Workshop on Model Order Reduction
of Transport-dominated Phenomena
Berlin, May 19–20, 2015

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

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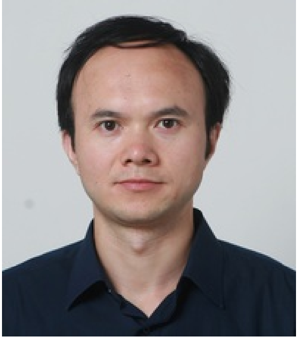
Outline

Collaborators

Lihong Feng



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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

$$E(t,\mu)\frac{\mathrm{d}x}{\mathrm{d}t} = A(t,\mu)x + f(x,\mu),$$

or

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

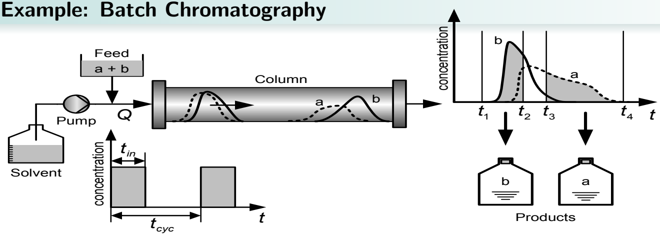
$x, x^k \in \mathcal{W}^n \subset \mathbb{R}^n$, $E, A \in \mathbb{R}^{n\times n}$, n is large.

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

Motivation

Motivating Example: Batch Chromatography



Principle of batch chromatography for binary separation.

Motivation

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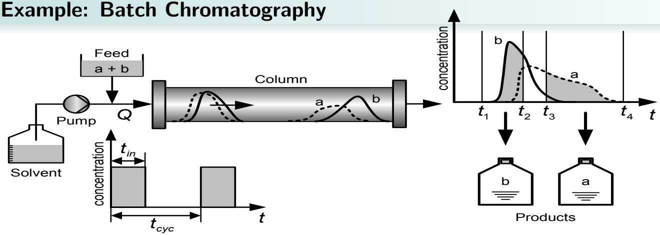

Principle of batch chromatography for binary separation.

$$\begin{cases} \dfrac{\partial c_z}{\partial t} + \dfrac{1-\epsilon}{\epsilon}\dfrac{\partial q_z}{\partial t} = -\dfrac{\partial c_z}{\partial x} + \dfrac{1}{Pe}\dfrac{\partial^2 c_z}{\partial x^2}, & 0 < x < 1, \\ \dfrac{\partial q_z}{\partial t} = \dfrac{L}{Q/(\epsilon A_c)}\kappa_z(q_z^{\mathrm{Eq}} - q_z), & 0 \le x \le 1, \end{cases} \quad z = \mathrm{a, b}$$

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

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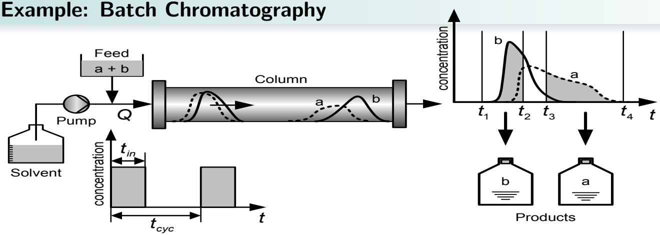

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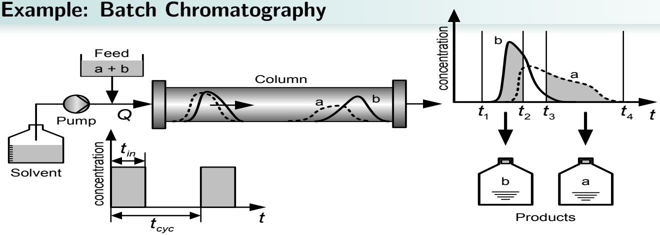

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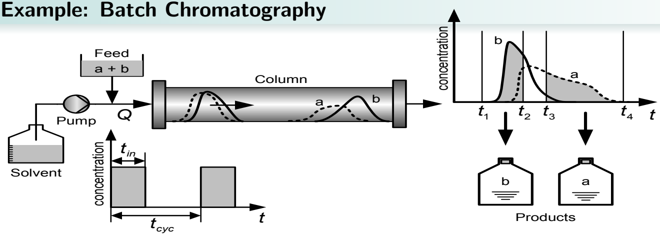

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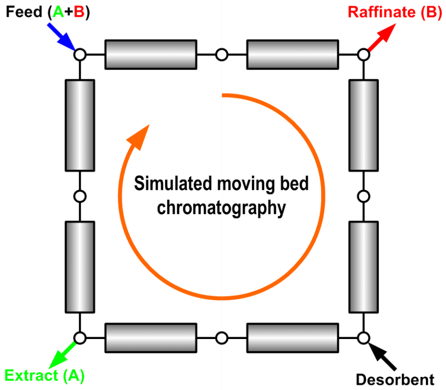
- A convection-dominated system, the Péclet number Pe is large.
- Requires long-time integration process.
- A nonlinear parametric coupled system, parameters $\mu := (Q, t_{\mathrm{in}})$.
- What are the optimal operating conditions?
  $\rightsquigarrow$ PDE constrained optimization.

