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# **A System to Evaluate Gas Network Capacities: Concepts and Implementation**

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# A System to Evaluate Gas Network Capacities: Concepts and Implementation

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## Abstract

In 2005 the European Union liberalized the gas market with a disruptive change and decoupled trading of natural gas from its transport. The gas is now transported by independent so-called *transmissions system operators* or TSOs. The market model established by the European Union views the gas transmission network as a black box, providing shippers (gas traders and consumers) the opportunity to transport gas from any entry to any exit. TSOs are required to offer the maximum possible capacities at each entry and exit such that any resulting gas flow can be realized by the network. The revenue from selling these capacities more than one billion Euro in Germany alone, but overestimating the capacity might compromise the security of supply. Therefore, evaluating the available transport capacities is extremely important to the TSOs.

This is a report on a large project in mathematical optimization, set out to develop a new toolset for evaluating gas network capacities. The goals and the challenges as they occurred in the project are described, as well as the developments and design decisions taken to meet the requirements.

## 1 Introduction

In the following, we will describe how disruptive changes in market regulation led to new challenges in the industry which sparked a project on how mathematical optimization can provide tools to deal with these new tasks. This article will give an overview of the run of the project and the choices made.

The results presented in this article were achieved as part of the *Forschungskooperation Netzo-optimierung* (ForNe) between Germany's largest TSO, Open Grid Europe GmbH (OGE, then E.ON Gas Transport) and Zuse Institute Berlin, Technische Universität Darmstadt, Friedrich-Alexander Universität Erlangen-Nürnberg, Universität Duisburg-Essen, Leibniz-Universität Hannover, Humboldt-Universität zu Berlin, Weierstrass-Institut für Angewandte Analysis und Stochastik, and later on the companies develOPT GmbH, and atesio GmbH.

The results of the project have been published in the book [KHPS15] and in several articles [GMSS15, RSSW16, SSW16a, FHH<sup>+</sup>11, PFG<sup>+</sup>14, SSW15a,

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SSW16b, GHHS16, JOP16, SL17]. Furthermore, the project resulted in several dissertations [Gei11, Mor13, Hum14, Hay16, Sch17, Sch13a, Wil14].

In this article, we report on some of the challenges and obstacles we encountered during the project. To the best of our knowledge, ForNe was at the time one of the largest applied research projects in mathematical optimization, with more than 40 people contributing. In the following, we describe how we tackled and solved upcoming problems, both mathematically and with the software tools developed, hoping that future projects might benefit from our experiences. Finally, the bilevel model for flow reallocations from Section 3.3.3 has not been published before. We included the description of flow relocations because it illustrates nicely how far we went from our initial belief that all we have to do is to route flows through a stationary network towards a tool that could try to cope with the complex reality created by the regulatory authorities.

The outline of the article is as follows. In the following section, we review the problem from the perspective of the TSO. Section 3 presents the mathematical models and methods from a high-level perspective, focusing on the interplay of the submodels for different aspects of the problem. In Section 4, we describe the architecture of the software and spotlight some parts of the implementation and the experiences we have made so far. We conclude and provide an outlook in Section 5.

## 2 The problem from the TSO's perspective

The problem that we were posed by our industry partner was motivated by a number of changes in the industry. We first outline the main change in the regulatory background that was at the core of the interest of our industry partner. We then describe the requirements that followed from these changes and the mathematical challenges that followed from these requirements.

### 2.1 Regulatory background

Until 2005, gas transport and supply in Europe was provided by an oligopoly of companies, owning and operating the network and trading gas. With more than 20% of the whole energy demand of Europe provided by natural gas, the European Union decided to introduce an active gas market. Therefore, in 2005 legislation was passed that gas trading and transport had to be done by mutual independent companies to ensure non-discriminatory access to the transport network for all traders [GGH<sup>+</sup>15]. This new legislation changed the operation and business model of the gas transport operators who, due to their high investment cost for natural gas pipeline networks usually became regional monopolies. Before, transport system operators (TSO) were part of an integrated organization and could plan the network operation and expansion together with the traders depending on long-term contracts with the suppliers and customers. Since then, the TSOs became independent and needed to plan under uncertainty about the gas flow situations resulting from short-term trading. Nevertheless, they have to ensure the safe and reliable operation of the transport network under these new circumstances.

In a simplified view, the EU regulations introduced the so-called *entry-exit model* with a virtual trading point as the basis of the capacity market. For each

network, a virtual trading point is introduced. All market participants need to buy capacity from the TSO to access this virtual trading point, i.e., suppliers need to buy *entry capacity*, demand customers need to buy *exit capacity*. Both capacities are offered independently. The preferred capacity product by the TSO is known as firm freely allocable capacity, i.e., the capacity bought by the customer, the *booking*, defines an upper bound on the amount of gas that can be induced or deduced from the network on a given day. After trading, the amount of capacity used is communicated to the TSO, the so-called *nomination*. The TSO may assume that the result of market operations is balanced in the sense that for a given day the total amount nominated at entries is equal to the total amount nominated at exits. The requirement for the TSO is now that it can provide the nominated amount of gas at the respective entries and exits by suitable transport and distribution of the gas in the network. To ensure this is possible, the TSO is allowed to restrict the amount of bookable capacity at each point in the network. A TSO may only sell capacity rights for which it can guarantee that each “likely and realistic” [Gas10, §9] gas flow complying with the capacity rights booked by all transport customers can technically be realized. Thus a TSO needs a way to check this requirement. We call this task the *verification of booked capacities*. In this article, we will discuss the development of a new system which supports the TSO in checking whether it can offer a given set of booked capacities without risking the security of supply.

## 2.2 Requirements and challenges

Mathematically, there are two major challenges:. First, one has to deal with the *uncertainty* of how transport customers use their capacity contracts, i.e., uncertainty about which gas flow situations have to be served by the network. Second, deciding *feasibility* of a given gas flow situation is, with the detail level required, a very difficult mixed-integer nonconvex nonlinear decision problem.

A central problem here is that while many flow situations might be legal, i.e., contractually possible, they are nevertheless not occurring in practice, either because they cannot be technically realized or because the necessary trades cannot be made. Furthermore, if we were to allow all contractually possible nominations, then only very small capacities would be possible. In fact, it might be that the system as a whole is infeasible, i.e., there is a flow situation which is impossible to fulfill.

Additionally, there are flow situations that occur very often whereas others situations are very rare. This difference makes it reasonable to also take the likelihood of the flow situations into account. From discussions, we know that most European TSOs use a similar approach as our industry partner is currently employing, i.e., generating “challenging” gas flow situations to cope with the uncertainty and checking these gas flow situations as we later describe here. Methods to generate “challenging” gas flow situations are described in, e.g., [BEG<sup>+</sup>15, SHDA15, HS16]. Usually, it is then concluded every nomination within the “convex hull” spanned by those extreme cases is feasible. Due to the non-convex properties of compressor stations, it can be shown that this assumption is mathematically not correct within the stationary model we employ.

