A Globally Convergent Method for Generalized Resistive Systems and its Application to Stationary Problems in Gas Transport Networks

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Keywords: Non-linear Systems, Globally Convergent Methods, Gas Transport Networks.

Abstract: We consider generalized resistive systems, comprising linear Kirchhoff equations and non-linear element equations, depending on the flow through the element and on two adjacent nodal variables. The derivatives of the element equation should possess a special signature. For such systems we prove the global non-degeneracy of the Jacobi matrix and the applicability of globally convergent solution tracing algorithms. We show that the stationary problems in gas transport networks belong to this generalized resistive type. We apply the tracing algorithm to several realistic networks and compare its performance with a generic Newton solver.

1 INTRODUCTION

Applied engineering problems often require to solve large systems of non-linear equations. While solving these systems, one cannot generally rely on the existence and the uniqueness of their solutions. Also, for the purpose of convergence one has to choose a starting point sufficiently close to the solution, to get into a basin of attraction of the iterative method used.

A surprising feature of some network problems is the existence of a unique solution and the availability of a globally convergent method, able to find the solution from an arbitrary starting point. This applies to systems of resistive type, comprising Kirchhoff's flow conservation conditions and element equations similar to Ohm's law in electrotechnics. For systems of this kind, written in a form $f(x)=0$, one can prove the non-degeneracy of the Jacobi matrix $J=\partial f/\partial x$ in the whole space of x. In other words, the mapping $y=f(x)$ is a diffeomorphism and every y has a single pre-image x. In particular, $y=0$ has a single pre-image x^*, in this way providing a unique solution of the system above. The solution can be found with the following algorithm:

Algorithm 1: Solution tracing.

```
start from an arbitrary point x_0;
take its image y_0 = f(x_0);
connect y_0 with the origin y = 0
by a straight line;
reconstruct pre-image of this line
in x-space.
```

The reconstruction of the pre-image of the line can be done, using, e.g., a homotopically stabilized Newton method (Allgower and Georg, 2003). The obtained line in x-space goes from the starting point x_0 to the solution x^* we are looking for.

In paper (Katzenelson, 1965) this idea has been used for the solution of continuous piecewise linear resistive systems. The system is composed of linear Kirchhoff equations and piecewise linear element equations of the form $f(P_{in}-P_{out},Q)=0$, relating a difference of nodal variables $P_{in}-P_{out}$ to the flow Q through the element. Continuity means that the mapping $y=f(x)$ as a whole is C^0-continuous, since the purpose is to approximate continuous element equations of general non-linear form. Resistiveness means that the element equation in every piece can be written as $P_{in}-P_{out}=RQ+Const$, where $R>0$ is the resistance, or, in more general way, that the derivatives of the element equation in every piece possess the following signature: $\nabla f=(+-)$. It is easy to show that under these conditions the Jacobian determinant $\det J$ of the system has the same sign in all pieces. Although this mapping is not a diffeomorphism anymore, it is a homeomorphism, every point y still has a single pre-image x. The linear system in every piece essentially coincides with the one appearing in Newton's step. The only necessary modification is that, whenever the step attempts to leave the piece, the algorithm should stop at the border:

Algorithm 2: Piecewise linear tracing.

```
do Newton's step using the current
Jacobi matrix;
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Clees, T., Hornung, N., Nikitin, I. and Nikitina, L.
A Globally Convergent Method for Generalized Resistive Systems and its Application to Stationary Problems in Gas Transport Networks.
DOI: 10.5220/0005958700640070
In *Proceedings of the 6th International Conference on Simulation and Modeling Methodologies, Technologies and Applications (SIMULTECH 2016)*, pages 64-70
ISBN: 978-989-758-199-1

```
if the solution leaves the piece:
   stop at the border;
   update the Jacobi matrix to
   the other side;
   proceed to the next piece;
else:
   return the solution.
```

The algorithm is globally convergent and comes to the solution in a finite number of steps.

In paper (Chien and Kuh, 1976) the condition that $\det J$ has to be of the same sign in all pieces has been relaxed. This condition has been imposed only on unbounded pieces, while in bounded ones $\det J$ can change sign and even vanish, producing a locally degenerate system. The tracing algorithm has been extended to process such cases, still providing convergence in a finite number of steps.

