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Improved optimization models for potential-driven network flow problems via ASTS orientations*

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Abstract

The class of potential-driven network flow problems provides important models for a range of infrastructure networks. For real-world applications, they need to be combined with integer models for switching certain network elements, giving rise to hard-to-solve MINLPs. We observe that on large-scale real-world *meshed* networks the relaxations usually employed are rather weak due to cycles in the network. To address this situation, we introduce the concept of *ASTS orientations*, a generalization of bipolar orientations, as a combinatorial relaxation of feasible solutions of potential-driven flow problems, study their structure, and show how they can be used to strengthen existing relaxations and thus provide improved optimization models. Our computational results indicate that ASTS orientations can be used to derive much stronger bounds on the flow variables than existing bound tightening methods. We also show that our proposed model extensions yield significant performance improvements for an existing state-of-the-art MILP model for large-scale gas networks.

1 Introduction

Network operators for utility and infrastructure networks face difficult planning and operational problems [BGS09, GHHV12, KHPS15, GMSS18]. Due to regulation and increasing cost pressure, but also due to the availability of powerful solvers, modern optimization methods are more and more applied to reduce cost and to improve the quality of planning and operation. The complexity of the considered optimization problems increases for several reasons, for instance because geographically bigger networks are considered or the detail level is increased. For instance, realistic network models for parts of the German gas network have more than 4000 nodes and almost 4500 arcs [SAB$^+$17]. For networks of this size, providing globally optimal solutions or at least good bounds for assessing solution quality is still a big challenge [GMSS18].

A key submodel for infrastructure networks for fluids, e.g., water and gas [Rag13, DLWB15, GHHV12], is the so-called *potential-driven nonlinear network flow*

*This paper extends the work presented in the working papers [HB18, BH18].

problem. This problem features a so-called *potential* π_u for each node $u \in V$, and the flow q_a of an arc $a \in A$ is related to the difference of the potential of its end nodes via an arc-specific *potential loss function* ϕ_a. Formally, the potential-driven network flow problem for a digraph $D = (V, A)$, supply vector q^{nom}, and bounds on the flow q_a and potential π_u is given by

$$\begin{aligned}
\min \quad & c^T(q, \pi, s) && && \text{(1a)}\\
q_v^{\text{nom}} + \sum_{a=uv \in A} q_a - \sum_{a=vu \in A} q_a &= 0 && \text{for all } v \in V, && \text{(1b)}\\
\pi_u - \pi_v &= \phi_a(q_a) && \text{for all } a \in A, && \text{(1c)}\\
\underline{q}_a \leq q_a &\leq \overline{q}_a && \text{for all } a \in A, && \text{(1d)}\\
\underline{\pi}_u \leq \pi_u &\leq \overline{\pi}_u && \text{for all } u \in V. && \text{(1e)}
\end{aligned}$$

An important property of this model is that the flow is always directed from higher to lower potential, i.e., the potentials induce an acylic orientation of the arcs. In other words: The network arising from a *feasible* flow by orienting each network arc in the direction of the flow over this arc contains no directed cycle.

This property is only implicit in the model for potential-driven network flows, i.e., it is not represented by an explicit constraint, but follows from the interplay of flow conservation and potential loss along an arc. Therefore, it is not reflected in the relaxations used to solve these nonlinear noncovex optimization problems. This is discussed in more detail in [HB18].

Our contribution This paper proposes to use the discrete structure arising from the combination of flow conservation and an acyclicity requirement for the flow to strengthen MINLP models and their relaxations that arise from potential-driven network flow problems. These strengthened models are particularly valuable when using global optimization methods on large networks. To this end, we introduce a combinatorial abstraction of feasible flows we call *ASTS orientation*. This combinatorial structure is implicit in otherwise purely continuous nonconvex models. Hence our approach enables to exploit the power of discrete global optimization techniques in this context. As real networks contain additional network elements that do not necessarily fit the potential-driven network flow framework, we consider a generic MINLP featuring the potential-driven network flow problem as a submodel. Moreover, we consider not only fixed demand vectors, but intervals for the demand at each source/sink. This is useful for situations where the demand is not fully fixed, e.g., due to mixing of gas qualities [GMSS15]. Moreover, this may be applied to analyze the difference in flow directions if large classes of demand vectors are possible [HHH$^+$15]. We provide an analysis of the structure of ASTS orientations and outline several ways to algorithmically exploit this structure. Our computational results indicate that this is very useful to tackle large-scale real-world networks.

Related work Potential-driven network flow problems have been considered at least since the 1970s [Mau77, CCH$^+$78] and are relevant for a variety of applications areas [HJ84]. Although *pure* potential-driven network flow problems (1) are nonconvex NLPs, their special structure enables the development of efficient solution techniques [CCH$^+$78, VMC15]. For network design problems, binary variables for enabling/disabling network elements are introduced, yielding MINLPs that are NP-hard [GPS$^+$19] and significantly harder to solve in practice [Rag13, HF13]. The same holds when the problem is extended by models for further (switchable) network elements to model network operation in detail [PFG$^+$15, KHPS15, GMSS18].

For the case of the potential network flow problem (1) with potential loss function $\phi_a(q_a) = c_a q_a |q_a|$, knowing the flow directions for all arcs enables the use of algebraic methods to e.g., solve certain stochastic optimization variants of the problem [GHHS16, GNS17]. Moreover, in many relevant cases the function describing the potential difference between two nodes is convex and fixed flow directions result in convex MINLP problems [Rag13]. Exploiting the structural results presented here in enumerating ASTS orientations [BH18] will support these lines of research.

To the best of our knowledge, there have been no attempts to exploit the acyclicity property as is done in this paper.

2 General model for potential-driven network flow problems

This section introduces the general model for potential-driven network flow problems that this paper is concerned with and provides some basic notation.

Let $G = (V, E)$ be a graph that represents the pipelines and other elements of the network the flow on which we seek to optimize. For the purpose of formulating our MINLP model we define $D = (V, A)$ to be the digraph arising by replacing each edge $e = \{u, v\}$ by a forward arc $a_e^+ = uv$ and a backward arc $a_e^- = vu$, i.e., $A = \{a_e^+, a_e^- \mid e \in E\}$. (We note that the theory developed in this paper also applies to multigraphs and multidigraphs, i.e., for networks with parallel pipelines, but for ease of notation and language we will speak of graphs and digraphs in the following.) We denote the arc set induced by an edge set $E' \subseteq E$ by $A[E'] := \{a \in \{a_e^+, a_e^-\} \mid e \in E'\}$. Analogously, we define the set $E[A']$ to be the edges corresponding to a set of arcs A'. To model network elements occuring in applications, we assume the edge set E is a partition of sets of potential-decreasing edges E_{dec}, potential-maintaining edges E_{mnt}, and generic edges E_{gen}. The operation of the potential-increasing and generic edges is described by feasible sets $F_e^{\text{dec}}, F_e^{\text{gen}} \subseteq \mathbb{R}^4_{\geq 0}$, that relate the feasible values of the inlet potentials π_u, the outlet potentials π_v and the flows $q_{a_e^+}$, $q_{a_e^-}$ on the arcs a_e^+, a_e^- for $e \in E_{\text{dec}}$. The feasible sets F_e^{dec} for $e = \{u, v\} \in E_{\text{dec}}$ are characterised by

$$\begin{aligned} F_e^{\text{dec}} \subseteq \{(\pi_u, \pi_v, q_{a_e^+}, q_{a_e^-}) \in \mathbb{R}^4_{\geq 0} \mid q_{a_e^+} - q_{a_e^-} > 0 \implies \pi_u > \pi_v, \\ q_{a_e^+} - q_{a_e^-} < 0 \implies \pi_u < \pi_v\}. \end{aligned} \tag{2}$$

For generic edges, there are no assumptions about the feasible set F_e^{gen}. Hence they cover all network elements not fitting our framework of potential-decreasing and -maintaining elements, e.g., compressors in gas networks or pumps in water networks. Potential-maintaining edges may be closed or open valves. In the open state the potential at their ends is equal, whereas in the closed state the flow is zero.

In practical applications the vast majority of edges is typically in E_{dec} and represents pipelines that can be modelled by a non-linear potential-loss function

$\phi_e\colon \mathbb{R} \to \mathbb{R}$ based on the edge flow $q_e := q_{a_e^+} - q_{a_e^-}$ with

$$\phi_e(q_e) > 0 \iff q_e > 0,$$
$$\phi_e(q_e) < 0 \iff q_e < 0,$$
$$\phi_e(q_e) = 0 \iff q_e = 0,$$

in which case the feasible set for edge $e = \{u, v\}$ is given by

$$F_e^{\text{dec}} = \{(\pi_u, \pi_v, q_{a_e^+}, q_{a_e^-}) \in \mathbb{R}^4_{\geq 0} \mid \pi_u - \pi_v = \phi_e(q_{a_e^+} - q_{a_e^-})\}.$$

The variables in our model are given by the flows $q_a \in \mathbb{R}_{\geq 0}$ on the arcs $a \in A$, the flows $q_u \in \mathbb{R}$ into and out of the nodes $u \in V$, representing sources and sinks, the potentials $\pi_u \in \mathbb{R}_{\geq 0}$ at the nodes $u \in V$, and variables $s_e \in \{0, 1\}$ that indicate whether a potential-maintaining edge $e \in E_{\text{mnt}}$ is open or closed. We also include upper and lower bounds for flows on arcs, flows into and out of nodes and the potentials at nodes, namely $\overline{q}_a$, $\underline{q}_a$, $\overline{q}_u$, $\underline{q}_u$, $\overline{\pi}_u$, and $\underline{\pi}_u$, respectively. This means in particular that in contrast to the models typically discussed in the literature we allow for nodes with flexible demands (i.e., nodes are not necessarily predetermined as sources or sinks with a given in- or out-flow) and develop our theoretical framework in the following sections accordingly.

The (linear) costs in our MINLP are represented by a cost vector $c \in \mathbb{R}^{|V|+|A|+|V|+|E_{\text{mnt}}|}$ that models the costs for flows in and out of a node, costs for flows along arcs, costs related to the potential at each node, and costs for opening or closing an edge in E_{mnt}. When required we will call a cycle $(u_0, u_1, \ldots, u_n, u_0)$, $u_0, u_1, \ldots, u_n \in V$, a negative-cost cycle if $\sum_{i=0}^{n-1} c_{u_i u_{i+1}} + c_{u_n u_0} < 0$, $\overline{q}_{u_i u_{i+1}} > 0$ for all $i = 0, 1, \ldots, n-1$, and $\overline{q}_{u_n u_0} > 0$. As each edge of the network is modelled by a forward and a backward arc in our MINLP, there may be solutions in which the model sends a flow through an edge in both directions. To exclude this unrealistic case for optimal solutions, we make the assumption throughout the paper that the cost vector is such that there are no negative 2-cycles, i.e. for all edges $e \in E$ if $c_{a_e^+} + c_{a_e^-} < 0$ then $\overline{q}_{a_e^+} = 0$ or $\overline{q}_{a_e^-} = 0$.