Motivation

Motivating Example: Simulated Moving Bed (SMB) Chromatography

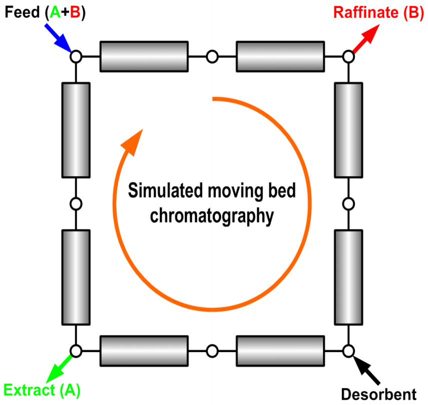


SMB chromatographic process with 4 zones and 8 columns.

Motivation

Motivating Example: SMB Chromatography

Governing equations are similar, but:



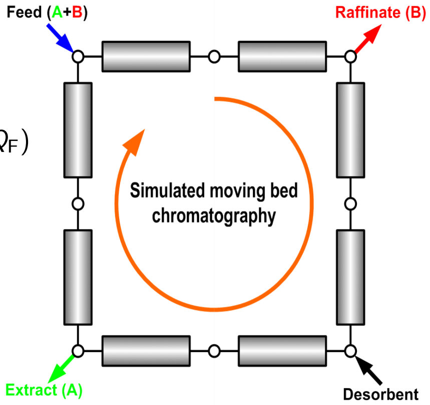
SMB chromatographic process with 4 zones and 8 columns.

Motivation

Motivating Example: SMB Chromatography

Governing equations are similar, but:

- More parameters, $\mu := (m_1, \ldots, m_4, Q_\mathsf{F})$
- Multi-switching system
- Cyclic steady state computation



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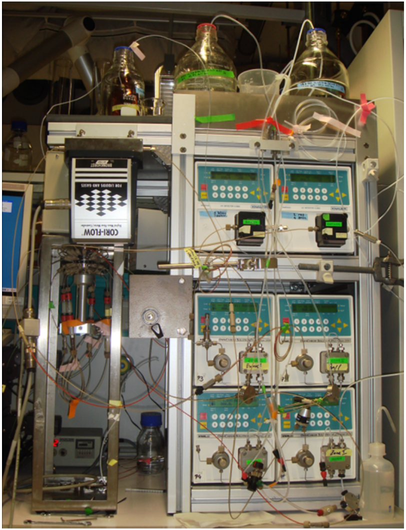
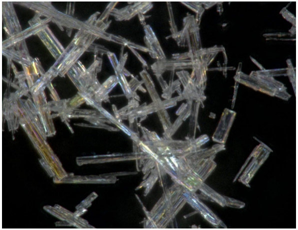
4-column SMB plant at MPI Magdeburg



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 roup) 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!

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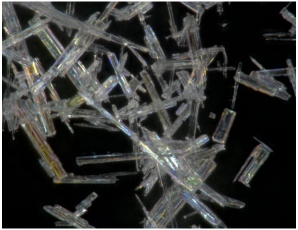

Seeberger and Seidel-Morgenstern were awarded the Humanity in Science Prize 2015 for this.

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MOR for Nonlinear Parametric Systems

Original full order system (FOM)

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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.

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Reduced-order model (ROM)

$$\hat{E}(t,\mu)\frac{\mathrm{d}z}{\mathrm{d}t} = \hat{A}(t,\mu)z + W^T f(Vz,\mu), \qquad \hat{x} := Vz,$$

or

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

$\hat{E} = W^T EV$, $\hat{A} = W^T AV$, $W, V \in \mathbb{R}^{n\times N}$, $z, z^k \in \mathbb{R}^N$, $N \ll n$.

Remarks

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.

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

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2. How to estimate the error in the quantities-of-interest, i.e., $\|y-\hat{y}\| \leq$? $\rightsquigarrow$ Output error bound.
3. How to efficiently construct the projection matrices V and W? $\rightsquigarrow$ Adaptive snapshot selection.

