

Universal Translation Algorithm for Formulation of Transport Network Problems

Anton Baldin, Kläre Cassirer, Tanja Clees, Bernhard Klaassen,
Igor Nikitin, Lialia Nikitina and Inna Torgovitskaia

Fraunhofer Institute for Algorithms and Scientific Computing, Schloss Birlinghoven, 53754 Sankt Augustin, Germany

Keywords: Complex Systems Modeling and Simulation, Non-Linear Systems, Applications in Energy Transport.

Abstract: The formulation of transport network problems is represented as a translation between two domain specific languages: from a network description language, used by network simulation community, to a problem description language, understood by generic non-linear solvers. A universal algorithm for this translation is developed, an estimation of its computational complexity given, and an efficient application of the algorithm demonstrated on a number of realistic examples. Typically, for a large gas transport network with about 10K elements the translation and solution of non-linear system together require less than 1 sec on the common hardware. The translation procedure incorporates several preprocessing filters, in particular, topological cleaning filters, which accelerate the solution procedure by factor 8.

1 INTRODUCTION

This short paper continues our previous work (Clees et al., 2016), where we discuss a general possibility for formulation of transport network problems as a translation between two abstract representations, a human-readable network description and a solver-specific code. This approach provides an open type of modeling, where both the network description and the physical laws defining the transport are completely in the hands of the user and can be given as plain text files. There is a universal translation procedure converting them to a problem description suitable for a given solver. In this approach one is not bound to any particular program and is flexible in the choice and experimentation with different solution kernels.

In state of the art, the solution of transport network problems combines well established modeling approaches with the standard solvers of non-linear systems. The network applications vary by the types of transported media: water supply (Rogalla and Wolters, 1994; Stevanovic et al., 2009), electric power transmission (Milano, 2015; Zimmerman and Murillo-Sanchez, 2015), gas transport networks (Scheibe and Weimann, 1999; Aymanns et al., 2008), etc. For each of them different types of network problems can be formulated: stationary, dynamical, feasibility, optimization, optimal control. All these prob-

lems can be represented in terms of non-linear programming (NLP), for which powerful solution algorithms are available (Bazaraa and Shetty, 1979; Bertsekas, 1999; Avriel, 2003; Fletcher, 2013). The algorithms are implemented in various software packages: MINOS (Murtagh and Saunders, 1978), SNOPT (Gill et al., 2005), IPOPT (Wächter and Biegler, 2006), KNITRO (Nocedal and Wright, 2006), COUENNE (Belotti et al., 2013). None of the approaches, however, provides a universal algorithm for formulation of transport network problem which would be independent on the type of transport media and a particular solver.

In spite of the variety of different possibilities, there is a common way of formulating the network problems, based on the fact that the network descriptions for all types are quite uniform. The networks are given as graphs with the properties, assigned per element. The physical laws, describing the propagation of properties over the graph, are given as equations and inequalities, assigned per element type. The equations can be written in the syntax of the target solver, e.g., in a form of expression trees (Gay, 2005) or a human-readable syntax of higher level systems, such as AMPL, Modelica, Mathematica, Matlab. Considering the network description as an abstract text and the list of physical laws as a dictionary, one can represent the problem formulation as a trans-

lation procedure between two formal languages (Harrison, 1978).

In the present paper we will describe an implementation of this idea, give detailed estimations of computational complexity, present several realistic examples and the results of performance tests. We will also discuss the aspects of multiphase solution procedure and a coupling of multiple network sectors. The translation procedure is straightforwardly implementable and highly parallelizable, allowing separate processing per every element.

In Section 2 the main translation algorithm is presented, its functionality is demonstrated on a simple example of the water supply network and its computational complexity is estimated. In Section 3 the filters are described, implementing the necessary pre- and postprocessing steps. In Section 4 several realistic examples are considered and the results of the corresponding performance tests are given.

2 THE ALGORITHM

The network (*NET*) is described by a set of *elements*, each of them is a set of *properties*, each specified by a map from the property *name* to the property *value*, of the form `prop=val`. The names and values can be generally represented as character strings.

Translation matrix (TM) is a set of rules defining *variables* and *equations*, applied when the elements match a specified pattern. The pattern is given also as a set of properties of the form `prop=val`. If this set is a subset of properties in the element, the rule is applied to the element.

