Model Order Reduction of Parametrized Nonlinear Evolution Equations with Applications in Chromatography

Peter Benner

Max Planck Institute for Dynamics of Complex Technical Systems
Magdeburg, Germany
Email: benner@mpi-magdeburg.mpg.de
Outline

1 Motivation
   • General set-up: nonlinear parametric systems
   • Motivating Examples

2 Model Order Reduction
   • Petrov-Galerkin Projection
   • Empirical Interpolation Method

3 Error Bound
   • Primal-only Error Bound
   • Primal-dual Output Error Bound

4 Basis Construction and Adaptive Snapshot Selection
   • POD-Greedy Algorithm
   • Adaptive Snapshot Selection

5 Numerical Results

6 Conclusions and Outlook
Collaborators

Lihong Feng

Yongjin Zhang

Andreas Seidel-Morgenstern

MPI Magdeburg
Computational Methods in Systems and Control (CSC)
Physical and Chemical Foundations of Process Engineering (PCF)
Motivation

General set-up: nonlinear parametric systems

Nonlinear Parametric Systems

\[ E(t, \mu) \frac{dx}{dt} = A(t, \mu)x + f(x, \mu), \]

or

\[ E(t^k, \mu)x^{k+1} = A(t^k, \mu)x^k + f(x^k, \mu), \]

\( x, x^k \in \mathcal{W}^n \subset \mathbb{R}^n, E, A \in \mathbb{R}^{n \times n}, n \) is large.

Often, the output \( y = g(x) \), or \( y = Cx \), is of interest \( \leadsto \) quantities-of-interest.

Multi-query context:
Solve the ODE system for many varying values of \( \mu \in \Omega \subset \mathbb{R}^d \), e.g., optimization, real-time control, inverse problems, \ldots
Motivation

Motivating Example: Batch Chromatography

Principle of batch chromatography for binary separation.
Principle of batch chromatography for binary separation.

\[
\begin{align*}
\frac{\partial c_z}{\partial t} + \frac{1 - \epsilon}{\epsilon} \frac{\partial q_z}{\partial t} &= - \frac{\partial c_z}{\partial x} + \frac{1}{Pe} \frac{\partial^2 c_z}{\partial x^2}, & 0 < x < 1, \\
\frac{\partial q_z}{\partial t} &= \frac{L}{Q/(\epsilon A_c)} \kappa_z (q^\text{Eq}_z - q_z), & 0 \leq x \leq 1,
\end{align*}
\]

- A convection-dominated system, the Péclet number $Pe$ is large.
Motivation

Motivating Example: Batch Chromatography

Principle of batch chromatography for binary separation.

\[
\begin{aligned}
\frac{\partial c_z}{\partial t} + \frac{1 - \epsilon}{\epsilon} \frac{\partial q_z}{\partial t} &= - \frac{\partial c_z}{\partial x} + \frac{1}{Pe} \frac{\partial^2 c_z}{\partial x^2}, & 0 < x < 1, \\
\frac{\partial q_z}{\partial t} &= \frac{L}{Q/(\epsilon A_c)} \kappa_z (q_z^{\text{Eq}} - q_z), & 0 \leq x \leq 1,
\end{aligned}
\]

- A convection-dominated system, the Péclet number $Pe$ is large.
- Requires long-time integration process.
Motivation

Motivating Example: Batch Chromatography

Principle of batch chromatography for binary separation.

\[
\begin{align*}
\frac{\partial c_z}{\partial t} + \frac{1 - \epsilon}{\epsilon} \frac{\partial q_z}{\partial t} &= -\frac{\partial c_z}{\partial x} + \frac{1}{Pe} \frac{\partial^2 c_z}{\partial x^2}, \\
\frac{\partial q_z}{\partial t} &= \frac{L}{Q/(\epsilon A_c)} \kappa_z(q_z^{Eq} - q_z),
\end{align*}
\]

- A convection-dominated system, the Péclet number $Pe$ is large.
- Requires long-time integration process.
- A nonlinear parametric coupled system, parameters $\mu := (Q, t_{in})$. 
Motivation

Motivating Example: Batch Chromatography

Principle of batch chromatography for binary separation.

\[
\begin{align*}
\frac{\partial c_z}{\partial t} + \frac{1 - \epsilon}{\epsilon} \frac{\partial q_z}{\partial t} &= -\frac{\partial c_z}{\partial x} + \frac{1}{Pe} \frac{\partial^2 c_z}{\partial x^2}, \\
\frac{\partial q_z}{\partial t} &= \frac{L}{Q/(\epsilon A_c)} k_{\kappa_z}(q_{E z}^z - q_z),
\end{align*}
\]

- A convection-dominated system, the Péclet number $Pe$ is large.
- Requires long-time integration process.
- A nonlinear parametric coupled system, parameters $\mu := (Q, t_{in})$.
- What are the optimal operating conditions?
  \[\mapsto\text{PDE constrained optimization.}\]
Motivation
Motivating Example: Simulated Moving Bed (SMB) Chromatography

SMB chromatographic process with 4 zones and 8 columns.
Governing equations are similar, but:

SMB chromatographic process with 4 zones and 8 columns.
Motivation

Motivating Example: SMB Chromatography

Governing equations are similar, but:

- More parameters, \( \mu := (m_1, \ldots, m_4, Q_F) \)
- Multi-switching system
- Cyclic steady state computation

SMB chromatographic process with 4 zones and 8 columns.
Motivation

4-column SMB plant at MPI Magdeburg
Motivation

SMB Chromatography — a practical application

Purified Artemisinin

- Artemisinin is the basic compound for producing the malaria medication Artesunate.
- New SMB-based process developed at MPI Magdeburg (PCF group) yields 99.5% purity (exceeding the limits set by WHO and FDA), based on new synthesis process invented by Peter Seeberger (MPI Colloids and Interfaces, Potsdam).
- Process can be easily implemented in low-cost plants in the countries where the plant Artemisia annua grows, mostly, in East Asia.
- Much cheaper than current anti-Malaria medication, and much higher degree of purity!
Motivation
SMB Chromatography — a practical application

Purified Artemisinin

Artemisinin is the basic compound for producing the malaria medication Artesunate.