On this basis, our MINLP looks as follows:

$$
\begin{aligned}
& \min\ c^T(q, \pi, s) && && \text{(3a)}\\
\text{s. t. } & q_v + \sum_{a=uv \in A} q_a - \sum_{a=vu \in A} q_a = 0 && \text{for all } v \in V, && \text{(3b)}\\
& (\pi_u, \pi_v, q_{a_e^+}, q_{a_e^-}) \in F_e^{\text{dec}} && \text{for all } e \in E_{\text{dec}}, && \text{(3c)}\\
& (\pi_u, \pi_v, q_{a_e^+}, q_{a_e^-}) \in F_e^{\text{gen}} && \text{for all } e \in E_{\text{gen}}, && \text{(3d)}\\
& s_e = 0 \implies q_{a_e^+} = q_{a_e^-} = 0 && \text{for all } e \in E_{\text{mnt}}, && \text{(3e)}\\
& s_e = 1 \implies \pi_u = \pi_v && \text{for all } e = \{u, v\} \in E_{\text{mnt}}, && \text{(3f)}\\
& s_e \in \{0, 1\} && \text{for all } e \in E_{\text{mnt}}, && \text{(3g)}\\
& \underline{q}_v \leq q_v \leq \overline{q}_v && \text{for all } v \in V, && \text{(3h)}\\
& 0 \leq \underline{q}_a \leq q_a \leq \overline{q}_a && \text{for all } a \in A, && \text{(3i)}\\
& 0 \leq \underline{\pi}_v \leq \pi_v \leq \overline{\pi}_v && \text{for all } v \in V. && \text{(3j)}
\end{aligned}
$$

The flow part q of a MINLP solution (q, π, s) naturally induces a digraph $D(E', q) := (V, A(q))$ for any edge subset $E' \subseteq E$ of the underlying graph G via

$$A(q) := \{a \in A[E'] \mid q_a > 0\}. \tag{4}$$

We say that the solution is *cyclic* if $D(E', q)$ contains a cycle and *acyclic* otherwise. Observe that an arc with $\overline{q}_a = 0$ is never in a cycle.

3 ASTS-orientations and their basic properties

We now define the theoretical concept that is central to this paper. It captures the discrete structure that arises from the combination of the flow conservation constraint and the acyclicity that follows from the fact that flow is always directed from higher to lower potential. Recall that an orientation of an underlying graph $G = (V, E)$ is a digraph $\tilde{D} = (V, \tilde{A})$ with $E = \{\{u, v\} \in V \times V \mid uv \in \tilde{A}\}$ and $uv \in \tilde{A} \iff vu \notin \tilde{A}$ for all $u, v \in V$.

Definition 1 Let $\tilde{D} = (V, \tilde{A})$ be a digraph with an underlying graph G, with $V_+, V_-, V_T \subsetneq V$ being disjoint sets of "sources", "sinks" and "transhipment nodes", respectively. We call the nodes in $V_F := V - V_+ - V_- - V_T$ "free nodes". A node $u \in V$ is said to satisfy the source-transhipment-sink-condition (STS-condition) with respect to (V_+, V_-, V_T, V_F) if

(i) $u \in V_+$ and there exists an arc $a = uv \in \tilde{A}$, or

(ii) $u \in V_-$ and there exists an arc $a = vu \in \tilde{A}$, or

(iii) $u \in V_T$ and there exist arcs $a_1 = vu, a_2 = uw \in \tilde{A}$, or

(iv) $u \in V_F$.

If all nodes $u \in V$ satisfy the STS-condition and $\tilde{D}$ is acyclic, $\tilde{D}$ is called an ASTS-orientation of G with respect to (V_+, V_-, V_T, V_F), and G is said to have an ASTS-orientation.

A subgraph $G_0 = (V_0, E_0)$ of G is said to have an ASTS-orientation with respect to (V_+, V_-, V_T, V_F) if there exists an orientation $\tilde{D}_0$ of G_0 such that $\tilde{D}_0 = (V_0, \tilde{A}_0)$ is an ASTS-orientation of G_0 with respect to $(V_+ \cap V_0, V_- \cap V_0, V_T \cap V_0, V_F \cap V_0)$. □

Note that ASTS-orientations are a generalization of bipolar orientations (see e.g., [dFOdMR95] for the concept of bipolar orientations). Moreover, there exists a bijection between the set of all ASTS-orientations of a graph G with $V_F = \varnothing$ and the bipolar orientations of the extended graph that arises from adding to G a "supersource" s that is adjacent to all sources, a "supersink" t that is adjacent to all sinks, and an edge $\{s, t\}$.

The following theorem characterizes graphs that allow for an ASTS-orientation.

Theorem 1 *Let $G = (V, E)$ be a graph with node set V, $V_+ \subsetneq V$, $V_- \subsetneq V$ and $V_T \subsetneq V$ disjoint sets of sources, sinks and transhipment nodes, respectively, and $V_F := V - V_+ - V_- - V_T$ the set of free nodes.*

Then the following four statements are equivalent:

(i) G has an ASTS-orientation $\tilde{D} = (V, \tilde{A})$ with respect to (V_+, V_-, V_T, V_F).

(ii) (path characterization) *Every node $u \in V$ is on a path from a source or a free node to a sink or a free node.*

(iii) (block characterization) *All components of G contain at least two free nodes or two out of the three node types "source", "sink" and "free node", and the leaves of the block tree of each of the components of G correspond to blocks that have a source, sink or free node other than the cut vertex of the block.*

(iv) (completion characterization) *There exists a subgraph of each component of G that has an ASTS-orientation, and for every ASTS-orientation $\tilde{D}_0 = (V_0, \tilde{A}_0)$ of some subgraph $G_0 = (V_0, E_0)$ of G there exists an orientation $\tilde{A}_1$ of the edges $E \setminus E_0$ such that $\tilde{D} = (V, \tilde{A}_0 + \tilde{A}_1)$ is an ASTS-orientation of G with respect to (V_+, V_-, V_T, V_F).* □

PROOF We will prove the theorem in the following order:

$$(i) \implies (ii) \implies (iii) \implies (ii) \implies (iv) \implies (i).$$

$(i) \implies (ii)$ Let $\tilde{D} = (V, \tilde{A})$ be an ASTS-orientation of G with respect to (V_+, V_-, V_T, V_F). We choose a node $u \in V$. If u is a node without incoming arcs, i.e., a source or a free node, we follow a directed path via outgoing arcs, starting from V. As $\tilde{D}$ is acyclic we will not return to a node we have already visited, and because G is finite, the directed path will end at a node that has no outgoing arcs, i.e., a node that is a sink or a free node. Similarly, if u is a node without outgoing arcs, i.e., a sink or a free node, we can follow a directed path from u via incoming arcs until we find a source or a free node. If u is a node with both outgoing and incoming arcs, we can construct one directed path to a source or free node and another directed path to a sink and a free node, where the acyclicity of $\tilde{D}$ ensures that the two paths are node-disjoint. Since we can carry out this procedure for any node, all nodes are on a directed path from a source or a free node to a sink or a free node. Now (ii) follows from considering the graph underlying $\tilde{D}$.

$(ii) \implies (iii)$ We show the contrapositive. Clearly, if G has components that do not contain two free nodes or two out of the three node types "source", "sink" and "free node", condition (ii) cannot be satisfied. Moreover, if a block of a graph is a leaf of the block tree graph and all nodes other than the cut-node of the block are transhipment nodes, a path from any of these nodes to a source, sink or free node must contain the cut-node. Hence, no node of the block, except possibly the cut-node itself, is on a path from a source or free node to a sink or free node.

$(iii) \implies (ii)$ Let $u \in V$ be a node of G. W.l.o.g. we will assume that u is in a component with a source and a sink and show that u is on a path from a source to a sink.[1] Now if u is a source (sink) itself, it is clearly on a path from a source to a sink as it is connected with the sink (source) that exists in its component of G. Therefore, in the following let u be neither a source nor a sink. We distinguish between three cases.

[1]If u is in a component with a source, a free node and no sink, or in a component with a sink, a free node and no source, or in a component with no sources, no sinks and two free nodes, the same line of argument will work to show that u is on a path from a source to a free node, or on a path from a free node to a sink, or on a path from a free node to a free node, respectively.

Case 1: The node u is in a block of G that has both a source and a sink. By virtue of the 2-connectedness of the block there exist two internally disjoint paths from u to a source and two internally disjoint paths from u to a sink. As a consequence, u must be on a path from a source to a sink.

Case 2: The node u is in a block that has either a source or a sink. We assume w.l.o.g. that the block has a source. If the block is a leaf of the block tree graph of G, the source is not the cut-node of the block due to condition (iii). If the block is not a leaf of the block tree graph, we will assume for the moment that the source is not a cut-node of the block. Now, since each component of G has a source and a sink, the block must have a cut-node that is connected with a sink in a different block. Then, due to the 2-connectedness of blocks, there exist two internally disjoint paths from u to the source and from u via the cut-node to the sink, with the latter being the case only if u is not the cut-node itself. In either case u is on a path from a source to a sink.

Now let us consider the case where our block is not a leaf of the block tree graph and the source is a cut-node of our block. Then the block contains at least two cut-nodes and one of the other cut-nodes of the block must be providing us with a path to a source or a sink in a further block, otherwise the block tree graph of G would have a leaf without source or sink. If the cut-nodes provide us with a path to a sink, there clearly exists, again due to the 2-connectedness of blocks, a path from the block's source to a sink that passes through u. If the cut-nodes only provide us with a path to another source, there must be another sink in a block that is accessible via the cut-node that is a source, otherwise the component that u is a node of would not have a sink. As a consequence, u is again on a path from a source to a sink.

Case 3: The node u is in a block without source and sink. Then u cannot be in a block that is a leaf of the block tree graph and therefore the block in which u is located contains at least two cut-nodes (one of which may be u itself). All cut-nodes must be on a path from u to a source or from u to a sink, otherwise the block tree graph of G would have a leaf without both source and sink. Moreover, due to the fact that all components of G have both a source and a sink, one of the cut-nodes must be on a path from u to a source and a different cut-node must be on a path from u to a sink. As a consequence, since a block is 2-connected, u must be on a path from a source to a sink.