The rules defining the variables have a form `var=prop`. When the rule is applied, a new variable v_i is introduced and the property `prop= v_i` is inserted in the given element.

The rules defining the equations have a form `eq=expr`, where `expr` contains a mathematical formula for the equation in the target syntax. The formula has constant, non-modifiable parts and variable parts. The variable parts are marked up by square brackets, containing the property names, in the form `[prop]`. When the rule is applied, the property is found in the given element, replaced by the corresponding `val` and the brackets are removed. As a result, the corresponding variables and constants from the given element become substituted into the equation. Algorithmically, this can be done as follows.

Algorithm (universal translator):

```
variables:
  foreach element in NET
    for all matching var prototypes in TM
```

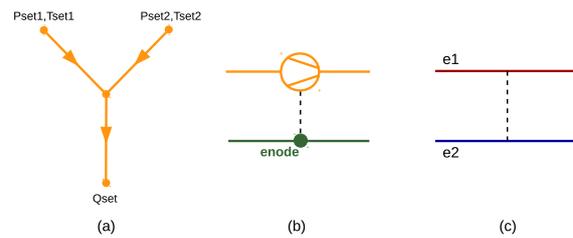


Figure 1: Examples of networks. From left to right: simple water network with three pipes, coupling between the edge in gas network and the node in power network, coupling between two edges.

```
define variables (v0,v1,...)
put them to element (prop=v0,...)
```

```
equations:
  foreach element in NET
    for all matching eq prototypes in TM
      find [props] in element description
      substitute their vals into the equation
      stream the equation
```

Let us show the work of the algorithm on the following example. The test network is displayed on Fig. 1 left. It is intentionally simple, for illustration purposes.

Example 1.1: water network (NET)

```
# nodes
class=n,name=n1,type=pset,pset=7
class=n,name=n2,type=pset,pset=5
class=n,name=n3,type=demand
class=n,name=n4,type=qset,qset=30
# edges
class=e,name=p1,type=p,node1=n1,node2=n3,R=0.3
class=e,name=p2,type=p,node1=n2,node2=n3,R=0.05
class=e,name=p3,type=p,node1=n3,node2=n4,R=0.1
```

The network description contains topological representation of the graph in the form of connections (`node1,2`). It also specifies water supply pressures (`psets`), output flow (`qset`) and hydraulic resistances of the pipes (`R`).

Example 1.2: translation matrix for water networks with laminar flow (TM)

```
# variables with start values
class=n, var=P, var0=1
class=e, type=p, var=Q, var0=0

# Kirchhoff law
class=n, type=demand, eq="[sumadj][Q]"
class=n, type=qset, eq="[sumadj][Q]-[qset]"
class=n, type=pset, eq="[P]-[pset]"

# equations of elements (linear resistors)
class=e, type=p,
  eq="[P@node1]-[P@node2]-[R]*[Q]"
```

The translation matrix introduces for every node (class=n) the pressure variable P with the starting value 1, for every pipe (class=e, type=p) the flow variable Q with the starting value 0. The equations incorporate Kirchhoff law written for every node. It is represented by an operator [sumadj], implementing a sum of flows in edges adjacent to a given node, with the signs specified by the incidence matrix of the graph:

$$[\text{sumadj}][Q]_n = \sum_e I_{ne} Q_e. \quad (1)$$

The incidence matrix I is internally evaluated using given connectivity data. The other equations describe linear pressure drops according to the given resistances. A reference operator is used to define pressure in end nodes: [P@node1,2].

The application of translation algorithm gives the following output.

Example 1.3: water network problem (PRO)

```
7 7                #nvars,neqs
v0-7              #eq0
v1-5              #...
v4+v5-v6
v6-30
v0-v2-0.3*v4
v1-v2-0.05*v5     #...
v2-v3-0.1*v6     #eq6
```

This is the list of the equations (represented by their left hand sides). It is ready for solution by such solvers as Mathematica and Matlab, accepting the expressions in human readable form. The equations can be also retranslated in the other formats, suitable for a particular solver. Here are the same equations in NLP format (explained further in Sec. 3.3).

