MYNTS: Multi-phYsics NeTwork Simulator

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Abstract: We present a generic approach for the simulation of transport networks, where the steps of physical modeling and numerical simulation are effectively separated. The model is described by a list of physical equations and inequalities as problem constraints for non-linear programming (NLP). This list is translated to the language of expression trees and is made accessible for the numerical solution by standard NLP solvers. Various problem types can be solved in this way, including stationary and transient network simulation, feasibility analysis and energy-saving optimization. The simulation is provided for different disciplines, such as gas transport, water supply and electric power networks. We demonstrate the implementation of this approach in our multiphysics network simulator.

1 INTRODUCTION

The simulation of transport networks in civil engineering becomes increasingly important for the planning and stable operation of modern infrastructure. Many software systems exist for the solution of specialized problems in the simulation of gas transport networks (Scheibe and Weimann, 1999; Aymanns et al., 2008), water supply (Rogalla and Wolters, 1994; Stevanovic et al., 2009), electric power transmission (Milano, 2015; Zimmerman and Murillo-Sanchez, 2015), etc. Our purpose is to develop a universal system capable of solving all problems of this kind, as well as of providing for them an energetically efficient optimal solution. The system has to be maximally open in terms of mathematical modeling and numerical solver, allowing the user to extend the system by new element types and new conditions and to upgrade it by modern highly efficient algorithms.

The possibility of such a universal solution follows from the great similarity of the considered problems. Indeed, different network disciplines represent the network topology as a graph on which problems of the following types are formulated:

- stationary problems – systems of non-linear equations $f(x) = 0$;
- transient problems – differential-algebraic equations, DAEs, $f(x, \dot{x}) = 0$;
- feasibility problems – find (any) solution of the system of equations and inequalities $f(x) = 0$, $g(x) \geq 0$;
- constrained optimization – find min $h(x)$ such that $f(x) = 0$, $g(x) \geq 0$.

Note that constrained optimization is the most general formulation, while the three others represent its particular cases: stationary problems – in the absence of the inequalities $g(x) \geq 0$ and with a trivial objective function $h(x)$ one has to solve only non-linear systems $f(x) = 0$; the sequential solution of non-linear systems represents a process of (semi-)implicit integration of a DAE; feasibility problems also belong to constrained optimization, where one can select an arbitrary objective function.

In its most general form constrained optimization is also known as non-linear programming, NLP, for which, since the 1970s, many efficient algorithms have been developed (Bazaraa and Shetty, 1979; Bertsekas, 1999; Avriel, 2003; Fletcher, 2013) and implemented in a number of software packages (Murtagh and Saunders, 1978; Gill et al., 2005; Wächter and Biegler, 2006; Nocedal and Wright, 2006; Belotti et al., 2013). Nowadays the solution of the above listed problems is as easy as the solution of a linear sparse system, one only needs to represent the problem in a standard form, accepted by the corresponding software package. Continuing this analogy, the solution of a linear sparse system requires to specify the system matrix in a triplet, a column or a row