New SMB-based process developed at MPI Magdeburg (PCF group) yields 99.5% purity (exceeding the limits set by WHO and FDA), based on new synthesis process invented by Peter Seeberger (MPI Colloids and Interfaces, Potsdam).

Process can be easily implemented in low-cost plants in the countries where the plant *Artemisia annua* grows, mostly, in East Asia.

Model plant built in Vietnam.

Much cheaper than current anti-Malaria medication, and much higher degree of purity!

Seeberger and Seidel-Morgenstern were awarded the Humanity in Science Prize 2015 for this.


MOR for Nonlinear Parametric Systems

Original full order system (FOM)

\[ E(t, \mu) \frac{dx}{dt} = A(t, \mu)x + f(x, \mu), \]

or

\[ E(t^k, \mu)x^{k+1} = A(t^k, \mu)x^k + f(x^k, \mu), \]

\( x, x^k \in \mathcal{W}^n \subset \mathbb{R}^n, E, A \in \mathbb{R}^{n \times n}, n \) is large.

Often the output \( y = g(x) \), or \( y =Cx \) is of interest.
MOR for Nonlinear Parametric Systems

Original full order system (FOM)

\[ E(t, \mu) \frac{dx}{dt} = A(t, \mu)x + f(x, \mu), \]

or

\[ E(t^k, \mu)x^{k+1} = A(t^k, \mu)x^k + f(x^k, \mu), \]

\( x, x^k \in \mathcal{W}^n \subset \mathbb{R}^n, E, A \in \mathbb{R}^{n \times n}, n \) is large.

Often the output \( y = g(x) \), or \( y = Cx \) is of interest.

Reduced-order model (ROM)

\[ \hat{E}(t, \mu) \frac{dz}{dt} = \hat{A}(t, \mu)z + W^T f(Vz, \mu), \quad \hat{x} := Vz, \]

or

\[ \hat{E}(t^k, \mu)z^{k+1} = \hat{A}(t^k, \mu)z^k + W^T f(Vz^k, \mu) \quad \hat{x}^k := Vz^k, \]

\( \hat{E} = W^T E V, \hat{A} = W^T A V, W, V \in \mathbb{R}^{n \times N}, z, z^k \in \mathbb{R}^N, N \ll n. \)
Let \( \hat{y}(t, \mu) \) be the approximate output of interest. Arising questions are:

1. How to deal with the nonlinearity and/or non-affinity, i.e., efficiently compute \( W^T f(Vz, \mu) \) or \( W^T f(Vz^k, \mu)? \)

2. How to estimate the error in the quantities-of-interest, i.e., \( \|y - \hat{y}\| \leq \? \)?

3. How to efficiently construct the projection matrices \( V \) and \( W \)?

\( \Rightarrow \) EIM.
Let $\hat{y}(t, \mu)$ be the approximate output of interest. Arising questions are:

1. How to deal with the nonlinearity and/or non-affinity, i.e., efficiently compute $W^T f(Vz, \mu)$ or $W^T f(Vz^k, \mu)$? $\leadsto$ EIM.

2. How to estimate the error in the quantities-of-interest, i.e., $\|y - \hat{y}\| \leq ? \leadsto$ Output error bound.
Let $\hat{y}(t, \mu)$ be the approximate output of interest. Arising questions are:

1. How to deal with the nonlinearity and/or non-affinity, i.e., efficiently compute $W^T f(Vz, \mu)$ or $W^T f(Vz^k, \mu)$? $\rightsquigarrow$ EIM.

2. How to estimate the error in the quantities-of-interest, i.e., $\|y - \hat{y}\| \leq ?$ $\rightsquigarrow$ Output error bound.

Empirical Interpolation Method (EIM)

Idea: construct a basis of interpolation functions (vectors), and use an affine expression to approximate $W^T f(Vz, \mu)$, i.e.,

$$W^T f(Vz, \mu) \approx W^T U \beta(z, \mu).$$

Precomputed

Different methods have been proposed to construct the basis $U \in \mathbb{R}^{n \times M}$ and the corresponding coefficients $\beta(z, \mu)$:

Empirical interpolation method (EIM)

[BARRAULT/MADAY/NGUYEN/PATERA ’04]

Missing point estimation (MPE)

[ASTRID/WEILAND/WILLCOX/BACKX ’08, FASSBENDER/VENDL ’11]

Discrete empirical interpolation method (DEIM)

[CHATURANTABUT/SORENSEN ’10]

Empirical operator interpolation

[DROHMANN/HAASDONK/OHLBERGER ’12]
MOR for Nonlinear Parametric Systems

Original full order system (FOM)

\[ E(t, \mu) \frac{dx}{dt} = A(t, \mu)x + f(x, \mu), \]

or

\[ E(t^k, \mu)x^{k+1} = A(t^k, \mu)x^k + f(x^k, \mu). \]

Reduced-order model (ROM)

\[ \hat{E}(t, \mu) \frac{dz}{dt} = \hat{A}(t, \mu)z + W^T f(Vz, \mu), \quad \hat{x} := Vz, \]

or

\[ \hat{E}(t^k, \mu)z^{k+1} = \hat{A}(t^k, \mu)z^k + W^T f(Vz^k, \mu) \quad \hat{x}^k := Vz^k, \]

\[ \hat{E} = W^T EV, \quad \hat{A} = W^T AV, \quad W, V \in \mathbb{R}^{n \times N}, \quad z, z^k \in \mathbb{R}^N, \quad N \ll n. \]
Original full order system (FOM)

\[ E(t, \mu) \frac{dx}{dt} = A(t, \mu)x + f(x, \mu), \]

or

\[ E(t^k, \mu)x^{k+1} = A(t^k, \mu)x^k + f(x^k, \mu). \]