We decided on a different approach. Using a combination of historic flow data on the exists and worst-case assumptions on the entries, we generate a huge number of flow situations, many of them average. Then, using scenario

reduction, we reduced the number of nominations to a manageable size. As a result of the reduction, the final nominations could be augmented by probabilities. This allowed setting a target range of, e.g., 98%, instead of requiring to solve all generated nominations.

Additionally, the regulatory framework contains the concept of capacity zones which are conglomerations of nodes which are jointly nominated. From the trader’s perspective, these zones are treated like a single node. The TSOs has the freedom to shift flow arbitrarily between the nodes in the zone. This freedom cannot be represented well in purely node based approaches which are therefore unnecessarily conservative.

Checking for technical feasibility can either be done using simulation tools and expert knowledge (augmented by automated tools) or by optimization-based methods, e.g., [vdH04]. The physical models underlying these methods are either very detailed, if using simulation tools, or have to be suitably simplified. Our goal here was to provide a fully unified methodology which allows us to incorporate more and more market information to also deal with future capacity contracts and market-based mechanisms. We demonstrate the flexibility of our approach in Section 3.3.3 by showing how to incorporate another contract type, flow reallocation options.

Each of the generated and reduced nomination scenarios is then separately checked for *technical feasibility*: Is it possible to operate the network within the technical limits, possibly using the flow reallocation options? The problem of answering this question is called *validation of nominations*.

Since we generate a comparatively large number of nominations to sample the solutions space, a fully automatized optimization-based system to validate the feasibility of nominations was needed. During the course of the project, we encountered several further details, especially of the German gas transport market, which made extensions of the approach necessary. In addition to the problem aspects described in [KHPS15], the models and methods have been extended to cover the following:

- Dealing with different types of gas with different calorific values [GMSS15] since gas is paid by energy content.
- Support for flow reallocation options and flow rebalancing. This is important as flow reallocation options are a flexible mechanism that may be used to offer more transmission capacity without the need for network expansion. The modeling of flow reallocation options is described in Section 3.3.3.

It is a difficult decision whether first to ensure correctness of a complex model and then work on increasing the size of the networks that can be handled, or to go the other way around and first ensure that networks of the necessary size can be computed, possibly rather imprecise and with features missing, and then try to improve precision and level of detail. Over the course of the project, we iterated several times between these two directions.

### 3 Our approach to the problem

In this section, we describe how we approached the problem. In most parts, we will only sketch the approach; for details, we give references to the literature.

An important goal of this section is to show, how the requirements evolved during our solution process and how the “textbook” mathematical models need to be adapted to yield solutions that are usable in practice.

### 3.1 The basic setup

We model the topology of a gas network with a directed graph  $G = (V, A)$ . The set of entries is denoted by  $V_+$ , the set of exits by  $V_-$ , and their union by  $V_\pm$ . The arcs are often referred to as *network elements*.

The mathematical models we developed, address two distinct aspects: The *usage of the network* by traders for their gas trading and the *operation of the network* by the TSO. In principle, network usage may be modeled by a set of gas flow situations. We model a particular gas flow situation as a balanced vector of inflows and outflows  $P^{\text{ext}} = (P_u^{\text{ext}})_{u \in V_\pm}$  and call such a vector a *nomination*.

Apart from the entities of interest, the transmission capacities, many more details need to be considered. We found the following technical and contractual constraints to be important when verifying booked capacities, therefore, our approach has to take these aspects into account:

**capacity contracts** Capacity contracts define limits on the amounts of gas that are injected or withdrawn, may be subject to additional constraints or conditions.

**historical gas flows** Gas flow measurements may be used for predicting future gas flows where appropriate.

**network topology and devices** A gas network is modeled as a graph with arcs of different types representing pipes, valves, control valves and compressor units.

**operational constraints** The operation of a network is subject to a range of constraints like bounds for the pressure, the joint operation of several network elements, and complex flow bounds for certain paths in the network.

**different gas qualities** Gas from different sources differs in its composition, resulting, e.g., in different calorific values. Since the capacity rights and the gas market are defined in terms of thermal power, the mixing of different calorific values needs to be taken into account to ensure proper power supply at the exits.

**flow reallocation options** A TSO may have contracted options to adjust the flow at certain nodes to support operating the network reliably.

**flow rebalancing** As we deal with stationary models, adjusting the flow at one node using a flow reallocation option requires an adjustment at other nodes to maintain the balance of injected and withdrawn gas.

Now, considering fixed inflows is not sufficient in view of flow reallocation options and the resulting necessity to model flow rebalancing according to the market. We thus consider *nomination scenarios*, consisting of a nomination and a *market preference vector*  $(w_u)_{u \in V_\pm}$  that describes the relative attractivity of entries and exits by weights. The nomination and the market preference vector

Variable	Index Set	Meaning
$P_u^{\text{ext}} \in \mathbb{R}_{\geq 0}$	$u \in V_{\pm}$	Desired inflow/outflow at each entry/exit in terms of thermal power.
$w_u \in \mathbb{R}$	$u \in V_{\pm}$	Weight of each entry/exit, describing the attractiveness of injecting/withdrawing gas at this particular node. We call the vector $(w_u)_{u \in V_{\pm}}$ the <i>market preference vector</i> .
$P_u^{\text{eff}} \in \mathbb{R}_{\geq 0}$	$u \in V_+$	Effective inflow at each entry in terms of thermal power after employing reallocation options and flow balancing.
$P_u \in \mathbb{R}_{\geq 0}$	$u \in V_-$	Outflow at each exit in terms of thermal power according to the flow and calorific value arriving at this exit. The goal is to operate the network such that we have $P_u = P_u^{\text{ext}}$ for all $u \in V_-$ .
$q_a \in \mathbb{R}$	$a \in A$	Mass flow for each arc/network element. A non-negative value indicates flow in the direction of the arc, a negative value flow in the opposite direction.
$H_{c,u} \in \mathbb{R}_{\geq 0}$	$u \in V$	Calorific value at each network node.
$p_u \in \mathbb{R}_{\geq 0}$	$u \in V$	Pressure at each network node.
$s_a \in \{0, 1\}^{k_a}$	$a \in A_{\text{active}}$	Vector of switching decisions for each active element. The number of switching variables $k_a$ depends on the type of the network element.

Table 1: Overview of the variables used to model network usage and network operation.

are the variables of the models and methods used to derive a set of nomination scenarios that capture potential gas flow situations.

