Model reduction for optimal control problems in field-flow fractionation

Tatjana Stykel and Carina Willbold
Universität Augsburg

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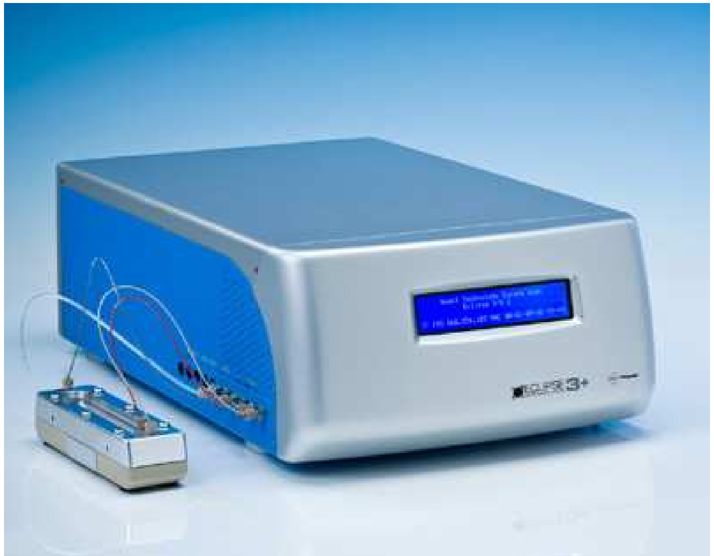
Outline

- Asymmetric flow-field-flow fractionation
- Optimal control problem
  - Stokes-Brinkman equations
  - advection-diffusion equations
- Discretization in space
- Model order reduction
  - IRKA for Stokes-type systems with many inputs/outputs
  - POD-DEIM approximation of nonlinear systems
- Numerical results
- Conclusions

Asymmetric flow-field-flow fractionation (AF^4)

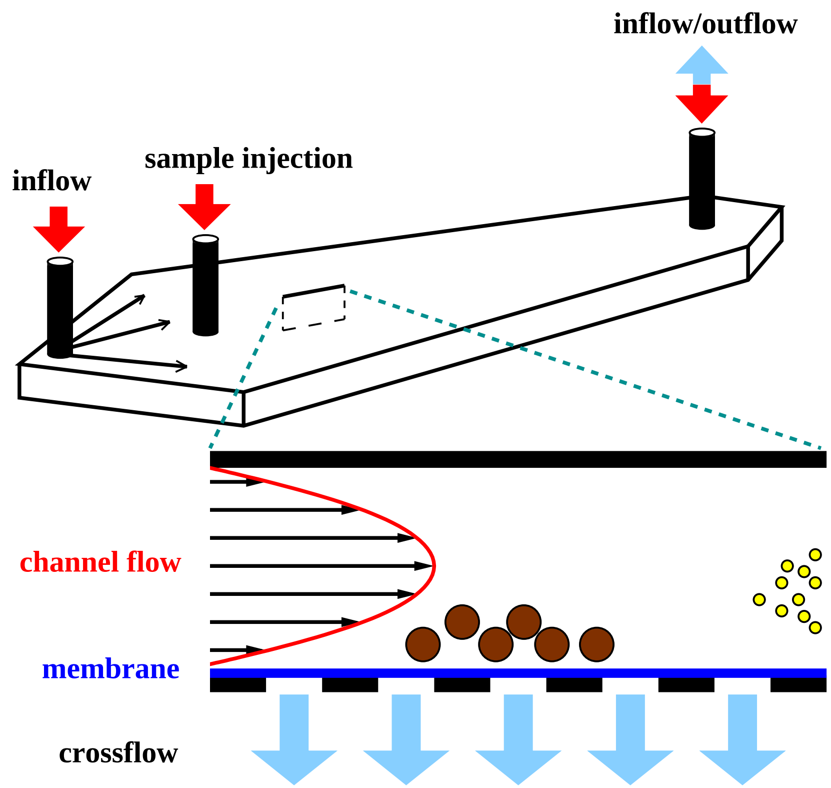


Wyatt Technology Europe GmbH

Separation of particles of different size in microfluidic flows

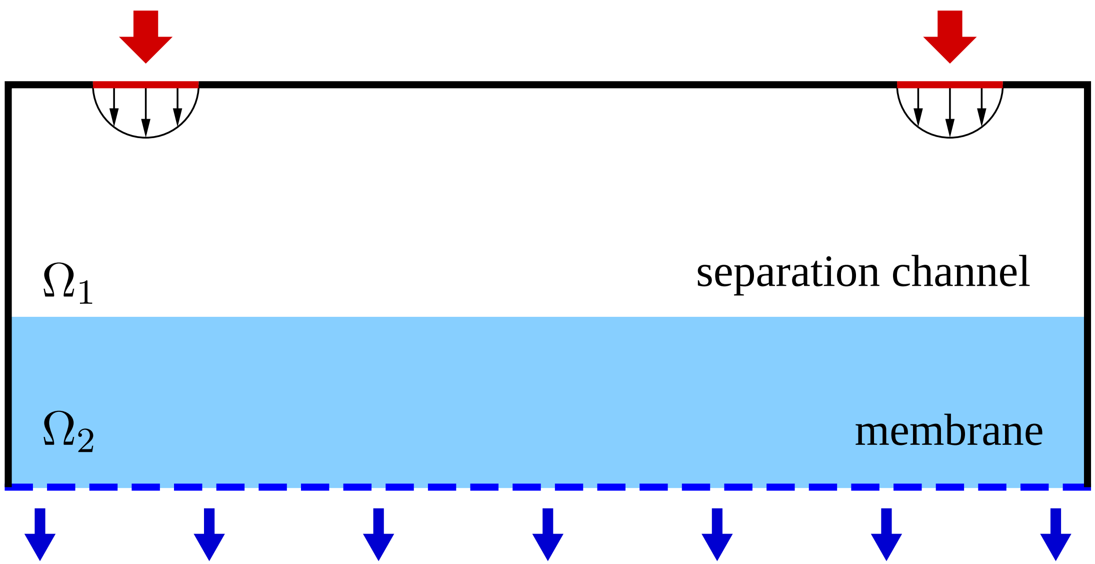
- injection
- focusing
- elution

[Giddings'66]