Example 1.4: water network problem (NLP)

```
7 7                #nvars,neqs
o1 v0 7           #eq0
o1 v1 5           #...
o54 3 v4 v5 o16 v6
o1 v6 30
o1 o1 v0 v2 o2 0.3 v4
o1 o1 v1 v2 o2 0.05 v5 #...
o1 o1 v2 v3 o2 0.1 v6 #eq6
```

The solver returns the answer, which can be mapped again to the NET form.

Example 1.5: water network problem solution

```
name=n1,P=7
name=n2,P=5
name=n3,P=4
name=n4,P=1
name=p1,Q=10
name=p2,Q=20
name=p3,Q=30
```

Complexity estimation for the algorithm is $O(Nelem Nprop Neq)$, where $Nelem$ – number of elements, $Nprop$ – number of properties per element, Neq – number of equations per element. It is identical with the complexity of matrix multiplication

$$NET * TM = PRO \quad (2)$$

where $NET(Nelem,Nprop)$, $TM(Nprop,Neq)$, $PRO(Nelem,Neq)$ are matrices of given dimensions. If the problem had only one type of elements and were linear, it were really specified by a matrix multiplication with the operations count given above. For non-linear problems the same estimation with average values holds, $Nprop$ – average number of properties per equation, Neq – average number of equations per element.

It is important to note that a particular representation of NET and TM structures as a simple list of properties, e.g., NetList (Clees et al., 2016) or in other format plays no role for the algorithm. These formats are different implementations for the same abstract structure (sets of maps) used to represent the network. On the implementation level, the readers of NET and TM have to be separated from the algorithms working on abstract structures, which can be conveniently represented by set and map containers of C++ Standard Template Library (STL). This allows to use efficient search and set-theoretical algorithms available in STL. On the other hand, the syntax of TM is flexible and is completely in user hands. One can define the other names for the properties in NET and adopt TM accordingly. One can also change the syntax of the equations in TM according to the solver language. In this way the format independence of the main algorithm is achieved.

The translation algorithm is highly parallelizable. The processing loops can be per-element separated and proportionally accelerated by the usage of multiprocessor architectures.

3 THE FILTERS

The network description often requires an additional preprocessing. Also an adaptation to a particular solver can be necessary. This can be done by specialized modules for filtering the data.

3.1 Topological Filters

Topological cleaning filters are required for the networks containing subgraphs disconnected from any source. For instance, in gas and water networks, such sources are pressure and temperature supplies (Pset,

Tset). Also the elements with vanishing or small resistance bear a problem. The loops formed from such elements have unstable flow balance. In both cases the corresponding network problems are ill-defined and can lead to a solver failure. Topological cleaning filters can recognize such parts and remove them at an early stage.

Topological reduction filters provide a deeper network optimization. When the edge elements are described by physical profiles, entering into the element equations, their serial and parallel connections also possess a computable common physical profile. Tree-like connections with given flows (Qsets) in the leaves can be contracted to the root with a single Qset. These operations are encountered in theory of generalized series-parallel graphs (SPG/GSPG), (Eppstein, 1992; Korneyenko, 1994) and their practical application allows to reduce the networks significantly, by a factor upto 100 (Clees et al., 2018b).

3.2 Classification Filters

The particular applications should decide which elements belong to nodes, edges (class=n,e) as necessary for the work of topological filters, Kirchhoff sum operator, etc. Additional classification could be necessary. For instance, in gas transport networks the decision, whether a node is Pset, is taken on the basis of a complicated logic, involving the presence of gas composition (gasmix). This evaluation can be spared for the main translation module and transferred to a specialized filter. Other examples of classification will be given below in Section 4.

3.3 Retranslation Filters

Particular solvers can require a special coding, different from human readable form suitable for TM. For instance, such solvers as IPOPT, SNOPT, MINOS use special NLP input (Gay, 2005), based on Polish prefix notation (PPN) of all formulae and a unified encoding of all variables, numerical constants and operators. Using a quadratic pipe law as an example (Clees et al., 2016):

$$\text{pow}(P@node1, 2) - \text{pow}(P@node2, 2) - R * Q * \text{abs}(Q) = 0$$

written in PPN form:

$$- - \text{pow } P@node1 \ 2 \ \text{pow } P@node2 \ 2 \ * \ * \ R \ Q \ \text{abs } Q$$

using encoding rules:

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

one obtains an equivalent expression:

$$o1 \ o1 \ o5 \ v1 \ n2 \ o5 \ v2 \ n2 \ o2 \ o2 \ n0.1 \ v3 \ o15 \ v3$$

In the same way all equations in the system have to be encoded. An important observation is that such encoding becomes much more efficient when applied to TM rather than to PRO, see Figure 2. It is similar to retranslating a short dictionary to another language and its usage for the translation of a long document. The complexity of direct retranslation of the problem increases linearly with the size of network, as $O(NET)$, while the performance of retranslation of TM depends only on its size, as $O(TM)$, which is much faster in practical applications.

In our implementation, the retranslation is done by a specialized filter `preNLP`. When applied to TM, the bracketed `[prop]` parts are left unchanged and used further for direct substitution by the main translation algorithm `utrans`. Certain postprocessing operations are also required, such as inserting a header, forming a structural Jacobian, providing starting point, etc. They are done by the `postNLP` filter, as shown schematically in Figure 2.

4 EXAMPLES OF USAGE

4.1 Multiphase Problems

Figure 3 top shows a typical one-phase solution procedure. The necessary translation is done once, the result is passed to the NLP solver and the answer is again encoded to NET form with the `x2net` filter.

The applications can require multiple phases, e.g., distribution of flows in the water network can be used to compute the temperature distribution.

Example 2.1: water network description for temperature mix

```
# nodes
class=n,name=n1,ttype=tset,tset=280
class=n,name=n2,ttype=tset,tset=300
class=n,name=n3,ttype=demand
class=n,name=n4,ttype=demand
# edges
class=e,name=p1,node1=n1,node2=n3,
Q=10,qtype=1,in=n1
class=e,name=p2,node1=n2,node2=n3,
Q=20,qtype=1,in=n2
```

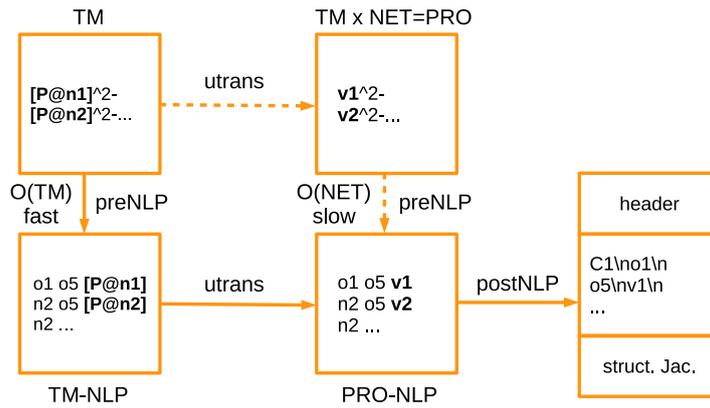


Figure 2: Retranslation of the problem to NLP form. The translation path, shown by solid lines, is much faster than the one shown by dashed lines.

```
class=e, name=p3, node1=n3, node2=n4,
    Q=30, qtype=1, in=n3
```

Example 2.2: translation matrix for temperature mix in water networks

```
# variables
class=n, var=T
class=e, var=T
# equations
class=n, ttype=tset, eq="[T]-[Tset]"
class=n, ttype=demand, eq="[summix][Q][T]-[T]"
class=e, qtype=1, eq="[T]-[T@in]"
class=e, qtype=0,
    eq="[T]-([T@node1]+[T@node2])/2"
```

In the corresponding workflow, displayed on Figure 3 bottom, the classification filter `wtmix` is used to set in NET `ttype` fields at nodes, `qtype` and `in` fields at edges. In TM the temperature variables are assigned to nodes and edges. The field `ttype` is used to distinguish between the temperature sources and intermediate nodes. In the intermediate nodes an operator `[summix]` implements a mixture of the temperature from the adjacent edges with the weights depending on the flows:

$$[\text{summix}][Q][T]_n = \sum_e w_{ne} T_e, \quad (3)$$

$$w_{ne} = u_{ne} / \sum_e u_{ne}, \quad u_{ne} = \max(I_{ne} Q_e, 0).$$

It is similar to `[sumadj]` operator, but effectively involves only incoming flows with $I_{ne} Q_e > 0$ and uses them for weighting. The physical meaning of the mix equation is that the weighted sum of incoming temperatures in edges equals to the temperature in the node.

