Mixed-Integer Partial Differential Equation Constrained Optimization

Armin Fügenschuh

(joint work with F. Gnegel, M. Hagel, S. Leyffer, M. Stiemer)

An area of research that recently gained momentum is the inclusion of continuous physical phenomena described by ODEs or PDEs into discrete decision processes as an additional type of constraints. For instance, Fügenschuh et al. [4, 3] describe network flow problems in which the transport equations are included, Koch et al. [7] and Hahn et al. [6] combine gas dynamics with discrete decisions related to the control of natural gas networks, and Frank et al. [2] consider the shortest path problem together with the heat equation. We will refer to this class of problems as *Mixed-Integer PDE-Constrained Optimization (MIPDECO)* problems, a term introduce in [8]; this notion includes ODEs as a one-dimensional special case of PDEs.

Classical mixed-integer linear programs have a finite number of constraints, for instance, one for each node or each arc of a finite graph structure. In contrast, differential equations are defined on continuous domains, they have to be valid at infinitely many points. In the numerical treatment of PDEs as well as in the field of Optimal Control, it is common practice to find a finite system that approximates the solution with high accuracy. A possible way for solving MIPDECO problems is thus to adapt known approximation techniques for PDEs in order to obtain an approximation with only finitely many constraints and variables. A common approach is to use finite-difference methods, which replaces the differential operators with suitable difference equations on a finite and regular grid. The approximated function values on the grid are then included in the MIPDECO formulation as additional variables, and the difference equations are additional constraints. The downside of this approach is that even moderately fine grids – by PDE-numerics standards – lead to a huge number of variables and constraints – by mixed-integer programming standards. Thus the solution of the linear programming relaxation (the root node of the evolving branch-and-bound-tree) of such an instance can take multiple hours or may not even finish on a state-of-the-art numerical solver (such as Cplex). Even in the case of linear systems (for instance, resulting from approximations of the heat equation, the wave equation, or the transport equation) numerical issues uncommon for MILPs derived for combinatorial problems have to be taken into account. For example, the standard bounds strengthening routines in the presolve phase of the aforementioned solvers may result in a false certificate of infeasibility [1].

In the case of linear PDEs, it is sometimes possible to transfer the solution of the PDE into a preprocessing step. That is, it can be efficient to solve the PDE for a basis of the control space and apply the principle of superposition to obtain solutions by linear combinations of the basis [2, 5]. In addition to that, splitting the solution process of the PDE and the MILP has the additional benefit that other solution methods, such as Galerkin methods (in particular, finite element methods) can be applied more readily.

We illustrate these ideas for the convection-diffusion equation, where an additional vector of variables $w = (w_1, w_2, \ldots, w_n) \in \mathbb{R}^n$ representing a control is included in the righthand side. In full, we consider the following PDE system:

$$u_t(x,t) - \vec{c} \cdot \nabla u(x,t) - d\Delta u(x,t) = y(x,t,w) \qquad \forall\,(x,t) \in \Omega \times (0,T), \tag{1a}$$

$$\frac{\partial}{\partial \vec{n}} u(x,t) = h_R(u_R - u(x,t)) \qquad \forall\,(x,t) \in \partial\Omega \times (0,T), \tag{1b}$$

$$u(x,0) = u_0(x) \qquad \forall\, x \in \Omega. \tag{1c}$$

Here Ω is a sufficiently regular domain in which the time depending temperature distribution u is studied. Further given are: a constant outer temperature u_R on the boundary $\partial\Omega$, a coefficient h_R for the heat transfer over the boundary, a temperature distribution $u_0(x)$ at time 0, and further constants $\vec{c}, d$. The function y on the righthand side expresses the influence of w on the continuous dynamics. We assume that y depends linearly on w. Then there exist functions y_i for all $i \in \{1, \ldots, n\}$, such that

$$y(x,t,w) = \sum_{i=1}^{n} w_i y_i(x,t).$$

By the principle of superposition the solution of the PDE can then be expressed as

$$u(x,t) = u_{\text{inh}}(x,t) + \sum_{i=1}^{n} w_i \hat{u}_i(x,t), \tag{2}$$

where u_{inh} (inh for inhomogeneous) is the solution of (1a) for $w = (0,0,\ldots,0)$ (which implies $y = 0$), and each $\hat{u}_i$ is the solution of (1a) for $y = y_i, u_R = 0$, and $u_0(x) = 0$.