Stokes-Brinkman equations

$$
\begin{aligned}
\rho\,\frac{\partial \boldsymbol{v}}{\partial t} - \nu \Delta \boldsymbol{v} + \nu \chi_{\Omega_2} \kappa^{-1} \boldsymbol{v} + \nabla p &= 0 && \text{in} \quad (\Omega_1 \cup \Omega_2) \times (0,T) \\
\nabla \cdot \boldsymbol{v} &= 0 && \text{in} \quad (\Omega_1 \cup \Omega_2) \times (0,T) \\
\boldsymbol{v}(\cdot, 0) &= \boldsymbol{v}_0 && \text{in} \quad \Omega_1 \cup \Omega_2 \\
\boldsymbol{v} &= \boldsymbol{v}_{\text{in}}^{(i)} && \text{on} \quad \Gamma_{\text{in}}^{(i)} \times (0,T),\ i = 1,2 \\
\boldsymbol{v} &= 0 && \text{on} \quad \Gamma_{\text{lat}} \times (0,T) \\
\nu \nabla \boldsymbol{v} \cdot \mathbf{n}_{\Gamma_{\text{bot}}} - p\, \mathbf{n}_{\Gamma_{\text{bot}}} &= 0 && \text{on} \quad \Gamma_{\text{bot}} \times (0,T)
\end{aligned}
$$



Advection-diffusion equations

$$
\begin{aligned}
\frac{\partial c_k}{\partial t} - \nabla \cdot D_k \nabla c_k + \boldsymbol{v} \cdot \nabla c_k &= 0 && \text{in} \quad \Omega_1 \times (0,T) \\
c_k(\cdot,0) &= c_{k,0} && \text{in} \quad \Omega_1 \\
D_k \nabla c_k \cdot \mathbf{n}_{\partial\Omega_1} - c_k \boldsymbol{v} \cdot \mathbf{n}_{\partial\Omega_1} &= 0 && \text{on} \quad \partial\Omega_1 \times (0,T) \\
& && \qquad k = 1,\ldots,K
\end{aligned}
$$

Optimal control problem: focusing phase

minimize $\quad \mathcal{J}(\boldsymbol{v}, p, \boldsymbol{c}, \boldsymbol{u}) = \dfrac{1}{2}\|\boldsymbol{c}(\cdot, T) - \boldsymbol{c}^{\rm foc}\|^2_{\mathbb{L}_2(\Omega_1)}$

s.t. $\boldsymbol{v}$ and p satisfy the Stokes-Brinkman equations,

$\boldsymbol{c} = [\,c_1, \,\ldots, \,c_K]^T$ satisfies the advection-diffusion equations

Control:

$$\boldsymbol{u} = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \in \mathcal{U}_{\textsf{ad}} = \left\{ \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \in \mathbb{R}^2_+ \;:\; u_j^{\min} \le w_j \le u_j^{\max}, \; j = 1, 2 \right\}$$

$$\boldsymbol{v}_{\textsf{in}}^{(i)}(x) = \begin{bmatrix} (-1)^{i+1} u_i (x_2 - a_1)(a_2 - x_2) \\ 0 \end{bmatrix}, \quad i = 1, 2$$

First-order optimality conditions

- Adjoint Stokes-Brinkman equations

$$
\begin{aligned}
-\rho\frac{\partial \boldsymbol{w}}{\partial t} - \nu\Delta\boldsymbol{w} + \nu\chi_{\Omega_2}\kappa^{-1}\boldsymbol{w} + \nabla q &= \boldsymbol{f} && \text{in} \quad (\Omega_1\cup\Omega_2)\times(0,T)\\
\nabla\cdot\boldsymbol{w} &= 0 && \text{in} \quad (\Omega_1\cup\Omega_2)\times(0,T)\\
\boldsymbol{w}(\cdot,T) &= 0 && \text{in} \quad \Omega_1\cup\Omega_2\\
\boldsymbol{w} &= 0 && \text{on} \quad (\Gamma_{\text{in}}^{(1)}\cup\Gamma_{\text{in}}^{(2)}\cup\Gamma_{\text{lat}})\times(0,T)\\
\nu\nabla\boldsymbol{w}\cdot\mathbf{n}_{\Gamma_{\text{bot}}} - q\,\mathbf{n}_{\Gamma_{\text{bot}}} &= 0 && \text{on} \quad \Gamma_{\text{bot}}\times(0,T)
\end{aligned}
$$

- Adjoint advection-diffusion equations

$$
\begin{aligned}
-\frac{\partial d_k}{\partial t} - \nabla\cdot D_k\nabla d_k - \boldsymbol{v}\cdot\nabla d_k &= 0 && \text{in} \quad \Omega_1\times(0,T)\\
d_k(\cdot,T) &= c_k^{\text{foc}} - c_k(\cdot,T) && \text{in} \quad \Omega_1\\
D_k\nabla d_k\cdot\mathbf{n}_{\Gamma_d} &= 0 && \text{on} \quad \partial\Omega_1\times(0,T)
\end{aligned}
$$

[Hoppe/Jahny/Peter'12]

Semidiscretized optimal control problem

minimize $\quad \mathcal{J}_h(\boldsymbol{v}_h, \boldsymbol{p}_h, \boldsymbol{c}_h, \boldsymbol{u}) = \dfrac{1}{2}\|\boldsymbol{c}_h(T) - \boldsymbol{c}_h^{\mathrm{foc}}\|^2$

subject to

- the semidiscretized Stokes-Brinkman equations

$$\begin{bmatrix} E_{11} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{v}}_h \\ \dot{\boldsymbol{p}}_h \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v}_h \\ \boldsymbol{p}_h \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \boldsymbol{u},$$
$$E_{11}\boldsymbol{v}_h(0) = \boldsymbol{v}_h^0$$

