma_1 \leq \|\mathbf{e}_\mathbf{y}(\boldsymbol{\mu})\| \leq \Delta_{\mathbf{y},\mathsf{ER},1} + \gamma_1$$

where $\Delta_{\mathbf{y},\mathsf{ER},1} := \left| \left(\mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\right)^{\mathsf{T}} \mathbf{r}_{\mathsf{pr}}\right|$ and $\gamma_1 := \left|\left(\mathbf{x}_{\mathsf{du}} - \mathbf{V}_{\mathsf{du}}\widehat{\mathbf{x}}_{\mathsf{du}}\right)^{\mathsf{T}}\mathbf{r}_{\mathsf{pr}}\right|$.

- Estimator:

$$\|\mathbf{e}_\mathbf{y}(\boldsymbol{\mu})\| \lessapprox \Delta_{\mathbf{y},\mathsf{ER},1}$$

Theorem (simplified) [Feng/B. '19, Feng/B. '21]

The norm of the true output error $\mathbf{e}_{\mathbf{y}}(\boldsymbol{\mu}) = \mathbf{y}(\boldsymbol{\mu}) - \widehat{\mathbf{y}}(\boldsymbol{\mu})$ can be bounded as follows:

$$\Delta_{\mathbf{y},\mathsf{ER},2} - \gamma_1 - \left| \left(\mathbf{V}_d \widehat{\mathbf{e}}_{\mathsf{du}}\right)^{\mathsf{T}} \mathbf{r}_{\mathsf{pr}} \right| \leq \|\mathbf{e}_{\mathbf{y}}(\boldsymbol{\mu})\| \leq \Delta_{\mathbf{y},\mathsf{ER},2} + \gamma_2$$

where $\Delta_{\mathbf{y},\mathsf{ER},2} := \left| \left(\mathbf{V}_{\mathsf{du}} \widehat{\mathbf{x}}_{\mathsf{du}}\right)^{\mathsf{T}} \mathbf{r}_{\mathsf{pr}} \right| + \left| \left(\mathbf{V}_d \widehat{\mathbf{e}}_{\mathsf{du}}\right)^{\mathsf{T}} \mathbf{r}_{\mathsf{pr}} \right|$ and $\gamma_2 := |(\mathbf{e}_{\mathsf{du}} - \mathbf{V}_d \widehat{\mathbf{e}}_{\mathsf{du}})^{\mathsf{T}} \mathbf{r}_{\mathsf{pr}}|$.

- Estimator:

$$\|\mathbf{e}_{\mathbf{y}}(\boldsymbol{\mu})\| \lessapprox \Delta_{\mathbf{y},\mathsf{ER},2}$$

$\rightarrow$ $\Delta_{\mathbf{y},\mathsf{ER},2}$ is sharper than $\Delta_{\mathbf{y},\mathsf{ER},1}$

$\rightarrow$ $\Delta_{\mathbf{y},\mathsf{ER},2}$ involves solving extra linear system

- Repeated computation of the error estimators (such as $\Delta_{\mathbf{y},\mathrm{ER},1}$, $\Delta_{\mathbf{y},\mathrm{ER},2}$) can be expensive for **multi-parameter systems** or problems having a **wide parameter range**
- [Feng et al. '23][6] proposes an **early-stopping strategy** to improve offline efficiency of the greedy algorithm
- **Save additional FOM solves** needed for evaluating the error estimator

[6] L. Feng, L. Lombardi, G. Antonini, and P. Benner. Multi-fidelity error estimation accelerates greedy model reduction of complex dynamical systems. *Int. J. Numer. Methods. Engrg.*, 124(23):5312–5333, 2023

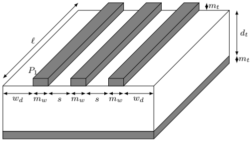
Error estimators for steady systems

Multi-fidelity error estimator: Application to time-delay systems

Co-planar microstrip:

- Time-delay system with $d = 168$ delays.
- Linear parametric system in the frequency-domain.
- $N = 16,644$ and $f \in [0,\ 10]$GHz.

$$\sum_{j=0}^{d} E_j \dot{x}(t - \tau_j) = \sum_{j=0}^{d} A_j x(t - \tau_j) + Bu(t), \qquad \forall\ t \geq 0$$
$$y(t) = Cx(t),$$



Method	Iter.	Runtime (min)	n	Valid.err
standard, $\lvert\Xi\rvert = 30$	11	50.7	132	8.5×10^{-4}
bi-fidelity, add only, $\lvert\Xi_c\rvert = 10$	11	27.6	132	0.0033
bi-fidelity, add-remove, $\lvert\Xi_c\rvert = 10$	11	26.5	132	8.2×10^{-4}
multi-fidelity, add only, $\lvert\Xi_c\rvert = 10$	11	21.6	132	0.0033
multi-fidelity, add-remove, $\lvert\Xi_c\rvert = 10$	11	20.1	132	8.2×10^{-4}

