Model reduction based optimal control for field-flow fractionation

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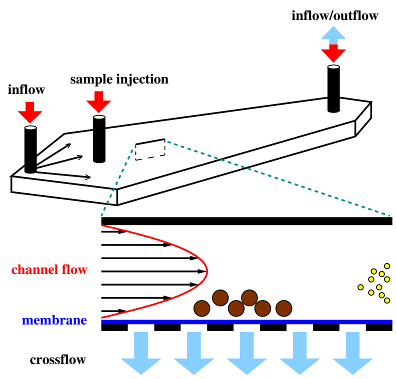
We discuss the application of model order reduction to optimal control problems governed by coupled systems of the Stokes-Brinkman and advection-diffusion equations. Such problems arise in field-flow fractionation processes for the efficient and fast separation of particles of different size in microfluidic flows. Our approach is based on a combination of interpolatory projection methods and POD-DEIM techniques for model reduction of the semidiscretized optimality system. Numerical results demonstrate the properties of this approach.

1 The optimal control problem



Field-flow fractionation (FFF) is a family of techniques for the separation of particles and macromolecules in microfluidic flows. Asymmetric flow-field-flow fractionation (AF^4) is the most used variant of the FFF techniques, where the separation of particles takes place in a thin channel Ω_1 with a permeable membrane Ω_2 as shown in the left figure. The separation process includes three steps: injection, focusing and elution. At the first step, the liquid is injected through the two inflow tubes at the bottom of the channel. There is a crossflow through the membrane and outflow at the bottom boundary Γ_{bot}. When the flow is balanced, the analyte is injected. The goal of the focusing phase is to concentrate the analyte in a thin band and move it in a carrier fluid towards the bottom of the channel. The separation of the particles occurs then in the elution phase, when a parabolic flow profile is created within the channel. The smaller particles are transported much more rapidly along the channel and eluted earlier than the larger ones.

The flow of the incompressible fluid in the channel is described by the Stokes-Brinkman equation

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

where $\mathbf{v}$ is the velocity vector, p is the pressure, $\mathbf{v}_0$ is the initial velocity, $\Gamma_{\text{in}}^{(i)}$, $i=1,2$, are the inflow boundaries on the top of the channel, $\mathbf{v}_{\text{in}}^{(i)}$ are the inflow velocities, ρ, ν and K denote the density, the viscosity of the liquid and the permeability of the membrane, respectively, χ_{Ω_2} is the characteristic function of the subdomain Ω_2 and $\Omega=\Omega_1\cup\Omega_2$.

To describe the transport of the analyte in the domain Ω_1 we use the advection-diffusion equations

$$\begin{aligned}
\frac{\partial c_m}{\partial t} - \nabla\cdot D_m\nabla c_m + (\mathbf{v}-\mathbf{v}_m)\cdot\nabla c_m &= 0 && \text{in} \quad \Omega_1\times(0,T),\\
c_m(\cdot,0) &= c_{m,0} && \text{in} \quad \Omega_1,\\
D_m\nabla c_m\cdot\mathbf{n}_{\partial\Omega_1} - c_m\mathbf{v}\cdot\mathbf{n}_{\partial\Omega_1} &= 0 && \text{on} \quad \partial\Omega_1\times(0,T),
\end{aligned} \tag{2}$$

where c_m is the concentration of the m-th analyte, $m=1,\ldots,M$, $D_m>0$, $\mathbf{v}_m$ and $c_{m,0}$ are the diffusion coefficient, the lift and the initial concentration, respectively.

During the focusing phase the following optimal control problem arises:

$$\text{minimize} \qquad J(\mathbf{z},\mathbf{u}) = \frac{1}{2}\|\mathbf{c}(\cdot,T)-\mathbf{c}^{foc}\|^2_{0,\Omega_1} + \frac{\beta}{2}\int_0^T \|\mathbf{u}\|^2 dt,$$

where $\mathbf{z}=[\mathbf{v}^T,p,\mathbf{c}^T]^T$ with $\mathbf{c}=[c_1,\ldots,c_M]^T$ satisfies the coupled system (1) and (2), $\mathbf{u}$ contains the control parameters describing the inflow and $\mathbf{c}^{foc}=[c_1^{foc},\ldots,c_M^{foc}]^T$ is a desired concentration. This optimal control problem was investigated in [3]. The computation of the optimal solution using, for example, gradient descent techniques requires the numerical solution of the state equations (1) and (2) and the adjoint systems at every iterative step.