$(ii) \implies (iv)$ By assumption every node is on a path from a source or free node to a sink or free node. Clearly, by orienting one such path from the source or the free node to a sink or the free node, we obtain an ASTS-orientation of a subgraph of G. Now let $\tilde{D}_0 = (\tilde{A}_0, V_0)$ be any ASTS-orientation of some proper subgraph of G. We will procede in two steps.

In the first step we will extend $\tilde{D}_0$ to an ASTS-oriented digraph whose underlying graph is still G and that contains all sources, sinks and free nodes in V, provided the latter is not the case yet. In the second step we will show that, provided the graph underlying our ASTS-oriented digraph contains all sources, sinks and free nodes is a proper subgraph of G, we can always find a path on the remaining unoriented edge set of G that can be oriented to provide a larger ASTS-oriented digraph. Statement (iv) then follows by induction on the remaining unoriented edge set.

Step 1 For each component of G all edges of which are in $E - E_0$ we enlarge the digraph $\tilde{D}_0$ by connecting, with the sinks in their components (or free nodes in their components, if there is no sink in a certain component), all sources that are not yet in the node set of our digraph, using directed paths whose internal nodes are not in the node set of our digraph either. The prodecure is as follows: for each source, we take an arbitrary path on G from the source to a sink (or to a free node, if necessary), which is possible due to (ii), and orient, into the direction away form the source, either the subpath from the source to the first node of the existing digraph or, if this is not possible because none of the nodes of the path is on the digraph, the entire path from the source to a sink (or to a free node, if necessary). In a similar fashion we add all remaining sinks to our digraph: by orienting edges that connect these sinks to the closest node of our existing digraph or by directly connecting them with a source (or a free node, if there is no source in the component). Finally, we add all remaining free nodes to our digraph: if a component has a source or a sink, we can orient the edges on a path to the nearest node on our digraph arbitrarily, either away from the free node or towards the free node. If a component has neither a source or a sink, we choose two free nodes, connect one with a directed path to the other, and connect the remaining free nodes to an existing node of our digraph in an arbitrary fashion, either away from the free node or towards it. The resulting enlarged digraph has an underlying graph that is a subgraph of G, has a node set that includes all sources, sinks and free nodes of G, and is ASTS-oriented (note that we did not create any directed cycle because we did not connect any two nodes that were already in the node set of our digraph).

Step 2 We will now show that given an ASTS-oriented digraph $\tilde{D}_0$ with an underlying proper subgraph G_0 of G and with a node set that includes all sources, sinks and free nodes of G, we can always find a path P with edges from $E - E_0$, with distinct endnodes in V_0, and with all other nodes being in $V - V_0$ that can be oriented such that the digraph that arises from adding the oriented path to $\tilde{D}_0$ again yields an ASTS-oriented digraph.

We pick an arbitrary edge from $E - E_0$. If both endnodes of this edge are in V_0, this edge is our path P. Otherwise, we extend this edge to a path by adding edges from $E - E_0$ until we have a path P with two distinct endnodes both of which are in V_0. This is always possible because of (ii) and since all sources, sinks and free nodes are in V_0 according to the construction in Step 1. We denote the endnodes of P by $u, v \in V_0$ and the inner nodes of P by $V' \subseteq V - V_0$.

We now orient P as a directed path, i.e. from one endnode to the other such that each internal node of the path is both head and tail of an arc, and denote the arcs of the directed path by $\tilde{A}'$. For constructing our orientation we observe that, as $\tilde{D}_0$ is acyclic and u and v are nodes of $\tilde{D}_0$, there is

(a) no directed path on $\tilde{D}_0$ from u to v and no directed path from v to u, or

(b) there is a directed path from u to v, but not from v to u, or

(c) there is a directed path from v to u, but not from u to v.

In case (a) we choose an arbitrary orientation for our directed path. In cases (b) and (c) we orient the path such that it has the same orientation as the existing path. As a consequence the orientation $\tilde{D}' = (V_0 \cup V', \tilde{A}_0 \cup \tilde{A}')$ that results from adding the arcs and nodes of the directed path to $\tilde{D}_0$ will be acyclic, too. (Note that by construction of P, only the endnodes of P are in V_0, and therefore orienting P cannot create any cycle containing an internal node of P.) As the STS-condition is already satisfied at the endnodes $u, v \in V_0$ and we have oriented the path P to form a directed path, the inner nodes of the path and hence the digraph $\tilde{D}'$ altogether also satisfy the STS-condition. Hence the resulting digraph $\tilde{D}' = (V_0 \cup V', \tilde{A}_0 \cup \tilde{A}')$ is ASTS-oriented.

$(iv) \implies (i)$ This is trivially the case. ∎

We have seen in the previous theorem that not all graphs admit an ASTS-orientation. The block characterization of Theorem 1 implies that even if a graph does not have an ASTS-orientation, this may be the case for a subgraph. This raises the question of whether we can find a maximal subgraph of a given graph G that allows for an ASTS-orientation. Indeed, successively removing blocks from G will lead to such a maximal subgraph.

Definition 2 Let $\mathcal{C}$ be the set of all components of a graph $G = (V, E)$ with node subsets (V_+, V_-, V_T, V_F). For a component $C = (V_C, E_C) \in \mathcal{C}$ let $V_C^1 \subseteq V_C$ be the set of the vertices of all blocks of C that are removed from C if we sucessively remove those blocks that correspond to leaves of the block tree graph of C without source, sink or free node other than the cut vertex of the block, however without removing the cut vertices that connect these blocks with the remaining graph. If the subgraph of C induced by $(V_C \setminus V_C^1) \cup (V_C \cap V_C^1)$ is a single block without at least two free nodes or two out of the three node types "source", "sink" and "free node", we define $V_C^2 := V_C \setminus V_C^1$, otherwise $V_C^2 := \varnothing$.

The set $V_{C,\text{out}} := V_C^1 \cup V_C^2$ is called the outer vertex set of C, the set $V_{C,\text{in}} := (V_C \setminus V_{C,\text{out}}) \cup (V_C \cap V_{C,\text{out}})$ the inner vertex set of C, the set $V_{\text{out}} := \bigcup_{C \in \mathcal{C}} V_{C,\text{out}}$ the outer vertex set of G, and the set $V_{\text{in}} := \bigcup_{C \in \mathcal{C}} V_{C,\text{in}}$ the inner vertex set of G. We refer to the edge set induced by V_{out} as $E_{\text{out}} \subseteq E$ and to the edge set induced by V_{in} as $E_{\text{in}} \subseteq E$. Further let $A_{\text{in}} := A[E_{\text{in}}] \subseteq A$ and $A_{\text{out}} := A[E_{\text{out}}] \subseteq A$ be the arc sets corresponding to the inner and outer edge sets, respectively. □

This definition is justified by the following insight.

Corollary 1 *Let $G = (V, E)$ be a graph with node subsets (V_+, V_-, V_T, V_F) and V_{in} and V_{out} the inner and outer vertex sets of G, respectively.*

(i) There is no subgraph of G that contains a vertex from $V_{\text{out}} \setminus V_\in$ and has an ASTS-orientation with respect to (V_+, V_-, V_T, V_F).

(ii) The subgraph of G induced by V_{in} is the maximal subgraph of G to have an ASTS-orientation with respect to (V_+, V_-, V_T, V_F). □

Proof As no vertex in V_{out} is, by construction, on a path from a source or a free node to a sink or a free node, statement (i) follows from the path characterization of Theorem 1. Statement (ii) follows from (i) by taking into account that the subgraph induced by V_{in} has an ASTS-orientation according to the block characterization of Theorem 1. ∎

4 ASTS orientations as combinatorial relaxations for potential-driven network flow problems

In the following we will consider the relationship between ASTS-orientations and the solutions of MINLP (3) on subsets $A' \subseteq A$ of the arc set. Addressing the more general case of subsets $A' \subseteq A$ will allow for a more flexible application of our theoretical framework. We may, for example, wish to disregard arcs in $A[E_{\text{gen}}]$ due to their specific properties, or computational reasons may suggest considering subgraphs of the original graph separately.

Definition 3 For a digraph $D = (V, A)$ for MINLP (3) and a corresponding inner vertex set V_{in}, an arc subset $A' \subseteq A_{\text{in}}$ is called a region. The vertex set $V' \subseteq V$ of the region is the vertex set induced by A', i.e. $V' := V[A']$, and the sources, sinks, transshipment nodes and free nodes of a region are given by:

$$\underline{q}_v^{A'} := \underline{q}_v + \sum_{a=uv\in A\setminus A'} \underline{q}_a - \sum_{a=vu\in A\setminus A'} \overline{q}_a, \tag{5a}$$

$$\overline{q}_v^{A'} := \overline{q}_v + \sum_{a=uv\in A\setminus A'} \overline{q}_a - \sum_{a=vu\in A\setminus A'} \underline{q}_a, \tag{5b}$$

$$V'_+ := \{v \in V' \mid \underline{q}_v^{A'} > 0\}, \tag{5c}$$

$$V'_- := \{v \in V' \mid \overline{q}_v^{A'} < 0\}, \tag{5d}$$

$$V'_T := \{v \in V' \mid \underline{q}_v^{A'} = \overline{q}_v^{A'} = 0\} \text{ and} \tag{5e}$$

$$V'_F := V' - V'_+ - V'_- - V'_T. \tag{5f}$$

□

The following lemma justifies our definition of sources, sinks and transshipment nodes of a region by showing that these function as sources, sinks and transshipment nodes for a region when considering the solutions of MINLP (3).

Lemma 1 *Let $G = (V, E)$ be a digraph for MINLP (3) and A' a region with sources, sinks, transshipment nodes and free nodes V'_+, V'_-, V'_T and V'_F, respectively.*

Then in any feasible solution (q, π, s) to MINLP (3)

(i) for all $u \in V'_+$ there exists an arc $a = uv \in A'$ with $q_a > 0$ for some $v \in V'$,

(ii) for all $u \in V'_-$ there exists an arc $a = vu \in A'$ with $q_a > 0$ for some $v \in V'$, and

(iii) for all $u \in V'_T$ there exists an arc $a_1 = vu \in A'$ with $q_{a_1} > 0$ for some $v \in V'$ iff there exists an arc $a_2 = uw \in A'$ with $q_{a_2} > 0$ for some $w \in V'$. □

Proof Let u be in V'_+. With (5c), (5a) and the node demand bounds (3h) and the flow bounds (3i), we obtain

$$\begin{aligned} 0 < \underline{q}_u^{A'} &= \underline{q}_u + \sum_{a=uv\in A\setminus A'} \underline{q}_a - \sum_{a=vu\in A\setminus A'} \overline{q}_a \\ &\le q_u + \sum_{a=uv\in A\setminus A'} q_a - \sum_{a=vu\in A\setminus A'} q_a, \end{aligned}$$

which, due to the flow conservation (3b) is equal to

$$= - \sum_{a=uv\in A'} q_a + \sum_{a=vu\in A'} q_a.$$

Now statement (i) follows with $q_a \geq 0$ for all $a \in A$. Statement (ii) follows analogously. For $u \in V'_T$ we proceed from (5e) in the same fashion as above, but once with (5a) and once with (5b). Using the node demand bounds (3h), the flow bounds (3i) and the flow conservation (3b) we obtain two inequalities that imply $\sum_{a=vu \in A'} q_a = \sum_{a=uv \in A'} q_a$. Then statement (iii) again follows from $q_a \geq 0$ for all $a \in A$. ■

We can now relate the solutions of MINLP (3) to the ASTS-orientations on regions of the arc set. The following theorem shows that under suitable conditions there exist ASTS-orientations that are compatible with the flow on regions. This result provides the reason why studying ASTS-orientations is useful when considering the potential-based network flow problem of MINLP (3).