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.,

$$W^T f(Vz,\mu) \approx \underbrace{W^T U}_{\text{Precomputed}} \; \beta(z,\mu).$$

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]

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

$$\hat{E}(t,\mu)\frac{\mathrm{d}z}{\mathrm{d}t} = \hat{A}(t,\mu)z + \underline{W^T U}\beta(z,\mu),$$

or

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

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

Error Bound

Consider the evolution scheme,

$$\begin{aligned} E(t^k,\mu)x^{k+1} &= A(t^k,\mu)x^k + f(x^k,\mu), \\ y^{k+1} &= Cx^{k+1}. \end{aligned}$$

The reduced-order model (ROM):

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

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/Haasdonk/Ohlberger '12, Zhang/Feng/Li/Benner '14]

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

$$\|e^1(\mu)\| \leq \eta^1_{N,M}(\mu) := \mathtt{R}^{(0)}_{\mathsf{F},\mu},$$

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

where

$$\mathtt{R}^{(i)}_{\mathsf{F},\mu} = \left\| E(t^i,\mu)^{-1} r^{i+1}(\mu) \right\|, \quad i = 0, \ldots, k-1,$$

$$\mathtt{G}^{(j)}_{\mathsf{F},\mu} = \left\| E(t^j,\mu)^{-1} A(t^j,\mu) \right\| + L_f \left\| E(t^j,\mu)^{-1} \right\|, \quad j = i+1, \ldots, k-1.$$

Primal-only Error Bound (Cont.)

Output Error Bound

Theorem (Output Error Bound 1) [Zhang/Feng/Li/Benner '14]

Under the assumptions of Prop. 1, we have:

$$\|e_{\mathrm{O}}^{k+1}(\mu)\| \leq G_{\mathrm{O},\mu}^{(k)} \eta_{N,M}^{k}(\mu) + ||C|| ||E(t^k,\mu)^{-1} r^{k+1}(\mu)||,$$

where

$$G_{\mathrm{O},\mu}^{(k)} = ||CE(t^k,\mu)^{-1} A(t^k,\mu)|| + L_f ||CE(t^k,\mu)^{-1}||.$$

Primal-dual Output Error Bound

"Dual" system and the reduced "dual" system

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

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

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Residual of the reduced dual system:

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

Recall residual of the ROM:

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

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Define an auxiliary vector,

$$\begin{aligned}\tilde{r}^{k+1}(\mu) &:= A(t^k,\mu)x^k + f(x^k,\mu) - E(t^k,\mu)\hat{x}^{k+1}\\ &= E(t^k,\mu)x^{k+1} - E(t^k,\mu)\hat{x}^{k+1}.\end{aligned}$$

Primal-dual Output Error Bound (Cont.)

Theorem (Output Error Bound 2) [Zhang/Feng/Li/Benner '15]

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

$$\|e_O^k(\mu)\| \leq \tilde{\Delta}^k(\mu), \qquad k = 1, \ldots, T_n,$$

where

$$\tilde{\Delta}^k(\mu) := \Phi^k(\mu)\|\tilde{r}^k(\mu)\|,$$
$$\Phi^k(\mu) \ = \|E(t^{k-1}, \mu)^{-T}\|\|r_{\mathrm{du}}^k(\mu)\| + \|\hat{x}_{\mathrm{du}}^k(\mu)\|.$$

Primal-dual Output Error Bound (Cont.)

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Define

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

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

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

Primal-dual Output Error Bound (Cont.)

Efficient Output Error Estimation: Case 1

Corollary 1 [Zhang/Feng/Li/Benner '15]

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

1. $\{\|\tilde{r}^k(\mu)\|\}$: $\exists\, \alpha \in \mathbb{R}^+$, s.t.,
$$\alpha \le \|\tilde{r}^{k+1}(\mu)\|/\|\tilde{r}^k(\mu)\| \quad \forall\, k = 1, \dots, T_n - 1;$$
2. $f(\cdot, \mu)$ is Lipschitz continuous, i.e., $\exists\, L_f \in \mathbb{R}^+$, s.t.,
$$\|f(x_1, \mu) - f(x_2, \mu)\| \le L_f \|x_1 - x_2\|, \quad \forall\, x_1, x_2 \in \mathcal{W}^n;$$
3. $L_f < \alpha/\|E(t^k, \mu)^{-1}\|$.