In the edge the temperature is generally (`qtype=1`) defined as the temperature in the upstream node `T@in`. The exception is zero flow case (`qtype=0`), where the

half-sum of temperature at end nodes is taken. This is done to regularize the problem in subgraphs with zero flows. The fields `qtype` and `in` are set by the `wtmix` filter using the available flow distribution.

The resulting problem in the second phase is linear and is solved in one iteration by the solver.

Example 2.3: water temperature mix solution

```
name=n1, T=280
name=n2, T=300
name=n3, T=293.33
name=n4, T=293.33
name=p1, T=280
name=p2, T=300
name=p3, T=293.33
```

4.2 Multisectoral Problems

The concept of universal translation can be naturally extended to process the networks with multiple sectors, also with coupling between them.

Example 3: translation matrix for multisectoral coupling

```
# variables
class=n, sector=gas, var=P
class=e, sector=gas, var=Q
class=n, sector=water, var=P
class=e, sector=water, var=Q
class=n, sector=power, var=U
class=e, sector=power, var=I
...

# equations
class=e, sector=gas, type=p,
    eq=[P@node1]*abs([P@node1])
    -[P@node2]*abs([P@node2])
    -[R]*[Q]*abs([Q])
class=e, sector=power, type=r,
```

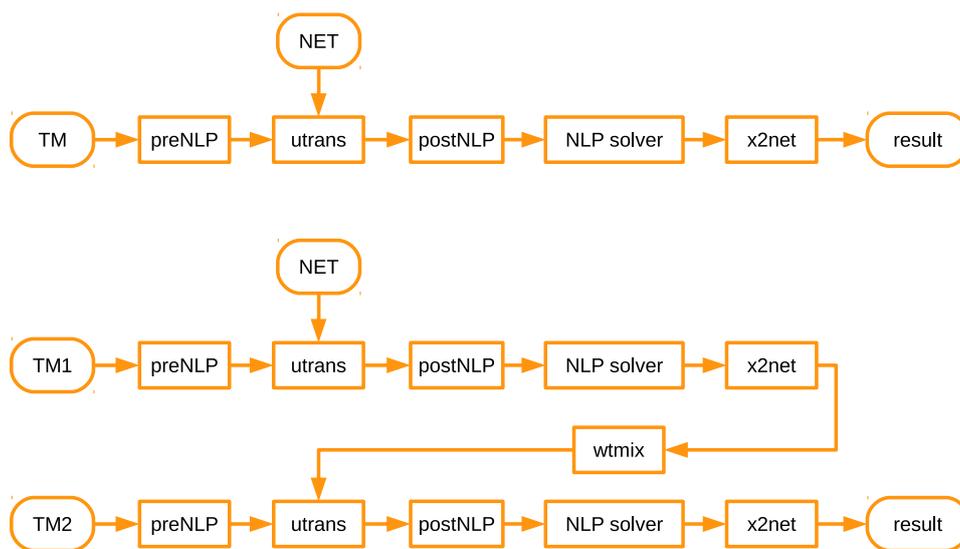


Figure 3: Solution workflows: one-phase on the top, two-phase at the bottom.

```

eq=[U@node1]-[U@node2]-[R]*[I]
class=e, sector=water, type=p,
eq="[P@node1]-[P@node2]-[R]*[Q]"
class=e, sector=gas, type=c, drive=E,
eq=[Q]
-efun([P@node1],[P@node2],[U@node])
...

```

Here three sectors (gas, power, water) are introduced. The coupling between power and gas is implemented using a cross-referencing. The typical network is shown on Figure 1 middle. The compressor element in the gas network has an equation, depending on the voltage variable $[U@enode]$ in the node of the power network. For the reference the field $[enode]$ in the compressor is used. Similar construction can be used to define the coupling between edge elements, as shown on Figure 1 right, for modeling of heat exchangers, power transformers, etc.