Use Empirical Interpolation to efficiently compute \( W^T f(Vz, \mu) \)

\[ \hat{E}(t, \mu) \frac{dz}{dt} = \hat{A}(t, \mu)z + W^T U \beta(z, \mu), \]

or

\[ \hat{E}(t^k, \mu)z^{k+1} = \hat{A}(t^k, \mu)z^k + W^T U \beta^k(z, \mu). \]

The fast computation can be achieved by the strategy of offline-online decomposition, i.e., \( \hat{E}, \hat{A} \) and \( W^T U \) can be precomputed once \( V, W, U \) are obtained.
Consider the evolution scheme,

\[ \begin{align*}
E(t^k, \mu)x^{k+1} &= A(t^k, \mu)x^k + f(x^k, \mu), \\
y^{k+1} &= Cx^{k+1}.
\end{align*} \]

The reduced-order model (ROM):

\[ \begin{align*}
\hat{E}(t^k, \mu)z^{k+1} &= \hat{A}(t^k, \mu)z^k + W^T f(Vz^k, \mu), \\
\hat{y}^{k+1} &= CVz^{k+1}.
\end{align*} \]

Here, \( \hat{E}(t^k, \mu) = W^T E(t^k, \mu) V \), \( \hat{A}(t^k, \mu) = W^T A(t^k, \mu) V \), \( \hat{x}^k := Vz^k \) approximates \( x^k \), \( k = 0, \ldots, T_n \).

Define the residual:

\[ r^{k+1}(\mu) := A(t^k, \mu)\hat{x}^k + f(\hat{x}^k, \mu) - E(t^k, \mu)\hat{x}^{k+1}. \]

We have the following error estimations.
Primal-only Error Bound
Field Variable Error Bound

Theorem (Error Bound 1)

[DROHMANN/HAA SDONK/OHLBERGER ’12, ZHANG/FENG/LI/BENNER ’14]

Let $e^k(\mu) := x^k - \hat{x}^k$ and $e^k_O(\mu) := y^k - \hat{y}^k$ be the error for the solution and the output at time step $t^k$, respectively. Under certain assumptions, we have:

\[
\|e^1(\mu)\| \leq \eta^1_{N,M}(\mu) := R^{(0)}_{F,\mu},
\]
\[
\|e^k(\mu)\| \leq \eta^k_{N,M}(\mu) := R^{(k-1)}_{F,\mu} + \sum_{i=0}^{k-2} \left( \prod_{j=i+1}^{k-1} G^{(j)}_{F,\mu} \right) R^{(i)}_{F,\mu}, \quad k = 2, \ldots, T_n.
\]

where

\[
R^{(i)}_{F,\mu} = \|E(t^i, \mu)^{-1} r^{i+1}(\mu)\|, \quad i = 0, \ldots, k - 1,
\]
\[
G^{(j)}_{F,\mu} = \|E(t^j, \mu)^{-1} A(t^j, \mu)\| + L_f \|E(t^j, \mu)^{-1}\|, \quad j = i + 1, \ldots, k - 1.
\]
Theorem (Output Error Bound 1) [Zhang/Feng/Li/Benner '14]

Under the assumptions of Prop. 1, we have:

\[ \| e_O^{k+1}(\mu) \| \leq G_O^{(k)} \eta_{N,M}^{k}(\mu) + \| C \| \| E(t^k, \mu)^{-1} r^{k+1}(\mu) \|, \]

where

\[ G_O^{(k)} = \| CE(t^k, \mu)^{-1} A(t^k, \mu) \| + L_f \| CE(t^k, \mu)^{-1} \|. \]
Primal-dual Output Error Bound

"Dual" system and the reduced "dual" system

\[ E(t^k, \mu)^T x_{du}^{k+1} = -C^T, \quad W_{du}^T E(t^k, \mu)^T V_{du} z_{du}^{k+1} = -W_{du}^T C^T. \]

Here, \( \hat{x}_{du}^k := V_{du} z_{du}^k \) approximates \( x_{du}^k, k = 1, \ldots, T_n. \)
Primal-dual Output Error Bound

"Dual" system and the reduced "dual" system

\[ E(t^k, \mu)^T x_{du}^{k+1} = -C^T, \quad W_{du}^T E(t^k, \mu)^T V_{du} z_{du}^{k+1} = -W_{du}^T C^T. \]

Here, \( \hat{x}_{du}^k := V_{du} z_{du}^k \) approximates \( x_{du}^k, k = 1, \ldots, T_n. \)

Residual of the reduced dual system:

\[ r_{du}^{k+1}(\mu) := -C^T - E(t^k, \mu)^T \hat{x}_{du}^{k+1}. \]

Recall residual of the ROM:

\[ r^{k+1}(\mu) := A(t^k, \mu) \hat{x}^k + f(\hat{x}^k, \mu) - E(t^k, \mu) \hat{x}^{k+1}. \]
"Dual" system and the reduced "dual" system

\[
E(t^k, \mu)^T x_{du}^{k+1} = -C^T, \quad W_{du}^T E(t^k, \mu)^T V_{du} z_{du}^{k+1} = -W_{du}^T C^T.
\]

Here, \(\hat{x}_{du}^k := V_{du} z_{du}^k\) approximates \(x_{du}^k\), \(k = 1, \ldots, T_n\).