- the semidiscretized advection-diffusion equations

$$\begin{aligned} \big(E_1 + E_2(\boldsymbol{v}_h)\big)\dot{\boldsymbol{c}}_h &= A(\boldsymbol{v}_h)\boldsymbol{c}_h, \\ E_1\boldsymbol{c}_h(0) &= \boldsymbol{c}_0 \end{aligned}$$

Projected gradient method

$\boldsymbol{u}^{(\nu)}$

$$E_0 \dot{\boldsymbol{x}} = A_0 \boldsymbol{x} + B \boldsymbol{u}^{(\nu)}, \quad \boldsymbol{y} = C\boldsymbol{x}$$

$\boldsymbol{y} = \boldsymbol{v}_h$

$$\big(E_1 + E_2(\boldsymbol{v}_h)\big)\dot{\boldsymbol{c}}_h = A(\boldsymbol{v}_h)\boldsymbol{c}_h$$
$$E_1 \boldsymbol{c}_h(0) = \boldsymbol{c}_h^0$$

$\boldsymbol{c}_h$

$$-\big(E_1 + E_2(\boldsymbol{v}_h)\big)^T \dot{\boldsymbol{d}}_h = A^T(\boldsymbol{v}_h)\boldsymbol{d}_h$$
$$E_1 \boldsymbol{d}_h(T) = \boldsymbol{c}_h^{\mathrm{foc}} - \boldsymbol{c}_h(T)$$

$\boldsymbol{d}_h$

$$-E_0^T \dot{\boldsymbol{z}} = A_0^T \boldsymbol{z} + C^T \boldsymbol{f}(\boldsymbol{c}_h, \boldsymbol{d}_h), \quad \boldsymbol{g} = B^T \boldsymbol{z}$$

$\boldsymbol{g}$

$$\boldsymbol{u}^{(\nu+1)} = \boldsymbol{u}^{(\nu)} - \gamma_\nu \boldsymbol{g} \in \mathcal{U}_{\text{ad}}$$

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Model reduction problem

Given a dynamical system

$$\begin{aligned} E(\boldsymbol{u})\,\dot{\boldsymbol{x}}(t) &= A(\boldsymbol{u})\,\boldsymbol{x}(t) + B\,\boldsymbol{u}(t) \\ \boldsymbol{y}(t) &= C\,\boldsymbol{x}(t) \end{aligned}$$

with $E, A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{l\times n}$.

Find a reduced-order model

$$\begin{aligned} \tilde{E}(\boldsymbol{u})\,\dot{\tilde{\boldsymbol{x}}}(t) &= \tilde{A}(\boldsymbol{u})\,\tilde{\boldsymbol{x}}(t) + \tilde{B}\,\boldsymbol{u}(t) \\ \tilde{\boldsymbol{y}}(t) &= \tilde{C}\,\tilde{\boldsymbol{x}}(t) \end{aligned}$$

with $\tilde{E}, \tilde{A} \in \mathbb{R}^{r\times r}$, $\tilde{B} \in \mathbb{R}^{r\times m}$, $\tilde{C} \in \mathbb{R}^{l\times r}$, $r \ll n$.

- preserve system properties
- small approximation error ($\|\tilde{\boldsymbol{y}} - \boldsymbol{y}\|$)
- numerically stable and efficient methods

MOR of the Stokes-Brinkman equations

$$\begin{bmatrix} E_{11} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{\boldsymbol{v}}_h \\ \dot{\boldsymbol{p}}_h \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{v}_h \\ \boldsymbol{p}_h \end{bmatrix} + \begin{bmatrix} B_1 \\ B_2 \end{bmatrix} \boldsymbol{u}, \qquad \boldsymbol{y} = \boldsymbol{v}_h$$

- differential-algebraic equation (DAE)

  $\hookrightarrow$ approximate the DAE system [Heinkenschloss et al.'08]

  $$E\,\dot{\boldsymbol{v}}_h = A\,\boldsymbol{v}_h + B\,\boldsymbol{u}, \qquad \boldsymbol{y} = C\,\boldsymbol{v}_h$$

  with $E = \Pi_l E_{11} \Pi_r, \quad A = \Pi_l A_{11} \Pi_r, \quad C = \Pi_r,$

  $$B = \Pi_l (B_1 - A_{11} E_{11}^{-1} A_{12} (A_{21} E_{11}^{-1} A_{12})^{-1} B_2),$$

  $$\Pi_l = I - E_{11}^{-1} A_{12} (A_{21} E_{11}^{-1} A_{12})^{-1} A_{21}, \quad \Pi_r = E_{11} \Pi_l E_{11}^{-1}$$

- large number of outputs ($C = \Pi_r \in \mathbb{R}^{n_v, n_v}$)

  $\hookrightarrow$ interpolatory $\mathbb{H}_2$ optimal approximation [Gugercin et al.'08]

- $sE - A$ is singular for all $s \in \mathbb{C}$

  $\hookrightarrow$ take a *reflexive inverse* $(sE - A)^-$ with respect to Π_r and Π_l

IRKA for the Stokes-Brinkman equation

Input: $E, A, B, C,\ \{\sigma_j\}_{j=1}^r,\ \{b_j\}_{j=1}^r,\ \{c_j\}_{j=1}^r$. **Output:** $\tilde{E}, \tilde{A}, \tilde{B}, \tilde{C}$