In paper (Griewank et al., 2015) the continuous piecewise linear mappings were represented in a so called *max-min form.* Further, using for max-min functions their definition in terms of absolute values:

$$\begin{aligned} &f(x) = \max_i \min_j a_{ij}^T x + b_{ij}, \\ &\max(x,y) = (x+y+|x-y|)/2, \\ &\min(x,y) = (x+y-|x-y|)/2, \end{aligned} \tag{1}$$

continuous piecewise linear systems have been transformed to systems combining globally linear functions and absolute value functions. The paper discusses the relation of such systems with linear complementarity problems (LCPs) and Karush-Kuhn-Tucker (KKT) conditions and presents a number of algorithms for their solution, converging in a finite number of steps.

The general relationship between physical laws and underlying topological structure of the systems is well discussed in works (Kron, 1945; Bulgakov et al., 2005; Tonti, 2013; Shai, 2001). In the present paper we will concentrate on particular aspects of non-linear transport networks and extend the solution tracing algorithm from (Katzenelson, 1965; Chien and Kuh, 1976) to a wider class of problems, which we will call generalized resistive systems. The systems contain linear Kirchhoff equations and non-linear element equations of the form $f(P_{in}, P_{out}, Q) = 0$. The element equations depend separately on the nodal variables P_{in}, P_{out} and the flow Q. The derivatives should possess a signature $\nabla f = (+--)$. In Section 2 we will show that systems of this kind have a non-degenerate Jacobi matrix and the solution tracing algorithm can be used for them, preserving its global convergence property. In Section 3 we will apply this algorithm to the solution of stationary problems in gas transport networks. These networks include so called control elements, possessing piecewise linear element equations of generalized resistive type. We use a max-min form of these equations and their regularized absolute value representation. We perform tests on a number of realistic networks and show the stability of the algorithm.

2 GENERALIZED RESISTIVE SYSTEMS

We will consider systems of the form:

$$\sum_e I_{ne} Q_e = Q_n^{(s)}, \; f_e(P_{in}, P_{out}, Q_e) = 0, \tag{2}$$

where indices $n = 1...N$ denote the nodes and $e = 1...E$ the edges of the network graph, I_{ne} is an incidence matrix of the graph, Q_e are flows through the edges, $Q_n^{(s)}$ are source/sink contributions, localized in supply/exit nodes, P_n are nodal variables (pressure, voltage, etc. – dependent on the context). The element equations possess derivatives of the signature:

$$\begin{aligned} &\partial f_e/\partial P_{in} > 0, \; \partial f_e/\partial P_{out} < 0, \\ &\partial f_e/\partial Q_e < 0. \end{aligned} \tag{3}$$

The Jacobi matrix of the system has the form:

$$J = \begin{pmatrix} 0 & I \\ \tilde{I}^T & -R \end{pmatrix}, \tag{4}$$

where $\tilde{I}$ contains derivatives $\partial f_e/\partial P_n$ of the element equations and R is a diagonal matrix containing positive entries $-\partial f_e/\partial Q_e$. Note that $\tilde{I}$ has the same pattern and the signs of entries as I. After elementary transformations we have

$$\det J = \prod_e (-R_e) \; \det I R^{-1} \tilde{I}^T. \tag{5}$$

The matrix $\tilde{L} = I R^{-1} \tilde{I}^T$ has sizes $N \times N$ and possesses a pattern and signs of entries identical with the Laplacian matrix $L = I\, I^T$. For the graphs containing several connected components both matrices have a block-diagonal structure, where we can select one block and further consider $L, \tilde{L}$ corresponding to one connected component. Both matrices have one zero eigenvalue, corresponding to an obvious eigenvector $v = (1...1)$. The difference between L and $\tilde{L}$ is that L is symmetric and v is its left and right eigenvector, while $\tilde{L}$ is not symmetric and v is its left eigenvector. This degeneracy is related to the structure of the incidence matrix, i.e., every column of I contains only two entries $+1$ and -1, so that the sum of entries in every column vanishes.

Are there any other vectors annulating $\tilde{L}$ from the left?