Residual of the reduced dual system:

\[
r_{du}^{k+1}(\mu) := -C^T - E(t^k, \mu)^T \hat{x}_{du}^{k+1}.
\]

Recall residual of the ROM:

\[
r^{k+1}(\mu) := A(t^k, \mu) \hat{x}^k + f(\hat{x}^k, \mu) - E(t^k, \mu) \hat{x}^{k+1}.
\]

Define an auxiliary vector,

\[
\tilde{r}^{k+1}(\mu) := A(t^k, \mu) x^k + f(x^k, \mu) - E(t^k, \mu) \hat{x}^{k+1} - E(t^k, \mu) x^{k+1}.
\]
Theorem (Output Error Bound 2) [Zhang/Feng/Li/Benner ’15]

Assume that $E(t^k, \mu)$ is invertible, then the output error $e^k_O(\mu) := y^k - \hat{y}^k$ satisfies

$$\|e^k_O(\mu)\| \leq \tilde{\Delta}^k(\mu), \quad k = 1, \ldots, T_n,$$

where

$$\tilde{\Delta}^k(\mu) := \Phi^k(\mu)\|\tilde{r}^k(\mu)\|,$$

$$\Phi^k(\mu) = \|E(t^{k-1}, \mu)^{-T}\| \|r^k_{du}(\mu)\| + \|\hat{x}^k_{du}(\mu)\|. $$
Assume that $E(t^k, \mu)$ is invertible, then the output error $e^k_O(\mu) := y^k - \hat{y}^k$ satisfies

$$\|e^k_O(\mu)\| \leq \tilde{\Delta}^k(\mu), \quad k = 1, \ldots, T_n,$$

where

$$\tilde{\Delta}^k(\mu) := \Phi^k(\mu)\|\tilde{r}^k(\mu)\|,$$

$$\Phi^k(\mu) = \|E(t^{k-1}, \mu)^{-T}\|\|r^k_{du}(\mu)\| + \|\hat{x}^k_{du}(\mu)\|.$$

Define

$$\rho^k(\mu) := \frac{\|\tilde{r}^k(\mu)\|}{\|r^k(\mu)\|}.$$

It can be shown that $\rho^k(\mu)$ is bounded, i.e.,

$$\underline{\rho}^k(\mu) \leq \rho^k(\mu) \leq \bar{\rho}^k(\mu).$$
Corollary 1

Under the assumptions of Theorem 1, for all $\mu \in \mathcal{P}$, assume that

1. $\{\|\tilde{r}^k(\mu)\|\} \colon \exists \alpha \in \mathbb{R}^+, \text{s.t.},$
   \begin{align*}
   \alpha & \leq \|\tilde{r}^{k+1}(\mu)\|/\|\tilde{r}^k(\mu)\| \quad \forall \quad k = 1, \ldots, T_n - 1;
   \end{align*}

2. $f(\cdot, \mu)$ is Lipschitz continuous, i.e., $\exists L_f \in \mathbb{R}^+, \text{s.t.},$
   \begin{align*}
   \|f(x_1, \mu) - f(x_2, \mu)\| & \leq L_f \|x_1 - x_2\|, \quad \forall \quad x_1, x_2 \in \mathcal{W}^n;
   \end{align*}

3. $L_f < \alpha/\|E(t^k, \mu)^{-1}\|.$

Then

\[ \underline{\rho}^k(\mu) \leq \rho^k(\mu) \leq \bar{\rho}^k(\mu), \]

where $\underline{\rho}^k(\mu) = \frac{\alpha}{\alpha + L_f \|E(t^{k-2}, \mu)^{-1}\|}$, $\bar{\rho}^k(\mu) = \frac{\alpha}{\alpha - L_f \|E(t^{k-2}, \mu)^{-1}\|}$.

Remark: Assumption \#3 is reasonable when $\|E(t^k, \mu)^{-1}\| \lesssim 1.$
Primal-dual Output Error Bound (Cont.)

Efficient Output Error Estimation: Case 2

Corollary 2 [Zhang/Feng/Li/Benner ’15]

Under the assumptions of Theorem 1, for all $\mu \in \mathcal{P}$, assume that

1. $\{\|\tilde{r}^k(\mu)\|\}$: $\exists \alpha, \bar{\alpha} \in \mathbb{R}^+$, s.t.,
   $$\alpha \leq \frac{\|\tilde{r}^k(\mu)\|}{\|\tilde{r}^{k+1}(\mu)\|} \leq \bar{\alpha}, \quad \forall \ k = 1, \ldots, T_n - 1;$$

2. $f(\cdot, \mu)$ is bi-Lipschitz continuous, i.e., $\exists L_f, \bar{L}_f \in \mathbb{R}^+$, s.t.,
   $$L_f \|x_1 - x_2\| \leq \|f(x_1, \mu) - f(x_2, \mu)\| \leq \bar{L}_f \|x_1 - x_2\|, \quad x_1, x_2 \in \mathcal{W}_n;$$

3. $L_f > \alpha^{-1}/\|\mathcal{E}(t^k, \mu)^{-1}\|$.