Talk outline

Conclusion

Contributions

- We derived a posteriori error estimators for a variety of classes of systems, both linear and nonlinear
- We introduced a new error estimator applicable when the **time-discretization is unknown**, in addition to an **inf-sup-constant-free** error estimator and a **multi-fidelity** error estimator
- We employed error estimators for **adaptive basis updates** and **adaptive parameter sampling** leading to

  reduced offline costs and
  good generalization on unseen parameters

Outlook

- Error estimation for digital twins to enable *on-the-fly* model updates
- Certifying ML-based surrogate models via error estimation

Contributions

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Outlook

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- ☐ Certifying ML-based surrogate models via error estimation

Thank you for your attention!

Y. Zhang, L. Feng, S. Li, and P. Benner.
An efficient output error estimation for model order reduction of parametrized evolution equations.
SIAM J. Sci. Comput., 37(6):B910–B936, 2015

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IEEE Trans. Microw. Theory Techn., 71(11):4762–4777, 2023

L. Feng, L. Lombardi, G. Antonini, and P. Benner.
Multi-fidelity error estimation accelerates greedy model reduction of complex dynamical systems.
Int. J. Numer. Methods. Engrg., 124(23):5312–5333, 2023

S. Chellappa, L. Feng, and P. Benner.
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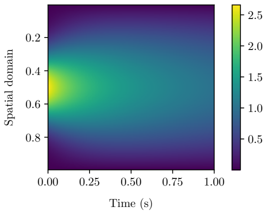
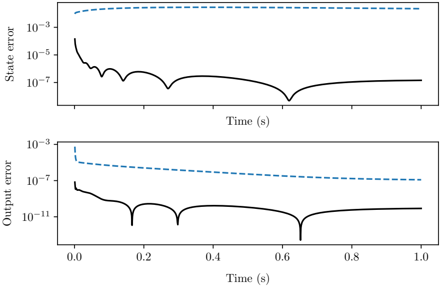
e-prints 2307.11138, arXiv, 2023

S. Chellappa, B. Cansiz, L. Feng, P. Benner, and M. Kaliske.
Fast and reliable reduced-order models for cardiac electrophysiology.
e-prints 2311.06164, arXiv, 2023

Backup slides

- FOM $\dot{\mathbf{x}} = \mathbf{A}\mathbf{x}$; solver: `scipy.integrate.odeint`
- POD ROM with $n = 12$
- To compute error estimator need $\mathcal{R}\left[\widetilde{\mathbf{x}}^k, \widetilde{\mathbf{x}}^{k-1}, \ldots, \widetilde{\mathbf{x}}^{k-s}\right]$ $\rightsquigarrow$ **unknown**
- Blue: estimated error without closure
  Orange: estimated error with closure term





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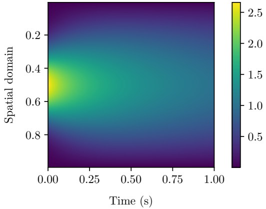
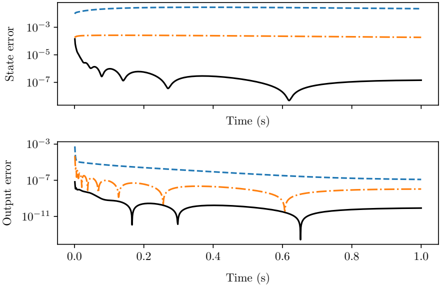
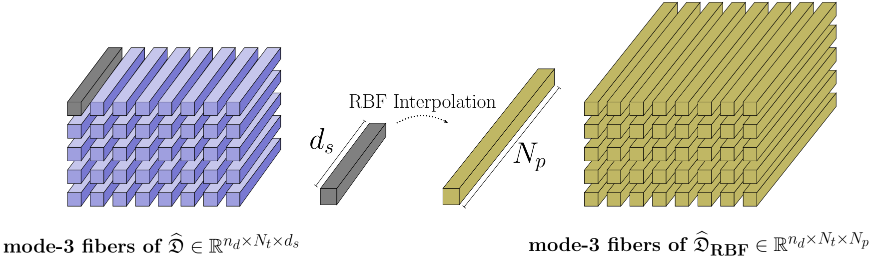
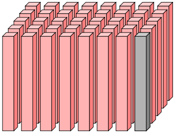




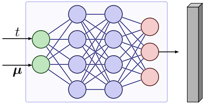


Approximation of the defect as a function of the parameter $\boldsymbol{\mu}$. The RBF interpolant learns an approximation of the defect vector over N_p samples, with interpolation occurring at d_s samples. We construct an individual RBF interpolant for each time and generalized spatial coordinate.

