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Model reduction for optimal control problems in field-flow fractionation

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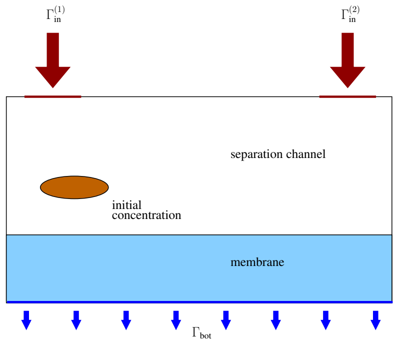
We discuss the application of model order reduction to optimal control problems governed by coupled systems of the Stokes-Brinkman and advection-diffusion equations. Such problems arise in field-flow fractionation processes for the efficient and fast separation of particles of different size in microfluidic flows. Our approach is based on a combination of balanced truncation and tangential interpolation 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 [3]. 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 partices 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

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

wnere $\mathbf{v}$ 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

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

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:

$$\text{minimize} \qquad J(\mathbf{y},\mathbf{u}) = \frac{1}{2}\|\mathbf{c}(\cdot,T)-\mathbf{c}^{foc}\|_{0,\Omega_1}^2 + \frac{\beta}{2}\int_0^T \|\mathbf{u}\|^2 dt, \tag{3}$$

where $\mathbf{y}=[\mathbf{v}^T,p,\mathbf{c}^T]^T$ 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 $\mathbf{c}^{foc}=[c_1^{foc},\ldots,c_M^{foc}]$ is a desired concentration. This optimal control problem was investigated in [5]. 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

The spatial discretization of the Stokes-Brinkman equation (1) using finite element methods lead to a descriptor system

$$E\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{y}(t) = [\, I_{n_v},\ 0\,]\,\mathbf{x}(t) = \mathbf{v}_h(t), \tag{4}$$

where $\mathbf{x} = [\mathbf{v}_h^T, \mathbf{p}_h^T]^T$, $\mathbf{v}_h = [v_{h,1}, \ldots, v_{h,n_v}]^T \in \mathbb{R}^{n_v}$ 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, we obtain bilinear control systems

$$E_m\dot{\mathbf{c}}_m(t) = A_m\mathbf{c}_m(t) + \sum_{j=1}^{n_v} v_{h,j}(t)N_{m,j}\mathbf{c}_m(t), \qquad \mathbf{y}_m(t) = C_m\mathbf{c}_m(t), \tag{5}$$

where $\mathbf{c}_m \in \mathbb{R}^{n_{c_m}}$ is the semidiscretized concentration vector of the m-th analyte, E_m and A_m are related to the diffusion term, and the matrices $N_{m,1}, \ldots, N_{m,n_v}$ are related to the advection term. Our goal is to approximate the systems (4) and (5) by reduced-order models that nearly have the same behaviour as the original systems. For model reduction of the semidiscretized Stokes-Brinkman equation (4) with many outputs, we use a combination of the balanced truncation method from [4] and the reduction technique from [2] specially developed for systems with many inputs or outputs. In order to compute a reduced-order model for the bilinear system (5), we want to apply the bilinear iterative rational Krylov algorithm (BIRKA) [1]. However, this algorithm requires an input matrix and A_m to be stable in the sense that all eigenvalues have negative real part. In our problem, the matrix A_m is singular and the input matrix is missing in (5). To tackle these problems, we first introduce a new state $\mathbf{z}_m(t) = \mathbf{c}_m(t) - \mathbf{w}$ with a fixed vector $\mathbf{w} \in \mathbb{R}^{n_{c_m}}$. Secondly, we add and substract a multiple $\alpha_m\mathbf{z}$ with $\alpha_m > 0$. As a result, we obtain new systems

$$\dot{\mathbf{z}}_m(t) = (A_m - \alpha_m I)\mathbf{z}_m(t) + \sum_{j=1}^{n_v+1} v_{h,j}(t)N_{m,j}\mathbf{z}_m(t) + B_m\mathbf{u}_m(t), \quad \mathbf{y}_m(t) = C_m\mathbf{z}_m(t) + C_m\mathbf{w}, \tag{6}$$

where $N_{m,n_v+1} = \alpha_m I$, $B_m = [\, N_1\mathbf{w},\ \ldots,\ N_{n_v}\mathbf{w},\ A_m\mathbf{w}\,]$ and $\mathbf{u}_m(t) = [v_{h,1}(t), \ldots, v_{h,n_v}(t), 1]^T$. In order to have few inputs, the vector $\mathbf{w}$ needs to be in the kernel of almost all matrices $N_{m,j}$. We were able to find $\mathbf{w}$ such that the matrix B_m has four colums.

We now present some results of numerical experiments. The bilinear system (6) of order 1976 was approximated by a reduced model of order 10 computed by the BIRKA. Figures 1(a) and (b) show the convergence history for the BIRKA and the relative error in the output for two different values of α.

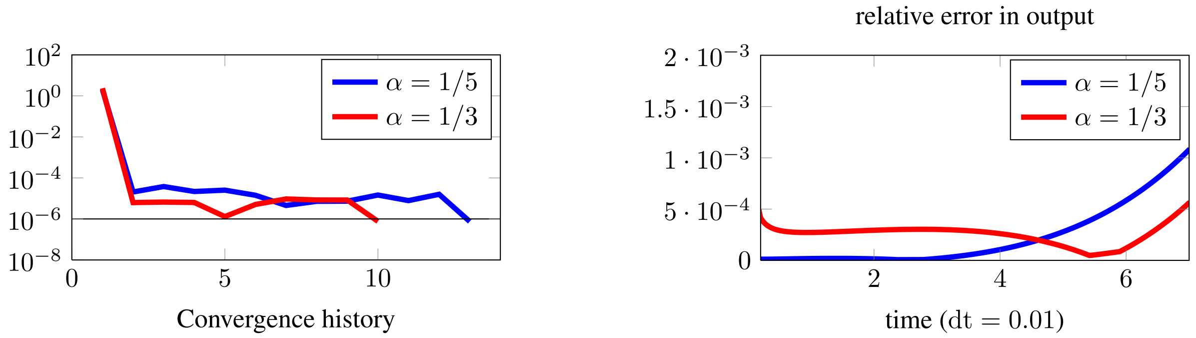

Fig. 1: (a) Convergence history for the BIRKA. (b) Evolution of the relative error.

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