Then

$$\underline{\rho}^k(\mu) \leq \rho^k(\mu) \leq \bar{\rho}^k(\mu),$$

where

$$\underline{\rho}^k(\mu) = \frac{1}{\alpha \bar{L}_f \|\mathcal{E}(t^{k-2}, \mu)^{-1}\| + 1}, \quad \bar{\rho}^k(\mu) = \frac{1}{\alpha L_f \|\mathcal{E}(t^{k-2}, \mu)^{-1}\| - 1}.$$

Remark: Assumption #3 is reasonable when $\|\mathcal{E}(t^k, \mu)^{-1}\|$ is large.
Recall that \( \| e_O^k(\mu) \| \leq \tilde{\Delta}^k(\mu) = \Phi^k(\mu) \| \tilde{r}^k(\mu) \| \), \( \rho^k(\mu) = \frac{\| \tilde{r}^k(\mu) \|}{\| r^k(\mu) \|} \), we have:

**Output Error Bound**

\[
\| e_O^k(\mu) \| \leq \Delta^k(\mu) := \Phi^k(\mu) \rho^k(\mu) \| r^k(\mu) \|.
\]
Recall that $\|e^k_O(\mu)\| \leq \Delta^k(\mu) = \Phi^k(\mu)\|\tilde{r}^k(\mu)\|$, $\rho^k(\mu) = \frac{\|\tilde{r}^k(\mu)\|}{\|r^k(\mu)\|}$, we have:

**Output Error Bound**

$$\|e^k_O(\mu)\| \leq \Delta^k(\mu) := \Phi^k(\mu)\rho^k(\mu)\|r^k(\mu)\|.$$  

**Estimating the Ratio $\rho^k(\mu)$**

$$\rho^k(\mu) \approx \rho_* := \frac{1}{T_n} \sum_{k=1}^{T_n} \rho^k(\mu_\star).$$

A computable output error estimation:

$$\|e^k_O\| \lesssim \Delta^k_{est}(\mu) := \rho_* \Phi^k(\mu)\|r^k(\mu)\|.$$  

Here, $\mu_\star$ is chosen to be the parameter, so that

$$\mu_\star = \arg\max_{\mu \in P} \psi(\mu), \quad \psi(\mu) = \frac{1}{T_n} \sum_{k=1}^{T_n} \Delta^k_{est}(\mu).$$
POD-Greedy Algorithm

How to compute $V$ ?

**Algorithm** POD-Greedy

| Input:  | $P_{\text{train}}, \mu_0, \varepsilon_{\text{RB}} (< 1)$. |
| Output: | Reduced Basis (RB): $V = [v_1, \ldots, v_N]$. |

1. Initialization: $N = 0$, $V = []$, $\mu_* = \mu_0$, $\psi(\mu_*) = 1$.
2. **while** $\psi(\mu_*) > \varepsilon_{\text{RB}}$ **do**
3. Compute the trajectory $X := [x^1(\mu_*), \ldots, x^{T_n}(\mu_*)]$.
4. **POD process:**
   - If $N \neq 0$, compute $x^k(\mu_*) := x^k(\mu_*) - \text{Proj}_{\mathcal{W}}[x^k(\mu_*)]$, $k = 1, \ldots, T_n$.
   - Do SVD for $X$: $X = Q\Sigma F^T$, $v_{N+1} := Q(:, 1)$.
   - Enrich $V$: $V = [V, v_{N+1}]$, $\mathcal{W} := \text{colspan}\{V\}$.
5. $N = N + 1$.
6. Find $\mu_* := \arg \max_{\mu \in P_{\text{train}}} \psi(\mu)$.
7. **end while**

**Remark:** When $T_n$ is large, adaptive snapshot selection can be applied.
Adaptive Snapshot Selection (ASS)

The idea of ASS is to discard the redundant linear information in the trajectory earlier, before the POD process.

- $S_A$: selected snapshots subspace,
- $x$: to be tested,
- $\phi(S_A, x)$: an indicator to measure the linear dependency of $S_A$ and $x$, e.g.,
  \[ \phi(S_A, x) = \angle(S_A, x). \]
- $x$ is taken as a new snapshot only when $x$ is “sufficiently” linearly independent from $S_A$, i.e., $\phi(S_A, x) > \varepsilon_{ASS}$. 

**Algorithm Adaptive Snapshot Selection** [Zhang/Feng/Li/Benner ’14]

**Input:** \( \{x^k\}_{k=1}^{T_n}, \varepsilon_{\text{ASS}} \).

**Output:** Selected snapshot matrix \( S_A = [x^{k_1}, \ldots, x^{k_\ell}] \).

1. Initialization: \( j = 1, k_j = 1, S_A = [x^{k_j}] \).
2. for \( k = 2, \ldots, T_n \) do
3. if \( \phi(S_A, x^k) > \varepsilon_{\text{ASS}} \) then
4. \( j = j + 1 \).
5. \( k_j = k \).
6. \( S_A = [S_A, x^{k_j}] \).
7. end if
8. end for
### Algorithm Adaptive Snapshot Selection

[Zhang/Feng/Li/Benner '14]

**Input:** \( \{x^k\}_{k=1}^{T_n}, \varepsilon_{\text{ASS}} \).

**Output:** Selected snapshot matrix \( S_A = [x^{k_1}, \ldots, x^{k_\ell}] \).

1. Initialization: \( j = 1, \ k_j = 1, \ S_A = [x^{k_j}] \).
2. for \( k = 2, \ldots, T_n \) do
3. if \( \phi(S_A, x^k) > \varepsilon_{\text{ASS}} \) then
4. \( j = j + 1 \).
5. \( k_j = k \).
6. \( S_A = [S_A, x^{k_j}] \).
7. end if
8. end for

**Remark:** a relaxed condition \( \phi(S_A, x^k) = \angle(x^{k_j}, x^k) \) can be employed for an efficient implementation.
**ASS-POD-Greedy Algorithm**