Then
$$\underline{\rho}^k(\mu) \le \rho^k(\mu) \le \bar{\rho}^k(\mu),$$
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. $\{\|\tilde{r}^k(\mu)\|\}$: $\exists\, \underline{\alpha},\ \bar{\alpha} \in \mathbb{R}^+$, s.t.,
$$\underline{\alpha} \leq \|\tilde{r}^k(\mu)\|/\|\tilde{r}^{k+1}(\mu)\| \leq \bar{\alpha}, \quad \forall\, k = 1, \ldots, T_n - 1;$$
2. $f(\cdot, \mu)$ is bi-Lipschitz continuous, i.e., $\exists\, \underline{L}_f,\ \bar{L}_f \in \mathbb{R}^+$, s.t.,
$$\underline{L}_f \|x_1 - x_2\| \leq \|f(x_1, \mu) - f(x_2, \mu)\| \leq \bar{L}_f \|x_1 - x_2\|, \quad x_1, x_2 \in \mathcal{W}^n;$$
3. $\underline{L}_f > \underline{\alpha}^{-1}/\|(E(t^k, \mu)^{-1}\|$.

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

Remark: Assumption #3 is reasonable when $\|E(t^k, \mu)^{-1}\|$ is large.

Primal-dual Output Error Bound (Cont.)

Efficient Output Error Estimation

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

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

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

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

A computable output error estimation:

$$\|e_O^k\| \lesssim \Delta_{\text{est}}^k(\mu) := \rho_\star\Phi^k(\mu)\|r^k(\mu)\|.$$

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

$$\mu_\star = \arg\max_{\mu\in\mathcal{P}}\psi(\mu), \quad \psi(\mu) = \frac{1}{T_n}\sum_{k=1}^{T_n}\Delta_{\text{est}}^k(\mu).$$

POD-Greedy Algorithm

How to compute V ?

Algorithm POD-Greedy [Haasdonk/Ohlberger '08]

Input: $\mathcal{P}_{\text{train}}$, μ_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**

Remark: When T_n is large, adaptive snapshot selection can be applied.

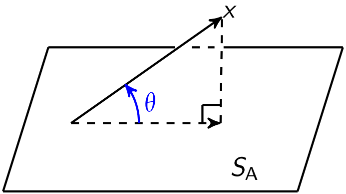
Adaptive Snapshot Selection (ASS)

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., $\phi(S_A, x) > \varepsilon_{ASS}$.



Adaptive Snapshot Selection (cont.)

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

Input: $\{x^k\}_{k=1}^{T_n}$, ε_{ASS}.
Output: Selected snapshot matrix $S_{\text{A}} = [x^{k_1}, \dots, x^{k_\ell}]$.

```
Initialization: j = 1, k_j = 1,  S_A = [x^{k_j}].
for k = 2, ..., T_n do
    if φ(S_A, x^k) > ε_ASS then
        j = j + 1.
        k_j = k .
        S_A = [S_A, x^{k_j}].
    end if
end for
```

Adaptive Snapshot Selection (cont.)

