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Adjoint-based error control for the simulation and optimization of gas and water supply networks

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ABSTRACT

In this work, the simulation and optimization of transport processes through gas and water supply networks is considered. Those networks mainly consist of pipes as well as other components like valves, tanks and compressor/pumping stations. These components are modeled via algebraic equations or ODEs while the flow of gas/water through pipelines is described by a hierarchy of models starting from a hyperbolic system of PDEs down to algebraic equations. We present a consistent modeling of the network and derive adjoint equations for the whole system including initial, coupling and boundary conditions. These equations are suitable to compute gradients for optimization tasks but can also be used to estimate the accuracy of models and the discretization with respect to a given cost functional. With these error estimators we present an algorithm that automatically steers the discretization and the models used to maintain a given accuracy. We show numerical experiments for the simulation algorithm as well as the applicability in an optimization framework.

1. Introduction

The flow of gas or drinking water through networked pipelines is of particular interest not only in the engineering community but also for the network operators in the real market. Many challenges arise from running a gas transmission or water supply network. Gas or water, which is fed in by multiple suppliers, has to be routed through the network to meet the consumers' demands. At the same time, the operational costs of the network like energy consumption of compressor and pumping stations or contractual penalties have to be minimized. This leads to an optimal control problem on a network. Further, since some of the network components like valves or compressor/pumping stations also have an `on/off` option, binary decisions are introduced to the optimization. This mixed integer aspect is not considered within this work and the corresponding `on/off` decisions are assumed to be given.

In the field of optimization and simulation of gas and water supply networks, there has been a lot of research over the past years, see for example [1–10]. There are already existing software packages that may simulate and optimize the gas flow through networks. One well-known representative is the software package SIMONE [11], which is able to simulate the flow through gas transmission networks using steady-state as well as transient models. However, for the optimization task, which is promoted as *operational* and *long-term optimization*, only stationary models are taken into account. In [2,7,1], non-linear

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programs (NLPs) are applied to solve the optimal control problem. For the solution of the underlying partial differential equation (PDE), an implicit Euler method is employed and a two-point discretization in space having the two endpoints of a pipe is defined a priori. A mixed-integer linear program (MILP) is introduced in [5,6], where the binary decisions can also be optimized. Nevertheless, the same two-point discretization is prescribed in advance. In [10], a mixed-integer nonlinear program (MINLP) that makes use of an implicit box scheme [12] is proposed. A MILP model is derived from this, in which combinatorial constraints are handled and the non-linearities are approximated by piecewise linear functions. This approach is combined with a classical sequential quadratic program (SQP) solver with a continuous treatment of the combinatorial constraints. While within [10] the piecewise linear functions are adaptively refined, the discretization in time and space is still chosen a priori and fixed.

Since the behaviour of gas and water supply networks may be dynamic and thus changes both in space and time, an automatic control of the accuracy of the simulation is beneficial. Duality-based methods, as they are commonly used in continuous optimization, are developed for example in [13–16]. There, goal-oriented a posteriori error estimation is used for space and time adaptive finite element approximations of the incompressible Navier–Stokes equations.

The flow of gas or water through pipeline networks may be described by qualitatively different models based on the Euler equations. Thus, a further possibility to achieve a compromise between the accuracy of the simulation and the computational costs is to use simplified models in regions with low activity, while sophisticated models have to be used in regions, where the dynamical behaviour has to be resolved in more detail. In [17–19], we derived an algorithm to adaptively control model and discretization errors with techniques from [14] for gas supply networks. In [20,21], we applied the concept of a posteriori error control to simulation tasks for gas and water supply networks. Within the cited references, only simulation tasks have been considered and an outlook to an efficient optimization framework with adaptive error control is given. The realization of the latter is the main contribution of this article.

To solve optimization tasks, we build upon an SQP solver which needs function evaluations and gradient information – second derivative information is computed with a BFGS update formula. One advantage of the applied solution technique is that we are directly able to consider various constraints. Further, many procedures already occurring in the computation of the applied adjoint-based error estimators for simulations can directly be used for the computation of gradient information for the optimization. However, an additional difficulty arises here due to possible changes in the spatial discretization between single time blocks of the adaptive simulation algorithm. While we only needed the adjoint within such blocks for error estimation, one needs the adjoint for the entire time horizon for the computation of gradient information. Thus, the underlying transformations describing refinements or coarsenings of the spatial discretization have to be incorporated in the adjoint equations and the entire system needs to be solved efficiently.

Besides academical examples, the presented framework also covers a wide range of special requirements occurring in many applications (like the conditions in Section 7.3). Here, it is important to note that the applied adaptive algorithm altogether leads to a reduction of the computation time, since the local application of simpler models and coarser discretizations throughout the optimization procedure saves more than the computational costs of the error estimation. Further, it is worth noting that the user of the optimization framework only has to prescribe a single desired tolerance, which is a strong argument regarding the practical acceptance.

In this work, we begin with a short description of the modeling aspects of gas and water supply networks in Section 2. In Section 3, we formally deduce adjoint equations, which are used to get a posteriori error estimators for the model as well as the spatial and temporal discretization errors. The adjoint-based error estimators are currently implemented in a first-discretize way, which is described in Section 4. The adaptive error control strategy as developed in [17–19] is shortly summarized in Section 5. In Section 6, the efficient computation of gradient information based on a first-discretize adjoint approach to solve optimization tasks is described. Results for simulation and optimization scenarios are given in Section 7.

2. Modeling

In this section, we give an overview of the modeling of gas and water supply networks. Starting with some general aspects of network modeling, we will then describe the key components of either type of network.

2.1. General aspects

The flow of gas or water through pipelines is a directed quantity, which can be adequately described in one space dimension. Hence, we model gas and water supply networks as a directed graph $\mathcal{G} = (\mathcal{J}, \mathcal{V})$ with arcs $\mathcal{J}$ and vertices $\mathcal{V}$ (nodes, branching points).

In both types of networks, the set of arcs $\mathcal{J}$ contains pipes. In the case of gas transport, the considered networks also consist of compressor stations, valves and control valves, while we have pumping stations, valves and tanks in water supply networks.

For the pipes, the underlying dynamics of gas/water may be described by a hierarchy of models. The most complex ones consist of a hyperbolic system of partial differential equations (PDEs), other models result from making simplifying assumptions. Each arc in the network that is modeled via PDEs is defined as an interval $\left[x_j^a, x_j^b\right]$ with $x_j^a < x_j^b, j \in \mathcal{J}_{\text{PDE}}$, where $\mathcal{J}_{\text{PDE}} \subseteq \mathcal{J}$ contains all arcs modeled with PDEs.