For the models and methods for the operation of the network that are used to validate a nomination scenario, the nomination, and the market preference vectors are, of course, the parameters. At the exits, the goal is to obtain exactly the outflows specified in the nomination. For the entries, however, flow reallocation options may be used to change the inflows specified by the nomination to aid network operation. In this case, flow rebalancing adjusts the flows at the remaining entries such that the overall inflow/outflow balance is maintained and entries with a higher weight are used up to their booked capacities as much as possible. Moreover, there are several other quantities that need to be considered to model the technical and physical constraints of network operation.

Table 1 shows the variables used to model network usage and network operation, respectively.

### 3.2 Models and methods for verifying booked capacities

As summarized in the introduction, the entry/exit model enables the gas traders to easily deal with the task of transporting gas. All they need to do is to book sufficient entry or exit capacities (depending on their role) some time in advance and to sell or buy gas at the virtual trading point. Since the gas is sold to/bought from a market participant in the same network, this transaction is automatically



balanced, so from the market perspective, everything is fine.

The TSO, however, needs to provision the network and/or limit the bookable capacities such that the desired gas transport can be realized. To do this, it is necessary to understand and model how the capacities may be used by the traders and which gas flow situations may arise. The gas withdrawn from most of the exits is consumed and thus follows certain demand patterns. Due to this, the offtake at these exits is quite predictable. The remaining exits are, e.g., storages and interconnection points to adjacent networks. As for entries, their flows depend very much on the gas market and are thus hard to predict. Moreover, the flows at these entries and exits may be highly correlated in a way that adversely affects network operation. For instance, it may happen that very few entries supply a large share of the exits and that the gas needs to be transported over long distances, requiring much compression power.

### 3.2.1 An approach based on Mathematical Programming

As already mentioned, the regulation requires a TSO only to sell capacity rights for which it can guarantee that each *likely and realistic* gas flow situation complying with the capacity rights can technically be realized. Thus one of the first tasks of the project was to formalize this requirement.

Most exits correspond to gas consumers with a certain gas demand, which can be predicted well based on past observations. Moreover, the gas for a particular consumer can only be withdrawn from the network at a particular exit. In contrast, there is much flexibility on the entry side: Usually, the gas supply for a single gas demand situation can be provided in many ways by the entries. The particular distribution of the supply among the entries may change on a day-to-day basis, depending on market prices, and is thus hard to predict.

This dichotomy motivated the following formalization for the problem of verifying booked capacities. The gas flow at the predictable exits is modeled by a random variable  $\xi$ . Moreover, for a given gas demand situation  $s$ , let  $\mathcal{B}(s)$  be the set of gas flow situations with demands given by  $s$  that comply with the booked capacity rights, i.e., all gas flows are within limits specified by the capacity rights. Finally, let  $\mathcal{T}$  be the set of gas flow situations that can technically be realized. The problem of verifying booked capacities can now be phrased as: Is the probability that *any* gas flow situation is technically feasible at least a certain probability level  $\alpha$ ? Or, formally, does the condition

$$\mathbb{P}_\xi[\mathcal{B}(\xi) \subseteq \mathcal{T}] \geq \alpha \quad (1)$$

hold? This expresses the idea that a given (stochastic) exit demand can be met by many supply patterns and that it should be very likely that *any* supply pattern results in technically feasible operation.

To devise an algorithm that answers this question approximately, we use discretization twice. First, we replace the random variable  $\xi$  by a finite set of demand samples  $\{s_1, \dots, s_M\}$ . Second, for each sample  $s_i$ , we sample a set  $\{P_1^{\text{ext}}, \dots, P_N^{\text{ext}}\}$  of gas flow situations from  $\mathcal{B}(s_i)$ . For each gas flow situation  $P_j^{\text{ext}}$ , we check technical feasibility (i.e., decide  $P_j^{\text{ext}} \in \mathcal{T}$ ) using our methods for nomination validation (see Section 3.3). By counting the number of samples  $s_i$  for which *all* gas flow situations  $\{P_1^{\text{ext}}, \dots, P_N^{\text{ext}}\}$  are technically feasible, we obtain an estimate for the left-hand side of (1). In this way, we reduced the task of verifying booked capacities to nomination validation.

To make this approach work, we need to detail the abstract concepts used. First, we need a stochastic model for the random variable  $\xi$  describing the demands. This is obtained from the data using methods outlined in Section 3.2.2. Second, we need a model for  $\mathcal{B}(s)$ , i.e., gas flow situations matching a certain demand vector  $s$ , and a method to sample from this set. This is sketched in Section 3.2.3. Finally and most importantly, we need a method for nomination validation, which is explained in Section 3.3. For all of these ingredients, a lot of details needed to be worked out.

In contrast to the original approach of our industry partner, this idea leads to much less conservative gas flow situations. It also provides much better coverage of potential gas flow situations. However, these two properties are achieved by considering much more gas flow situations, which necessitates an automatic method for nomination validation. As the selection of the considered gas flow situations is based on random sampling, there is no “scenario idea” for a single gas flow situation, i.e., it has no particular meaning. Thus it is hard for planners to analyze a certain gas flow situation and to judge its overall relevance.

### 3.2.2 Analysing historical flow data

Transmission system operators measure the amount of gas injected to or withdrawn from the network for every entry and exit, respectively. They are legally obliged to use this data in their capacity models to consider *likely and realistic* flow situations for their network. This section summarizes the approach for obtaining distributional models from historical data about gas flows, which is described in full detail in [HHL<sup>+</sup>15a].

The exit flows often depend on the *local temperature* in the particular geographical area (see Fig. 1 for examples). To avoid modeling the temperature distributions within Germany, we chose a pragmatic approach and introduced a network-wide *reference temperature*. This reference temperature is determined, for each day, as a weighted average of the local temperatures of several locations in Germany. To further simplify the modeling of the temperature dependency of gas demand, we divide the temperature range into *temperature classes*. Each temperature class should be small enough to treat the temperature as constant within this temperature class. Thus the goal is to have one distributional model for each temperature class, reflecting the temperature dependency by different distributional models.

To account for correlations between the gas flows it is desirable to use multivariate stochastic models as far as possible. Moreover, (multivariate) normal distributions are particularly interesting, as a wide range of techniques has been developed for working with them. Thus the aim was to identify a hopefully large share of the exit flows to be normally distributed.

In a first attempt, the temperature classes and the type of distribution for each exit have been determined manually. This was done by partitioning the temperature range in intervals such that each interval contains a sufficient number of samples. The exits have been classified into various types, by using visual inspection of the historical gas flow data, complemented by hypothesis tests for normal distributions. This process was very tedious but provided valuable insights into the data.