$$(v\tilde{L})_{n'} = \sum_{n,e} v_n I_{ne} R_e^{-1} \tilde{I}_{n'e}$$
$$= v_{n'} d_{n'} - \sum_{n \neq n'} v_n u_{nn'} = 0, \quad (6)$$
$$d_{n'} = \sum_e I_{n'e} R_e^{-1} \tilde{I}_{n'e}, \; u_{nn'} = -\sum_e I_{ne} R_e^{-1} \tilde{I}_{n'e}.$$

Here we separate diagonal and non-diagonal contributions and see from the sign patterns of I and $\tilde{I}$ that $d_{n'} > 0$, while $u_{nn'} > 0$ if $n \neq n'$ are connected by an edge and $u_{nn'} = 0$ otherwise. Also, from the annulation of the matrix by $v = (1...1)$ we have

$$d_{n'} = \sum_{n \neq n'} u_{nn'}. \quad (7)$$

Thus we have

$$\sum_{n \neq n'} (v_{n'} - v_n) u_{nn'} = 0. \quad (8)$$

Let us consider a maximal entry $v_{n'} \geq v_n$ for all $n \neq n'$. The above condition gets LCP form, satisfied only if

$$(v_{n'} - v_n) u_{nn'} = 0, \quad (9)$$

i.e., for connected nodes $v_{n'} = v_n$ must be satisfied. In this way the maximal value propagates to all connected nodes in the graph, leading to the conclusion that $v_n = \text{Const}$ is the only solution. Therefore, only the vectors proportional to $v = (1...1)$ are the left annulators of $\tilde{L}$.

To eliminate the degeneracy, one has to remove (at least) one Kirchhoff equation in the connected component and fix the corresponding nodal variable to a constant value. Physically this corresponds to the creation of an entry point for the flow and setting a pressure (voltage, etc.) value there: $P_n = \text{Const}$ for $n \in Pset$. On matrix level it corresponds to the removal of (at least) one row from the matrices $I, \tilde{I}$ and the corresponding row and column from $L, \tilde{L}$. Searching the left annulators of $\tilde{L}$, we obtain a similar system but with $v_n = 0$ for $n \in Pset$ and the equations with $n' \notin Pset$. We come to the conclusion that the maximal value $v_{n'}$ propagates to all connected nodes $\notin Pset$ and to their neighbours $\in Pset$, where $v_n = 0$ is set. Thus, the maximal value $v_{n'} = 0$. Similarly, considering the propagation of the minimal value, we also have $v_{n'} = 0$. Therefore, $v = 0$ is the only solution, the matrix $\tilde{L}$ does not have non-zero annulators and $\det \tilde{L} \neq 0$.

Further, it is easy to show that $\det \tilde{L} > 0$. The standard Laplacian matrix L is symmetric and positive semi-definite. Removing the $Pset$ nodes makes it strictly positive definite, so that $\det L > 0$. Considering a linear homotopy

$$\hat{I}(\lambda) = I(1-\lambda) + \tilde{I}\lambda, \; \hat{R}(\lambda) = 1 \cdot (1-\lambda) + R\lambda,$$
$$\hat{L}(\lambda) = I \hat{R}^{-1}(\lambda) \hat{I}^T(\lambda), \quad (10)$$
$$\hat{L}(0) = L, \; \hat{L}(1) = \tilde{L},$$

during the transition $\lambda \in [0,1]$ all matrices have the same sign pattern as at the beginning and at the end of the path. We know that $\det L > 0$. If $\det \tilde{L} < 0$, we can find a point in between where $\det \hat{L}(\lambda) = 0$, i.e., find a degenerate matrix in the considered class of matrices, which, as we have just proven, does not exist. Thus, $\det \tilde{L} > 0$.

Finally, we conclude that $\det J$ does not vanish and has a sign $(-1)^E$ defined only by the number of edges in the connected component. In particular, when piecewise linear element equations are considered, $\det J$ has the same sign in all pieces.

We note that "purely" resistive systems, with element equations dependent on the difference of nodal variables, form a special subclass of generalized resistive systems, whose element equations can depend on nodal variables separately. This special subclass corresponds to $\tilde{I} = I$ and a symmetric Jacobi matrix. Our main conclusion is that the generalized resistive systems can be treated in pretty the same way as resistive ones, although their Jacobi matrix is not symmetric anymore. Particularly, for piecewise linear systems one can apply tracing algorithms from (Katzenelson, 1965; Chien and Kuh, 1976), providing convergence in a finite number of steps. For non-linear systems one can use a homotopic version of the algorithm (Allgower and Georg, 2003) together with other stabilization strategies, such as backtracking line search (Press et al., 1992) and its high-order versions (Wächter and Biegler, 2006). For piecewise smooth systems one can use a combination of those:

Algorithm 3: Piecewise smooth tracing.