1. $V = [\,(\sigma_1 E - A)^{-} B b_1,\ \ldots,\ (\sigma_r E - A)^{-} B b_r\,]$,
   $W = \left[\,(\sigma_1 E^T - A^T)^{-} C^T c_1,\ \ldots,\ (\sigma_r E^T - A^T)^{-} C^T c_r\,\right]$,
2. **while** (not converged)
   a) $\tilde{E} = W^T E V$, $\quad \tilde{A} = W^T A V$, $\quad \tilde{B} = W^T B$, $\quad \tilde{C} = CV$
   b) $\tilde{A} x_j = \lambda_j \tilde{E} x_j$, $\quad y_j^* \tilde{A} = \lambda_j y_j^* \tilde{E}$, $\quad y_j^* \tilde{E} x_i = \delta_{ij}$, $\ i, j = 1, \ldots, r$
   c) $\sigma_j = -\lambda_j$, $\quad b_j^T = y_j^* \tilde{B}$, $\quad c_j = \tilde{C} x_j$, $\ j = 1, \ldots, r$
   d) $V = [\,(\sigma_1 E - A)^{-} B\, b_1,\ \ldots,\ (\sigma_r E - A)^{-} B\, b_r\,]$,
   $W = \left[\,(\sigma_1 E^T - A^T)^{-} C^T c_1,\ \ldots,\ (\sigma_r E^T - A^T)^{-} C^T c_r\,\right]$

   end while
3. $\tilde{E} = W^T E V$, $\quad \tilde{A} = W^T A V$, $\quad \tilde{B} = W^T B$, $\quad \tilde{C} = CV$

[Gugercin/St./Wyatt'13]

MOR of the advection-diffusion equations

Goal: approximate the dynamical system

$$E(\boldsymbol{v}_h)\,\dot{\boldsymbol{c}} = A(\boldsymbol{v}_h)\,\boldsymbol{c}$$

Method: proper orthogonal decomposition (POD)

- Compute the snapshot matrix $\boldsymbol{C} = [\,\boldsymbol{c}(t_1), \ldots, \boldsymbol{c}(t_k)\,]$.
- Compute the SVD $\boldsymbol{C} = [U,\, U_0]\begin{bmatrix} \Sigma & \\ & \Sigma_0 \end{bmatrix}[V,\, V_0]^T$.
- Compute the reduced-order model

$$U^T E(\boldsymbol{v}_h) U\,\dot{\widetilde{\boldsymbol{c}}} = U^T A(\boldsymbol{v}_h) U\,\widetilde{\boldsymbol{c}}$$

$\hookrightarrow$ Evaluation of $E(\boldsymbol{v}_h)$ and $A(\boldsymbol{v}_h)$ for different $\boldsymbol{v}_h$ is required!

Discrete empirical interpolation method (DEIM)

Goal: approximate $\boldsymbol{f}(t) \in \mathbb{R}^n$ by projection $\boldsymbol{f}(t) \approx W\tilde{\boldsymbol{f}}(t)$, $W \in \mathbb{R}^{n\times k}$

- Compute the snapshot matrix $\boldsymbol{F} = [\,\boldsymbol{f}(t_1), \ldots, \boldsymbol{f}(t_q)\,]$.
- Compute the SVD $\boldsymbol{F} = [W,\, W_0]\begin{bmatrix} \Sigma & \\ & \Sigma_0 \end{bmatrix}[V,\, V_0]^T$.
- Select k rows of $W \in \mathbb{R}^{n\times k}$ $\hookrightarrow$ $P^T W$ with $P = [\boldsymbol{e}_{r_1}, \ldots, \boldsymbol{e}_{r_k}\,]$
- Determine $\tilde{\boldsymbol{f}}(t)$ from $P^T\boldsymbol{f}(t) = P^T W\tilde{\boldsymbol{f}}(t)$.

$\hookrightarrow$ DEIM approximation $\boldsymbol{f}(t) \approx W(P^T W)^{-1}P^T\boldsymbol{f}(t)$ with the error bound

$$\|\boldsymbol{f}(t) - W(P^T W)^{-1}P^T\boldsymbol{f}(t)\| \le \|(P^T W)^{-1}\|_2 \|(I - WW^T)\boldsymbol{f}(t)\|$$

[Chaturantabut/Sorensen'10]

Matrix DEIM

Goal: approximate $F(\boldsymbol{v})$ s.t. $F(\boldsymbol{v}) \approx \sum_{j=1}^{k} W_j \tilde{f}_j(\boldsymbol{v})$, $W_j \in \mathbb{R}^{n\times n}$, $\tilde{f}_j \in \mathbb{R}$

$\Longleftrightarrow$ approximate $\boldsymbol{f}(\boldsymbol{v}) = \mathrm{vec}(F(\boldsymbol{v})) \in \mathbb{R}^{n^2}$ by projection

$\boldsymbol{f}(\boldsymbol{v}) \approx W\tilde{\boldsymbol{f}}(\boldsymbol{v})$ with $W = [\,\mathrm{vec}(W_1), \ldots, \mathrm{vec}(W_k)\,] \in \mathbb{R}^{n^2\times k}$

$\tilde{\boldsymbol{f}}(\boldsymbol{v}) = [\,\tilde{f}_1(\boldsymbol{v}),\ \ldots,\ \tilde{f}_k(\boldsymbol{v})\,]^T \in \mathbb{R}^k$

- Compute the snapshots $F_1 = F(\boldsymbol{v}_1), \ldots, F_q = F(\boldsymbol{v}_q) \in \mathbb{R}^{n\times n}$

  $\hookrightarrow$ $\boldsymbol{F} = [\,\mathrm{vec}(F_1), \ldots, \mathrm{vec}(F_q)\,] \in \mathbb{R}^{n^2\times q}$ is the snapshot matrix for $\boldsymbol{f}(\boldsymbol{v})$

- Compute the eigenvalue decomposition

$$\boldsymbol{F}^T\boldsymbol{F} = \begin{bmatrix} \langle F_1, F_1\rangle_F & \cdots & \langle F_1, F_q\rangle_F \\ \vdots & \ddots & \vdots \\ \langle F_q, F_1\rangle_F & \cdots & \langle F_q, F_q\rangle_F \end{bmatrix} = [V,\ V_0] \begin{bmatrix} \Lambda & \\ & \Lambda_0 \end{bmatrix} [V,\ V_0]^T$$

