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## PDE-constrained optimization models for scientific processes

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We survey a number of practical applications of PDE-constrained optimization problems across science and engineering.

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Inspired by literature such as [6], we wish to give an impression of the wide applicability of PDE-constrained optimization across the scientific disciplines. Although far from exhaustive, we provide examples of problems with varying structure and motivation. A key challenge in the field of numerical linear algebra would be to investigate solvers for such problems, for example applying work carried out on “all-at-once” iterative methods accelerated by saddle point preconditioners for the solution of steady [8] and time-dependent [7] problems.

Attempting to unify the notation from the literature, in order to achieve consistent derivation of all problems considered, we denote  $\mathbf{x}$  as a spatial variable throughout, with  $t$  the time variable on an interval  $(0, T)$ ,  $\beta$  (or variants of this notation with subscripts) as one or more regularization parameters, and  $\Omega$  the spatial domain with boundary  $\partial\Omega$ . We apply the convention that  $y$  (and sometimes additionally  $z$ ) denote *state variables* (or *PDE variables*),  $\hat{y}$  (and  $\hat{z}$ ) are *desired states*, with  $u$  the *control variable*. Bold lower-case letters are used to denote vectors. The aim is to make clear the overarching structures that these formulations have in common, and how the problem statements may be adapted to address specific scientific challenges.

Six applications of PDE-constrained optimization, summarized from literature covering a number of fields, are given below:

▷ **Monge–Kantorovich mass transfer problem** (see [4] and [6, Section 4.3]): Here, one wishes to find a mapping from one bounded density function to another (these correspond to  $y_0$  and  $\hat{y}$  in the problem formulation below) that is optimal in a suitable sense, by minimizing the *Kantorovich distance* between the two functions. Discussed in [4] and [6, Section 4.3] was the equivalence of this formulation, and that of solving a problem of the form:

$$\min_{y, \mathbf{u}} \frac{1}{2} \int_{\Omega} (y(\mathbf{x}, T) - \hat{y}(\mathbf{x}))^2 d\Omega + \frac{\beta T}{2} \int_0^T \int_{\Omega} y \|\mathbf{u}\|^2 d\Omega dt \quad \text{s.t.} \quad y_t + \nabla \cdot (y\mathbf{u}) = 0 \quad \text{in } \Omega \times (0, T),$$

with initial condition  $y = y_0$  at  $t = 0$ . Here, the state  $y$  denotes a time-dependent density field, with the control  $\mathbf{u} = [u_1(\mathbf{x}, t), u_2(\mathbf{x}, t)]^T$  a velocity field.

▷ **Inverse acoustic wave propagation** (see [2, Section 3.1]): One wishes to minimize over the  $L^2$  norm the difference between an observed state and that predicted by the PDE model for acoustic wave propagation:

$$\min_{y, u} \frac{1}{2} \sum_{j=1}^{N_r} \int_0^T \int_{\Omega} (y - \hat{y})^2 \delta(\mathbf{x} - \mathbf{x}_j) d\Omega dt + \beta \int_{\Omega} (|\nabla u|^2 + \epsilon)^{1/2} d\Omega \quad \text{s.t.} \quad y_{tt} - \nabla \cdot (u \nabla y) = f \quad \text{in } \Omega \times (0, T),$$

coupled with boundary condition  $u \nabla y \cdot \mathbf{n} = 0$ , and initial conditions  $y = y_t = 0$  at  $t = 0$ . One builds a profile of the state  $y$ , based on the observed pressure  $\hat{y}(\mathbf{x}, t)$  at  $N_r$  receivers in an acoustic medium on a space-time domain. The receivers correspond to points  $\mathbf{x}_j$ , prescribed on the boundary of the domain, with  $f(\mathbf{x}, t)$  a known acoustic energy source,  $u(\mathbf{x})$  the squared acoustic velocity distribution, and  $\epsilon > 0$  a (small) parameter.

▷ **Optimal control of chemical processes** (see [3]): One wishes to “control” a chemical reaction in some sense, by solving:

$$\begin{aligned} \min_{y, z, u} & \frac{\beta_y}{2} \int_0^T \int_{\Omega} (y - \hat{y})^2 d\Omega dt + \frac{\beta_z}{2} \int_0^T \int_{\Omega} (z - \hat{z})^2 d\Omega dt \\ & + \frac{\beta_{y,T}}{2} \int_{\Omega} (y(\mathbf{x}, T) - \hat{y}_T)^2 d\Omega + \frac{\beta_{z,T}}{2} \int_{\Omega} (z(\mathbf{x}, T) - \hat{z}_T)^2 d\Omega + \frac{\beta_u}{2} \int_0^T \int_{\partial\Omega} u^2 ds dt \\ \text{s.t.} & \quad y_t - D_y \nabla^2 y + k_y y = -\gamma_y y z, \quad z_t - D_z \nabla^2 z + k_z z = -\gamma_z y z \quad \text{in } \Omega \times (0, T), \end{aligned}$$

with boundary conditions  $D_y \frac{\partial y}{\partial n} + b(\mathbf{x}, t, y) = u$  and  $D_z \frac{\partial z}{\partial n} + \xi z = 0$ , initial conditions  $y = y_0$  and  $z = z_0$  at  $t = 0$ , and box constraints  $u_a \leq u \leq u_b$  imposed on the control variable, belonging to  $L^\infty(\partial\Omega \times (0, T))$ . This is therefore a *boundary control problem*. Here,  $D_y, D_z, \gamma_y, \gamma_z, k_y, k_z, \xi$  denote (nonnegative) constants. The state variables relate to concentrations of reactants (with one possibly denoting a temperature), with the control relating to the rate at which a chemical is fed into the reaction mechanism, as one also wishes to minimize the “cost” of carrying out the reaction.

