Mixed-Integer PDE-Constrained Optimization

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Many complex scientific and engineering applications can be formulated as optimization problems constrained by partial differential equations (PDEs) with both continuous and integer decision variables. This new class of mathematical problems, called mixed-integer PDE-constrained optimization (MIPDECO) [4], must overcome the combinatorial challenge of integer decision variables combined with the numerical and computational complexity of PDE-constrained optimization.

Examples of MIPDECO include the remediation of contaminated sites and the maximization of oil recovery, which involve flow through porous media and the optimization of wellbore locations and optimal flow rates [2], and operational schedules [1]. Related applications also arise in the optimal scheduling of shale-gas recovery [6]. Next-generation solar cells face complicated geometric and discrete design decisions to achieve perfect electromagnetic performance [5]. In disaster-recovery scenarios, such as oil spills [7], and hurricanes [3], resources must be scheduled to mitigate the disaster while adjusting to the underlying dynamics for accurate forecasts. Other science and engineering examples include the design, control, and operation of wind farms and gas networks.

Each of these applications combine discrete decision variables with complex multiphysics simulation. Until recently, these grand challenge problems have been regarded as computationally intractable. Formally, we state a mixed-integer PDE-constrained optimization problem as

$$\begin{array}{llll} & \underset{u,w}{\text{minimize}} & \mathcal{F}(u,w) & \\ (1) & \text{subject to} & \mathcal{C}(u,w) & = 0, \\ & & \mathcal{G}(u,w) & \leq 0, \\ & & u & \in \mathcal{D}, \text{ and } w \in \mathbb{Z}^p \text{ (integers),} \end{array}$$

which is defined over a domain Ω. We use x, y, z to indicate spatial coordinates of the domain Ω and t to denote time. The objective function of (1) is $\mathcal{F}$, $\mathcal{C}$ are the equality constraints, and $\mathcal{G}$ are inequality constraints. The equality constraints include the PDEs as well as boundary and initial conditions. We denote the continuous decision variables of the problem by $u(t, x, y, z)$, which includes the PDE states, controls, or design parameters. We denote the integer variables by $w(t, x, y, z)$, which may include design parameters that are independent of (t, x, y, z). Thus, in general, problem (1) is an infinite-dimensional optimization problem, because the unknowns, (u, w), are functions defined over the domain Ω, although we avoid a formal discussion of function spaces in this paper.

We review existing approaches for solving these problems, and we highlight their computational and mathematical challenges. We introduce a benchmark set for this class of problems and present some early numerical experience using both mixed-integer nonlinear solvers and nonlinear rounding heuristics.

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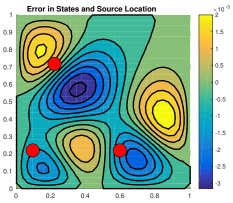

$$
\begin{array}{lll}
\underset{u,w}{\text{minimize}} & \displaystyle\frac{1}{2}\int_{\Omega}(u-\bar{u})^2 d\Omega & \text{Least-squares fit} \\
\text{subject to} & \displaystyle -\Delta u = \sum_{k,l} w_{kl} f_{kl} \text{ in } \Omega & \text{Poisson eqn.} \\
& \displaystyle \sum_{k,l} w_{kl} \leq S \ , \ w_{kl} \in \{0,1\} & \text{source budget}
\end{array}
$$

Figure 1. Formulation and solution of a simple source inversion model.

One example of our benchmark problems is a simple source inversion problem based on Laplace's equation with Dirichlet boundary conditions, which is motivated by groundwater flow applications. The goal is to match observations, $\bar{u} \in \Omega$ by selecting possible sources from a set of possible sources using binary variables. We prefer the use of binary variables, because an alternative formulation, which models the source location as continuous variables, results nonlinear (i.e. nonconvex) constraints. We discretize the PDE with a five-point finite difference stencil using an equidistant meshsize of $h = 1/32$, and we limit the number of sources to $S = 3$. The resulting discretized problem is a convex mixed-integer quadratic program. We solve the discretized problem using MINOTAUR's branch-and-bound solver, which searches 759 nodes in 69s of CPU time on an Intel i7 core. Figure 1 shows the optimal selection of sources as red dots and the deviation from $\bar{u}$, as well as the problem formulation.

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