$\hookrightarrow$ $W = \boldsymbol{F} V \Lambda^{-1/2} = \left[\,\sum_{i=1}^{q} \mathrm{vec}(F_i) v_{i1},\ \ldots,\ \sum_{i=1}^{q} \mathrm{vec}(F_i) v_{ik}\,\right]$

$\hookrightarrow$ $W_j = \sum_{i=1}^{q} F_i v_{ij}$, $j = 1, \ldots, k$

Matrix DEIM

- Select k rows of W $\hookrightarrow$ P^TW with $P = [\boldsymbol{e}_{r_1}, \ldots, \boldsymbol{e}_{r_k}] \in \mathbb{R}^{n^2 \times k}$

$$\hookrightarrow \quad P^TW = \begin{bmatrix} (W_1)_{i_1,j_1} & \cdots & (W_k)_{i_1,j_1} \\ \vdots & \ddots & \vdots \\ (W_1)_{i_k,j_k} & \cdots & (W_k)_{i_k,j_k} \end{bmatrix} \quad \text{with} \quad \begin{array}{c} r_1 = nj_1 + i_1 \\ \vdots \\ r_k = nj_k + i_k \end{array}$$

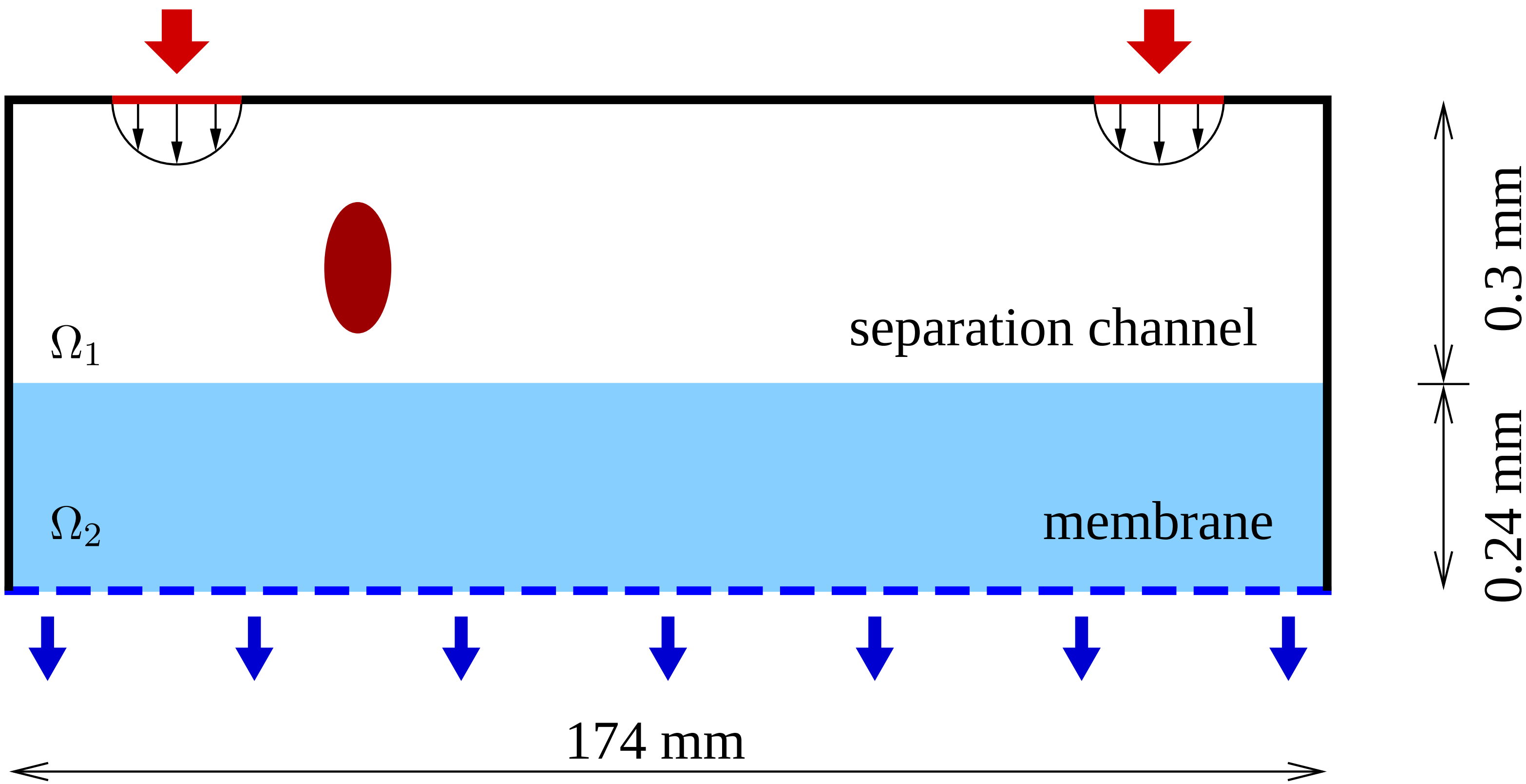
- Determine $\tilde{\boldsymbol{f}}(t)$ from $P^T\mathrm{vec}(F(\boldsymbol{v})) = P^TW\tilde{\boldsymbol{f}}(t)$

$$\hookrightarrow \quad \tilde{\boldsymbol{f}}(t) = (P^TW)^{-1} \begin{bmatrix} (F(\boldsymbol{v}))_{i_1,j_1} \\ \vdots \\ (F(\boldsymbol{v}))_{i_k,j_k} \end{bmatrix} = \begin{bmatrix} \tilde{f}_1(\boldsymbol{v}) \\ \vdots \\ \tilde{f}_k(\boldsymbol{v}) \end{bmatrix}$$