4.3 Realistic Network Problems

For the validation, we have applied the developed algorithms for solving a number of realistic network problems, received from our industrial partners. The smallest test cases are shown on Figure 4. The gas transport network N1, shown in the top image, contains about a hundred of nodes and edges, has two Pset supplies (shown by rhombi) and three Qset exits (n76, n80, n91, shown by triangles). The bottom image shows a water cooling network NSR/KLT72 of comparable complexity. The other, medium-sized gas network N2 contains about a thousand nodes and edges, while the largest considered gas network N3 has about five thousand nodes and edges.

To assess the performance of the algorithm, we se-

lect as a measure the timing of translation and solution steps for the networks of different complexity. The results of the tests are collected in Table 1. Solution for these gas networks is performed in two phases. First, all compressors and regulators are set in special mode with their goals enforced, providing linear element equations. The result is used as a starting point for the second phase, with compressors and regulators set to their actual element equations. The solution can be also done in one phase but the solution in two phases appears to be empirically faster. The timing in the table is given per one phase.

In comparison with our previous numerical experiments (Clees et al., 2018a), the translation procedure now includes topological cleaning algorithms, which for the largest network N3 accelerate the solver procedure by a factor about 8. With this acceleration the solver procedure now requires a CPU time comparable with the translation time.

In more details, the gas compressors in these tests were considered in frames of the so called *free model*. In this model the compressors attempt to satisfy specified goals, such as fixed output pressure or throughput flow, while the restrictions on revolution number and power of the drive are not imposed. Consideration of these restrictions is possible in frames of the *advanced model* (Clees et al., 2018b). Its implementation requires an additional filter, transforming individual characteristics of the compressor to tabulated functions, representing the extended element equation.

Further, the tests were performed with a gas of *constant composition and temperature*. Implementation of the mix procedure for gas is analogous to the

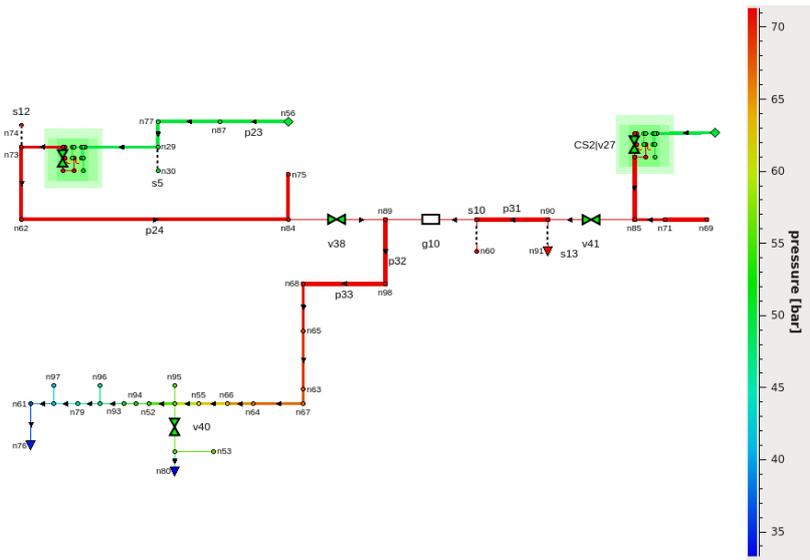


Figure 4: Realistic test networks: gas network N1 on the top, water cooling network NSR/KLT72 at the bottom.

above described mix step for water networks, requiring to upgrade the solution procedure by one more phase. The implementation of the gas mix phase and the advanced model of compressors is on the way.

5 CONCLUSIONS

We have presented the formulation of transport network problems as a translation between two formal languages. As input one has a network description in a form of a graph with properties and a configurable set of translation rules, corresponding to physical equations of transport, given per element type. As output one has a problem description given as a system of non-linear equations in a form, suitable for the

chosen solver.

A universal translation algorithm has been developed, possessing computational complexity linear in the number of elements in the graph, the number of properties per element and the number of equations per element type. The processing can be separated element-wise and allows massive parallelization.

A number of realistic examples has been used to test operability and performance of the algorithm, including water supply, cooling circuits, gas transport, power networks, as well as multisectoral couplings. Typically, for a large gas transport network with about 10K elements the translation and solution of non-linear system together require less than 1 sec. The translation procedure incorporates several preprocessing filters, in particular, topological cleaning filters,

Table 1: Performance of translation and solution phases for various networks.

network	nodes	edges	translation, sec	solution, sec
N1	100	111	0.04	0.02
N2	931	1047	0.15	0.24
N3	4466	5362	0.39	0.42

(timing for 3 GHz Intel i7 CPU 8 GB RAM workstation)

which accelerate the solution procedure by factor 8.