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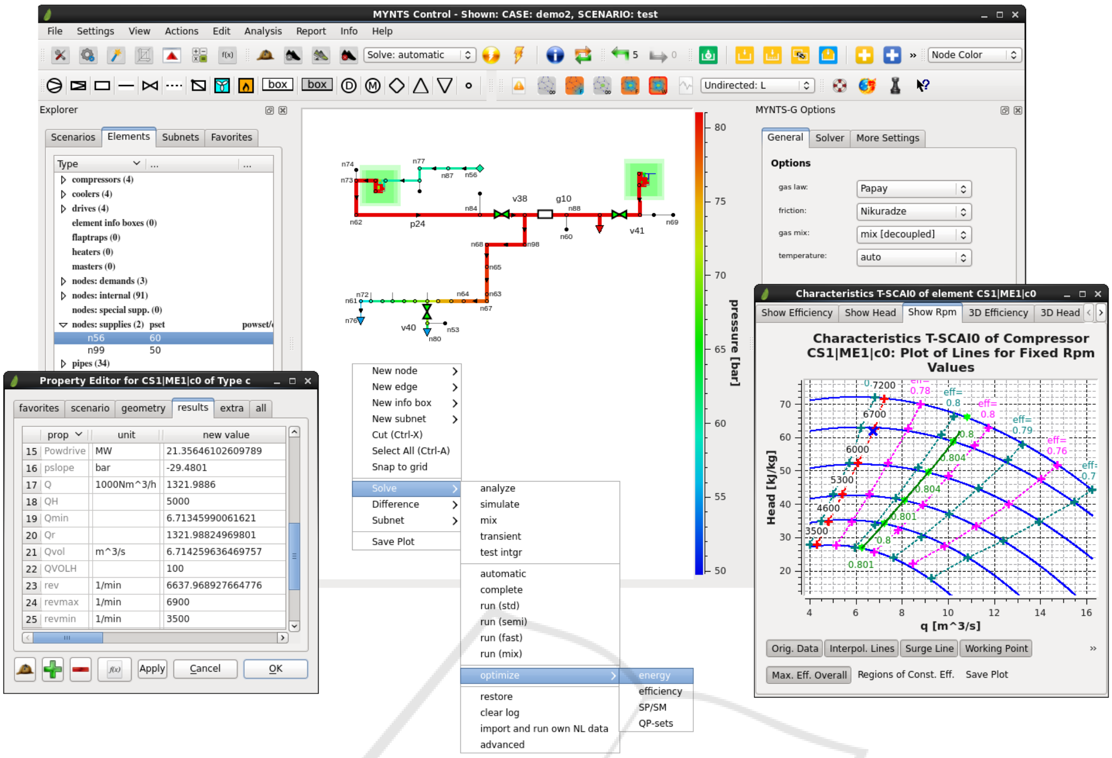


Figure 1: Gas transport network simulation in Mynts.

compressed form, while NLP solvers accept systems of non-linear equations in the form of so-called expression trees (Gay, 2005). This de facto standard is supported by many existing NLP solvers, while newly developed algorithms can be easily equipped with the necessary interface. In this way the mathematical modeling becomes effectively separated from the solution algorithms, providing the required flexibility and modularity of the software.

The same transport network problem can have various representations: a human-readable description of the network (e.g. in NetList format, used in practice for solution of real-life problems for gas, water and electric power transport (Baumanns et al., 2012; Clees, 2012; Clees, 2016; Clees et al., 2016a; Clees et al., 2016b)), formats understandable only by simulation kernels (e.g. NL (Gay, 2005)), there is also an intermediate level of modeling languages (such as AMPL (Fourer et al., 2002), Modelica (Modelica, 2012)). Well designed simulator should be able to translate the problem between its different representations and do it fast for large realistic problems. In this paper we describe the algorithms suitable for this purpose.

Related work: in (Clees, 2012) we present general concepts common for all types of transport network problems, in (Clees, 2016) we describe the gas part of our simulator applied for parameter studies in gas transport networks, in (Clees et al., 2016a; Clees et al., 2016b) the detailed modeling of water cooling networks is given. Our advancement reported in the present paper is the development of general algorithms for formulation and solution of transport network problems based on their representation in NLP form. In the first place, we have the task to translate between different problem encodings, i.e., between a human-readable description of the transport network problem and the language understood by NLP solvers. We tackle these aspects in Section 2. Different approaches for solving NLPs are discussed in Section 3. Our system Mynts with its main components and examples of usage is presented in Section 4.

2 PROBLEM FORMULATION

Network problems can be presented as a list of elements (nodes, edges), containing a topological definition (in the form of an incidence matrix, i.e., every edge should refer to the two nodes it connects to) and a set of properties used for problem formulation (e.g., node coordinates, pipe length, diameter, etc). For instance, a gas transport problem can have the following form.