Theorem 2 *Let $D = (V, A)$ be a digraph for MINLP (3), $G = (V, E)$ be the underlying graph, and $A_{\text{in}} \subseteq A$ and $A_{\text{out}} \subseteq A$ be the arc sets corresponding to the inner and outer edges sets, respectively. Further, let $A' \subset A_{\text{in}}$ be a region of D with vertex set V', sources V'_+, sinks V'_-, transshipment nodes V'_T and free nodes V'_F, and let V'_{in} and V'_{out} be the inner and outer vertex sets of the region, respectively, with corresponding arcs sets A'_{in} and A'_{out}. If*

(a) $A_{\text{gen}} \cap (A' \cup A_{\text{out}}) = \varnothing$ and

(b) $[A_{\text{mnt}} \cap (A' \cup A_{\text{out}})] \setminus \{a \in A \mid \overline{q}_a = 0\}$ does not contain a negative-cost cycle

there exists for every solution (q, π, s) to MINLP (3) another solution to MINLP (3) with the same or a lower objective function value such that

(i) $q_a = 0$ for all $a \in A_{\text{out}} \cup A'_{\text{out}}$,

(ii) for each component (V_C, A_C) of $(V'_{\text{in}}, A'_{\text{in}})$, there exists an ASTS-orientation $\tilde{D}_C = (V_C, \tilde{A_C})$ of the corresponding underlying undirected component (V_C, E_C) with respect to $(V'_+ \cap V_C, V'_- \cap V_C, V'_T \cap V_C, V'_F \cap V_C)$ with

$$a_1 \in \tilde{A_C} \implies (q_{a_1} \geq 0 \text{ and } q_{a_2} = 0) \qquad \forall e \in E_C \text{ and } \{a_1, a_2\} = \{a_e^+, a_e^-\}. \tag{6}$$

□

Proof In a first step we consider all cycles in our solution (q, π, s), i.e., the cycles in the digraph $D(A' \cup A_{\text{out}}, q)$ induced by q. For cycles with length 2, we can construct, due to our assumption about the cost function in Section Section 2, a solution q' to (3) with lower or equal objective function value such that $q'_{a_e^+} = 0$ or $q'_{a_e^-} = 0$ for all $e \in E$. Regarding cycles with length greater than 2, if such a cycle is in $A' \cup A_{\text{out}}$, it does not contain any arc from A_{gen} by the assumptions of the present theorem. Due to property (2) of the feasible set F_e^{dec} and constraint (3c), the arcs on the cycle cannot contain arcs from A_{dec} either. Accordingly each arc on the cycle is in A_{mnt}, which by assumption does not contain any cycles with negative total cost. Therefore we can reduce the flow along each cycle such that the flow on one arc of the cycle becomes 0, without increasing the objective function value and without affecting feasibiliy regarding the potential bounds, since flows on arcs in A_{mnt} do not affect the potential. As a consequence, this new solution q'' to MINLP (3) is acyclic on A'.

Second, by construction of A_{out} and of A'_{out}, no node in $V_{\text{out}} \setminus V_{\text{in}}$ and no node in $V'_{\text{out}} \setminus V'_{\text{in}}$ is on a path from a source or a free node to a sink or a free node. Hence we can reduce the flows on arcs in A_{out} and on arcs in A'_{out} to 0, obtaining a solution q''' to MINLP (3) with lower or equal objective function value for which statement (i) of the theorem holds. Note that q''' is still acyclic on A'.

Third, let (V_C, A_C) be a component of $(V'_{\text{in}}, A'_{\text{in}})$ and (V_C, E_C) its underlying graph. Then (V_C, E_C) has an ASTS-orientation by construction of $(V'_{\text{in}}, A'_{\text{in}})$ due to Corollary 1. We consider the subgraph $(V_{>0,C}, E_{>0,C})$ of (V_C, E_C) defined by the non-zero flows on the component (V_C, A_C), i.e.,

$$\begin{aligned} E_{>0,C} &:= \{e \in E_C \mid \exists a \in \{a_e^+, a_e^-\} \colon q'''_a > 0\}, \\ V_{>0,C} &:= V_C[E_{>0,C}]. \end{aligned}$$

If $V_{>0,C} = \varnothing$, any arbitrary ASTS-orientation of (V_C, E_C) trivially satisfies (6), so let us assume $V_{>0,C} \neq \varnothing$ for the remainder of this proof. Let $\tilde{D}_{>0,C} = (V_{>0,C}, \tilde{A}_{>0,C}) := D(E_{>0,C}, q''')$ be the digraph induced by q'''. Since $q'''_{a_e^+} = 0$ or $q'''_{a_e^-} = 0$ for all $e \in E$ the digraph $\tilde{D}_{>0,C}$ is in fact an orientation of $(V_{>0,C}, E_{>0,C})$. We observe that (6) holds on the subgraph $\tilde{A}_{>0,C}$. Moreover, this orientation is certainly acylic as q''' is acyclic. For all $v \in V_{>0,C} \cap V'_+$, Lemma 1 and (4) imply that v has an out-arc on $\tilde{A}_{>0,C}$. Analogously Lemma 1 and (4) imply that all $v \in V_{>0,C} \cap V'_-$ have in-arcs on $\tilde{A}_{>0,C}$. Finally, it follows from Lemma 1 and (4) that all $v \in V_{>0,C} \cap V'_T$ have both out- and in-arcs on $\tilde{A}_{>0,C}$. Hence $\tilde{A}_{>0,C}$ is an ASTS-orientation of the subgraph $(V_{>0,C}, E_{>0,C})$ with respect to

$$(V_{>0,C} \cap V'_+, V_{>0,C} \cap V'_-, V_{>0,C} \cap V'_T, V_{>0,C} \cap V'_F).$$

Fourth, as we know that (V_C, E_C) has an ASTS-orientation by construction of $(V'_{\text{in}}, A'_{\text{in}})$ and we have just constructed an ASTS-orientation on the subgraph $(V_{>0,C}, E_{>0,C})$ of (V_C, E_C), we can extend this orientation to an ASTS-orientation $(V_C, \tilde{A}_C)$ of (V_C, E_C) with respect to

$$(V_C \cap V'_+, V_C \cap V'_-, V_C \cap V'_T, V_C \cap V'_F)$$

due to the completion characterization of Theorem 1. Since $q_{a_e^+} = q_{a_e^-} = 0$ for all edges $e \in E_C \setminus E_{>0,C}$, i.e., the edges oriented during this extension process, (6) now holds on all of $(V_C, \tilde{A}_C)$. ∎

Remark 1 The previous Theorem has shown that under suitable conditions every solution to MINLP (3) corresponds to an ASTS-orientation. Clearly, the converse is not true since node, flow or potential bounds may prevent an ASTS-orientation from having a corresponding solution to MINLP (3). □

5 Decomposition results for ASTS orientations

The graphs underlying network optimization problems are often highly structured. In this section we explore various ways to exploit structure to describe the set of ASTS orientations for a large region of the network by the sets of ASTS orientations for smaller regions. This is useful algorithmically as the number of ASTS orientations and hence the computational effort to handle them grows exponentially[2] with the number of arcs involved.

5.1 Decomposition based on pre-oriented edges

Computational results on real-world data indicate that the flow direction for a large share of the edges can be determined using standard preprocessing techniques. This suggests to consider ASTS orientations for the remaining edges only. To study this, we need some further concepts.

Definition 4 Let $G = (V, E)$ be a graph and $\overrightarrow{A} \subseteq A[E]$ be orientations for a given subset (i.e., $a_1 = uv \in \overrightarrow{A} \implies \nexists a_2 = vu \in \overrightarrow{A}$). The graph $G^0 = (V^0, E^0)$ that arises from removing the oriented edges from G, i.e., $E^0 := E \setminus E[\overrightarrow{A}]$, $V^0 := V[E^0]$, is called the *residual graph of* G *with respect to* $\overrightarrow{A}$. We denote the components of G^0 by $G_i = (V_i, E_i)$. The set of nodes $\overline{V_i}$ in V_i that are incident to arcs in $\overrightarrow{A}$, i.e., the set

$$\overline{V_i} := \{u \in V_i \mid \exists a = uv \in \overrightarrow{A} \text{ or } \exists a = vu \in \overrightarrow{A}\}, \tag{7}$$

is called the *boundary of the component* G_i. An orientation $\tilde{D}_i = (V_i, \tilde{A}_i)$ of G_i induces, by virtue of

$$\overline{A}_i := \{uv \mid u \neq v \in \overline{V_i},\ \exists u\text{-}v\text{-path on } \tilde{D}_i\}, \tag{8}$$

a digraph $\overline{D_i} = (\overline{V_i}, \overline{A}_i)$ on the boundary $\overline{V_i}$, called the *skeleton of* $\tilde{D}_i$, that indicates the mutual reachability of nodes in the boundary of G_i in the orientation $\tilde{D}_i$. □

Remark 2 Note that a skeleton may have, for some $u, v \in V$, both arcs uv and vu. Clearly, such a skeleton is not a skeleton of an ASTS-oriented $\tilde{D}_i$. □

The next concept describes ASTS-orientations on the components G_i that are compatible with the arcs in $\overrightarrow{A}$. The idea here is that the existing arcs in $\overrightarrow{A}$ contribute to satisfying the STS-condition at the nodes of G. As a consequence, when taking into account the arcs in $\overrightarrow{A}$ we need fewer restrictions on the orientations of the components G_i to produce an ASTS-orientation of G. For a transhipment node in some component G_i with an emanating arc in $\overrightarrow{A}$, for example, the STS-condition is already satisfied when there is an arc on D_i going towards the transhipment node, i.e., it is sufficient to classify the transshipment node as a sink on D_i if we would like to satisfy the STS-condition at this node on D. Similarly, to provide another example, a source on G with an emanating arc in $\overrightarrow{A}$ can be classified as a free node on its component G_i if we would like to ensure that the STS-condition is satisfied on D. In this way we can reduce the problem of constructing an ASTS-orientation on a graph with a set of pre-oriented edges $\overrightarrow{A}$ to the general problem of constructing an ASTS-orientation on a graph.