In the course of the project, it became apparent that the distributional

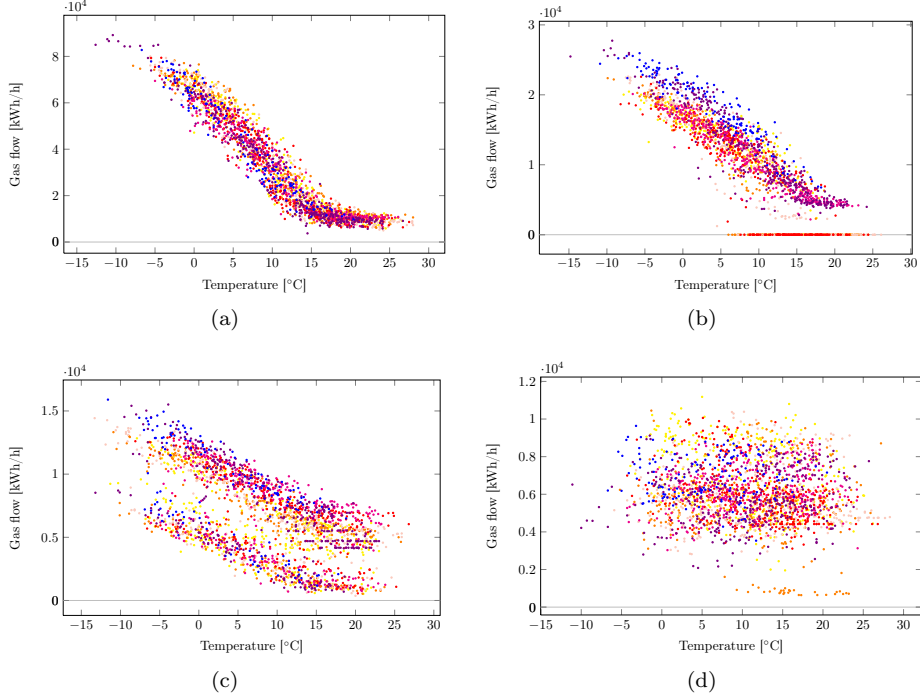


Figure 1: Plots showing the daily gas demand for four selected exits. The indicated temperature is the local temperature at the exit location.

models have to be updated according to new data on a regular basis. We thus developed an automated approach that determines suitable temperature classes and for each exit a best-fitting distribution from a certain class of parametric (univariate) distributions. The portfolio of candidate distributions also contains univariate normal distributions. For all exits modeled by univariate normal distributions (usually a large share of the exits), multivariate normal distributions are obtained by complementing the univariate marginal distributions with the correlation matrix computed from the data. The visualization methods used in the manual process have been very valuable in guiding the development and debugging of this automated process.

### 3.2.3 Constructing nominations for nomination validation

In addition to simple capacity rights for single entries and exits, there are much more constraints on the gas flow situation that may occur in practice. We already mentioned zone capacity rights, i.e., limits for the total amount of flow injected or withdrawn from a set of entries or exits. Some parts of the gas network are co-owned and may be used by several TSO. Similar to the situation with entries, it is uncertain how the other TSO are using their share of the capacity of those parts of the network. On top of this, it is in the interest of the TSO to use a “tight” model of relevant gas flow situations, i.e., to exclude as many gas unrealistic gas flow situations as possible, as this allows to obtain higher capacities that can be offered to the market.

It was thus evident that a model for  $\mathcal{B}(s)$  would be on the one hand, rather complex and on the other hand should provide certain flexibility for expressing requirements and restrictions from practice. We thus choose MILP as a modeling framework and devised a generic model for capacity rights. This model can be used by the industry partner to formulate the conditions and constraints of a wide range of capacity products. In particular, the model can handle zones and more general dependencies between flows at several nodes.

Creating that model was an interactive process that took more than a year. The communication was done based on technical papers with model details and lots of examples. Luckily, some network planners were mathematicians with modeling experience, so they could judge the suitability of the model and provide valuable feedback. The detailed examples created during the discussion have later been used as acceptance tests to check the expected behavior of the model.

### 3.3 Models and methods for nomination validation

It turned out that the main task in our project would be to solve the problem of validating nominations. To solve this task taking into account the different possibilities of the TSO to an acceptable level of accuracy turned out to be harder than we initially thought. At the end, we used a variety of methods that work together in one software system.

The task in the nomination validation problem is to determine whether there is a feasible control for the gas network serving a nomination scenario given by the vector  $(P_u^{\text{ext}})_{u \in V_{\pm}}$  of desired in- and outflows. Control in this setting means technical measures (using compressors, valves, etc.) and non-technical measures (here: flow reallocation options).

To solve this very complex problem, we ended up addressing three different problem aspects by a separate layer of modeling.

1. The operational capabilities of a gas network are described by the topology of the network and the characteristics of each of the network elements. These aspects can conveniently be modeled in terms of the mass flow  $q_a$  of each network element, the pressure  $p_u$  at each node, and the switching decisions  $s_a$  for each active elements. The basic assumption here is that the gas flow situation in terms of mass flows is given and fixed.
2. The next layer deals with the fact that the capacity contracts are not concluded in terms of mass flow  $(q_u^{\text{ext}})_{u \in V_{\pm}}$ , but instead in terms of thermal power  $(P_u^{\text{ext}})_{u \in V_{\pm}}$ . This makes it necessary to model a simple form of gas mixture.
3. Using flow reallocation options and the resulting re-balancing are market-based mechanisms. These effects are modeled as a bilevel problem with a linear second level problem, providing effective inflows  $(P_u^{\text{eff}})_{u \in V_{+}}$  at each entry. This bilevel model depends on the market preference vector  $(w_u)_{u \in V_{\pm}}$  that governs the re-balancing and the desired in- and outflow vector  $(P_u^{\text{ext}})_{u \in V_{\pm}}$ .

These three model layers are solved by an integrated method that is summarized in Fig. 2. We will use the rest of this subsection to outline the different parts.