**How to compute $V$ ?**

**Algorithm POD-Greedy**  
[Haasdonk/Ohlberger '08]

**Input:** $\mathcal{P}_{\text{train}}, \mu_0, \varepsilon_{\text{RB}}(< 1)$.

**Output:** Reduced Basis (RB): $V = [v_1, \ldots, v_N]$.

1. **Initialization:** $N = 0$, $V = [], \mu_\star = \mu_0$, $\psi(\mu_\star) = 1$.
2. **while** $\psi(\mu_\star) > \varepsilon_{\text{RB}}$ **do**
3. **Compute the trajectory** $X := [x^1(\mu_\star), \ldots, x^{T_n}(\mu_\star)]$.
4. **POD process:**
   - If $N \neq 0$, compute $x^k(\mu_\star) := x^k(\mu_\star) - \text{Proj}_{\mathcal{W}}[x^k(\mu_\star)]$, $k = 1, \ldots, T_n$.
   - Do SVD for $X$: $X = Q\Sigma F^T$, $v_{N+1} := Q(:, 1)$.
   - Enrich $V$: $V = [V, v_{N+1}]$, $\mathcal{W} := \text{colspan}\{V\}$.
5. $N = N + 1$.
6. **Find** $\mu_\star := \arg \max_{\mu \in \mathcal{P}_{\text{train}}} \psi(\mu)$.
7. **end while**
ASS-POD-Greedy Algorithm

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>ASS-POD-Greedy</th>
<th>[Zhang/Feng/Li/Benner '14]</th>
</tr>
</thead>
</table>

**Input:** \( P_{\text{train}}, \varepsilon_{RB} (< 1) \)

**Output:** Reduced Basis (RB): \( V = [v_1, \ldots, v_N] \)

1. Initialization: \( N = 0, V = [], \mu_* = \mu_0, \psi(\mu_*) = 1. \)
2. **while** \( \psi(\mu_*) > \varepsilon_{RB} \) **do**
3. Compute the trajectory \( X := [x^1(\mu_*), \ldots, x^{T_n}(\mu_*)], \)
   apply ASS to get: \( X_{\text{ASS}} := [x^{k_1}(\mu_*), \ldots, x^{k_\ell}(\mu_*)] \) \( (\ell \ll T_n). \)
4. **POD process:**
   If \( N \neq 0 \), compute \( x^{k_j}(\mu_*) := x^{k_j}(\mu_*) - \text{Proj}_{W}[x^{k_j}(\mu_*)], j = 1, \ldots, \ell. \)
   Do SVD for \( X_{\text{ASS}}: X_{\text{ASS}} = Q\Sigma F^T, v_{N+1} := Q(:, 1). \)
   Enrich \( V: V = [V, v_{N+1}], W := \text{colspan}\{V\}. \)
5. \( N = N + 1 \)
6. Find \( \mu_* := \arg \max_{\mu \in P_{\text{train}}} \psi(\mu). \)
7. **end while**
Numerical Examples:

1. Linear convection-diffusion equation
2. Burgers’ equation
3. Batch chromatography
4. Continuous SMB chromatography
Example 1: Linear Convection-diffusion Equation

Primal-dual Error Bound/Estimation: Proposed vs. Existing

\[ u_t = q_1 u_{xx} + q_2 u_x - q_2, \quad x \in (0, 1), \quad t \in (0, 1], \]
\[ y = \frac{1}{|\Omega_0|} \int_{\Omega_0} u(t, x) \, dx, \]
\[ \mu := (q_1, q_2), \quad \mathcal{P} = [0.1, 1] \times [0.5, 5], \]
\[ n = 800, \quad T_n = 100. \]

Error bound decay during RB extension.

ErrorBound-1: [Grepl/Patera’05], ErrorBound-2: proposed.
Example 1: Linear Convection-diffusion Equation

Behavior of $\rho_*$

Behavior of the average ratio $\rho_* = \frac{1}{T_n} \sum_{k=1}^{T_n} \rho_k^{\mu_*}$ during the RB construction process for the linear convection-diffusion equation.
Example 1: Linear Convection-diffusion Equation

Behavior of the Ratio $\frac{\|\tilde{r}^{n+1}\|}{\|\tilde{r}^n\|}$

Behavior of the ratio $\frac{\|\tilde{r}^{n+1}\|}{\|\tilde{r}^n\|}$ in the time trajectory corresponding to different RB dimensions for the linear convection-diffusion equation.
Example 2: Burgers’ Equation

Error Bound/Estimation: Primal Only vs. Primal-dual

\[
  u_t + \left( \frac{u^2}{2} \right)_x = \nu u_{xx} + 1, \quad x \in (0, 1), \quad t \in (0, 2],
\]

\[
  y = u(t, 1; \nu),
\]

\[
  \nu \in \mathcal{P} = [0.05, 1], \quad n = 500, \quad T_n = 1000.
\]

Error bound decay during RB extension.

ErrorBound-1: primal only, ErrorBound-2: primal-dual.
Example 2: Burgers’ Equation

Behavior of $\rho_*$

Behavior of the average ratio $\rho_* = \frac{1}{T_n} \sum_{k=1}^{T_n} \rho^k(\mu_*)$ during the RB construction process for the Burgers’ equation.
Example 2: Burgers’ Equation

Behavior of the Ratio \( \| \tilde{r}^{n+1} \| / \| \tilde{r}^n \| \)

Behavior of the ratio \( \| \tilde{r}^{n+1} \| / \| \tilde{r}^n \| \) in the time trajectory corresponding to different RB dimensions for the Burgers’ equation.
Example 3: Batch Chromatography

Principle of batch chromatography for binary separation.
Example 3: Batch Chromatography

Principle of batch chromatography for binary separation.

\[
\begin{align*}
A_{c}^{k+1} &= B_{c}^{k} + d_{z}^{k} - \tau h_{z}^{k} \\
q_{z}^{k+1} &= q_{z}^{k} + \Delta t h_{z}^{k} \\
c_{z}^{k}, q_{z}^{k} &\in \mathbb{R}^{n}, \tau = \frac{1 - \epsilon}{\epsilon} \Delta t
\end{align*}
\]

\[
\begin{align*}
\hat{A}_{c} a_{c}^{k+1} &= \hat{B}_{c} a_{c}^{k} + d_{0}^{k} \hat{d}_{c} - \tau \hat{H}_{c} \beta_{z}^{k} \\
a_{q}^{k+1} &= a_{q}^{k} + \Delta t \hat{H}_{q} \beta_{z}^{k} \\
a_{c}^{k}, a_{q}^{k} &\in \mathbb{R}^{N}, \beta_{z}^{k} \in \mathbb{R}^{M}
\end{align*}
\]

The parameter \( \mu = (Q, t_{in}) \).
Example 3: Batch Chromatography

Performance of the ASS for Basis Generation

Illustration of the generation of CRBs ($W_a$, $W_b$) at the same error tolerance ($\varepsilon_{CRB} = 1.0 \times 10^{-7}$) with different thresholds for ASS.