[2]Observe that ASTS orientations can be used to solve the NP-hard longest path problem.

Definition 5 Let $G = (V, E)$ be a graph with node subsets (V_+, V_-, V_T, V_F) and let $\overrightarrow{A}$ be a given subset of edge orientation as above, $G_i = (V_i, E_i)$ the components of the residual graph of G with respect to $\overrightarrow{A}$, and $\overline{V_i}$ the boundaries of G_i. An orientation $\tilde{D}_i = (V_i, \tilde{A}_i)$ of G_i is called an *ASTS-orientation relative to* $\overrightarrow{A}$ if it is an ASTS-orientation of G_i with respect to $(V_+^i, V_-^i, V_T^i, V_F^i)$ given by

$$V_+^i := (V_+ \cap V_i) \setminus \overline{V_i} \cup \{u \in \overline{V_i} \cap (V_+ \cup V_T) \mid \exists a = vu \in \overrightarrow{A}, \nexists a = uw \in \overrightarrow{A}\} \tag{9a}$$

$$V_-^i := (V_- \cap V_i) \setminus \overline{V_i} \cup \{u \in \overline{V_i} \cap (V_- \cup V_T) \mid \exists a = uv \in \overrightarrow{A}, \nexists a = wu \in \overrightarrow{A}\} \tag{9b}$$

$$V_T^i := (V_T \cap V_i) \setminus \overline{V_i}, \tag{9c}$$

$$V_F^i := V_i - V_+^i - V_-^i - V_T^i. \tag{9d}$$

□

We can now give a characterization of ASTS-orientations on G that respect the given subset $\overrightarrow{A}$ of oriented edges.

Theorem 3 *Let $G = (V, E)$ be a graph with node subsets (V_+, V_-, V_T, V_F) and $\overrightarrow{A}$, G_i, $\overline{V_i}$ be as in the preceding definition. Moreover, let $\tilde{D}_i = (V_i, \tilde{A}_i)$ be orientations of the components G_i. Then the overall digraph $\tilde{D} = (V, \overrightarrow{A} \cup \bigcup \tilde{A}_i)$ is an ASTS-orientation of G with respect to (V_+, V_-, V_T, V_F) if and only if*

(i) Each $\tilde{D}_i$ is an ASTS-orientation relative to $\overrightarrow{A}$,

(ii) the graph on V that arises when the arcs in $\overrightarrow{A}$ are added to the union of the skeletons of the orientations $\tilde{D}_i$, i.e., the graph

$$\overline{D} := (\bigcup \overline{V_i} \cup V \setminus \bigcup V_i, \overrightarrow{A} \cup \bigcup \overline{A}_i), \tag{10}$$

is acyclic, and

(iii) the nodes in $V \setminus \bigcup V_i$, i.e., the nodes of G that are only incident to arcs in $\overrightarrow{A}$, satisfy the STS-condition with respect to (V_+, V_-, V_T, V_F). □

Proof With the concepts defined above, the proof is a mere technical exercise.

$\Longrightarrow$ Let the overall digraph $\tilde{D} = (V, \overrightarrow{A} \cup \bigcup \tilde{A}_i)$ be an ASTS-orientation. We will show that the three conditions of the proposition are true.

(i) Since all nodes of $\tilde{D}$ satisfy the STS-condition, so do all nodes of the orientations $\tilde{D}_i$ that are not incident to any arc in $\overrightarrow{A}$, i.e., all nodes in $V_i \setminus \overline{V_i}$. For the nodes in $\overline{V_i}$, i.e., the nodes on the boundaries of the components G_i, we will look at the four sets $V_+^i \cap \overline{V_i}, V_-^i \cap \overline{V_i}, V_T^i \cap \overline{V_i}$ and $V_F^i \cap \overline{V_i}$ separately. Nodes in $V_+^i \cap \overline{V_i}$ are, by definition, also in $V_+ \cup V_T$, i.e., they have an outgoing arc on $\tilde{D}$. However, they have, also by definition, no outgoing arc in $\overrightarrow{A}$. Hence the outgoing arc must be in $\tilde{A}_i$, i.e., nodes in $V_+^i \cap \overline{V_i}$ are sources on $\tilde{D}_i$. With a similar line of argument we can see that all nodes in $V_-^i \cap \overline{V_i}$ are sinks on

$\tilde{D}_i$. As nodes in V_T^i are not in the boundary of G_i, the set $V_T^i \cap \overline{V_i}$ is empty, and, finally, nodes in $V_F^i \cap \overline{V_i}$ are free nodes, i.e., they satisfy the STS-condition automatically. Altogether, we have established that all nodes in $\bigcup \overline{V_i}$ satisfy the STS-condition. As $\tilde{D}$ is acyclic, the subgraphs $\tilde{D}_i$ must be acyclic, too. Hence the digraphs $\tilde{D}_i$ are ASTS-orientations with respect to $(V_+^i, V_-^i, V_T^i, V_F^i)$.

(ii) By definition of the skeletons $\overline{\tilde{D}_i}$, the nodes of $\overline{D}$ are reachable by the same nodes in $\bigcup \overline{V_i}$ as they are on $\tilde{D}$. As a consequence, the acyclicity of $\tilde{D}$ implies the acyclicity of $\overline{D}$.

(iii) As $\tilde{D}$ is an ASTS-orientation, the nodes that are only incident to arcs in $\overrightarrow{A}$ satisfy the STS-condition. Moreover, as $(V, \overrightarrow{A})$ is a subgraph of $\tilde{D}$, it must be acyclic.

$\Longleftarrow$ We assume the three conditions are true. Then $\tilde{D}$ is acyclic because the orientations $\tilde{D}_i$ and the graph $\overline{D}$ are acyclic (conditions (i) and (ii)). We can see directly from the definition of the sets V_+^i, V_-^i, V_T^i and V_F^i that the nodes in $\bigcup V_i \setminus \overline{V_i}$ satisfy the STS-condition on $\tilde{D}$ due to condition (i), while the nodes in $V \setminus \bigcup V_i$ satisfy the STS-condition on $\tilde{D}$ due to condition (iii) of the proposition. It remains to show that the nodes in $\bigcup \overline{V_i}$ satisfy the STS-condition on $\tilde{D}$. We will look at the nodes in the sets $V_+ \cap \overline{V_i}, V_- \cap \overline{V_i}, V_T \cap \overline{V_i}$ and $V_F \cap \overline{V_i}$ separately. The nodes in $V_+ \cap \overline{V_i}$ are in V_+^i if they have an arc in $\overrightarrow{A}$ going towards them, but no emanating arc in $\overrightarrow{A}$. Due to condition (i), these nodes have an emanating arc on $\tilde{D}_i$, i.e., they satisfy the STS-condition on $\tilde{D}$. The nodes in $V_+ \cap \overline{V_i}$ are in V_F^i if they have an emanating arc in $\overrightarrow{A}$. In this case they satisfy the STS-condition on $\tilde{D}$ automatically. For the nodes in $V_- \cap \overline{V_i}$ a similar line of arguments applies. The nodes in $V_T \cap \overline{V_i}$ are in V_+^i, V_-^i, or V_F^i depending on the arcs in $\overrightarrow{A}$ that are incident to them. If they have an arc in $\overrightarrow{A}$ emanating from them, but no arc in $\overrightarrow{A}$ towards them, they are in V_-^i. Then condition (i) ensures that they have an arc going towards them on $\tilde{D}_i$. Accordingly, they satisfy the STS-condition on $\tilde{D}$. Analogously, condition (i) ensures that also the nodes in $V_T \cap \overline{V_i}$ that are in V_+^i fulfill the STS-condition on $\tilde{D}$. The remaining nodes in $V_T \cap \overline{V_i}$ are in V_F^i because they have both an arc in $\overrightarrow{A}$ that emanates from them and an arc in $\overrightarrow{A}$ going towards them, which is why they satisfy the STS-condition on $\tilde{D}$ ab initio. Finally, the nodes in V_F trivially satisfy the STS-condition on $\tilde{D}$. ■

5.2 Decomposition into blocks

The components arising from a set of pre-oriented edges $\overrightarrow{A}$ according to Definition 4 may still be rather large. However, as graphs for real-world networks are rather sparse they may be decomposed further. A natural next step is to consider decompositions into blocks.

Theorem 4 *Let $G = (V, E)$ be a graph with node set V, $V_+ \subsetneq V$, $V_- \subsetneq V$ and $V_T \subsetneq V$ disjoint sets of sources, sinks and transhipment nodes, respectively, and $V_F := V - V_+ - V_- - V_T$ the set of free nodes. Furthermore, let V_c be the set of all cut vertices of G, $\mathcal{B}$ the set of all blocks of G, and $\tilde{D}_B = (V_B, \tilde{A}_B)$ orientations of the blocks $B \in \mathcal{B}$. Then the digraph $\tilde{D} = (V, \bigcup_{B \in \mathcal{B}} \tilde{A}_B)$ is an ASTS-orientation of G with respect to (V_+, V_-, V_T, V_F) if and only if* *(i) for all $B \in \mathcal{B}$ the orientations $\tilde{D}_B$ are ASTS-orientations with respect to*

$$((V_+ \cap V_B) \setminus V_c, (V_- \cap V_B) \setminus V_c, (V_T \cap V_B) \setminus V_c, (V_F \cap V_B) \cup V_c), \text{ and}$$

(ii) the cut vertices V_c of G satisfy the STS-condition with respect to (V_+, V_-, V_T, V_F). $\square$

Proof $\Longrightarrow$ If $\tilde{D} = (V, \bigcup_{B\in\mathcal{B}} \tilde{A}_B)$ is an ASTS-orientation with respect to (V_+, V_-, V_T, V_F), the digraphs $(V_B, \tilde{A}_B)$ are acyclic. As the nodes in V_+, V_- and V_T satisfy the STS-condition on $\tilde{D}$, the nodes in $(V_+ \cap V_B) \setminus V_c$, $(V_- \cap V_B) \setminus V_c$ and $(V_T \cap V_B) \setminus V_c$ satisfy the STS-conditions on $\tilde{D}_B$ for sources, sinks and transshipment nodes, respectively, and condition (ii) holds. The nodes in $((V_F \cap V_B) \cup V_c)$ satisfy the STS-condition for free nodes trivially.