Network base description:

```
# Nodes
n, name="n56", H=5.2, X=14400, Y=10800
n, name="n99", H=0, X=18471.821, Y=10670.833
....
# Pipes
p, name="p11", node1="n93", node2="n94",
   L=7900.0, D=0.5, k=0.02
p, name="p12", node1="n94", node2="n52",
   L=4700.0, D=0.5, k=0.02
....
# Compressors
c, name="CS1|ME1|c0", node1="CS1|ME1|n2",
   node2="CS1|ME1|n3"
c, name="CS1|ME2|c0", node1="CS1|ME2|n4",
   node2="CS1|ME2|n5"
....
```

For user convenience, this description can be divided into sections where the properties for a *class* of problems are listed (base) and where problem *variations* are set (scenario). They can also be stored in separate files.

Network scenario description:

```
name="n56", PSET=50, gasmix="gas1"
name="n99", PSET=60, gasmix="gas2"
name="n76", QSET=300
name="n91", QSET=1000
name="CS1|ME1|c0", MODE="PO", SPO=80,
   model="advanced", cchar="T-SCAI0",
   echar="P-SCAI0"
name="CS1|ME2|c0", MODE="M", SM=500,
   model="advanced", cchar="T-SCAI1",
   echar="P-SCAI1"
```

A scenario for a gas transport problem typically contains pressure settings in supply nodes (PSET), outflow settings in exit nodes (QSET), references to gas composition (gasmix), compressor mode settings, such as output pressure (SPO) and output flow (SM), a model of operation (advanced or free), a reference to characteristics of compressor (cchar) and its driving engine (echar), etc. Any properties can be added, they should only make sense in the context of the considered discipline.

The discipline description is a list of translation rules, which allow to compose variables, equations and inequalities given per element.

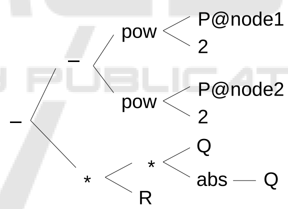
Network discipline description:

```
# Variables
for every node:
  var P,rho,T,...
  # pressure, density, temperature
for every edge:
  var Q... # flow
for every compressor:
  var Rev,Perf,Had...
  # revolutions per minute, power,
  # adiabatic enthalpy difference
.....
# Equations
for every node:
  eq gas_law(rho,P,T, gasmix,...)=0
for every pipe:
  eq pipe_law(P@node1,P@node2,Q, L,D,...)=0
.....
```

Here the section of variables extends the list of properties per given element by new properties whose values will be computed in the network simulation. Equation prototypes combine the properties with expressions representing the underlying physical laws. Gas transport simulation can use several types of laws for gas compressibility, pressure drop in pipes and compressor working conditions, in more detail considered in Section 4. They can also be extended by the user, by specifying a formula per element or a class of elements. Let us demonstrate this by defining a quadratic pipe law (Mischner et al., 2011) by the equation:

```
pow(P@node1,2)-pow(P@node2,2)-R*Q*abs(Q)=0
```

A translation utility represents this equation in the form of an *expression tree:*



then, using the correspondence

P@node1	P@node2	Q	R	2
v1	v2	v3	n0.1	n2
pow	abs	*	-	
o5	o15	o2	o1	

the tree is traversed by the left-hand rule and encoded in *Polish prefix notation (PPN)*:

```
o1 o1 o5 v1 n2 o5 v2 n2 o2 o2 v3 o15 v3 n0.1
```

In the obtained representation of the expression tree the leaves are variables (v...) and constants (n...), while the branches are operators (o...). A representation in the form of an expression tree makes equations suitable for automatic differentiation using the chain rule. A detailed description of the encoding procedure can be found in (Gay, 2005). The interface supports more than 70 basis operators and a possibility to extend them by arbitrary user defined functions. PPN encoded expression trees are the language which many NLP solvers understand.