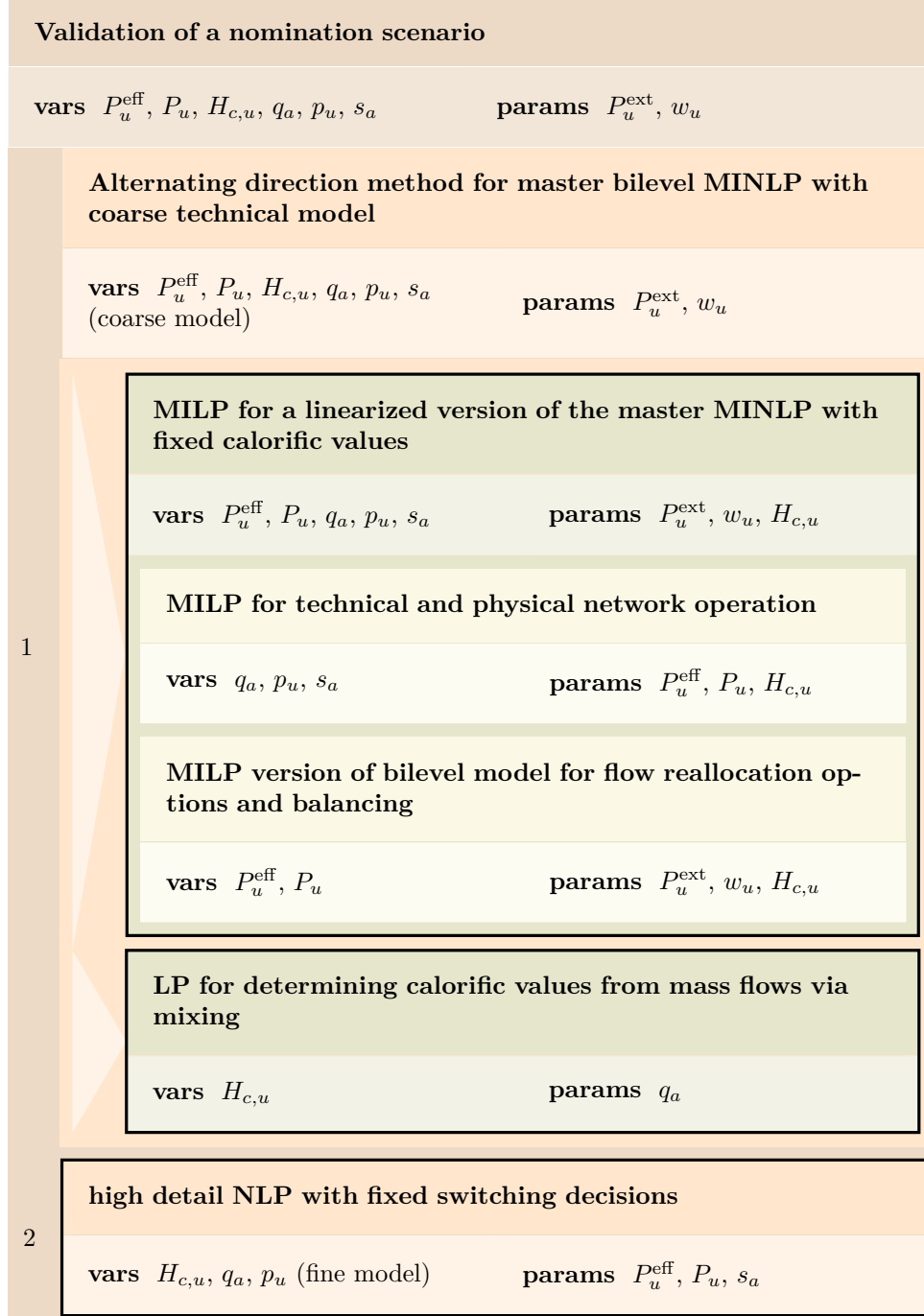


Figure 2: Structure of the models and methods used by nomination validation for checking a single nomination scenario. The models marked with thick lines are solved by an off-the-shelf solver as part of the overall method.

### 3.3.1 Technical and physical network operation: Nomination validation for flow nominations

At the beginning of the project, we started with a classical approach to validating nominations. We took a standard physical model, using mass flow and pressure as the main state variables to describe the physical behavior of the network. We then used a simple model for the pressure drop on pipes

$$p_v^2 = \left( p_u^2 - \Lambda |q| q \frac{e^S - 1}{S} \right) e^{-S} \quad (2)$$

with suitable constants  $\Lambda$  and  $S$  (see [KHPS15, p. 27]), modeled compressors rather coarsely and tried to solve the resulting MINLP using standard techniques.

We briefly outline the most important aspects of our modeling to indicate the complexity of the MINLP model used at this point. Our basic assumptions concerning the gas physics are the following.

- We consider a stationary gas flow situation given as a vector of balanced in- and outflows in terms of mass flow.
- We consider the isothermal case, i.e., we neglect the change of temperature due to the various physical effects involved. The model is based on a constant mean temperature calculated as a flow-weighted average according to the injected gas qualities.
- We ignore the mixing of gas and assume all parameters (molar mass, calorific value, norm density, pseudocritical pressure and temperature, molar heat capacity) of the gas to be constant with the value given by the respective flow-weighted average as for the temperature. (Calorific values will be handled specially by the method described in Section 3.3.2.)
- The so-called  $z$ -factor describing the deviation from a real gas is assumed to be constant along a network element.

Under these assumptions, we can model the pressure drop in pipes using the equation (2).

This flow in the network can be controlled by so-called *active elements*. A particularly simple one is a *valve*, which allows the gas to either flow or not.

To compensate for the pressure loss in the network, the TSO uses *compressors*. Typically the TSO operates a number of compressor stations at various points in the network, where a number of compressors are placed. The energy expenditure in these compressor stations accounts for the majority of the operating costs of the TSO. In coarse models, the only parameters of interest are bounds on the in- and outflow of the station and the maximum absolute and relative pressure increase that can be obtained. For a detailed physical model, one needs to take into account that a compressor consists of a compressor machine, which compresses the gas and a compressor drive, which powers the compressor machine. We do not go into detail of compressor modeling in this section but refer to the chapter [FGG<sup>+</sup>15] and the paper [SSW15a]. We note, however, that a detailed compressor model leads to a nonlinear nonconvex system of constraints.

In addition to the constraints for operating each network element, there are further constraints for the joint operation of the active elements. We model these via so-called *subnetwork operation modes* which specify a set of joint switching states for each element in a subnetwork. Typically, such a subnetwork corresponds to a bigger physical entity like a compressor or control valve station.

The model sketched is a very complex MINLP model combining many non-convex constraints for the pressure drop on pipes/resistors and the operating ranges of compressor machines and drives with sophisticated switching decisions for the active elements and the subnetwork operation modes.

The result of a simple MINLP approach was not satisfying at all. We could only solve very small instances and even on those the error compared to simulation results was unacceptable. This meant that we needed to come up with an approach that was tailored to the problem. We will only sketch this approach as this forms a large part of [KHPS15], for an overview over the underlying physics set, see [FGG<sup>+</sup>15], for a short overview over the models and solution approaches, see [SKMP15].

The main idea to overcome this was a two-stage approach:

1. In the first stage, we use a simplified physical and technical model to obtain switching decisions for operating the network.
2. The second stage uses these switching decisions to determine refined controls in the detailed and accurate physical and technical model.

As the second stage does not involve any integer variables anymore, it is addressed by the NLP method described in [SSW15c].

The first stage, however, is still necessarily a nonconvex MINLP as the non-linear pressure loss in pipes cannot be meaningfully simplified further. Therefore, we developed the following four distinct approaches exploiting different properties to tackle the hard problem of finding feasible switching decisions.