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2 Model reduction techniques

A spatial discretization of the Stokes-Brinkman equation (1) using Taylor-Hood P2/P1 finite element method leads to a linear time-invariant descriptor system

$$E\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{y}(t) = [\, I_{n_v},\ 0\,]\, \mathbf{x}(t) = \mathbf{v}_h(t), \tag{3}$$

where $\mathbf{x} = [\mathbf{v}_h^T, \mathbf{p}_h^T]^T$, $\mathbf{v}_h \in \mathbb{R}^{n_v}$ and $\mathbf{p}_h \in \mathbb{R}^{n_p}$ are the semidiscretized velocity and pressure vectors, the matrix E is singular, but the pencil $\lambda E - A$ is regular. If we discretize the advection-diffusion equations (2) in space using SUPG finite elements, we obtain the time-varying systems

$$M_m(\mathbf{v}_h)\dot{\mathbf{c}}_{m,h}(t) = A_m(\mathbf{v}_h)\mathbf{c}_{m,h}(t), \quad m = 1, \ldots, M, \tag{4}$$

where $\mathbf{c}_{m,h} \in \mathbb{R}^{n_{c_m}}$ is the semidiscretized concentration vector of the m-th analyte. Our goal is now to approximate systems (3) and (4) and their adjoints by reduced-order models that nearly have the same behaviour as the original systems. For model reduction of the semidiscretized Stokes-Brinkman equation (3) and its adjoint, we use the interpolatory projection method based on the IRKA algorithm adapted for descriptor systems [2]. In order to compute a reduced-order model for the advection-diffusion (4) and its adjoint, we apply a combination of proper orthogonal decomposition (POD) [4] and discrete empirical interpolation (DEIM) [1].

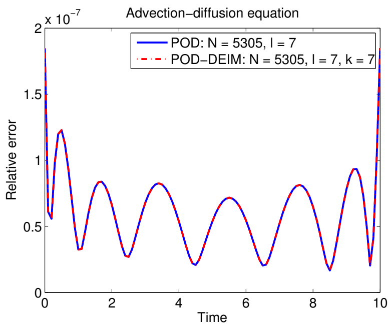
Consider the semidiscretized advection-diffusion equation (4). Let $V \in \mathbb{R}^{n_{c_m}, \ell}$ be a POD projection matrix. Then the reduced-order model has the form $V^T M_m(\mathbf{v}_h) V \dot{\tilde{\mathbf{c}}} = V^T A_m(\mathbf{v}_h) V \tilde{\mathbf{c}}$, where an efficient evaluation of the nonlinear matrix-valued functions $V^T M_m(\mathbf{v}_h) V$ and $V^T A_m(\mathbf{v}_h) V$ for different $\mathbf{v}_h$ is required if we want to solve the reduced model numerically.

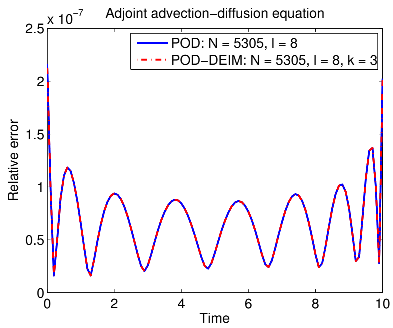
Given a general parameter-dependent matrix $F(\boldsymbol{\xi}) \in \mathbb{R}^{n \times n}$ with $\boldsymbol{\xi} \in \mathbb{R}^n$, we aim to find an approximation