In terms of general theory (Harrison, 1978) all these representations belong to *formal languages*, being sets of strings of symbols, constrained by specific rules. The network description and the lists of equations in human-readable or NLP format define different formal languages, while the description of the discipline provides a means for translation, in a way:

$$\textit{discipline} * \textit{network description} = \textit{NLP}.$$

Algorithmically, this can be done as follows.

Algorithm 1: Problem translation.

```
read network graph (base and scenario);
read vars and eqs prototypes (discipline);
translate eqs prototypes to NLP format
  with placeholders for vars and consts;
loop over element:
  create vars per element according
    to the discipline description;
  place them into the graph as sequentially
    numbered ids (v1...vn);
loop over element:
  create eqs per element according to
    the discipline description;
  substitute actual vars and consts
    to the placeholders;
output the eqs.
```

Since the main part of the algorithm is a straightforward substitution (stamping), it requires $O(N+E)$ operations, where N and E are the numbers of nodes and edges in the network graph, respectively.

3 PROBLEM SOLUTION

In the field of applied optimization the problems are often subdivided into two parts: simulation and optimization. Simulation solves the part of the problem defined by equations $f(x,y)=0$ with respect to some part of the variables y, while the remaining variables x are considered as constant parameters. Then optimization is applied to the objective function $h(x,y)$, with respect to the variables x, while y is permanently updated for the given x using the simulation. Algorithmically this can be expressed as follows.

Algorithm 2: Optimization on top of the simulation.

```
define y(x):
  solve f(x,y) w.r.t. y;
  return y;
optimize h(x,y(x)) w.r.t. x.
```

An alternative is to use NLP algorithms which solve the optimization and simulation parts simultaneously.

Algorithm 3: NLP.

```
optimize h(x,y) w.r.t. (x,y) s.t. f(x,y)=0.
```

The first variant is often used if the simulation and/or the optimization are considered as blackbox algorithms, e.g., if simulation $y(x)$ is encapsulated in a proprietary software tool. In this case one is reduced to applying the first algorithm indeed. The second variant composes a unified system of equations $f(x,y)=0$ and optimality conditions for $h(x,y)$, which are solved simultaneously by means of superconvergent methods (usually a stabilized Newton's method). The first algorithm finds, for every value of x, an exact solution of the system $f(x,y)=0$. This is completely superfluous for intermediate optimization steps when x is only an approximation to the optimum. For the second algorithm the precision of the solution for the equations and the precision of the optimality conditions are improved simultaneously in the solution process, so that a precise solution of the simulation problem is obtained only at the last step, being also the optimal one. For the first algorithm the required computational effort can be estimated as $O(Nsim\ Nopt)$, where $Nsim$ is the number of iterations per simulation and $Nopt$ is the number of optimization steps. The second algorithm solves a unified system, which is almost entirely composed of the equations from the simulation part, so that the overhead related to the optimality conditions is usually small and the overall effort becomes $O(Nsim)$. Thus, NLP algorithms definitely win in performance and, therefore, they are our preferred choice.

The possibility to represent gas network simulations in NLP form has been earlier discussed in (Schmidt et al., 2015a), where the mathematical modeling of gas transport networks has been considered in great detail. However, the implementation (Schmidt et al., 2015b) used the simplest possible NLP version, a penalty method, taking a cumulative norm of the residuals of the physical equations as single objective function. This approach admits a violation of the physical constraints (gas laws, etc). Although the global minimum of this objective coincides with the solution for feasible problems, there is danger that the solution process gets stuck in a local minimum and the physical solution will be lost. Also, one cannot simply add a real objective there, like the total power of all compressors in energy optimization, since the improvement of the objective would be achieved at the cost of the violation of the physical equations. Fortunately, this is easy to correct and in our implementation all physical equations are set as equality constraints $f(x) = 0$ and, at solutions, are satisfied exactly.