**MILP approach** This approach [GMMS15] transforms the MINLP into a MILP model using a general technique given by [GMMS12] building on prior work. This MILP is a relaxation of our original MINLP. Advantages of this technique include: a priori guarantees on the error of the solution with respect to the underlying MINLP model, certification of infeasibility of the original MINLP, independence of the MILP solver used. Extensions of this technique have been discussed in, e.g., [GMS13, Gei11, Mor13, DGK<sup>+</sup>11, GKL<sup>+</sup>11].

**Specialized MINLP approach** This approach [HFH<sup>+</sup>15] uses a somewhat coarser MINLP formulation. This allows using a specialized algorithm that is implemented in the general-purpose MINLP solver framework SCIP [Ach09, VG16]. Advantages of this technique include: certification of infeasibility with respect to the coarsened MINLP, short computation times due to tight integration with the solver.

**Reduced NLP heuristic** This heuristic [GSS15] reformulates the MINLP as a coarse NLP. The formulation chosen leads to very small NLPs which allows checking a large number of discrete settings in a short time. To reduce the number of settings to test, first a transshipment problem is solved on an aggregated graph and then analyzed. The advantages of

this technique include: Adaptability to a specific network, computation speed. Extensions of this technique to the case of random loads have been discussed in [GHHS16].

**MPEC heuristic** This heuristic [SSW15b] reformulates all discrete decisions as complementarity constraints and uses standard regularization approaches to solve the resulting NLPs. Advantages of this technique include: computation speed, very detailed physical model. Extensions of this technique have been discussed in, e.g., [RSSW16, Sch13b, Sch15, SSW13].

The second stage model can now be used to generate solutions for models that have much higher physical fidelity than the models used in the first stage, see [SSW15c, SSW15a, SSW16a].

There are, however, difficulties when certifying infeasibility. The MIP approach and the specialized MINLP approach can certify feasibility for their models, as the MIP approach uses a relaxation of a MINLP, it automatically provides also an infeasibility certificate for this MINLP. What to do, however, if the second stage cannot find a solution? What do we report in this case? Here, it was very important to enter into discussions with our industry partner as they needed to get familiar with the possibilities and limitations of our approach without being overloaded with technical details. We refer to the discussion in [JSSW15]. One additional point was that the industry partner was interested to get more information than just the report that an instance was infeasible. Can the infeasibility be explained? This lead to structural results [JOP16] that allowed to localize infeasibilities that can be derived using network flow techniques and bound strengthening.

As reported in [HHL<sup>+</sup>15b], all four approaches have their strengths and combining them provides a very powerful solver for the nomination validation problem. When considering the extensibility regarding different calorific values and the use of flow reallocation options (and hence nonconstant in- and outflows in terms of mass flow), however, the MILP approach turned out to be most flexible and robust.

### 3.3.2 Handling of different gas sources: Nomination validation for power nominations

At the start of our project, we started with models that are close to the models found in the mathematical literature. In these models, the state of the gas in a pipe is described through the variables pressure  $p$ , density  $\rho$ , velocity  $v$ , and gas temperature  $T$ . In the stationary and isothermal case and using further simplifications, it is sufficient to use the state variables pressure  $p$  and mass flow  $q$ . The mass flow, however, is not a quantity that is relevant for the practitioner: Most of the results of internal calculations are given in volumetric flow at standard conditions and all contracts are stated in terms of thermal power  $P$  delivered. We worked under the assumption that we could easily convert our results from mass flow to these quantities. For the first conversion, we assumed that during normal operation the gas density in a pipe is roughly constant, so that a linear relation between mass flow and volumetric flow at standard conditions holds. For the second conversion, we assumed that the “gas quality” is equal at all entry nodes, specifically that the calorific value  $H_c$  is constant, so that  $P_u = H_c q_u$ . Close to the end of the project, we found out,



after prodding by our industry partner, that the second assumption was often severely violated. Even though, the industry partner has two distinct networks for gas with low calorific value and high calorific value, the differences in gas quality in these networks are still non-negligible. So, we had to come up with a method that allowed us to incorporate the effects of different calorific values in our model without losing all of the work that had been done for the case of fixed gas quality. We note that the mixing problems that occur, even without taking into account the gas physics, are very challenging; they are known as (generalized) pooling problems for which rich literature exists (for a survey, see [MF09]). In our case, we had two major difficulties to overcome:

- The coupling between the thermal power, the mass flow, and the calorific value introduces (many) nonconvex bilinear constraints.
- In the considered gas networks, for many arcs, the flow direction is not known beforehand and depends on the network control. This leads to non-smoothness, as the mixing condition discriminates between ingoing and outgoing arcs (w.r.t. flow), which is to be decided by the model.

To tackle this additional layer of complexity, a tailored method was developed, which we outline here. For more details, we refer to [GMSS15]. The method alternately solves the following two models that arise as restrictions of the master MINLP model. In this model, we use as the objective function the weighted deviation of the  $P_u$  from the desired outflows  $P_u^{\text{ext}}$ .

- In the first model, the calorific values  $H_{c,u}$  are fixed, and we optimize with respect to the network controls.
- In the second model, all other variables are fixed, and we optimize with respect to the calorific values  $H_{c,u}$ .

The first model is a slight variation of the MINLP described above, which can be solved with the MILP approach. The second model is an LP which can be readily solved using standard solvers. If this does not yield an acceptable solution, we change the weights of the different nodes: Nodes with large deviation get a larger weight.

We were, however, not satisfied with the ad-hoc nature of our solution approach. This motivated us to try to develop a better understanding, why our method worked. We were able to give a convergence theory for our method and show a connection to classical feasibility pump heuristics [GMSS17a]. We have also extended the method such that we can use more detailed compressor models [GMSS17b] in the nomination validation.

Overall, this major difficulty motivated us to develop new methods and prove interesting theorems.

### 3.3.3 Flow reallocations and market behavior

As a result of the algorithm of the preceding section, we came across quite a number of nominations that were infeasible, but could be made feasible in regular operation. This was because we had not taken into account non-technical measures the TSO can take. The main measures are so-called *flow reallocation options* that the TSO can conclude with its transportation customers, i.e., the

traders. If any flow reallocation options are available, the amount of gas injected into the network may be changed by the TSO after nomination.

We consider three types of flow reallocation options, all acting on entry nodes only:

**Increase** The TSO may increase the amount of flow above the nominated value.

**Decrease** The TSO may decrease the amount of flow below the nominated value.

**Distribution** The TSO may decrease the flow at one entry and simultaneously increase the flow at another entry by the same amount, staying balanced.

Increase and decrease introduce an imbalance between injection and withdrawal, leading to infeasibility in stationary models of gas flow. Therefore, the nomination is *rebalanced* according to the preferences of the traders (here understood as a unified agent). Here, the capacity contracts need to be taken into account. Furthermore, the use of flow reallocation options *protects* certain nodes from the influence of the traders.