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

Input: $\{x^k\}_{k=1}^{T_n}$, ε_{ASS}.
Output: Selected snapshot matrix $S_\text{A} = [x^{k_1}, \ldots, x^{k_\ell}]$.

```
Initialization: j = 1, k_j = 1, S_A = [x^{k_j}].
for k = 2, ..., T_n do
    if φ(S_A, x^k) > ε_ASS then
        j = j + 1.
        k_j = k .
        S_A = [S_A, x^{k_j}].
    end if
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: $\mathcal{P}_{\text{train}}$, μ_0, $\varepsilon_{\text{RB}}(< 1)$.
Output: Reduced Basis (RB): $V = [v_1, \dots, v_N]$.

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 $X := [x^1(\mu_\star), \dots, x^{T_n}(\mu_\star)]$.
4: POD process:
If $N \neq 0$, compute $x^k(\mu_\star) := x^k(\mu_\star) - \text{Proj}_{\mathcal{W}}[x^k(\mu_\star)]$, $k = 1, \dots, T_n$.
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

POD-Greedy + ASS

Algorithm ASS-POD-Greedy [ZHANG/FENG/LI/BENNER '14]

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

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 $X := [x^1(\mu_\star), \ldots, x^{T_n}(\mu_\star)]$,

apply ASS to get: $X_{\text{ASS}} := [x^{k_1}(\mu_\star), \ldots, x^{k_\ell}(\mu_\star)]$ $(\ell \ll T_n)$.

4: POD process:

If $N \neq 0$, compute $x^{k_j}(\mu_\star) := x^{k_j}(\mu_\star) - \text{Proj}_{\mathcal{W}}[x^{k_j}(\mu_\star)]$, $j = 1, \ldots, \ell$.

Do SVD for X_{ASS}: $X_{\text{ASS}} = Q\Sigma F^T$, $v_{N+1} := Q(:, 1)$.

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**

Numerical Results

Numerical Examples:

1. Linear convection-diffusion equation
2. Burgers' equation
3. Batch chromatography
4. Continuous SMB chromatography

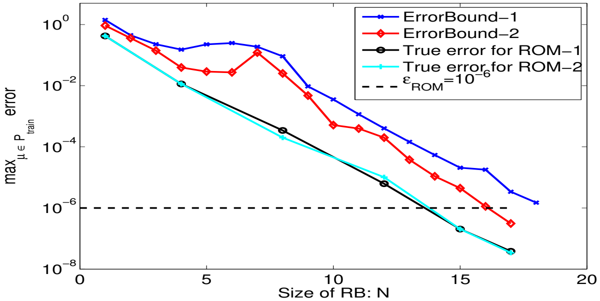
Example 1: Linear Convection-diffusion Equation

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

$$u_t = q_1 u_{xx} + q_2 u_x - q_2, \qquad x \in (0,1), \quad t \in (0,1],$$

$$y = \frac{1}{|\Omega_0|} \int_{\Omega_0} u(t,x)\,\mathrm{d}x, \qquad \Omega_0 = [0.495, 0.505],$$

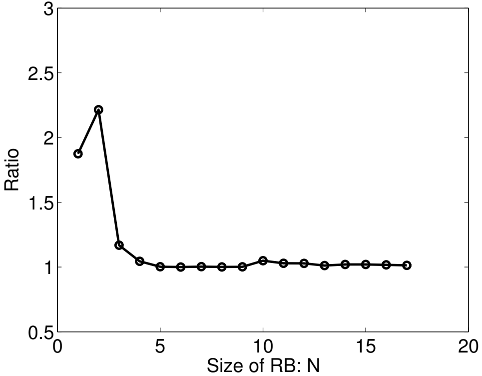
$$\mu := (q_1, q_2),\ \mathcal{P} = [0.1, 1] \times [0.5, 5], \qquad n = 800, \quad T_n = 100.$$



Error bound decay during RB extension.
ErrorBound-1: [Grepl/Patera'05], ErrorBound-2: proposed.

Example 1: Linear Convection-diffusion Equation

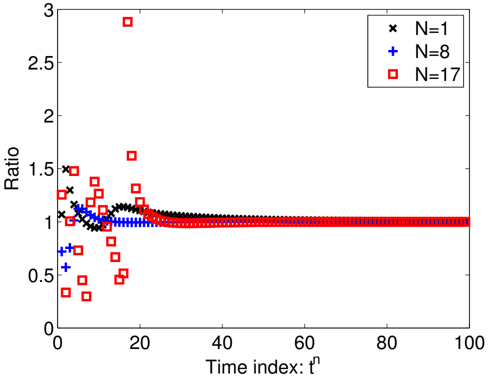
Behavior of $\rho_\star$



Behavior of the average ratio $\rho_\star = \frac{1}{T_n}\sum_{k=1}^{T_n} \rho^k(\mu_\star)$ during the RB construction process for the linear convection-diffusion equation.