For solving NLPs many efficient algorithms have been developed (Bazaraa and Shetty, 1979; Bertsekas, 1999; Avriel, 2003; Fletcher, 2013), e.g., those implemented in the optimization package Ipopt (Wächter and Biegler, 2006):

- an interior-point algorithm (also known as primal-dual barrier method) for the solution of generic NLPs with equations and inequalities;
- a line-search filter with second order corrections, serving as a stabilizer for Newton's method;
- an inertia correction method, driving the iterations towards a critical point of the desired type (e.g., minimum, not maximum, not saddle point);
- a feasibility restoration method, applying an emergency restart in the case that the convergence becomes too slow;
- an automatic initialization, appropriate problem scaling, interfaces to many sparse linear solvers, etc.

Our approach, using the translation of network problems to the standard NLP format, also allows to employ for their solution any other package, such as Snopt (Gill et al., 2005), Minos (Murtagh and Saunders, 1978), Knitro (Nocedal and Wright, 2006), etc. For the solution of mixed integer NLPs one can use Couenne (Belotti et al., 2013), while multiobjective optimization can be done with the approaches described in (Clees et al., 2015).

4 NETWORK SIMULATION IN MYNTS

The backbone of the system is formed by linear Kirchhoff equations and non-linear element equations, depending on the flow through an element and on its two adjacent nodal variables:

$$\sum_e I_{ne} Q_e = Q_n^{(s)}, \; f_e(P_{in}, P_{out}, Q_e) = 0, \quad (1)$$

where indices $n = 1...N$ denote the nodes and $e = 1...E$ the edges of the network graph, I_{ne} is the incidence matrix of the graph, Q_e are flows through the edges, $Q_n^{(s)}$ are source/sink contributions, localized in the supply/exit nodes, P_n are nodal variables (pressure, voltage, etc – depending on the discipline). For example, in gas transport networks the simplest pipe law has a quadratic form (Mischner et al., 2011):

$$f_e = P_{in}^2 - P_{out}^2 - R Q_e |Q_e|, \quad (2)$$

where R is a resistance coefficient, depending on pipe length L, diameter D, friction factor λ, temperature T, compression factor z and on pressure, temperature and density at normal conditions $(P_{norm}, T_{norm}, \rho_{norm})$:

$$R = \frac{16 \, \lambda \, L \, T \, z \, P_{norm} \, \rho_{norm}}{\pi^2 \, D^5 \, T_{norm}}. \quad (3)$$

System (1) describes a stationary network problem, while for dynamical (transient) problems additional terms with time derivatives are included. Specific for every medium, new equations can be introduced, relating additional nodal and element variables.

Modeling of gas transport networks in Mynts includes the following building blocks, described in detail in (Schmidt et al., 2015a; Mischner et al., 2011; CES, 2010):

- main elements: supplies, exits, pipes, valves, compressors, drives, regulators, resistors, shortcuts, flaptraps, heaters, coolers;
- gas laws: ideal, AGA, Papay, AGA8-DC92 (ISO standard);
- pressure drop in pipes: besides the quadratic law, more accurate Hofer and Nikuradze formulae are used;
- various models for compressors (turbo, piston) and their drives (gas turbine, steam turbine, gas motor, electro motor), with characteristic diagrams calibrated on real compressors;
- control logic of compressors and regulators, implemented in the form of control equations or inequalities, e.g., a compressor/regulator can have a control goal to keep fixed output pressure (SPO), input pressure (SPI) or flow value (SM);
- gas temperature: propagation over the network, including non-linear heat capacity, heat exchange with the soil, Joule-Thomson effect (temperature drop in gas due to free expansion through a valve, regulator, etc);
- gas composition: propagation and mixing (including detailed molar components and effective gas properties like critical temperature and pressure, calorific value, molar mass, etc).