In this operational view, decisions happen at three stages, sequentially, where each decision restricts the choices for the next stage.

1. The TSO decides about the usage of flow reallocation options.
2. The traders decide about the rebalancing of nominations.
3. The TSO decides the technical configuration.

One can now canonically formulate a multi-level optimization problem consisting of three levels, corresponding to the stages above. Taking into account that both the first and third levels are decided by the TSO and that the traders are ignorant about the technical details of the third level, the problem can be reduced to a bilevel problem.

$$\begin{aligned}
& \underset{x,y,z}{\text{minimize}} && h_0(z) && (3) \\
& \text{subject to} && f_1(x) \leq 0 \\
& && h_1(y, z) \leq 0 \\
& && \underset{y}{\text{maximize}} && g_0(y) \\
& && \text{subject to} && g_1(x, y) \leq 0
\end{aligned}$$

Here,  $x$  are the flow reallocation options,  $y$  is the nomination, and  $z$  is the network state. Within this formulation, the problem of nomination validation as described in Sections 3.3.1 and 3.3.2 is represented by the objective  $h_0(z)$  and constraints  $h_1(y^*, z)$ , given a fixed nomination  $y^*$ .

The “follower” problem of (3) can be seen as a network flow problem on a particular graph where flow is routed from nodes representing the nominated values to nodes representing the effective flow values at the entries. The  $y$  variables take the role of the flow with  $x$  acting as arc capacities. Hence, flow on some arcs is fixed or bounded by the leaders decisions. The objective of the follower is to maximize sum of the effective flow values  $P_u^{\text{eff}}$  weighted by the market preference vector  $(w_u)_{u \in V_{\pm}}$

The bilevel problem in (3) can be transformed to a single-level optimization problem via the equivalent KKT reformulation of the follower problem [CMS07]. This leads again to an LP and an additional complementarity constraint. This complementarity constraint  $\lambda_a \perp y_a$  can be expressed, e.g., as a special ordered set of type 1 in a MIP solver. Furthermore, binary variables in the leader mark the application of flow relocation to the nodes. They are used ensure consistency of the options that are used and to enable and disable particular constraints in the follower problem.

In summary, this reformulation allows us to incorporate these non-technical measures into our overall approach. We have seen that even minor changes in the problem setting can lead to huge changes in the mathematical model and the needed algorithms. We would not have been able to react to the changing requirements and even notice the need for such a change if we had not had a flexible software system that allowed for rapid feedback. This is the topic of the next section.

## 4 Architecture of the ForNe System and current implementation

The software that was developed in the project consists of two parts: The computing core and the user interface. Computing core and user interface together constitute what we call the *ForNe System*. The computing core implements the models mentioned above, providing algorithms for the validation of flow and power nominations. The user interface offers several means to interact with the ForNe System and orchestrates the solution of high-level subproblems within the validation of flow nominations and the verification of booked capacities.

Changing requirements and specifications are a common challenge in applied (research) projects. Before describing the architecture and some implementation details of the ForNe System, we want to review the history of the system and how it changed over the course of the project. We hope that the discussion of both the evolution of the requirements as well as our final solution can be helpful for future projects with similar requirements.

### 4.1 Changing requirements during the project

The requirements on the system were subject to major changes during the project. Starting as a platform to show our results and generate transparency between researchers and practitioners, it turned into a Software-as-a-Service (SaaS) platform to provide different interfaces to the various tools developed in the project.

The availability of gas network data was one key driver for the evolution of the system. At the beginning of the project, several artificial networks topologies covering major aspects of the network allowed to develop and test the first optimization models and algorithms. The first real planning scenarios from our industry partner created the need to discuss solutions and also the solution methods in more detail. To provide a platform for these discussions, the first user interface was developed in the form of an HTML based web interface. Therein it was possible to upload data and start a computation for the validation of a nomination. This computing job was then executed on the server, and

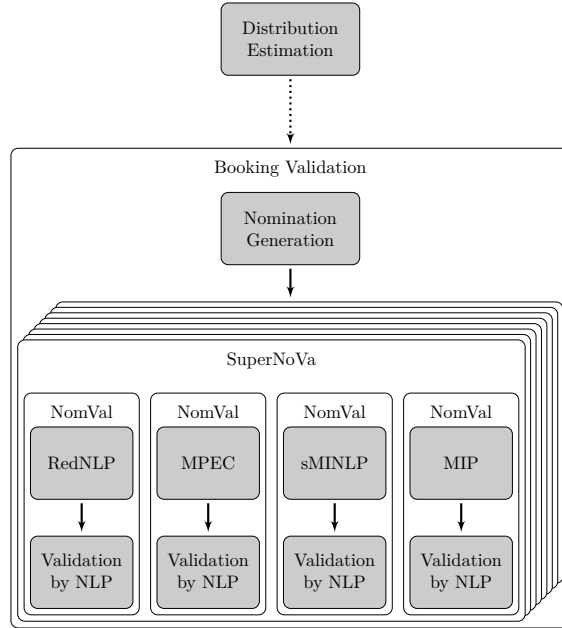


Figure 3: Overview of the architecture for a booking validation. Components with a white background are handled by the user interface and components with a gray background by the computing core.

the output of the computing core was streamed to the user. This approach created the transparency that was needed to create trust in our methods as the industry partner could experiment with the data, follow the solution process, and independently examine the results.

Provided with this new tool, an increasing number of planning scenarios was generated, which frequently had to be recomputed as models and methods improved. At the latest when the scenario sampling approach for the validation of a booking was introduced, the system did not scale. Our solution shifted from a synchronous streaming solution to an asynchronous approach where instances are composed and then submitted to a computing cluster where they are processed as soon as the required hardware capacity is available. This allowed to massively scale the number of jobs the system could handle. The results also became persistent and could be retrieved by several persons. Several interfaces to facilitate interaction of the system with humans and machines were introduced.

With this background on the evolution of the system, we now focus on the features and the architecture of the current ForNe System.

## 4.2 Features and architecture

The ForNe System can compute solutions for several kinds of problems with the main objective to verify booked capacities. The different problem types are realized by *applications* with a predefined set of input data and parameters and expected results. This allows combining apps to realize more workflows with the advantage that each step can also be executed in isolation.

As an example, Fig. 3 provides an overview of the process of the verification

of booked capacities assuming the nominations are validated using the SuperNoVa approach. Each box represents one application in the ForNe System. Boxes with a gray background represent functionality that is implemented in the computing core which is only wrapped into an application. In a first step, a distribution model is estimated from the measured data as described in Section 3.2.2. The resulting distribution is written to a file and can be used to verify different variants of booked capacities, i.e., in the assessment of which capacities can be published and which capacity requests accepted. The dashed arrow depicts this human interaction. The validation of a booking is a process in two steps which is managed by the user interface. First, a number of nomination scenarios is generated as described in Section 3.2.3; a feature that is also implemented in the computing core. Then, these nominations are validated in parallel.