Example 1: Linear Convection-diffusion Equation

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

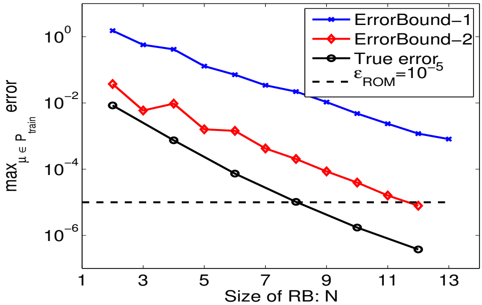


Behavior of the ratio $\frac{\|\tilde{r}^{n+1}\|}{\|\tilde{r}^n\|}$ in the time trajectory corresponding to different RB dimensions for the linear convection-diffusion equation.

Example 2: Burgers' Equation

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

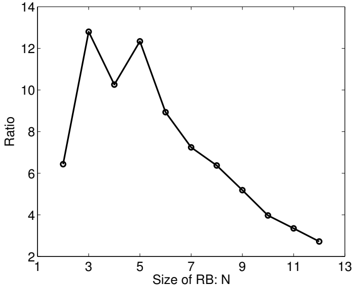
$$u_t + (\frac{u^2}{2})_x = \nu u_{xx} + 1, \quad x \in (0,1), \quad t \in (0,2],$$
$$y = u(t,1;\nu),$$
$$\nu \in \mathcal{P} = [0.05, 1], \quad n = 500, \quad T_n = 1000.$$



Error bound decay during RB extension.
ErrorBound-1: primal only, ErrorBound-2: primal-dual.

Example 2: Burgers' Equation

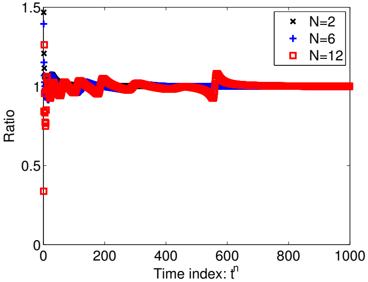
Behavior of $\rho_\star$



Behavior of the average ratio $\rho_\star = \frac{1}{T_n} \sum_{k=1}^{T_n} \rho^k(\mu_\star)$ during the RB construction process for the Burgers' equation.

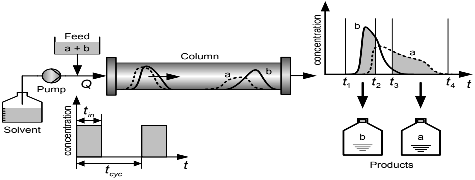
Example 2: Burgers' Equation

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



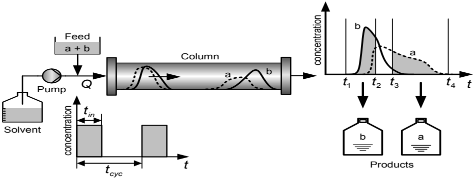
Behavior of the ratio $\frac{\|\tilde{r}^{n+1}\|}{\|\tilde{r}^n\|}$ in the time trajectory corresponding to different RB dimensions for the Burgers' equation.

Example 3: Batch Chromatography



Principle of batch chromatography for binary separation.

Example 3: Batch Chromatography



Principle of batch chromatography for binary separation.

FOM → **ROM**

$$\begin{cases} Ac_z^{k+1} = Bc_z^k + d_z^k - \tau h_z^k \\ q_z^{k+1} = q_z^k + \Delta t h_z^k \\ c_z^k, q_z^k \in \mathbb{R}^n, \tau = \dfrac{1-\epsilon}{\epsilon}\Delta t \end{cases}$$

$$\begin{cases} \hat{A}_{c_z} a_{c_z}^{k+1} = \hat{B}_{c_z} a_{c_z}^k + d_0^k \hat{d}_{c_z} - \tau \hat{H}_{c_z} \beta_z^k \\ a_{q_z}^{k+1} = a_{q_z}^k + \Delta t \hat{H}_{q_z} \beta_z^k \\ a_{c_z}^k, a_{q_z}^k \in \mathbb{R}^N, \beta_z^k \in \mathbb{R}^M \end{cases}$$

$n \gg N, M$

The parameter $\mu = (Q, t_{\text{in}})$.

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.

	ε_{ASS}	Dim. CRB (W_a	W_b)	Runtime [h]
no ASS	–	146	152	62.5 (-)
ASS	1.0×10^{-4}	147	152	6.05 (-90.3%)
ASS	1.0×10^{-3}	147	152	3.62(-94.2%)
ASS	1.0×10^{-2}	144	150	2.70 (-95.7%)

Example 3: Batch Chromatography