$\Longleftarrow$ Due to condition (i), for all $B \in \mathcal{B}$ the digraphs $\tilde{D}_B$ are acyclic, hence the tree property of the block tree implies that $(V, \bigcup_{B\in\mathcal{B}} \tilde{A}_B)$ is acyclic, too. As the nodes in $(V_+ \cap V_B) \setminus V_c, (V_- \cap V_B) \setminus V_c, (V_T \cap V_B) \setminus V_c$ and $(V_F \cap V_B) \setminus V_c$ satisfy the STS-conditions for sources, sinks, transshipment nodes and free nodes, respectively, for all $B \in \mathcal{B}$, so do all nodes in $V \setminus V_c$. The remaining nodes in V_c satisfy the STS-condition due to condition (ii). $\blacksquare$

The previous theorem provided a block decomposition for any ASTS-orientation of a given graph G. However, when solving MINLP (3) it is sufficient to consider only those ASTS-orientations that exist according to Theorem 2 and are compatible with a solution to MINLP (3) in the sense of (6). Moreover, the fact that decomposing a graph into blocks reveals the global tree structure of the graph (as captured in the block tree of the graph) provides additional information about the flows through cut vertices. Via a suitable definition of sources, sinks, transshipment nodes and free nodes relative to a block, this information further reduces the number of ASTS-orientations we need to consider for finding a solution to (3).

More precisely speaking, the flow through a cut vertex into a block B is entirely determined by the nodes in the blocks of the branch of the block tree that is connected with the node after removing B from the block tree. The following definition provides the necessary concepts.

Definition 6 In the setting of Theorem 2 let (V_C, A_C) be a component of A'_{in}, $V_c^C \subset V_C$ the set of all cut vertices of (V_C, E_C), $\mathcal{B}^C$ the set of all blocks of (V_C, E_C), T^C the block tree of (V_C, E_C), and for all blocks $B = (V_B, E_B) \in \mathcal{B}^C$ let $T_B^C := T^C - \{B\}$ be the forest we obtain by removing from T^C the node that respresents the block B. For a cut vertex v of a block B, i.e. $v \in V_c^C \cap V_B$, we define $G_{B,v}^C$ to be the subgraph of (V_C, E_C) that is the union of all blocks in the component of T_B^C that contain v. We call the node set $V(G_{B,v}^C)$ the *flow* *determining nodes relative to* v and

$$V^C_{+,B} := ((V'_+ \cap V_B) \setminus V^C_c) + \{v \in V^C_c \cap V_B \mid \sum_{u \in V(G^C_{B,v})} \underline{q}^{A'}_u > 0\}, \tag{11a}$$

$$V^C_{-,B} := ((V'_- \cap V_B) \setminus V^C_c) + \{v \in V^C_c \cap V_B \mid \sum_{u \in V(G^C_{B,v})} \overline{q}^{A'}_u < 0\}, \tag{11b}$$

$$V^C_{T,B} := ((V'_- \cap V_B) \setminus V^C_c) + \{v \in V^C_c \cap V_B \mid \sum_{u \in V(G^C_{B,v})} \underline{q}^{A'}_u = \sum_{u \in V(G^C_{B,v})} \overline{q}^{A'}_u = 0\}, \tag{11c}$$

$$V^C_{F,B} := V_B - V^C_{+,B} - V^C_{-,B} - V^C_{T,B}. \tag{11d}$$

the *sources, sinks, transhipment nodes and free nodes relative to* B. □

The following theorem shows that when restricting ourselves to ASTS-orientations that exist according to Theorem 2 we can further reduce the number of orientations that are worth considering in two ways: there are blocks for which we do not need to consider ASTS-orientations (statement (i)) and the number of ASTS-orientations that results from focussing on blocks is a subset of the ASTS-orientations that exist according to Theorem 2 (statement (ii)).

Theorem 5 *In the setting of Theorem 2 let* $B = (V_B, E_B) \in \mathcal{B}^C$ *be a block of a component* $C = (V_C, E_C)$ *and let* $\tilde{D} := (V_C, \tilde{A}_C)$ *be an ASTS-orientation of* C *that exists due to Theorem 2.*

(i) *If* B *is without any source and sink and has at most one free node, i.e.,*

$$V^C_{+,B} \cup V^C_{-,B} = \varnothing \textit{ and } |V^C_{F,B}| \leq 1, \tag{12}$$

then $q_a = 0$ *for all arcs* $a \in A[E_B]$.

(ii) *For all* $B \in \mathcal{B}^C$ *that do not satisfy* (12) *there exist ASTS-orientations* $\tilde{D}_B = (V_B, \tilde{A}_B)$ *with respect to* $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$ *such that* $\bigcup_{B \in \mathcal{B}^C} \tilde{A}_B$ *is equal to* $\tilde{A}_C$ *except for arcs with flow zero, i.e.*

$$\{a \in \bigcup_{B \in \mathcal{B}^C} \tilde{A}_B \mid q_a \neq 0\} = \{a \in \tilde{A}_C \mid q_a \neq 0\}. \tag{13}$$

Moreover, the union of the ASTS-orientations $\tilde{D}_B$ *is an ASTS-orientation with respect to* $(V'_+ \cap V_C, V'_- \cap V_C, V'_T \cap V_C, V'_F \cap V_C)$ *of the union of all blocks that do not satisfy* (12)*, and this ASTS-orientation satisfies* (6). □

Proof (i) Equations (12) imply that there cannot be any flows on the arcs of B except for cycles. This, however, is not possible because it would violate the fact that $\tilde{D}$ is acylic and satisfies (6) by assumption.

(ii) Let B be a block of (V_C, A_C) that does not satisfy (12). We consider the subgraph $(V_{>0,B}, E_{>0,B})$ of B defined by the non-zero flows on B, i.e.,

$$E_{>0,B} := \{e \in E_B \mid \exists a \in \{a^+_e, a^-_e\} \colon q_a > 0\},$$
$$V_{>0,B} := V[E_{>0,B}],$$

and define the orientation $\tilde{D}_{>0,B}$ to be the subgraph of $\tilde{D}$ induced by $V_{>0,B}$. If $V_{>0,B} = \varnothing$, any ASTS orientation on B with respect to $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$

trivially satisfies (13). Such an orientation must exist due to Corollary 1 since B does not satisfy (12). Hence we assume $V_{>0,B} \neq \varnothing$ in the following. If we can show that $\tilde{D}_{>0,B}$ is an ASTS orientation of B with respect to $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$, we can extend this orientation to an ASTS orientation of B due to the completion characterization of Theorem 1, which is possible by Corollary 1 since B does not satisfy (12). As all orientations $\tilde{D}_B$ constructed in this fashion certainly satisfy (13), we will have proved the first claim of Statement (*ii*).

We now show that $\tilde{D}_{>0,B}$ is indeed an ASTS orientation of B with respect to $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$. For a block B, orientation $\tilde{D}_{>0,B}$ is trivially acyclic since $\tilde{D}$ is acyclic. Regarding the STS-condition, we now consider the nodes in $V_{>0,B}$ that are *not* cut-vertices of B. Let $v \in V^C_{T,B}$ be such a node. Since v is not a cut-vertex of B, (11c) implies $v \in V'_T \cap V_C$. Therefore, as $v \in V_{>0,B}$, it must have both an outgoing and an incoming arc with postive flow in the solution of MINLP (3) due to Lemma 1. Hence it must have both an outgoing arc and an incoming arc on $\tilde{D}$, because of Eq. (6). But since these arcs have positive flow, their underlying edges are in $E_{>0,B}$. Accordingly, they are also arcs of $\tilde{D}_{>0,B}$. As we have choosen v to be in $V^C_{T,B}$, this means that v satisfies the STS-condition. Analogously we can show that *all* nodes in $V_{>0,B}$ that are *not* cut-vertices of B satisfy the STS-condition with respect to $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$.

Now let v be a node in $V_{>0,B}$ that *is* a cut-vertex of B. We consider the case $v \in V^C_{T,B}$. Being in $V_{>0,B}$, the node v must have an outgoing or an incoming arc in A_B with positive flow. Further, (11c) implies due to the tree structure of the block tree that v has, in any solution to MINLP (3), a net flow balance of 0 with respect to B. As a consequence, due to the flow conservation (3b), v must have both an outgoing and an incoming arc in A_B with positive flow. Hence, due to (6), v must have both an outgoing and an incoming arc on $\tilde{D}$. Since these arcs have positive flow, they are also arcs of $\tilde{D}_{>0,B}$, by construction. Hence, as v was assumed to be in $V^C_{T,B}$, it satisfies the STS-condition. Analogously it can be shown that *all* nodes in $V_{>0,B}$ that *are* cut-vertices of B satisfy the STS-condition with respect to $(V^C_{+,B}, V^C_{-,B}, V^C_{T,B}, V^C_{F,B})$ and we have proved the first claim of Statement (*ii*).

Regarding the second claim of Statement (*ii*), we observe that the union of the ASTS orientations $\tilde{D}_B$ we have constructed is certainly acyclic due to the tree structure of the block tree. Moreover, all nodes in V_C that are not cut-vertices of (A_C, E_C) are in $V^C_{+,B}$ iff they are in $V'_+ \cap V_C$, are in $V^C_{-,B}$ iff they are in $V'_- \cap V_C$, are in $V^C_{T,B}$ iff they are in $V'_T \cap V_C$, and are in $V^C_{F,B}$ iff they are in $V'_F \cap V_C$, i.e., they certainly satisfy the STS-condition on the union of the orientations $\tilde{D}_B$. Finally, we observe that the orientations $\tilde{D}_B$ satisfy (6) by our construction above. Hence all that remains to be shown is that the cut-vertices of (V_C, E_C) satisfy the STS-condition with respect to $(V'_+ \cap V_C, V'_- \cap V_C, V'_T \cap V_C, V'_F \cap V_C)$.

We consider a node $v \in V'_T \cap V_C$. We have to show that v has an incoming and an outgoing arc on the union of the orientations $\tilde{D}_B$. If there exists a block B with $v \in V^C_{T,B}$ or one block B_1 with $v \in V^C_{+,B_1}$ and another block B_2 with $v \in V^C_{-,B_2}$, this is trivially the case. Moreover, the cases $v \in V^C_{+,B}$ for all B with $v \in V_B$ and $v \in V^C_{-,B}$ for all B with $v \in V_B$ can be disregarded due to the definition of V'_T. What remains is the case in which v is a node of blocks B_i such that there exists an i with $v \in V^C_{F,B_i}$.