The interface for the ForNe System is highly extensible. Apart from these building blocks of the validation of a booking, several applications provide convenience functionality such as data conversion, data error checking and creation of visualizations. Moreover, several groups of applications provide advanced functionality not yet designed for productive use, e.g., for topology planning or capacity maximization.

Several interfaces are available to upload input data, start, stop, query the status and download the results of jobs. This includes an HTML-based web interface for human interaction, and an XML-based web API allows integration into the processes and infrastructure of our industry partner. The HTML interface also supports the upload of simple line based batch files where every line specifies one problem instance.

Most of the jobs are rather long running; ranging from several hours for the validation of a nomination to several days for the detailed validation of a booking. Proper job management has to ensure that the status and, upon termination, the results of a job are available and users are notified. Furthermore, the job has to support the abortion and in some cases also the continuation of jobs. Proper termination and restart have to be ensured for the problem types where several components are solved individually and in parallel such as SuperNoVa or booking validation.

### 4.3 Implementation Details

In this section, we provide some more technical details about the ForNe System.

The computing core is implemented in C++ using the framework Lamatto++ [GMM]. It includes appropriate data structures, parsing facilities, advanced data checks on a logical level that goes far beyond pure schema validation, preprocessing (e.g., flow and pressure propagation and network simplification), abilities to build various kinds of optimization models and algorithms developed in the project, and solution analysis. It contains interfaces to several solvers, including CPLEX [IBM], Gurobi [Gur], SCIP [Ach09, VG16], and Ipopt [WB06] (through GAMS [GAM]). Apart from the problems that are the focus of this paper, the computing core contains algorithms for several related problems such as for gas network topology extension for a single [FHH<sup>+</sup>11, Hum14] and multiple scenarios [Sch17, SL17], and capacity maximization [Hay16].

The user interface is implemented in Python and uses CherryPy [Che] as a web framework. A class hierarchy for problem types enables code reuse. Each

problem class contains a list of parameters and expected outputs from which the various interfaces and documentation are generated. This approach ensures high flexibility in the addition, modification, and deletion of parameters which can easily become time-consuming and error-prone without such infrastructure. Each problem class performs lightweight tasks directly and submits jobs to solve subproblems with the computing core to the cluster. For example, for each SuperNoVa four jobs are submitted to the cluster. Each of them determines the status of the SuperNoVa upon termination and possibly kills the remaining jobs as soon as the result of the SuperNoVa has been decided.

The computing cluster is hosted at the Zuse Institute Berlin and is managed by the cluster resources management system SLURM [YJG03]. Dependencies between jobs are used to trigger job evaluations and email notifications. Due to the limited length of the job queue (50 000 jobs in our installation), an additional job queue is implemented in the interface as this quickly becomes a bottleneck, e.g., if several bookings are to be validated in parallel.

## 5 Conclusions and outlook

By the end of the project, the software system described consists of about 300 000 lines of code and has been used to conduct extensive computational experiments, comprising several months of computing time on a cluster with more than 1500 cores located at ZIB. All in all, millions of nomination scenarios were generated and solved in parallel. The system proved to be reliable and robust enough to handle this large-scale workload.

To establish the usefulness of our new method the industry partner provided data for historical gas flows, capacity contracts and reallocation options, and the topology and technical parameters of several operational networks. This data was taken from the existing simulation-based process [BEG<sup>+</sup>15], which was semi-automatically converted to the respective input formats of the ForNe system, though due to the complexity of some of the models and their input data, parts of the input had to be generated manually.

It turned out that the initial quality of the input data was not sufficient to obtain results matching those of the established process. This resulted in many iterations with successively improved data. For finding and repairing data errors, researchers' experience and intimate knowledge of the implemented models and algorithms turned out to be indispensable.

Regarding the practical use of tools built on highly complex mathematical models, there are two conclusions from this observation. First of all, quality assurance for complex input data is crucial to obtain meaningful results and should be supported by tools (not just the data sanity checks of the optimization code) as far as possible. For use in practice, such tools need to be usable and appealing to the industrial users, i.e., without requiring a deep understanding of the underlying math. Secondly, it is necessary to provide, as far as possible, easily comprehensible means to understand the working of the underlying models and algorithms. Of course, this is very hard to achieve for general MIP/MINLP solvers, but the problem-specific high-level design of the algorithms often allows to derive insights from intermediate results. For instance, initial bound tightening combines input data from several sources, sometimes detecting infeasibility. With some additional effort, it is possible to indicate the set of data that lead

to certain bounds, helping to pinpoint the data inconsistency.

All in all, the computational experiments established the feasibility and power of the proposed approach. However, they also showed several possibilities for improvement. Most importantly, the physical-technical model used in the first stage of nomination validation to determine the discrete control decisions turned out to be often too optimistic, i.e., it fails to detect situations that are technically infeasible. Detailed investigations revealed the following potential sources for this behavior:

- The MILP relaxations used to model pressure-loss in pipes and resistors are sometimes quite weak. Improvements in the initial bound tightening process may help to overcome this.
- The compressor modeling in the first stage of nomination validation neglects the drives' maximum power that sometimes limits the network capacity. This issue is addressed by novel compressor models [HSW17] developed in a subproject of the CRC/Transregio 154 *Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks*.
- The relaxation arising from the alternating direction scheme for handling calorific values may be too coarse. In particular, due to its design, this scheme is not very powerful for proving technical infeasibility as it is not an exact approach. More sophisticated decomposition schemes might be useful to tackle this issue.

The running time necessary for validating a single nomination scenario should also be improved substantially: It is usually well below one hour, but sometimes exceeds four days. One possibility might be incorporating the ideas from the mentioned heuristic approaches in the current solver. There is also room for improving the overall running time of a booking validation by improving the order in which the corresponding nomination scenarios are validated. Preliminary experiments indicate that with a sufficient number of evaluated scenarios it might be possible to correctly decide the feasibility of similar scenario by fast machine-learning methods. On the other hand, this could be an indication that we were not aggressive enough regarding scenario reduction. Overall, it became clear that a substantial speed-up of the overall system can be achieved.

We hope that our methods can be extended to provide a full analysis of the entry/exit system in the future and allow for a fully automated calculation of welfare-optimal technical capacities. For steps in this direction, see [Hay16]. Another relevant and challenging research direction is to extend these methods (or devise entirely new ones) towards network design. The goal is to extend or adapt the existing network such that it can accommodate the gas flow situations expected in the future.

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