```
start from an arbitrary point x0;
take its image y0 = f(x0);
connect y0 with the origin y = 0
by a straight line;
select its homotopic subdivision {yi},
i = 0...k;
loop over i:  solve the system f(x) = yi
   repeat until convergence:
      update the Jacobi matrix;
      perform Newton's step;
      if the solution leaves the piece:
         stop at the border;
      apply backtracking line search;
      if still at the border:
         proceed to the next piece;
   end;
end.
```

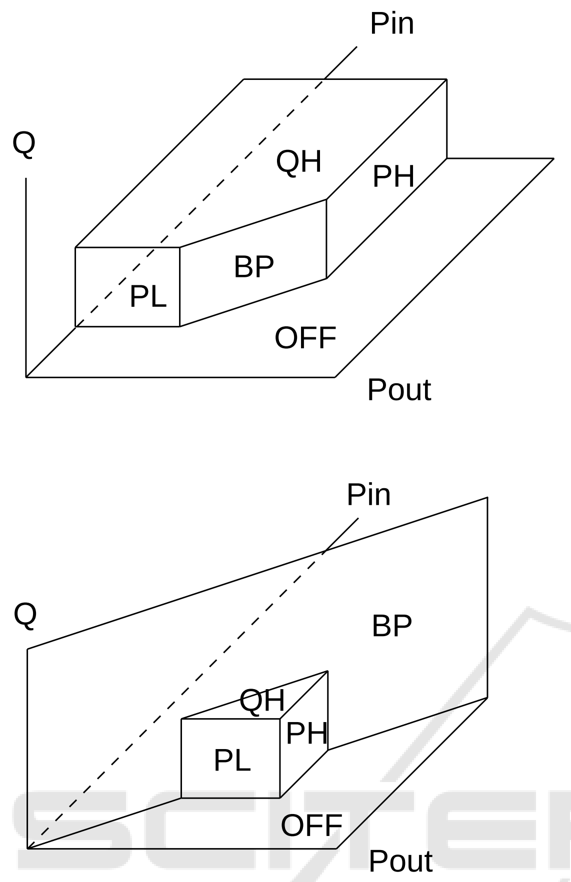

Figure 1: Control element diagrams. On the top: regulator, on the bottom: compressor.

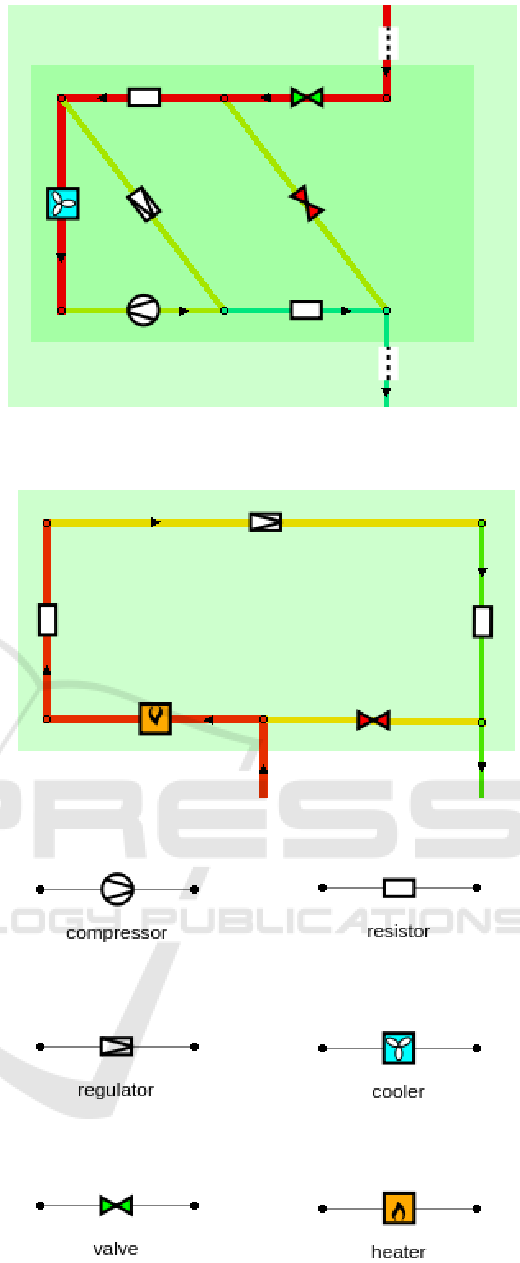

Figure 2: Gas transport network simulation in Mynts. On the top – closeup to a compressor station, on the middle – closeup to a regulator station, on the bottom – elements used.