Now the approximations of the functions on the righthand side of (2) are calculated in a preprocessing step. Hereto, a finite element method can be applied, for instance, which has the additional benefit that the basis functions can be evaluated at arbitrary points in the domain without further approximation techniques (i.e., not only at grid points), since finite element solutions are discrete functions that are naturally defined throughout Ω.

We then replace the system (1) by its approximative solution (2), and thus decouple the discretization of the PDE from the further solution process. Constraints defined for the whole domain, such as a state constraint

$$u(x,t) \geq 0, \qquad \forall (x,t) \in \Omega \times (0,T) \tag{3}$$

can be evaluated during the branch-and-bound solution process (technically, as lazy constraints) at a finite number of positions (x,t), and are added on demand in case one is violated. Since these constraints are dense in w_i (i.e., having many nonzero entries), it is not clear at first if this approach is computationally advantageous, and thus comparative numerical studies were carried out. The numerical results we obtained for two case studies – a wildfire hazard controlled by firefighters operating on a road network, and a contaminated subsurface water flow controlled by filtration stations – show a large reduction in computation time. It turned out that only very few lazy constraints were in fact generated, so that their density did no great harm to the solution process.

References

[1] A. Dittel, A. Fügenschuh, S. Göttlich, and M. Herty. MIP Presolve Techniques for a PDE-based Supply Chain Model. *Optimization Methods & Software*, 24(3):427–445, 2009.

[2] M. Frank, A. Fügenschuh, M. Herty, and L. Schewe. The Coolest Path Problem. *Networks and Heterogeneous Media*, 5(1):143–162, 2010.

[3] A. Fügenschuh, S. Göttlich, C. Kirchner, M. Herty, and A. Martin. Efficient Reformulation and Solution of a Nonlinear PDE-Controlled Flow Network Model. *Computing*, 85(3):245–265, 2009.

[4] A. Fügenschuh, M. Herty, A. Klar, and A. Martin. Combinatorial and Continuous Models and Optimization for Traffic Flow on Networks. *SIAM Journal on Optimization*, 16(4):1155–1176, 2006.

[5] F. Gnegel, M. Dudzinski, A. Fügenschuh, and M. Stiemer. Mixed Integer PDE Constrained Optimization for the Control of a Wildfire Hazard. In *Operations Research Proceedings 2017*, pages 483–488. Springer Verlag, Heidelberg, 2018.

[6] M. Hahn, S. Leyffer, and V. M. Zavala. Mixed-Integer PDE-Constrained Optimal Control of Gas Networks. Technical report, Argonne National Laboratory ANL/MCS-P7095-0817, 2017. Available at URL: https://wiki.mcs.anl.gov/leyffer/images/2/27/GasNetMIP.pdf (visited on 06/25/2018).

[7] T. Koch, B. Hiller, M. E. Pfetsch, and L. Schewe. *Evaluating gas network capacities.* Society for Industrial and Applied Mathematics (SIAM), Philadelphia, 2015.

[8] S. Leyffer. Mixed-Integer PDE-Constrained Optimization. In A. Wiegele L. Liberti, S. Sager, editor, *Mixed-integer Nonlinear Optimization: A Hatchery for Modern Mathematics*, volume 46/2015, pages 2738–2740. Mathematisches Forschungsinstitut Oberwolfach, 2015. DOI: 10.4171/OWR/2015/46.