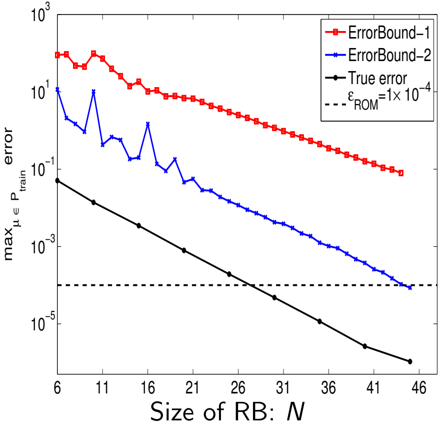
Performance of the ASS for Basis Generation

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

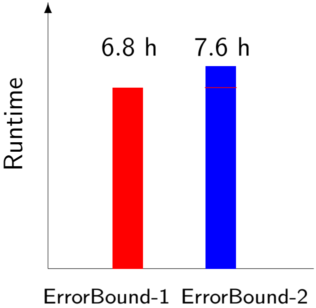
Algorithms	Runtime [h]
POD-Greedy	17.9
ASS-POD-Greedy	7.6 (−57.5%)

Example 3: Batch Chromatography

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



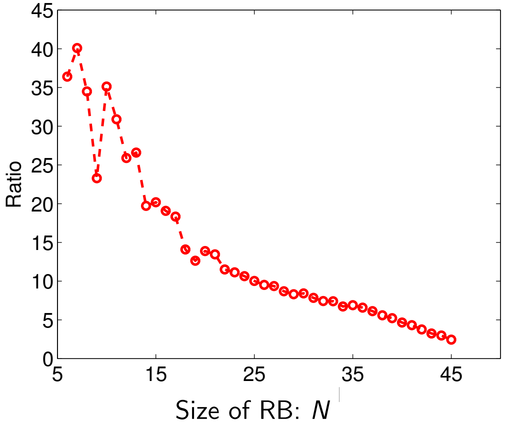
Error bound decay during RB extension.



Runtime for the RB construction.

Example 3: Batch Chromatography

Behavior of $\rho_\star$



Behavior of the average ratio $\rho_\star = \frac{1}{T_n}\sum_{k=1}^{T_n} \rho^k(\mu_\star)$ during the RB construction process for the batch chromatographic model.

Example 3: Batch Chromatography

ROM-based Optimization

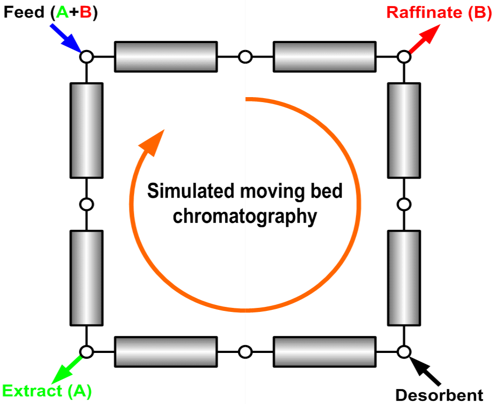
FOM-based Opt.:		ROM-based Opt.:
$\min_{\mu \in \mathcal{P}} \{-Pr(c_z(\mu), q_z(\mu); \mu)\},$ s.t. $Rec(c_z(\mu), q_z(\mu); \mu) \geq Rec_{\min},$ $c_z(\mu), q_z(\mu)$: solutions to FOM.	← Approx.	$\min_{\mu \in \mathcal{P}} \{-Pr(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu)\},$ s.t. $Rec(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Rec_{\min},$ $\hat{c}_z(\mu), \hat{q}_z(\mu)$: solutions to ROM.

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

Model	Obj. (Pr)	Opt. solution (μ)	#Iterations	Runtime [h]/SpF
FOM-Opt.	0.020264	$(0.0796, 1.0545)$	202	33.88 / -
ROM-Opt.	0.020266	$(0.0796, 1.0545)$	202	0.58 / 58

⋆ 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:

1. More parameters: $\mu := (m_1, \ldots, m_4, Q_F)$.
2. A multi-switching system: $x^0_{T+1} = P_s x^{T_n}_T$, T is the time period.
3. Cyclic steady state (CSS) computation, the system is simulated many time periods till the CSS is reached.
4. A parametric coupled system.

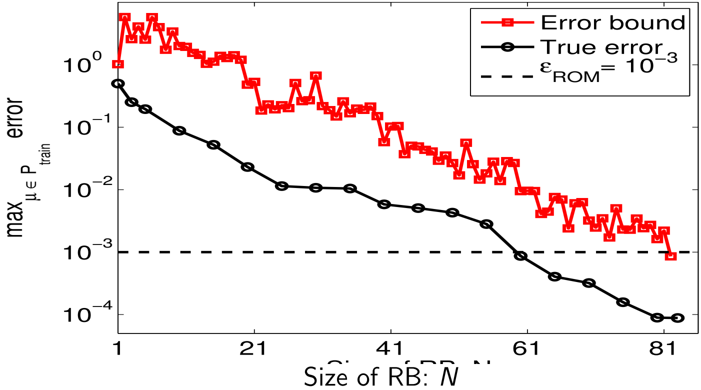
$$\text{FOM:} \quad \begin{cases} A_z(\mu)c_z^{k+1} = B_z(\mu)c_z^k + r_z^k + t_s\kappa_z q_z^k \\ q_z^{k+1} = (1 - t_s\kappa_z\Delta t)q_z^k + t_s\kappa_z H_z \Delta t c_z^k \end{cases}$$

$$\text{ROM:} \quad \begin{cases} \hat{A}_z(\mu)a_{c_z}^{k+1} = \hat{B}_z(\mu)a_{c_z}^k + \hat{r}_z + t_s\kappa_z \hat{D}_z a_{q_z}^k \\ a_{q_z}^{k+1} = (1 - t_s\kappa_z\Delta t)a_{q_z}^k + t_s\kappa_z H_z \Delta t \hat{D}_z^T a_{c_z}^k \end{cases}$$

$$\hat{A}_z(\mu) = V_{c_z}^T A_z(\mu) V_{c_z},\ \hat{B}_z(\mu) = V_{c_z}^T B_z(\mu) V_{c_z},\ \hat{r}_z = V_{c_z}^T r_z^k,\ \hat{D}_z = V_{c_z}^T V_{q_z}.$$

Example 4: SMB Chromatography