3 APPLICATION TO GAS TRANSPORT NETWORKS

The simulation of the gas transport networks is performed by the software Mynts (Multi-phYsics NeTwork Simulator, www.scai.fraunhofer.de) developed in our group. A small training network used here for experiments is shown in Fig. 3. It contains 100 nodes, 111 pipes and other connecting elements, two *Pset* sources, three *Qset* sinks. Detailed structure of compressor and regulator stations is shown on Fig. 2. We note that real life problems are much larger. In cooperation with our partners we solve stationary and transient problems for gas networks with thousands of elements.

Stationary problems in gas transport networks are described by a system (2) with element equations satisfying the resistivity conditions $\nabla f = (+--)$. Typical elements used in gas transport networks are listed below.

Pipes: in the simplest case can be represented by a quadratic resistive model (Mischner et al., 2011)

$$P_{in}|P_{in}| - P_{out}|P_{out}| = RQ|Q|, \qquad (11)$$

where P is a pressure, Q is a flow, R is a resistance coefficient, depending on diameter, length and friction characteristics of the pipe. For realistic modeling more complicated element equations can be used, based on friction models by Nikuradze, Hofer

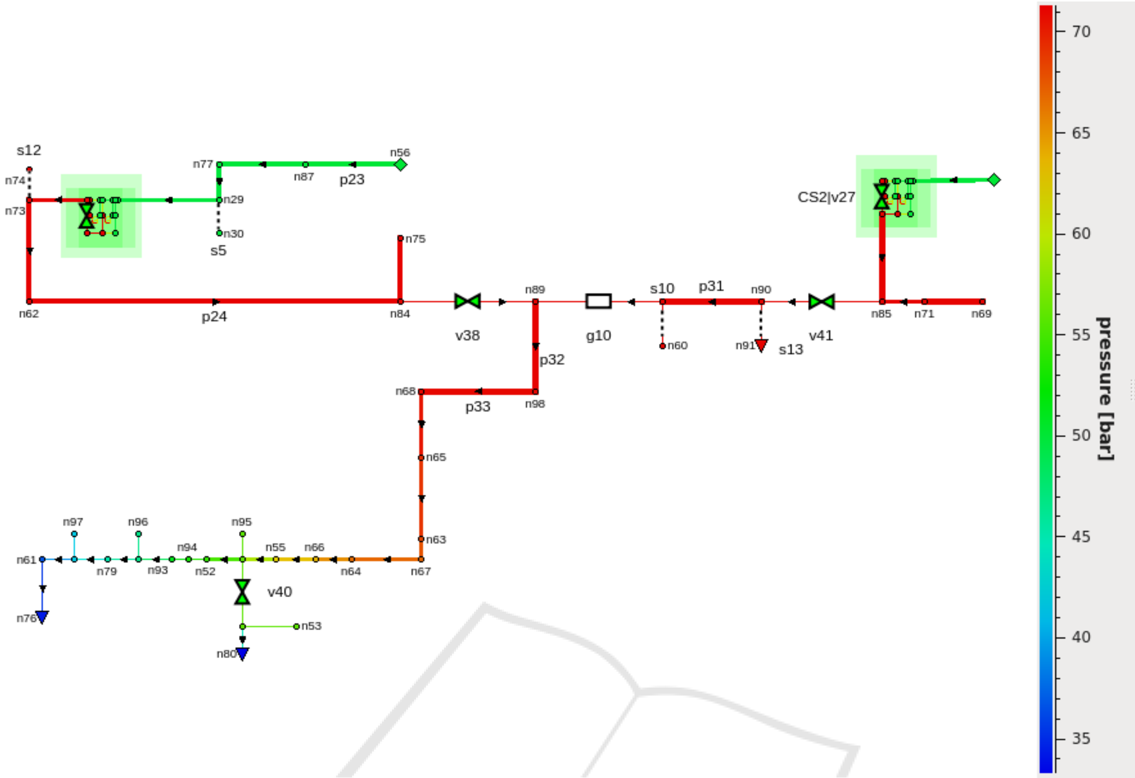

Figure 3: Gas transport network simulation in Mynts (cont'd). The network topology with the resulting pressure distribution, shown by color.