<table>
<thead>
<tr>
<th>$\varepsilon_{ASS}$</th>
<th>Dim. CRB ($W_a W_b$)</th>
<th>Runtime [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>no ASS –</td>
<td>146 152</td>
<td>62.5 (-)</td>
</tr>
<tr>
<td>ASS $1.0 \times 10^{-4}$</td>
<td>147 152</td>
<td>6.05 ($-90.3%$)</td>
</tr>
<tr>
<td>ASS $1.0 \times 10^{-3}$</td>
<td>147 152</td>
<td>3.62 ($-94.2%$)</td>
</tr>
<tr>
<td>ASS $1.0 \times 10^{-2}$</td>
<td>144 150</td>
<td>2.70 ($-95.7%$)</td>
</tr>
</tbody>
</table>
Example 3: Batch Chromatography

Performance of the ASS for Basis Generation

Comparison of the runtime for RB generation using the POD-Greedy algorithm with and without ASS.

<table>
<thead>
<tr>
<th>Algorithms</th>
<th>Runtime [h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>POD-Greedy</td>
<td>17.9</td>
</tr>
<tr>
<td>ASS-POD-Greedy</td>
<td>7.6 (−57.5%)</td>
</tr>
</tbody>
</table>
Example 3: Batch Chromatography

Error Bound/Estimation: Primal Only vs. Primal-dual

Error bound decay during RB extension.

Runtime for the RB construction.

6.8 h 7.6 h
Example 3: Batch Chromatography

Behavior of $\rho_*$

Behavior of the average ratio $\rho_* = \frac{1}{T_n} \sum_{k=1}^{T_n} \rho^k(\mu_*)$ during the RB construction process for the batch chromatographic model.
Example 3: Batch Chromatography
ROM-based Optimization

FOM-based Opt.:  
\[ \min_{\mu \in \mathcal{P}} \{-Pr(c_z(\mu), q_z(\mu); \mu)\}, \text{ s.t.} \]
\[ Rec(c_z(\mu), q_z(\mu); \mu) \geq Rec_{\text{min}}, \]
\[ c_z(\mu), q_z(\mu): \text{ solutions to FOM.} \]

ROM-based Opt.:  
\[ \min_{\mu \in \mathcal{P}} \{-Pr(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu)\}, \text{ s.t.} \]
\[ Rec(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Rec_{\text{min}}, \]
\[ \hat{c}_z(\mu), \hat{q}_z(\mu): \text{ solutions to ROM.} \]

Optimization based on the ROM \((N = 45)\) and the FOM \((n = 1500)\).

<table>
<thead>
<tr>
<th>Model</th>
<th>Obj. ((Pr))</th>
<th>Opt. solution ((\mu))</th>
<th>#Iterations</th>
<th>Runtime [h]/SpF</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOM-Opt.</td>
<td>0.020264</td>
<td>(0.0796, 1.0545)</td>
<td>202</td>
<td>33.88 / -</td>
</tr>
<tr>
<td>ROM-Opt.</td>
<td>0.020266</td>
<td>(0.0796, 1.0545)</td>
<td>202</td>
<td>0.58 / 58</td>
</tr>
</tbody>
</table>

⋆ The optimizer: NLOPT\_GN\_DIRECT\_L in NLopt package.
Example 4: SMB Chromatography

SMB chromatographic process with 4 zones and 8 columns.
Example 4: SMB Chromatography

Model Descriptions

A more complex system:

- More parameters: $\mu := (m_1, \ldots, m_4, Q_F)$.
- A multi-switching system: $x_T^0 = P_s x_T^n$, $T$ is the time period.
- Cyclic steady state (CSS) computation, the system is simulated many time periods till the CSS is reached.
- A parametric coupled system.

FOM:
\[
\begin{align*}
A_z(\mu)c_{zk}^{k+1} &= B_z(\mu)c_{zk}^k + r_z^k + t_s\kappa_z q_{zk}^k \\
q_{zk}^{k+1} &= (1 - t_s\kappa_z\Delta t)q_{zk}^k + t_s\kappa_z H_z\Delta t c_{zk}^k
\end{align*}
\]

ROM:
\[
\begin{align*}
\hat{A}_z(\mu)a_{cz}^{k+1} &= \hat{B}_z(\mu)a_{cz}^k + \hat{r}_z + t_s\kappa_z \hat{D}_z a_{qz}^k \\
\hat{a}_{qz}^{k+1} &= (1 - t_s\kappa_z\Delta t)\hat{a}_{qz}^k + t_s\kappa_z H_z\Delta t \hat{D}_z^T a_{cz}^k
\end{align*}
\]

$\hat{A}_z(\mu) = V_{cz}^T A_z(\mu) V_{cz}$, $\hat{B}_z(\mu) = V_{cz}^T B_z(\mu) V_{cz}$, $\hat{r}_z = V_{cz}^T r_z^k$, $\hat{D}_z = V_{cz}^T V_{qz}$. 
Example 4: SMB Chromatography

Error Behavior during the RB Construction Process

Error bound decay during RB extension.
Example 4: SMB Chromatography

Behavior of $\rho_*$

![Graph showing the behavior of the average ratio $\rho_*$](image)

Behavior of the average ratio $\rho_* = \frac{1}{T_n} \sum_{k=1}^{T_n} \rho^k(\mu_*)$ during the RB construction process for the SMB model.
Example 4: SMB Chromatography

ROM Validation

Runtime comparison of the detailed and reduced simulations over a validation set $\mathcal{P}_{\text{val}}$ with 200 random sample parameters. $\varepsilon_{\text{RB}} = 1 \times 10^{-3}$, $\varepsilon_{\text{ASS}} = 1 \times 10^{-5}$.