Training

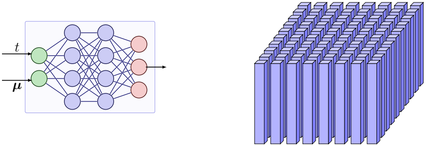


mode-1 fibers of $\widehat{\mathfrak{D}} \in \mathbb{R}^{n_d \times N_t \times d_s}$



Feedforward neural network

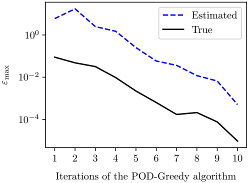
Inference



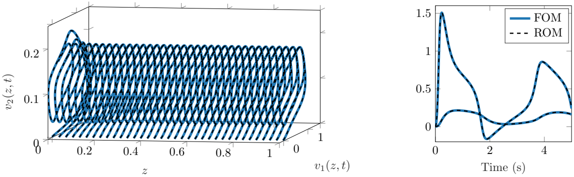
inference of mode-1 fibers of $\widehat{\mathfrak{D}}_{\mathbf{NN}} \in \mathbb{R}^{n_d \times N_t \times N_p}$

Approximation of the defect coefficients as a function of the inputs $(t, \boldsymbol{\mu})$. The neural network is trained based on data available at d_s parameter samples. In the inference stage, the neural network learns the approximation of the defect for all N_p parameter samples.

- $|\Xi_{\text{defect}}| = d_s = 21$
- ROM dimension $n = 30$
- FNN details:
  - 3 layers $(64, 64, 32)$
  - learning rate 0.002
  - Adam optimizer
  - 2000 epochs

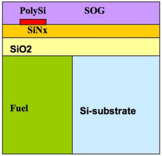


FHN equation: error (estimator) decay when using the SVD+FNN method to approximate the closure term.



FHN equation with SVD+FNN: performance at the test parameter $\boldsymbol{\mu} = (0.04, 0.0472)$
Left: Limit cycle behaviour; **Right:** output quantities.

- Linear heat transfer model in a mechanical device
- FOM dimension $N = 4257$, ROM tolerance $\texttt{tol} = 10^{-4}$
- Frequency domain input/output model; parameter $\boldsymbol{\mu} := (s, h_1, h_2, h_3)$
- $s \in \jmath 2\pi \cdot [10^{-2}, 10^{2}]$ and $\{h_i\}_{i=1}^{3} \in [1, 10^4]$



Test cases [7]

Test 1: Fixed training set

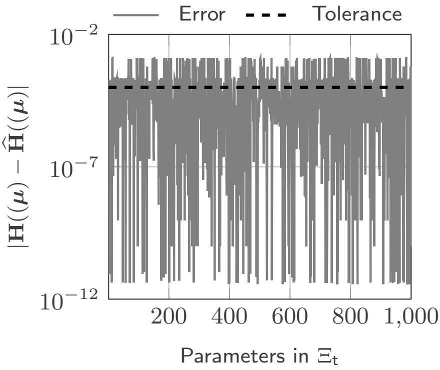
Training set (Ξ) with 5^4 log-sampled parameters

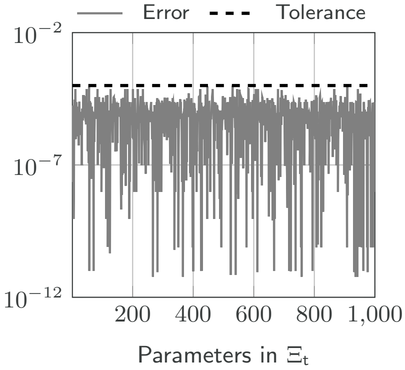
Test 2: Adaptive sampling (with RBF)

Coarse training set (Ξ_c) with 4^4 log-sampled parameters, Fine training set (Ξ_f) with 7^4 log-sampled parameters

Test set for validation: Test set (Ξ_t) with 1000 randomly chosen parameters from 8^4 log-spaced samples

[7] S. Chellappa, L. Feng, V. de la Rubia, and P. Benner. Adaptive interpolatory MOR by learning the error estimator in the parameter domain. In *Model Reduction of Complex Dynamical Systems*, volume 171 of *International Series of Numerical Mathematics*, pages 97–117. Birkhäuser, Cham, 2021





ROM size (n)	Time(s)
86	254

Fixed training set

ROM size (n)	Time(s)
85	162

Adaptive sampling