or Prandtl-Colebrook (Mischner et al., 2011; Schmidt et al., 2015).

Resistors: physically correspond to short pipe segments, described by the same quadratic formula, with R specified explicitly.

Valves: simple switching elements

$$P_{in} = P_{out} \quad \text{(open)}; \qquad (12)$$
$$Q = 0 \quad \text{(closed)}.$$

Regulators: control elements dropping pressure, physically correspond to a variable resistor, whose value is automatically adjusted to satisfy one of the following control goals: a fixed output pressure (SPO), a fixed input pressure (SPI) or a fixed flow value (SM). Being combined with the given upper and lower bounds: $PH = \min(SPO, POMAX)$, $PL = \max(SPI, PIMIN)$, $QH = \min(SM, MMAX)$, the element equation defines a polyhedral surface shown in Fig. 1, top. Here every face corresponds to the best possible satisfaction of the control goal, e.g., $P_{out} = PH$ (typical for SPO-mode), $Q = QH$ (typical for SM-mode), $P_{in} = P_{out}$ (bypass BP, equivalent to an open valve), $Q = 0$ (OFF, equivalent to a closed valve), etc. Like any piecewise linear equation, it can be represented in max-min form:

$$\max(\min(\min(\min(P_{in} - PL, -P_{out} + PH), -Q + QH), P_{in} - P_{out}), -Q) = 0. \qquad (13)$$

Compressors: control elements increasing pressure, they also have a resistive equation, similar to a battery with internal resistance in electrotechnics. They also can be configured to satisfy the control goals of SPO, SPI and SM type. The element equation defines a polyhedral surface shown in Fig. 1, bottom. The corresponding max-min form is:

$$\max(\max(\min(\min(P_{in} - PL, -P_{out} + PH), -Q + QH), P_{in} - P_{out}), -Q) = 0. \qquad (14)$$

Nodal equations: relate additional nodal variables, such as density ρ, temperature T etc., have the form of a gas law

$$P = f(\rho, T, \ldots) \ \text{ or } \ \rho = f^{-1}(P, T, \ldots), \quad (15)$$

using an approximation formula, such as AGA, Papay, ISO standard AGA8-DC92, etc. (Schmidt et al., 2015; CES, 2010). The physical stability of the medium requires that the functions f, f^{-1} increase monotonously w.r.t. the first argument, in this way supporting the existence and uniqueness of a solution.

In real scenarios further variables and equations are added, describing temperature distribution, gas composition, more detailed modeling of control elements, etc.

To provide a resistive property for all elements, their equations should be properly regularized. In pipe/resistor equations one needs to add a laminar term εQ to the right hand side, where ε is a small positive constant. This term provides non-degeneracy of the system and correct signature of the equation for $Q = 0$. Also the $\varepsilon(P_{in} - P_{out})$ term should be added to the left hand side to protect the system from similar problems at $P = 0$. Note that the absolute value function in the $Q|Q|$ and $P|P|$ terms has a different meaning: $Q|Q|$ provides the correct symmetry of the equation in reversal of the flow direction, while $P|P|$ removes a fold in the mapping and provides the existence and uniqueness of a solution everywhere in the space of variables, including the non-physical domain $P < 0$. Although the physical solution cannot be located in this domain, the tracing algorithm can wander there on intermediate iterations. Also, as we see below, this domain plays an important indicator role for the solution of feasibility problems.