<table>
<thead>
<tr>
<th>Simulations</th>
<th>Maximal error</th>
<th>Average runtime [s]/SpF</th>
</tr>
</thead>
<tbody>
<tr>
<td>FOM ($n = 800$)</td>
<td>$-$</td>
<td>338.71(-)</td>
</tr>
<tr>
<td>ROM ($N = 83$)</td>
<td>$1.1 \times 10^{-4}$</td>
<td>46.7 / 7</td>
</tr>
</tbody>
</table>
Example 4: SMB Chromatography

ROM-based Optimization

FOM-based Opt.:

\[
\min_{\mu \in \mathcal{P}} \left\{ -Q(\mu) \right\}, \quad \text{s.t.,}
\]
\[
Pu_{a,E}(c_z(\mu), q_z(\mu); \mu) \geq Pu_{a,\text{min}},
\]
\[
Pu_{b,R}(c_z(\mu), q_z(\mu); \mu) \geq Pu_{b,\text{min}},
\]
\[
Q_1 \leq Q_{\text{max}},
\]
\[
c_z(\mu), q_z(\mu): \text{solutions to FOM}.
\]

ROM-based Opt.:

\[
\min_{\mu \in \mathcal{P}} \left\{ -Q(\mu) \right\}, \quad \text{s.t.,}
\]
\[
\hat{Pu}_{a,E}(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Pu_{a,\text{min}},
\]
\[
\hat{Pu}_{b,R}(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Pu_{b,\text{min}},
\]
\[
\hat{Q}_1 \leq Q_{\text{max}},
\]
\[
\hat{c}_z(\mu), \hat{q}_z(\mu): \text{solutions to ROM}.
\]

\[\mathcal{P} = [4.2, 4.7] \times [2.5, 3.0] \times [3.5, 4.0] \times [2.2, 2.7] \times [0.05, 0.1],\]

\[Pu_{a,E} := \frac{\int_0^1 c_{a,\text{CSS}}(t) \, dt}{\int_0^1 c_{a,\text{CSS}}(t) \, dt + \int_0^1 c_{b,\text{CSS}}(t) \, dt}, \quad Pu_{b,R} := \frac{\int_0^1 c_{b,\text{CSS}}(t) \, dt}{\int_0^1 c_{a,\text{CSS}}(t) \, dt + \int_0^1 c_{b,\text{CSS}}(t) \, dt}.
\]

Constraints: \(Pu_{a,\text{min}} = 99.0\%, \quad Pu_{b,\text{min}} = 99.0\%, \quad Q_{\text{max}} = 0.50.\]
Example 4: SMB Chromatography

ROM-based optimization

Comparison of the optimization based on the ROM ($N = 83$) and FOM ($n = 800$), $\varepsilon_{\text{opt}} = 1 \times 10^{-4}$.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Objective</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$Q_F$</td>
<td>0.07</td>
<td>0.0745</td>
<td>0.0745</td>
</tr>
<tr>
<td>$m_1$</td>
<td>4.50</td>
<td>4.3269</td>
<td>4.3271</td>
</tr>
<tr>
<td>$m_2$</td>
<td>2.90</td>
<td>2.8599</td>
<td>2.8603</td>
</tr>
<tr>
<td><strong>Opt. solution</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$m_3$</td>
<td>3.50</td>
<td>3.6036</td>
<td>3.6039</td>
</tr>
<tr>
<td>$m_4$</td>
<td>2.30</td>
<td>2.3468</td>
<td>2.3685</td>
</tr>
<tr>
<td>$Q_F$</td>
<td>0.07</td>
<td>0.0745</td>
<td>0.0745</td>
</tr>
<tr>
<td><strong>Constraints</strong></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$P_{u_a,E}$</td>
<td>98.89%</td>
<td>99.00%</td>
<td>99.00%</td>
</tr>
<tr>
<td>$P_{u_b,R}$</td>
<td>99.49%</td>
<td>99.00%</td>
<td>99.00%</td>
</tr>
<tr>
<td>$Q_1$</td>
<td>0.4161</td>
<td>0.4997</td>
<td>0.4998</td>
</tr>
<tr>
<td><strong># Iterations</strong></td>
<td></td>
<td>71</td>
<td>79</td>
</tr>
<tr>
<td><strong>Runtime [h] / SpF</strong></td>
<td></td>
<td>5.13 / -</td>
<td>0.82 / 6</td>
</tr>
</tbody>
</table>

★ The optimizer: NLOPT\_LN\_COBYLA in NLopt package.
Conclusions and Outlook

Conclusions:

- An efficient output error estimation for MOR of nonlinear parametrized evolution equations is proposed.
- Adaptive Snapshot Selection (ASS) is proposed, so that the offline time is largely reduced.
- Application to convection dominated problems, e.g. batch chromatography and linear SMB chromatography, is presented.

Outlook:

- More reliable and efficient estimation of $\rho^k(\mu)$.
- Reduced basis methods for SMB chromatography with uncertainty quantification (UQ).
References