W.l.o.g we consider the case in which $v \in V^C_{+,B_j}$ for all $j \neq i$. Since all orientations $\tilde{D}_{B_j}$ are ASTS orientations and v thus satisfies the STS-conditions with respect to $v \in V^C_{+,B_j}$, this implies that v has an outgoing arc on all $\tilde{D}_{B_j}$. Moreover, by (11a), in our solution to MINLP (3) the node v has outgoing arcs with positive flow in all arc sets A_{B_j}. We can assume that v has no incoming arc on any $\tilde{D}_{B_j}$ because otherwise we have finished. Accordingly, v cannot have an incoming arc with positive flow in any A_{B_j} due to (6), which we know is satisfied by all orientations $\tilde{D}_B$. Hence in our solution to MINLP (3)

$$q_{vu} > 0 \text{ for all } vu \in A_{B_j} \text{ for all } j \neq i. \tag{14}$$

Now let us recall that we assumed $v \in V'_T \cap V_C$, i.e., by (5e) the node v has a flow balance of zero within the component C. In conjunction with (14) the flow conservation (3b) requires an arc $uv \in A_{B_i}$ with $q_{uv} > 0$. As all $\tilde{D}_B$ satisfy (6), this means that there exists an arc with head v on $\tilde{D}_{B_i}$, i.e., v has both an incoming and an outgoing arc on the union of the orientations $\tilde{D}_B$. Since $v \in V'_T \cap V_C$, we have proved that v satisfies the STS-condition with respect to $(V'_+ \cap V_C, V'_- \cap V_C, V'_T \cap V_C, V'_F \cap V_C)$.

As one can show analogously that *all* cut-vertices of (V_C, E_C) satisfy the STS-condition with respect to $(V'_+ \cap V_C, V'_- \cap V_C, V'_T \cap V_C, V'_F \cap V_C)$, we have finished proving Statement (*ii*). ■

Remark 3

1. The bounds for the node demands calculated in the previous Theorem 5 (and the classification of nodes into sources, sinks, transhipment nodes and free nodes building of these bounds) can be tightened significantly boundary combining the information about node demand bounds resulting from considering the block trees of the components of the subgraph (V'_{in}, A'_{in}) (as in the previous theorem) with node demand bounds that can be obtained from considering the block tree of the subgraph (V_{in}, A_{in}).
2. Algorithmically, it is faster to calculate $V^C_{+,B}$, $V^C_{-,B}$ and $V^C_{T,B}$ recursively starting from the leaves of the block tree than to sum up the demand bounds of all nodes of the blocks of the subgraphs $G^C_{B,v}$ (as in Theorem Theorem 5). □

6 Exploiting ASTS orientations algorithmically

Theorem 2 implies that given a suitable region A', the MINLP (3) complemented by the constraints

$$q_a = 0 \quad \text{for all } a \in A_{\text{out}} \cup A'_{\text{out}}, \tag{15a}$$

$$\{D(A', q) \text{ is an ASTS-orientation w.r.t. } (V_+, V_-, V_T, V_F)\} \tag{15b}$$

is equivalent to (3) in the sense that one of the two problems is feasible iff the other one is feasible and both problems have the same objective value. To formulate (15b) as a MILP constraint, we first introduce binary variables x_e for the flow direction of each edge $e \in E'_{\text{in}} := E[A'_{\text{in}}]$, where $x_e = 1$ means flow along a^+_e and $x_a = 0$ indicates flow along a^-_e. The coupling between these binary variables and the corresponding flow variables can be achieved via the big-M constraints

$$q_{a^+_e} \leq x_e \overline{q}_{a^+_e} \qquad \text{and} \qquad q_{a^-_e} \leq (1 - x_e)\overline{q}_{a^-_e}. \tag{16}$$

To model the requirements for an ASTS orientation, we employ a Dantzig-Wolfe approach: We (conceptually) enumerate all ASTS orientations and require that one of those is chosen. Of course, this approach will not work for large networks as we expect the number of ASTS orientations to grow exponentially in the number of arcs. For this reason, we consider a family $\mathcal{A} = \{A'_1, \ldots, A'_k\}$ of regions for which all ASTS orientations can be enumerated with reasonable effort. Each region A'_i is chosen such that it fulfills the requirements (a) and (b) of Theorem 2. Observe that in general this does not guarantee that an ASTS orientation for the entire set E_{in} is chosen. Let $\mathcal{O}_i$, $1 \leq i \leq k$, be the set of ASTS orientations for the edge set $E'_{i,\text{in}}$ corresponding to region A'_i. For each $\tilde{D}_j = (V_j, \tilde{A}_j) \in \mathcal{O}_i$ we introduce a binary variable $y^C_{\tilde{D}}$, where $\tilde{D}$ is selected iff $y^C_{\tilde{D}} = 1$. This requirement is formulated as

$$\sum_{\tilde{D}_j \in \mathcal{O}_i \,:\, a_e^+ \in \tilde{A}_j} y^C_{\tilde{D}} = x_e \quad \text{for all } e \in E'_{i,\text{in}}. \tag{17}$$

Adding constraints (15a), (16), and (17) for each region A'_i can be used to strengthen the MINLP model (3) or any relaxation of it. In particular, it can be used to strengthen the classical network flow subproblem of (3), which in turn can be used in an optimality-based bound tightening procedure (see Section 7.3). To this end, the resulting MILP model is minimized and maximized for each arc flow variable in turn to obtain stronger flow bounds.

The framework presented so far offers many algorithmic opportunities. Depending on the structure of the network and the values of the constants, one may, for example, wish to choose the following approach:

1. Determine the global outer edges according to Corollary 1.
2. Consider the region given by $A' := A[E_{\text{dec}}] \cup A[E_{\text{mnt}}]$.
3. Decompose the inner edges of the components of the region into blocks according to Theorem 5.
4. Decompose the blocks remaining according to Statement (*ii*) of Theorem 5 based on pre-oriented edges according to Theorem 3.
5. Decompose the resulting components into blocks according to Theorem 4.

For our computational proof of concept we will employ a somewhat lighter approach in the following, which is based on the ideas of Corollary 1, Theorem 3 and Theorem 4.

1. Determine the global outer edges E_{out}.
2. Consider the components of the graph consisting of those edges for which the flow bounds do not yet determine the flow direction.

   Consider the edge set of each of these components as a region and determine the local inner and outer edge sets E'_{in} and E'_{out}. Decompose the edge sets E'_{in} further into blocks and consider these blocks to make up the set of regions $\mathcal{A}$.

This scheme does not capture all constraints implied by considering ASTS orientations, as we do not exclude cycles through multiple regions (cf. (ii) of Theorem 3). However, there is already a significant computational impact as we will see in the next section.

7 Computational results

In order to investigate the computational potential of these ideas we consider gas network optimization instances used in the literature [KHPS15, SAB$^+$17]. We study the improvement in the bound tightening over existing problem-specific bound tightening techniques as well as the impact of strengthening optimization models by information due to ASTS orientations on the running time to solve the models.

7.1 Test instances

In order to benefit from analyzing possible ASTS orientations, the network has to feature several cycles. We therefore use the largest networks of the public GasLib [SAB$^+$17], GasLib-582 (version 2) and GasLib-4197, containing many cycles. These are complemented by non-public data for a real-world network HN-AB that has also been studied in [PFG$^+$15, KHPS15]. Although the networks GasLib-582 and HN-AB are of comparable size it has been observed [PFG$^+$15] that instances for HN-AB are harder to solve.

MINLP models for networks of this size (see Table 1) cannot be solved in reasonable time by current solvers [PFG$^+$15]. We therefore consider the MILP relaxation [GMMS15, GMMS12] of a certain gas network MINLP that has been successfully used to solve the GasLib-582 and HN-AB instances in [KHPS15].

In order to apply the theory we developed, we treated the network elements pipes and control valves as potential-decreasing edges, the network elements valves, resistors, and shortpipes as potential-maintaining edges, and compressor elements as generic edges. To match the MINLP model to these choices, we modified each network in the following way. First, the altitude of each network node is set to 0, hence all pipes are horizontal. Thus the potential drop function for a pipe is $\phi_a(q_a) = c\phi_a|\phi_a|$ for some constant c, fulfilling the requirement (2). Moreover, we replaced resistors by open valves. With this modified data, the MILP from [GMMS15] is a relaxation of a MINLP of the type (3).

For each instance (consisting essentially of a gas demand vector) we use the lamatto framework [Lam14] that has also been used in [GMMS12, GMMS15, GMSS15, GMSS18] to generate the MILP relaxation. It is crucial to note that this generation process includes a state-of-the-art bound tightening procedure summarized in [SKMP15]. Among other bound tightening techniques, this includes optimality-based bound tightening for the flows, i.e., minimizing and maximizing the flow over each arc subject to flow conservation constraints and flow bounds (either from the original input or derived via other bound tightening steps). This bound tightening is able to fix the flow direction on a large share of the network arcs, but there also remain large parts of the network where the flow direction cannot be fixed. As an objective, we chose to minimize the total amount of compressed gas, i.e., the sum of the flow variables through active compressor stations. The root node of each MILP model was solved with Gurobi 8.1 [GO19]; in the following, we consider only those instances which are not infeasible after the root node.

instance set		# arcs		# instances
	decreasing	maintaining	increasing	
GasLib-582	301	303	5	3545 (4227)
HN-AB	524	158	7	42 (43)
GasLib-4197	3657	797	12	2014 (2859)

Table 1: Statistics for the considered instance sets. The column "# instances" gives the number of "not infeasible" instances as described above and, in parantheses, the number of all instances.

7.2 Implementation and computational setup

The algorithms have been coded prototypically in Python. For the enumeration of ASTS orientations, a simple backtracking search is used. The enumeration is stopped as soon as at least 2000 ASTS orientations have been generated. For components with so many orientations, no orientations are considered in the following to avoid an unreasonable blowup of the MILP model used for OBBT as well the original MILP extended by the configuration model based on the enumerated orientations.

To measure the tightness of flow bounds for a network arc, we define the *flow range* to be the difference between the upper and the lower flow bound of that arc. In order to have an instance-independent tightness measure, the *relative flow range* is the flow range divided by *twice* the total inflow, i.e., the sum of the flows entering the network. Hence the relative flow range is in the interval $[0, 1]$. We use this to limit computation time for OBBT: the flow bounds for a variable are tightened only if the relative flow range is at least 2.5%. The MILP models during OBBT are solved using SCIP 6.0 [GBE$^+$18].

All computations were performed on machines with Intel Xeon E5-2670 CPUs with 2.5 GHz and 64 GB of RAM. The runtimes reported are for single threaded computations that use the machine exclusively.