Modeling of water networks strongly resembles the modeling of gas transport networks, except that a set of important simplifications can be applied. In Mynts it is assumed, e.g., that transient effects and the compressibility of the fluid do not play a role. Hence, the constitutive assumption, which relates the pressure to the density of a compressible fluid, is omitted. Moreover, only the temperature is considered as internal energy and only one phase of liquid water is being modeled. Mynts includes the following building

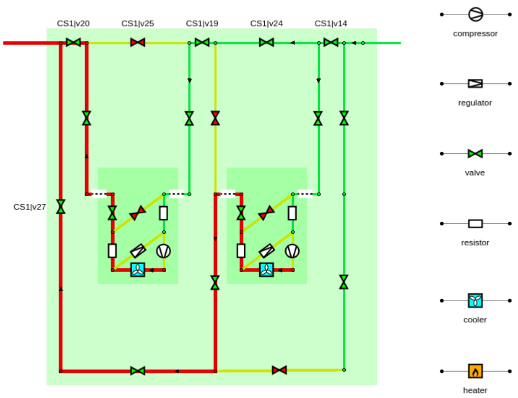


Figure 2: Gas transport network simulation in Mynts. Closeup to a compressor station.

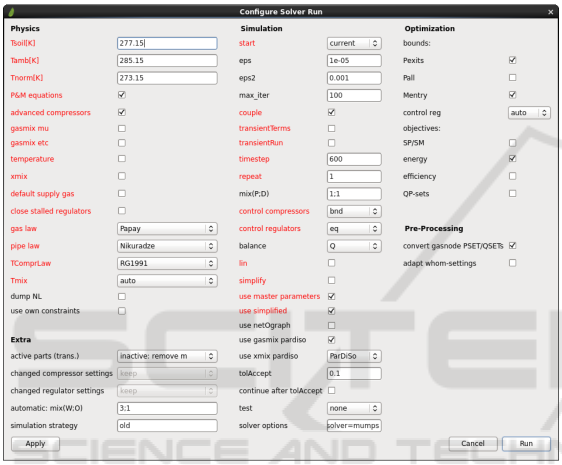


Figure 3: Gas transport network simulation in Mynts. Configuration of the solver.

blocks, which are described in detail in (Clees et al., 2016a; Clees et al., 2016b; Colburn, 1933; Colebrook, 1939; VDI/VDE, 1962; KSB AG, 2005; Brkić, 2011):

- main elements: supplies, exits, pipes, resistors, two-way and three-way valves, pumps and heat exchangers;
- pressure drop in pipes: Bernoulli's equation with friction including a variety of implementations for Colebrook's friction factor (more complex armatures are considered as simple resistors via their k_{vs}-values);
- models for regulated and unregulated pumps (including user defined characteristic curves), heat exchangers and two-way or three-way valves with linear and equal percentage characteristics;
- simple control via goals defined either for pump speed or valve lift, or – at arbitrary elements of the network – for pressure, pressure drop, flow rate or temperature;
- water temperature: propagation and mixing over the network, power supply and exit at dedicated elements, heat exchange with the environment and with other network elements.

Modeling of electric power networks (Herman, 2011; Milano, 2010):

- main elements: buses (generators, consumers, prosumers, internal) and branches (transmission lines, transformers and phase shifters, shortcuts);
- voltage drop in lines due to resistances (direct-current, DC) or impedances (alternating-current, AC): analogously to Ohm's law for DC circuits, the voltage drop in an AC circuit is the product of the current and the impedance of the circuit; electrical impedance is the vector sum of electrical resistance, capacitive reactance and inductive reactance;
- Norton scheme (admittance formulation): all constant impedance elements of the model are incorporated into a complex bus admittance matrix that relates the complex nodal current injections to the complex node voltages; similarly, the system branch admittance matrices relate the bus voltages to the vectors of branch currents at the from and to ends of all branches, respectively;
- various types of transformers, their parameters (e.g. tap ratio, phase shift) and connections (Delta, Wye, Wye-G).

Fig. 1 shows an example of a gas transport simulation in Mynts. The network, used here for illustration, contains 100 nodes, 111 pipes and other connecting elements. 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.

The color in Fig. 1 shows the pressure distribution in the network, which starts from 50 bar and 60 bar, respectively, at the two supply nodes, is increased to 80 bar by two compressor stations and then gradually falls to 55 bar at the exit nodes.