$\hookrightarrow$ MDEIM approximation $F(\boldsymbol{v}) \approx \sum_{j=1}^{k} W_j \tilde{f}_j(\boldsymbol{v})$

$\hookrightarrow$ POD-MDEIM approximation $U^TF(\boldsymbol{v})U \approx \sum_{j=1}^{k} U^TW_jU\tilde{f}_j(\boldsymbol{v})$

Numerical experiments



Numerical experiments

Model reduction of the Stokes-Brinkman equations

- dimensions of the original and reduced systems:

$$n = 20053, \quad m = 2, \quad n_v = 17708 \quad \hookrightarrow \quad r = 40$$

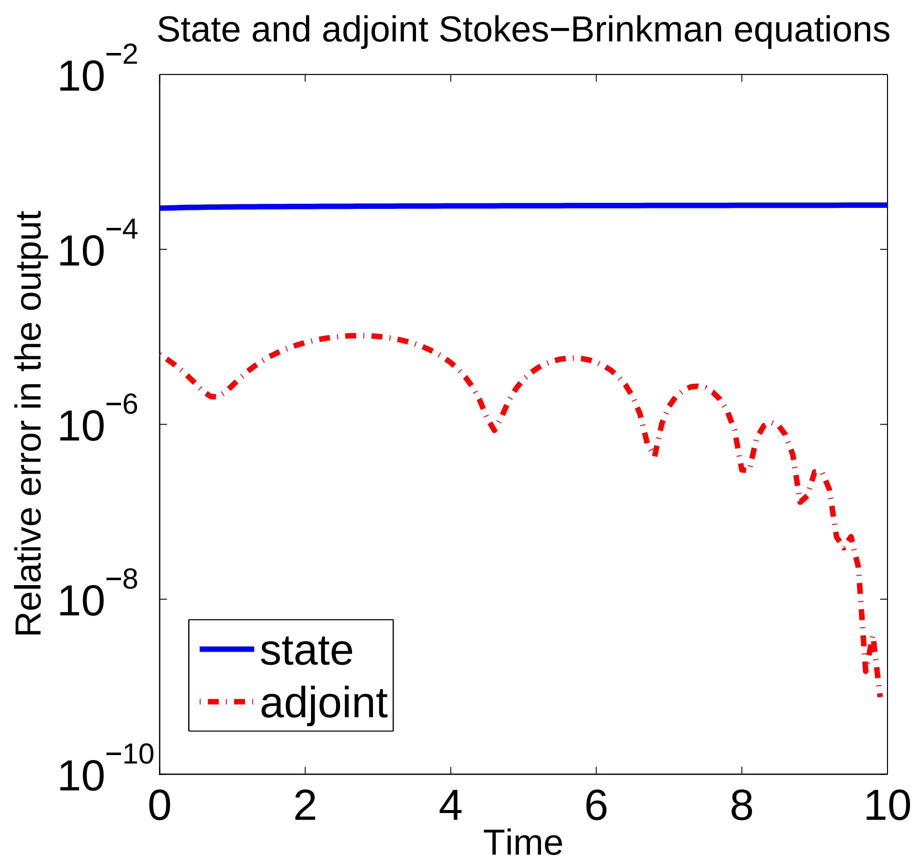
- simulation time:

  state equation

$$t_{orig} = 60.68 \text{ sec}$$
$$t_{red} = 0.12 \text{ sec}$$

  adjoint equation

$$t_{orig} = 62.97 \text{ sec}$$
$$t_{red} = 3.22 \text{ sec}$$

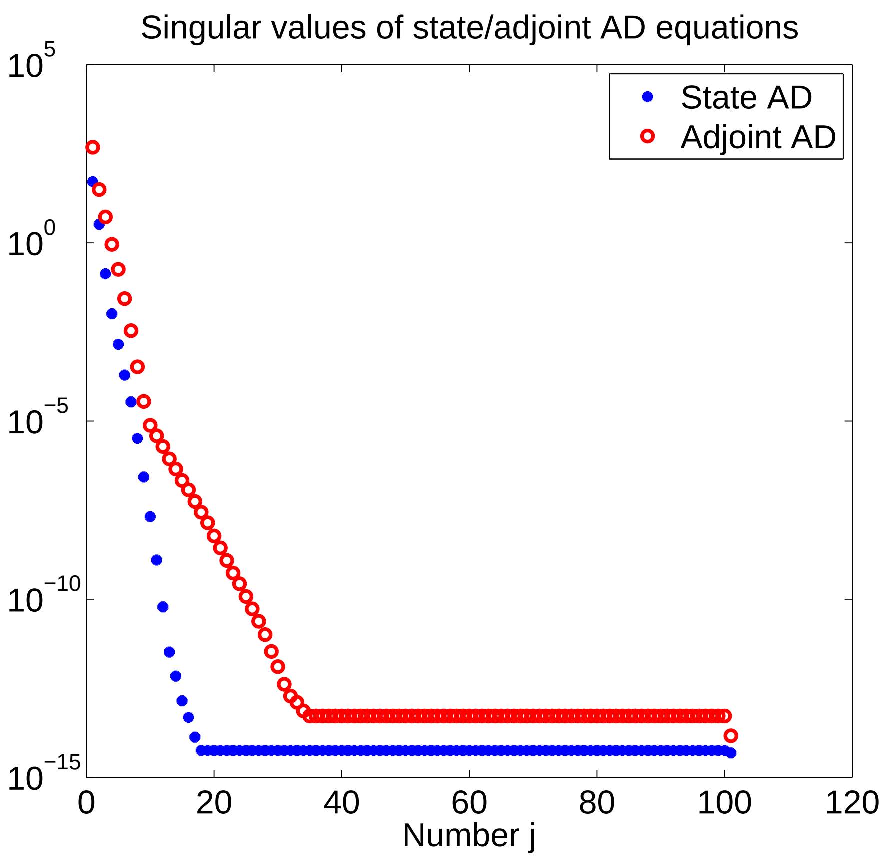


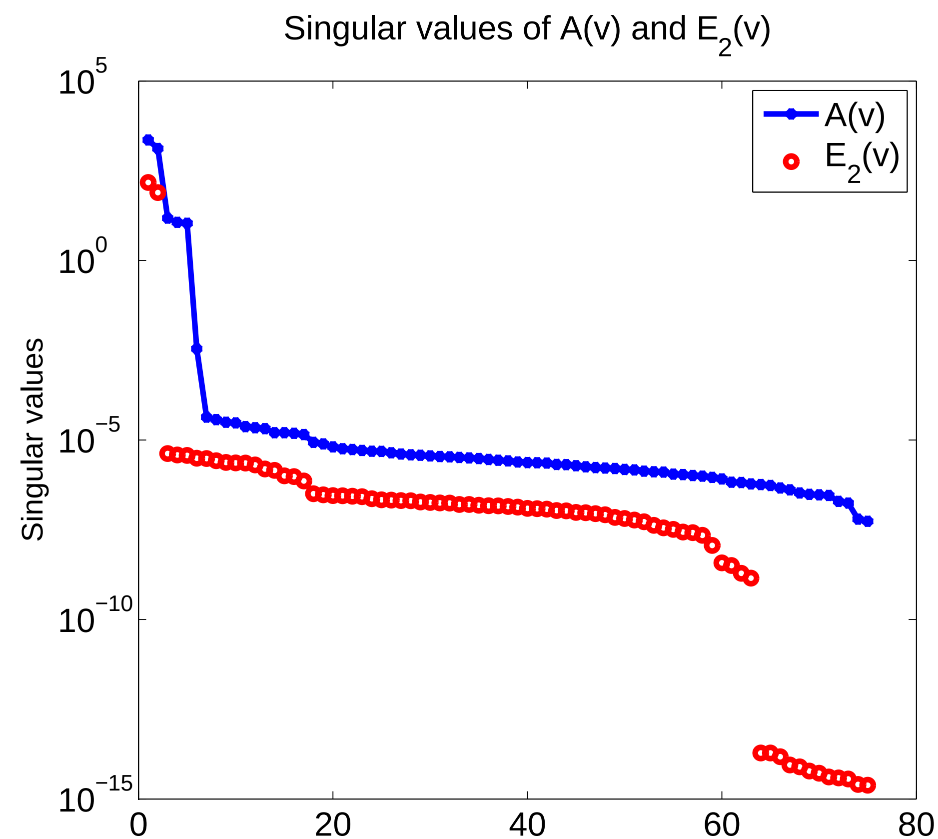
Numerical experiments

Model reduction of the state and adjoint advection-diffusion equations

- dimensions of the original and reduced systems:

$$n_c = 5305 \quad \hookrightarrow \quad r_{st} = 7,\ r_{adj} = 8,\ k(A) = 7,\ k(E_2) = 3$$