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▷ **Boundary control in chemotaxis** (see [9, Chapter 13]): Here, one solves the following minimization problem:

$$\begin{aligned} \min_{z, y, u} & \frac{1}{2} \int_{\Omega} (z(\mathbf{x}, T) - \widehat{z})^2 \, d\Omega + \frac{\beta_y}{2} \int_{\Omega} (y(\mathbf{x}, T) - \widehat{y})^2 \, d\Omega + \frac{\beta_u}{2} \int_0^T \int_{\partial\Omega} u^2 \, ds dt \\ \text{s.t.} & \quad z_t - D_z \nabla^2 z - \gamma_z \nabla \cdot \left( \frac{\nabla y}{(1+y)^2} z \right) = 0, \quad y_t - \nabla^2 y + k_y y - k_z \frac{z^2}{\eta + z^2} = 0 \quad \text{in } \Omega \times (0, T), \end{aligned}$$

with boundary conditions  $\frac{\partial y}{\partial n} + \gamma_y y = \gamma_y u$  and  $\frac{\partial z}{\partial n} = 0$ , initial conditions  $z = z_0$  and  $y = y_0$  at  $t = 0$ , and box constraints  $u_a \leq u \leq u_b$  imposed on the control variable. Here,  $z, y$  denote two *state variables*, corresponding to the bacterial cell density and chemoattractant concentration respectively, with the control  $u$  arising from a mixed boundary condition, and  $D_z, \gamma_z, \gamma_y, k_z, k_y, \eta$  (nonnegative) constants. One wishes to identify the behaviour of control such that the biological system acts in a way determined by the given desired states  $\widehat{z}, \widehat{y}$ .

▷ **Shape optimization in blood flow** (see [1]): Here, in one of many examples of flow control problems in fluid dynamics, one wishes to minimize the mechanical loading on blood particles, for instance to avoid damage of red blood cells. This is very important when designing prosthetic devices or artificial heart components, for example. One considers finding a shape  $\Omega$ , in the case where it can be parameterized by  $\alpha \in \mathcal{A}_{\text{ad}}$  for some admissible set  $\mathcal{A}_{\text{ad}}$ , which solves:

$$\begin{aligned} \min_{\mathbf{y}, z, \alpha} & \quad 2 \int_{\Omega_{\text{obs}}} \varepsilon(\mathbf{y}) : \varepsilon(\mathbf{y}) \, d\Omega_{\text{obs}} \\ \text{s.t.} & \quad \rho(\mathbf{y} \cdot \nabla \mathbf{y}) - \nabla \cdot \boldsymbol{\sigma}(\mathbf{y}, z) = \mathbf{0}, \quad \nabla \cdot \mathbf{y} = 0 \quad \text{in } \Omega, \end{aligned}$$

with observation region  $\Omega_{\text{obs}}(\alpha) \subset \Omega(\alpha)$ . Boundary conditions  $\mathbf{n} \cdot \boldsymbol{\sigma}(\mathbf{y}, z) = h$  on  $\partial\Omega_h$ ,  $\mathbf{y} = \mathbf{g}$  on  $\partial\Omega_g$ , are posed on disjoint segments of  $\partial\Omega$ , and the weak form of the PDEs is considered. The stress tensor  $\boldsymbol{\sigma}$  and viscous stress tensor  $\varepsilon$  are given by

$$\boldsymbol{\sigma}(\mathbf{y}, z) = -z\mathbf{I} + 2\mu\varepsilon(\mathbf{y}), \quad \varepsilon(\mathbf{y}) = \frac{1}{2}(\nabla\mathbf{y} + \nabla\mathbf{y}^\top),$$

with  $\mathbf{y}$  and  $z$  denoting velocity and pressure,  $\mu$  the dynamic viscosity (constant for a Newtonian fluid),  $\rho$  the fluid density, and  $\mathbf{I}$  the identity tensor.

▷ **Image denoising** (see [5]): Posed as a bilevel optimization problem, one is given a set of training pairs of images  $(f_k, \widehat{y}_k)$ ,  $k = 1, \dots, N$ , corresponding to a set of noisy images and (exact or approximate) ground truth images, and wishes to find weights  $u_i$  (each corresponding to a data fidelity model function  $\phi_i(y, f)$ ) that solve:

$$\min_{u_i \geq 0, i=1, \dots, d} \frac{1}{2} \sum_{k=1}^N \int_{\Omega} (\widetilde{y}_k - \widehat{y}_k)^2 \, d\Omega + \frac{\beta}{2} \sum_{i=1}^d \|u_i\|_X^2,$$

where  $\widetilde{y}_k$  itself solves the minimization problem:

$$\min_y |Dy|(\Omega) + \sum_{i=1}^d \int_{\Omega} u_i \phi_i(y, f_k) \, d\Omega, \quad |Dy|(\Omega) = \sup_{\mathbf{g} \in C_0^\infty(\Omega; \mathbb{R}^2), \|\mathbf{g}\|_\infty \leq 1} \int_{\Omega} y \nabla \cdot \mathbf{g} \, d\Omega,$$

for the given noisy images  $f_k$ . The idea is to find an “optimal weighting” of a (possibly large) number of noise models  $\phi_i$ . Here,  $X$  corresponds to  $\mathbb{R}$  if  $u_i$  denote scalar parameters, and a norm such as  $L^2(\Omega)$  if  $u_i(\mathbf{x})$  are distributed functions over  $\Omega$ . The subsequent investigation of optimality conditions, and the approximation of the total variation term  $|Dy|$  using Huber-type regularization [5], leads to a PDE-constrained optimization model for this imaging application.

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