Currently we are working on the extension of the translation procedure by the advanced modeling of gas compressors and mix phase for gas composition and temperature. Our further plans include the acceleration of the solver procedure by applying topological reduction algorithms and parallelization of translation procedure on multiprocessor architectures.

ACKNOWLEDGMENTS

This work is supported by German Federal Ministry for Economic Affairs and Energy, project BMWI-0324019A, MathEnergy: Mathematical Key Technologies for Evolving Energy Grids. This material is also based upon work supported by the German Bundesland North Rhine-Westphalia using fundings from the European Regional Development Fund, grant Nr. EFRE-0800063, project ES-FLEX-INFRA.

REFERENCES

- Avriel, M. (2003). *Nonlinear Programming: Analysis and Methods*. Dover Publishing.
- Aymanns, P. et al. (2008). Online simulation of gas distribution networks. *9th SIMONE Congress, October 15–17, 2008, Dubrovnik, Croatia*.
- Bazaraa, M. S. and Shetty, C. M. (1979). *Nonlinear programming: theory and algorithms*. John Wiley & Sons.
- Belotti, P. et al. (2013). Mixed-integer nonlinear optimization. *Acta Numerica*, 22:1–131.
- Bertsekas, D. P. (1999). *Nonlinear Programming*. Athena Scientific.
- Clees, T. et al. (2016). MYNTS: Multi-physics NeTwork Simulator. In *SIMULTECH 2016, July 29–31, 2016, Lisbon, Portugal*, pages 179–186. SCITEPRESS.
- Clees, T. et al. (2018a). Making Network Solvers Globally Convergent. *Advances in Intelligent Systems and Computing*, 676:140–153.
- Clees, T. et al. (2018b). Modeling of Gas Compressors and Hierarchical Reduction for Globally Convergent Stationary Network Solvers. *International Journal On Advances in Intelligent Systems, IARIA* (submitted).
- Eppstein, D. (1992). Parallel recognition of series-parallel graphs. *Information and Computation*, 98:41–55.
- Fletcher, R. (2013). *Practical Methods of Optimization*. John Wiley & Sons.
- Gay, D. M. (2005). *Writing .nl Files*. Technical Report, Sandia National Laboratories, Albuquerque.
- Gill, P. E. et al. (2005). SNOPT: An SQP algorithm for large-scale constrained optimization. *SIAM Review*, 47(1):99–131.
- Harrison, M. A. (1978). *Introduction to Formal Language Theory*. Addison-Wesley.
- Korneyenko, N. M. (1994). Combinatorial algorithms on a class of graphs. *Discrete Applied Mathematics*, 54:215–217.
- Milano, F. (2015). *PSAT Software*. faraday1.ucd.ie/psat.html.
- Murtagh, B. and Saunders, M. (1978). Large-scale linearly constrained optimization. *Mathematical Programming*, 14:41–72.
- Nocedal, J. and Wright, S. J. (2006). *Numerical Optimization*. Springer.
- Rogalla, B.-U. and Wolters, A. (1994). Slow transients in closed conduit flow – part I: Numerical methods. In Chaudhry, M. H. and Mays, L. W., editors, *Computer Modeling of Free-Surface and Pressurized Flows*, volume 274 of *NATO ASI Series*, pages 613–642. Springer, Netherlands.
- Scheibe, D. and Weimann, A. (1999). Dynamische Gasnetzsimulation mit GANESI. *GWF Gas/Erdgas*, (9):610–616.
- Stevanovic, V. D. et al. (2009). Prediction of thermal transients in district heating systems. *Energy Conversion and Management*, 50(9):2167–2173.
- Wächter, A. and Biegler, L. T. (2006). On the implementation of an interior-point filter line-search algorithm for large-scale nonlinear programming. *Mathematical Programming*, 106(1):25–57.
- Zimmerman, R. D. and Murillo-Sanchez, C. E. (2015). *Matpower 5.1 User's Manual*. www.pserc.cornell.edu/matpower.