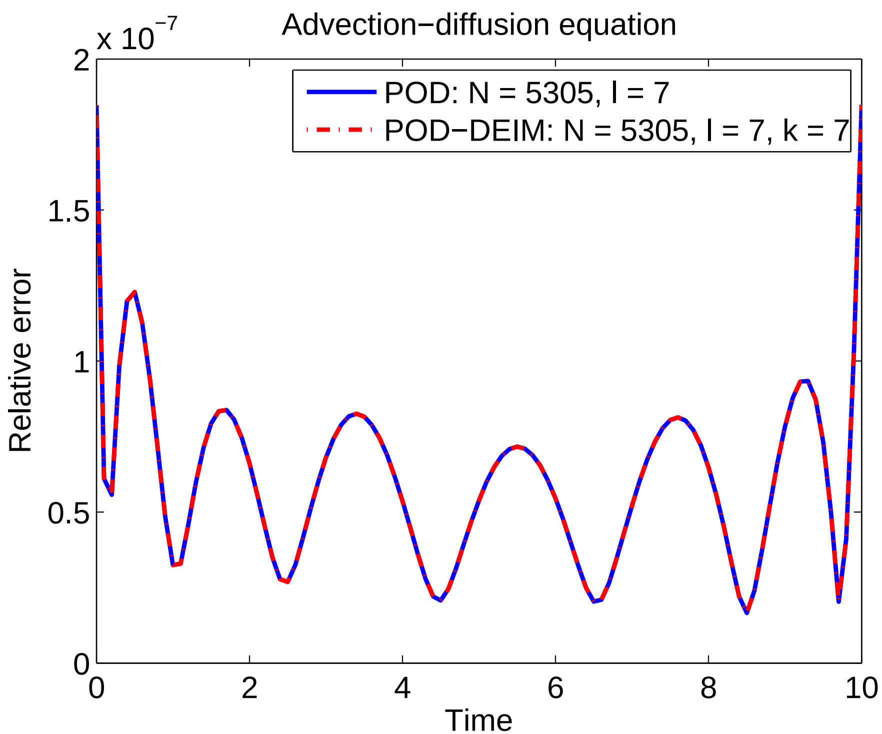


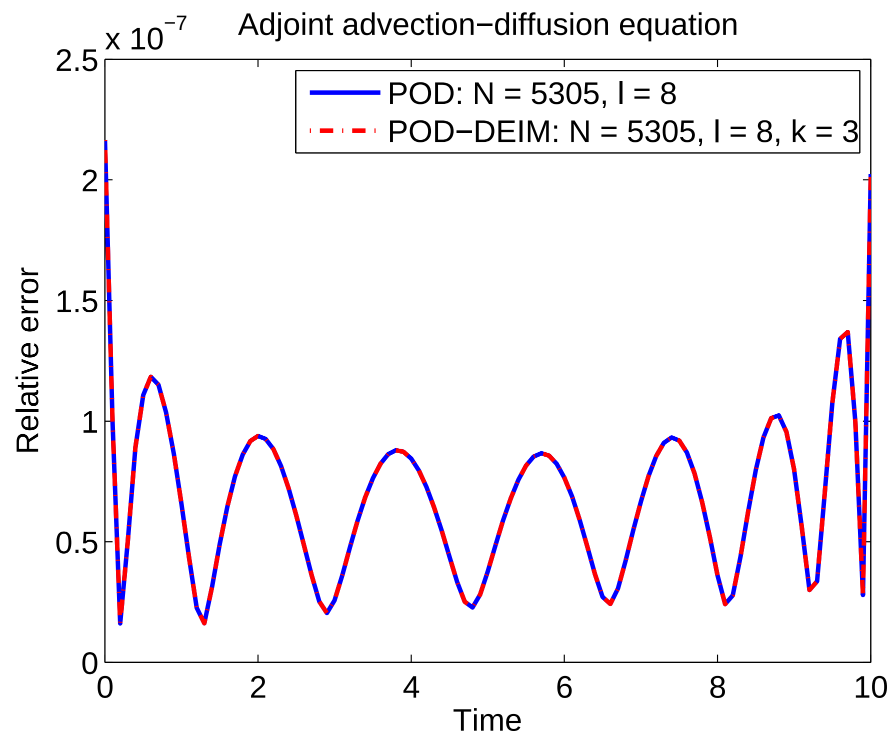


Numerical experiments

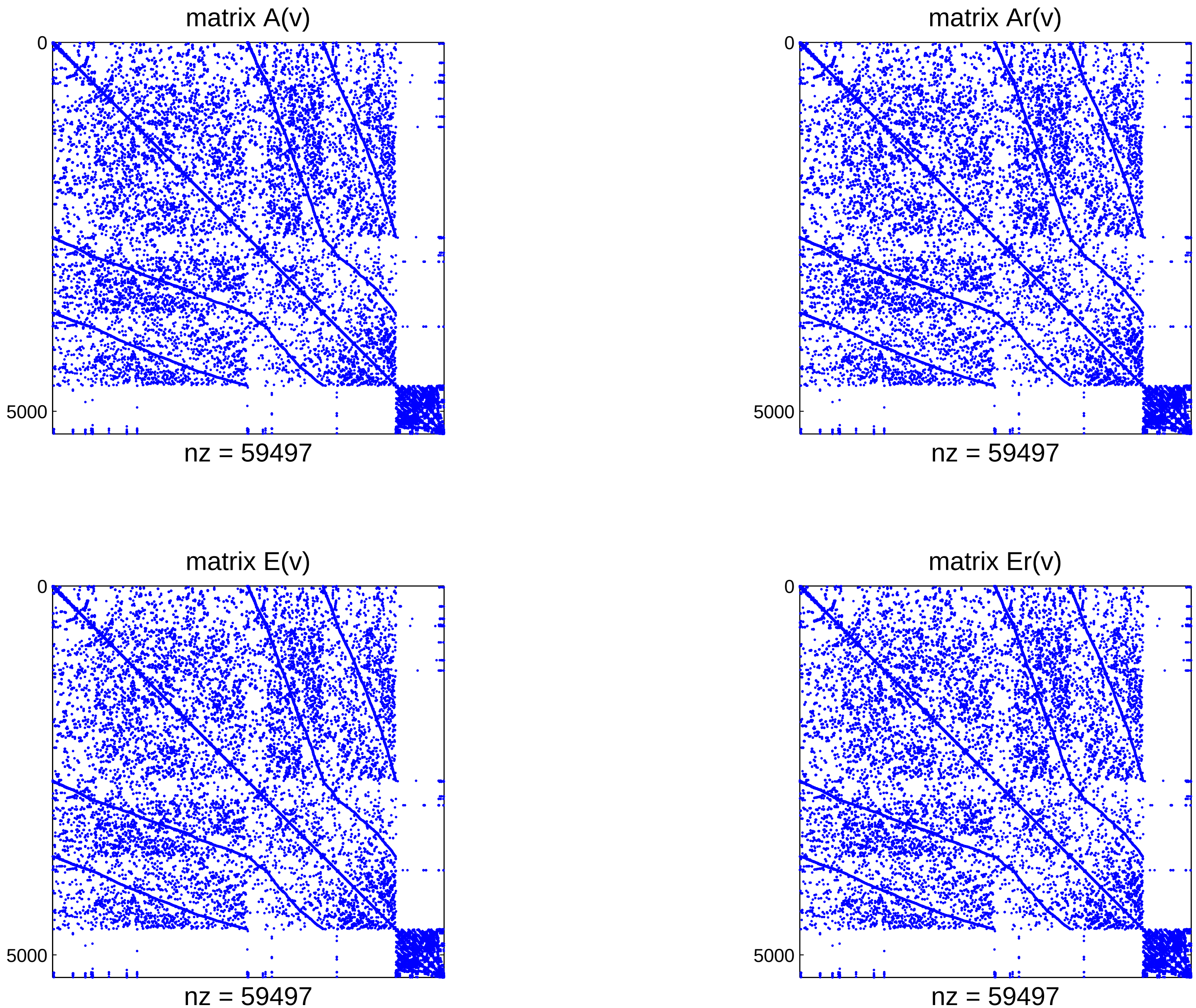
Model reduction of the state and adjoint advection-diffusion equations

- state equation: $t_{orig} = 11.15$ sec, $t_{red} = 0.03$ sec
- adjoint equation: $t_{orig} = 11.29$ sec, $t_{red} = 0.03$ sec





Numerical experiments



Conclusion

- Optimization problem in flow-field-flow fractionation
- IRKA for the semidiscretized Stokes-Brinkman equations
- POD-MDEIM for the semidiscretized advection-diffusion equations

Current work

- Optimal choice of the snapshots in POD-MDEIM
- Error estimates for the (sub)optimal control [Kammann et al.'12]
  - coupled system
  - semidiscretized Stokes-Brinkman equations $\longrightarrow$ DAE