For valves and control elements one should also introduce regularization terms to provide the resistive signature for every face of the element equation. Properly regularized equations have the form:

Valves:

$$P_{in} - P_{out} = \varepsilon Q \quad \text{(open)}; \qquad (16)$$
$$Q = \varepsilon(P_{in} - P_{out}) \quad \text{(closed)}.$$

Regulators:

$$\max(\min(\min(\min(P_{in} - \varepsilon P_{out} - \varepsilon Q - PL, \qquad (17)$$
$$\varepsilon P_{in} - P_{out} - \varepsilon Q + PH), \varepsilon(P_{in} - P_{out}) - Q + QH),$$
$$P_{in} - P_{out} - \varepsilon Q), \varepsilon(P_{in} - P_{out}) - Q) = 0.$$

Compressors:

$$\max(\max(\min(\min(P_{in} - \varepsilon P_{out} - \varepsilon Q - PL, \qquad (18)$$
$$\varepsilon P_{in} - P_{out} - \varepsilon Q + PH), \varepsilon(P_{in} - P_{out}) - Q + QH),$$
$$P_{in} - P_{out} - \varepsilon Q), \varepsilon(P_{in} - P_{out}) - Q) = 0.$$

Here the max-min functions can be transformed to an absolute value representation

$$\max(x, y) = (x + y + |x - y|)/2, \qquad (19)$$
$$\min(x, y) = (x + y - |x - y|)/2,$$

one can also use, for the absolute value function, its smooth regularization:

$$|x|_\varepsilon = \sqrt{x^2 + \varepsilon^2}. \qquad (20)$$

The obtained system belongs to the generalized resistive type and, therefore, it always has a unique solution. On the other hand, it can happen in real scenarios that they do not have a solution. The determination whether a solution for given conditions exists represents a so-called feasibility problem. Usually solutions disappear when one requires too much from the network, e.g., to transport a large amount of gas through a long pipe system with only one supply where Pset=10 bar and all compressors are switched off. There is no physical solution for such a scenario, while a solution of our generalized resistive system will exist. This solution, however, will be located in the non-physical domain, where some nodes have negative pressure. This can be used as an indicator of feasibility for the tested scenario.

Practically, observing the work of the algorithm, we often see that a solution goes to the non-physical domain, wandering there along complex trajectories. Finally it either returns to the physical domain if the problem is feasible or remains in the non-physical domain otherwise. Considering the solution as the function of a regularization parameter $x^*(\varepsilon)$ and removing the regularization $\varepsilon \to +0$, we observe that the solution for feasible problems will have a limit in the physical domain, while for infeasible ones it either has a limit in the non-physical domain or tends to infinity.

We note that ε-regularization is one possibility to provide global convergence of the tracing algorithm. The other possibility is a modification of the algorithm described in (Chien and Kuh, 1976), making it applicable also for degenerate Jacobi matrices encountered in bounded pieces. An investigation of this possibility is part of our further plans.

We have implemented the tracing algorithm in a test mode in our network simulator Mynts under the option solver_strategy=stable. Using a number of realistic scenarios from our partners, we have compared the performance of the algorithm vs. the option solver_strategy=standard, representing a generic Newton's solver. The results of our comparison are presented in Table 1. We see that the generic solver provides worse convergence and diverges in certain scenarios, while the tracing algorithm always converges, in agreement with its theoretical property. In these experiments we use the simplest version of the tracing algorithm with a trivial homotopic subdivision ($k = 1$) and the backtracking line search switched off. We see that already this version provides convergence in all considered scenarios. A study of the relationship between the performance of the algorithm and its homotopic and line search settings is planned.

Table 1: Gas transport network simulation, comparison of the two algorithms. For every network two scenarios are considered, different by numerical values of *Pset*, *Qset* and compressor/regulator *SM*, *SPO* settings. Divergent cases are marked as ’div’. Timings are given for a 3 GHz Intel i7 CPU.

network	nodes	edges	scenario	solver_strategy				feasible?
				standard		stable		
				iterations	time, sec	iterations	time, sec	
N1	100	111	S1	3	0.01	2	0.01	Y
			S2	57	0.17	4	0.02	Y
N2	931	1047	S1	11	0.27	8	0.25	Y
			S2	div	–	58	1.7	N
N3	4466	5362	S1	div	–	13	2.0	Y
			S2	47	6.5	14	1.9	Y

4 CONCLUSIONS

We have considered generalized resistive systems, comprising linear Kirchhoff equations and non-linear element equations of the form $f(P_{in}, P_{out}, Q) = 0$, possessing a signature $\nabla f = (+--)$. For such systems we have proven the global non-degeneracy of the Jacobi matrix and the applicability of globally convergent tracing algorithms. Considering stationary problems in gas transport networks, we have shown that the underlying equations can be rewritten in generalized resistive form. The piecewise smooth tracing algorithm has been applied to several realistic networks and its performance has been compared with a generic Newton solver. The generic solver provides slower convergence and fails in certain scenarios. The tracing algorithm has better performance and converges for all scenarios.

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