On the bottom right a characteristic diagram of one compressor is shown, where the horizontal axis refers to the volume flow through the compressor, the vertical axis to the adiabatic enthalpy difference, the blue parabolic curves correspond to fixed revolution numbers, the magenta and dark cyan lines to fixed adiabatic efficiency, the green line to maximal efficiency and the red line to the minimal possible throughput flow for the given pressure increase (the so-called *surge line*). The curves for the maximal and the minimal revolution numbers and the surge line define a working region of the compressor, where the working point must be located (shown by a blue cross, here located on the surge line). In addition, there is an upper limit for the power, provided by the compressor drive, and there are lower and upper limits on input and output pressure and flow, which together with other control equations and inequalities contribute to the whole NLP system.

The solution of the NLP system can either be performed as a "pure simulation" (solve>simulate) or as a simulation with optimization (solve>optimize). For the optimization the following objectives can be selected:

- energy: minimize the total power, provided by all drives;
- efficiency: maximize the average adiabatic efficiency for all compressors;
- SPSM: minimize the deviation from the prescribed pressure and flow conditions in compressors and regulators (SPO, SPI, SM);
- QP-sets: minimize the deviation from the prescribed flow settings (QSET) for supply nodes with the given pressure settings (PSET).

The energy optimization allows to achieve the best energy savings of the gas transport for a given network scenario. The efficiency optimization tries to set all compressors on their central green lines. The optimization of SPSM/QP-sets allows to control the distribution of load between compressors/suppliers.

Fig. 2 shows a closeup of a compressor station. It consists of two compressors, which by means of a special pattern of open and closed valves are connected parallel to each other. Each compressor has input and output resistors and is equipped with a cooler, compensating the temperature increase in the compressor, and a bypass regulator. This regulator is automatically opened if the working point reaches the surge line and provides an internal gas circulation to keep a constant output pressure for small outflows. There is also a bypass valve, which opens only if the compressor is shut down.

Fig. 3 shows a menu for detailed solver configuration. In particular, it allows to set various physical parameters, switch between the physical models, add transient terms, choose a solution method (e.g., the whole problem can be solved as a coupled system at once or in blocks using an iterative relaxation scheme), set the maximal number of iterations, the solver tolerance, select deep options to the solver, etc. The optimization part allows to select the above described objectives or their combinations.

The viewer visualizes the network hierarchically, switching automatically the level of detail suitable for the current zoom factor. The user can select a property shown on the graph by color or by the variable width of the edges and nodes, change the size and shape of visual elements, the detailization of the displayed information, etc.

Graphical user interface of Mynts is not only a network viewer, but also a scalable network editor. It allows to create and modify the network topology (new nodes/edges, connect, merge, split, etc) and also to edit the properties of the elements. For example, the left bottom menu in Fig. 1 shows the details of a compressor element, where the user can inspect different properties and modify the settings.

The detailed numbers on Mynts performance are given in our satellite paper (Clees et al., 2016c). In particular, solution of a realistic gas transport network scenario with 4466 nodes and 5362 edges requires 1.9sec on a 3 GHz Intel i7 CPU.

5 CONCLUSIONS

We have presented a generic approach for the simulation of transport networks. The main steps of physical modeling and numerical simulation are effectively separated. Input data for the modeling come in the form of lists representing the topology of the network, physical properties of the elements and a prototypical description of variables and constraints defining the discipline. A rapid algorithm translates the problem statement into the language of PPN encoded expression trees, making it accessible for the numerical solution by standard NLP solvers. The applicability of this approach has been demonstrated on various problem types, including stationary and transient network simulation, feasibility analysis and energy-saving optimization. The approach has been implemented in our multiphysics network simulator Mynts, supporting various disciplines, such as gas transport, water supply and electric power networks.

Our further plans include the support of other disciplines (steam engines, mechanical transmissions, pipelines in the chemical industry), the solution of cross-disciplinary problems and interfacing to other simulation kernels and modeling systems (Couenne, SCIP, Modelica).

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