7.3 Strengthening flow bounds

We start our evaluation by investigating the improvement of the bounds for the flow variables when performing OBBT using the MILP model consisting of the classical network flow constraints (3b), (3h), and (3i) complemented by the configuration models (17) for choosing an ASTS orientation in each selected region. As a benchmark, we compare against the bounds obtained by the lamatto bound tightening algorithm (described in [SKMP15]), in the following refered to as "lamatto BT". This algorithms performs, among others, classical bound tightening for the constraints of the network elements, as well as OBBT using the classical network flow problem. Our bound tightening procedure, "OBBT with orientations", performs OBBT using the MILP model explained above for each arc (with sufficiently high relative flow range, see above) starting from the flow bounds obtained by "lamatto BT".

To measure the strength of the flow bounds, we consider the distribution of the flow range values for each instance. We compare the flow range distribution of "lamatto BT" vs. "OBBT with orientations" by comparing their tails, i.e., for how many arcs the flow range exceeds certain thresholds. An example for

flow range	lamatto BT	OBBT with orientations	rel. improvement [%]
== 0.0	2739	2779	1.5
$\geq$ 1000.0	334	223	33.2
$\geq$ 2000.0	268	207	22.8
$\geq$ 3000.0	190	140	26.3
$\geq$ 4000.0	134	6	95.5
$\geq$ 5000.0	130	0	100.0
$\geq$ 6000.0	56	0	100.0

Table 2: Comparison of flow range distribution for GasLib-4197 instance `nomination_mild_1280.lp`. The first row gives the number of arcs for which the flow value has been fixed.

the GasLib-4197 instance `nomination_mild_1280.lp` is shown in Table 2. For instance, using "lamatto BT" there remain 56 arcs with a flow range of at least 6000 units, whereas "OBBT with orientations" reduces the flow range of all arcs below 5000 units.

We extend this kind of analysis to all instances of an instance set by considering for each instance the relative flow range as defined above. This allows us to use fixed thresholds for all instances; these thresholds are relative to the instance-specific total inflow. The results are shown in Table 3. It is evident that "OBBT with orientations" is very effective in improving the bounds for arcs with a large initial flow range. Moreover, for 1% to 2% additional arcs the flow can actually be fixed. Note that the bounds could be tightened further by iterating the lamatto bound tightening and our OBBT using ASTS orientations until no further improvement is possible.

7.4 Improved models for gas network operation

To investigate the computational impact of exploiting information derived from ASTS orientations, we consider the following three MILP variants:

"original" MILP model as generated using the lamatto framework

"original+bounds" extends the "original" model by bounds obtained via OBBT using feasible ASTS orientations

"original+bounds+orientations" extends "original+bounds" further by the configuration model (17) for these orientations

We use Gurobi 8.1 to solve these MILPs for each instance with a runtime limit of 3600 seconds. As the instances are numerically challenging, we used the Gurobi parameter `NumericFocus=3`. Each of the three MILP model variants is solved 5 times using distinct seeds; "runtime" in the subsequent evaluation refers to the average of the runtime of these 5 runs (using the time limit in case the instance has not been solved). Apart from GasLib-4197, all instances have been solved to optimality. Due to limited computational resources, we preliminarily selected a subset of 104 instances from GasLib-4197.

	min	0.25 quantile	median	0.75 quantile	max
== 0.0	0.0	0.0	2.2	2.2	3.3
≥ 0.1	10.9	16.4	16.4	16.4	19.3
≥ 0.2	10.9	11.5	11.5	16.4	19.3
≥ 0.3	10.9	11.5	11.5	11.5	32.5
≥ 0.4	10.9	11.5	11.5	11.5	32.5
≥ 0.5	19.0	29.4	29.4	31.7	69.1
≥ 0.6	35.3	47.6	47.6	47.6	58.3
≥ 0.7	35.3	47.6	52.4	52.4	52.4
≥ 0.8	35.3	41.2	41.2	52.4	68.8
≥ 0.9	35.3	41.2	45.2	58.3	75.9

(a) GasLib-582

	min	0.25 quantile	median	0.75 quantile	max
== 0.0	0.0	0.0	0.0	0.9	1.1
≥ 0.1	9.8	11.8	14.6	14.6	15.0
≥ 0.2	6.7	11.8	11.8	11.8	12.1
≥ 0.3	6.7	11.8	11.8	11.8	15.4
≥ 0.4	7.3	11.5	11.8	11.8	13.0
≥ 0.5	4.1	10.3	14.5	19.1	30.2
≥ 0.6	14.7	30.2	36.2	38.2	54.8
≥ 0.7	16.7	30.2	36.2	38.2	56.5
≥ 0.8	20.6	30.2	32.5	40.6	61.9
≥ 0.9	20.6	21.2	29.2	41.9	65.0

(b) HN-AB

	min	0.25 quantile	median	0.75 quantile	max
== 0.0	1.1	1.3	1.5	1.6	2.6
≥ 0.1	32.8	35.6	36.8	37.4	39.0
≥ 0.2	24.4	28.5	31.8	35.1	39.1
≥ 0.3	20.4	23.9	26.6	30.1	34.5
≥ 0.4	20.7	23.1	24.3	27.5	35.0
≥ 0.5	25.3	27.0	29.0	30.1	37.9
≥ 0.6	60.4	63.6	65.0	95.5	96.4
≥ 0.7	62.7	66.4	67.4	95.5	100.0
≥ 0.8	55.2	66.4	66.9	100.0	100.0
≥ 0.9	52.2	66.4	95.9	100.0	100.0

(c) GasLib-4197

Table 3: Comparison of the improvement of the relative flow range distribution over all considered instances of each instance set. The tables show the distribution of the reduction (in percentage of arcs) of the number of arcs whose relative flow range exceeds the given threshold. For instance, in the instance set GasLib-4197 the number of arcs with a relative flow range of at least 0.9 is reduced by at least 52.2%, 95.9% in the median, and at most 100%.

The results are summarized in the performance profiles [DM02] in Fig. 1. The performance profiles are restricted to “non-trivial” instances, i.e., those for which at least one of the models has a runtime of at least 10 seconds.

Only roughly one quarter of the GasLib-582 instances is “non-trivial” in this sense, showing that this instance set is rather easy to solve. The difference between the “original” and “original+bounds” models are negligible, with the performance of “original+bounds+orientations” being clearly inferior. This is expected, as the additional model complexity due to the configurations models for the orientations is overkill for the already easy instances.

For the HN-AB instance set, which is known to be harder than GasLib-582, 29 out of the 42 instances are “non-trivial”. Initially, “original” and “original+bounds” perform rather similar and close to the virtual best solver, with “original+bounds+orientations” being clearly outperformed. However, on harder instances both “original+bounds” and “original+bounds+orientations” outperform “original” with “original+bounds+orientations” being initially inferior, but becoming eventually superior.

All the studied GasLib-4197 are “non-trivial” and the effect observed already for HN-AB is even more pronounced: “original+bounds” consistently outperforms “original”, and is itself being outperformed by “original+bounds+orientations” for harder instances.

To summarize, our results clearly show that the harder the instances, the more beneficial it is to use the proposed extended models. We should mention, however, that with the current implementation the runtime gains are exceeded by the computation times for analysing ASTS orientations and, most importantly, for performing OBBT using the orientations.

8 Conclusions and further work

We proposed ASTS orientations as a combinatorial relaxation capturing essential properties of feasible solutions of potential-driven flow problems. Incorporating the restriction to ASTS orientations into established relaxations leads to tighter relaxations. Our computational results for large-scale gas networks indicate that there is a significant computational advantage if the considered instances are sufficiently hard. It is interesting to note that these substantial improvements can already be gained by considering small subgraphs only.

The theoretical framework for ASTS orientations presented in this paper offers further algorithmic opportunities that have not been investigated yet. For instance, we did not yet exclude cycles encompassing several undirected components as suggested by Theorem 3. Algorithmically, this can be done by separating such cycles. Another line of research is to develop efficient variants of OBBT based on ASTS orientations.

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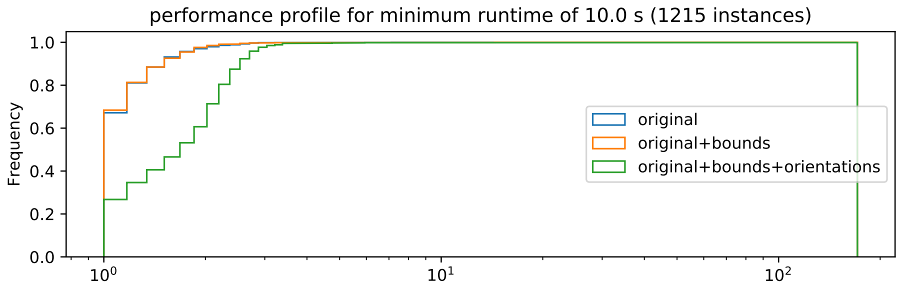
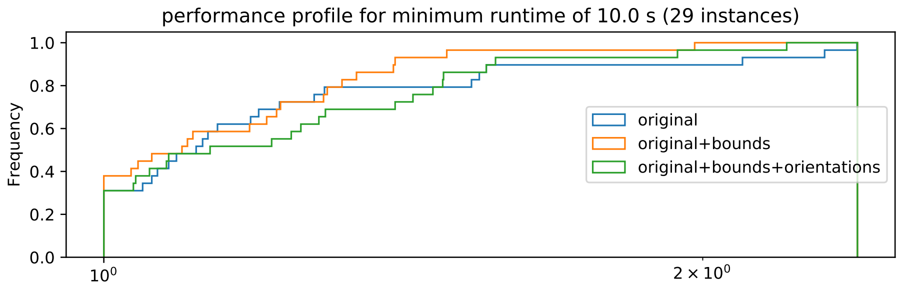
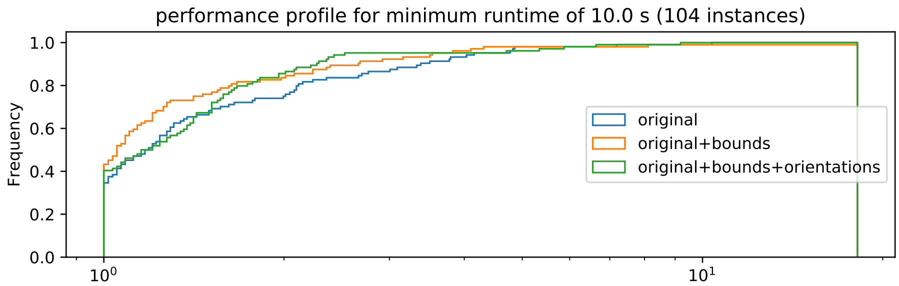


(a) GasLib-582



(b) HN-AB



(c) GasLib-4197

Figure 1: Performance profiles for the average running time of solving each MILP instance 5 times using Gurobi.

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