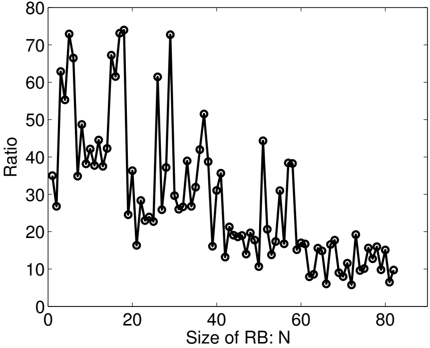
Error Behavior during the RB Construction Process



Error bound decay during RB extension.

Example 4: SMB Chromatography

Behavior of $\rho_\star$



Behavior of the average ratio $\rho_\star = \frac{1}{T_n}\sum_{k=1}^{T_n} \rho^k(\mu_\star)$ 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. $\varepsilon_{\text{RB}} = 1 \times 10^{-3}$, $\varepsilon_{\text{ASS}} = 1 \times 10^{-5}$.

Simulations	Maximal error	Average runtime [s]/SpF
FOM ($n = 800$)	–	338.71(-)
ROM ($N = 83$)	1.1×10^{-4}	46.7 / 7

Example 4: SMB Chromatography

ROM-based Optimization

FOM-based Opt.:		ROM-based Opt.:
$\min_{\mu\in\mathcal{P}} \{-Q_{\mathrm{F}}(\mu)\}, \quad$ s.t.,		$\min_{\mu\in\mathcal{P}} \{-Q_{\mathrm{F}}(\mu)\}, \quad$ s.t.,
$Pu_{a,\mathrm{E}}(c_z(\mu), q_z(\mu); \mu) \geq Pu_{a,\min}$,	← Approx.	$\hat{P}u_{a,\mathrm{E}}(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Pu_{a,\min}$,
$Pu_{b,\mathrm{R}}(c_z(\mu), q_z(\mu); \mu) \geq Pu_{b,\min}$,		$\hat{P}u_{b,\mathrm{R}}(\hat{c}_z(\mu), \hat{q}_z(\mu); \mu) \geq Pu_{b,\min}$,
$Q_1 \leq Q_{\max}$,		$\hat{Q}_1 \leq Q_{\max}$,
$c_z(\mu), q_z(\mu)$: solutions to FOM.		$\hat{c}_z(\mu), \hat{q}_z(\mu)$: solutions to ROM.

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

$$Pu_{a,\mathrm{E}} := \frac{\int_0^1 c^{\mathrm{E}}_{a,\mathrm{CSS}}(t)\,\mathrm{d}t}{\int_0^1 c^{\mathrm{E}}_{a,\mathrm{CSS}}(t)\,\mathrm{d}t + \int_0^1 c^{\mathrm{E}}_{b,\mathrm{CSS}}(t)\,\mathrm{d}t}, \quad Pu_{b,\mathrm{R}} := \frac{\int_0^1 c^{\mathrm{R}}_{b,\mathrm{CSS}}(t)\,\mathrm{d}t}{\int_0^1 c^{\mathrm{R}}_{a,\mathrm{CSS}}(t)\,\mathrm{d}t + \int_0^1 c^{\mathrm{R}}_{b,\mathrm{CSS}}(t)\,\mathrm{d}t}.$$

Constraints: $Pu_{a,\min} = 99.0\%, \quad Pu_{b,\min} = 99.0\%, \quad Q_{\max} = 0.50.$

Example 4: SMB Chromatography

ROM-based optimization

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

		Initial-guess	FOM-Opt.	ROM-Opt.
Objective	Q_{F}	0.07	0.0745	0.0745
Opt. solution	m_1	4.50	4.3269	4.3271
	m_2	2.90	2.8599	2.8603
	m_3	3.50	3.6036	3.6039
	m_4	2.30	2.3468	2.3685
	Q_F	0.07	0.0745	0.0745
Constraints	$Pu_{a,\text{E}}$	98.89%	99.00%	99.00%
	$Pu_{b,\text{R}}$	99.49%	99.00%	99.00%
	Q_1	0.4161	0.4997	0.4998
# Iterations			71	79
Runtime [h] / SpF			5.13 / -	0.82 / 6

⋆ 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).

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