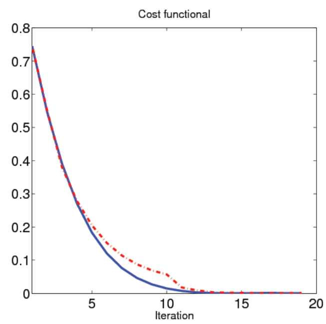
$$F(\boldsymbol{\xi}) \approx \sum_{j=1}^{k} U_j f_j(\boldsymbol{\xi}), \quad \text{where } U_j \in \mathbb{R}^{n \times n},\ f_j(\boldsymbol{\xi}) \in \mathbb{R} \text{ and } k \text{ is small.} \tag{5}$$

Then the product $V^T F(\boldsymbol{\xi}) V$ is approximated by $V^T F(\boldsymbol{\xi}) V \approx \sum_{j=1}^{k} (V^T U_j V) f_j(\boldsymbol{\xi})$, where the parameter-independent reduced matrices $V^T U_j V$ can be precomputed and stored, and only the evaluation of k components $f_j(\boldsymbol{\xi})$ is required. The approximation (5) can be obtained using the matrix DEIM approach as follows. For snapshots $F_1 = F(\boldsymbol{\xi}_1), \ldots, F_q = F(\boldsymbol{\xi}_q)$, we first construct a symmetric matrix $\mathcal{F} = [\mathcal{F}_{ij}]_{i,j=1}^q$ with $\mathcal{F}_{ij} = \langle F_i, F_j \rangle_F = \sqrt{\mathrm{tr}(F_j^T F_i)}$. Computing the eigenvalue decomposition $\mathcal{F} = [W, W_0]\mathrm{diag}(\Lambda, \Lambda_0)[W, W_0]^T$, we get the POD basis matrices $U_j = \sum_{i=1}^{q} F_i w_{ij}$, where w_{ij} are the entries of $W\Lambda^{-1/2} \in \mathbb{R}^{q \times k}$. The coefficient vector $\mathbf{f}(\boldsymbol{\xi}) = [f_1(\boldsymbol{\xi}), \ldots, f_k(\boldsymbol{\xi})]^T$ can then be determined as $\mathbf{f}(\boldsymbol{\xi}) = (P^T U)^{-1} P^T \mathrm{vec}(F(\boldsymbol{\xi}))$, where $\mathrm{vec}(F)$ is a vector obtained by stacking the columns of F below one another, $U = [\mathrm{vec}(U_1), \ldots, \mathrm{vec}(U_k)] \in \mathbb{R}^{n^2 \times k}$, $P = [\mathbf{e}_{r_1}, \ldots, \mathbf{e}_{r_k}] \in \mathbb{R}^{n^2 \times k}$ is a selector matrix computed from U using Greedy algorithm, and $\mathbf{e}_j$ denotes the j-th column of an identity matrix.

We now present some results of numerical experiments. The state and adjoint advection-diffusion equations of order 5305 were approximated by the POD models of order 7 and 8, respectively. We assembled 3 entries of $M_m(\mathbf{v}_h)$ and 7 entries of $A_m(\mathbf{v}_h)$. The first two figures below show the relative error in the approximate solutions, while the third figure demonstrates the convergence of the cost functional for the original and the reduced-order models in the gradient method.







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References

[1] S. Chaturantabut, D. Sorensen, Nonlinear model reduction via discrete empirical interpolation, SIAM J. Sci. Comput., 32(5), pp. 2737–2764, 2010.
[2] S. Gugercin, T. Stykel, S. Wyatt, Model reduction of descriptor systems by interpolatory projection methods. Preprint 03/2013, Institut für Mathematik, Universität Augsburg, 2013. Submitted for publication.
[3] R. H. W. Hoppe, M. Jahny, M. Peter, Optimal control of asymmetric flow field-flow fractionation, Manuscript, Universität Augsburg, 2012.
[4] M. Hinze, S. Volkwein, in *Dimension Reduction of Large-Scale Systems*, P. Benner, V. Mehrmann, D. Sorensen (eds.), Lecture Notes in Computational Science and Engineering 45 (Springer-Verlag, Berlin, 2005), pp. 261–306.