B4
A Jack of all trades? Solving stochastic mixed-integer nonlinear constraint programs

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Natural gas is one of the most important energy sources in Germany and Europe. In recent years, political regulations have led to a strict separation of gas trading and gas transport, thereby assigning a central role in energy politics to the transportation and distribution of gas. These newly imposed political requirements influenced the technical processes of gas transport in such a way that the complex task of planning and operating gas networks has become even more intricate.

There are many requirements to be met by gas network operators: They do not only have to guarantee a safe and reliable operation of the network, they also have to provide access for customers (e.g., gas traders, public services, industrial firms, power plants, and energy suppliers) under technical and economic conditions that are nondiscriminatory, transparent, and at competitive prices. Rejecting access to the network requires well-founded justification, such as specifying unavoidable costs caused by accepting a customer's request. These and other requirements call for technical and economic expertise in gas network planning far beyond current capabilities.

A key concept of the new framework of gas transport is the "Entry/Exit Model": capacities for injection and extraction of gas are sold through different and independent contracts. Customers do not have to specify anymore from which entry point to which exit point of the network the gas should be transported, the transport company has to guarantee that any combination of entry and exit points is technically feasible. The term "technical capacity" in political regulations is meant to denote the maximum capacity available at an entry or exit point in the gas network. Even if this concept is assumed to be reasonable, it is mathematically not well-defined, if one considers the requirement of arbitrary combinations between exits and entries as requested by the two-contract model. Thus, a basic theoretical and computational analysis of gas transport is needed [37] – not only by the network operators themselves: The regulatory bodies are also highly interested in such questions.

Mathematically, the combination of discrete decisions on the configuration of a gas transport network, the nonlinear equations describing the physics of gas, and the uncertainty in demand and supply yield large-scale and highly complex stochastic mixed-integer nonlinear optimization problems.

The MATHEON project *Optimization of Gas Transport* plays a key role in making available the necessary core technology to solve the mathematical optimization problems which model the topology planning and the operation of gas networks. The vision of the project has been to advance the rapid specification and efficient solution of mixed-integer nonlinear programs with chance constraints. This continues to have a broad impact on industrial and academic projects inside and outside of MATHEON. The mathematical optimization software developed by MATHEON scientists in this and in preceding projects has been successfully employed within MATHEON projects *Strategic Planning in Public Transport, Integrated Planning of Multi-layer Telecommunication Networks, Service Design in Public Transport, Symmetries in Integer programming, Improvement of the Linear Algebra Kernel of Simplex-based LP- and MIP-Solvers, Nonconvex Mixed-Integer Nonlinear Programming, Scheduling Techniques in Constant Integer Programming, Chip Design Verification with Constraint Integer Programming*, and *Combinatorial Optimization at Work*, hence crosslinking all domains of expertise within the application area "Networks".

The MATHEON project *Stable Transient Modeling and Simulation of Flow Networks* aims at modeling guidelines for flow networks guaranteeing stable partial differential-algebraic equation systems (PDAEs) and identifying prototype space and time discretizations to ensure stable numerical solutions for such network PDAEs.

An important aspect of the academic impact is the free availability of our framework. As a result of several years of research and development, it is now possible to download a complete state-of-the-art framework for mixed-integer linear and nonlinear programming in source code at http://scip.zib.de

The mutual research activities enabled many cooperations, both with industrial and academic partners. The *Forschungskooperation Netzoptimierung* (ForNe, http://www.zib.de/en/projects/current-projects/project-details/article/forne.html) takes a key role within our research network. Funded by the Open Grid Europe GmbH, ForNe connects scientists from University of Nürnberg-Erlangen, University of Duisburg-Essen, TU Darmstadt, Leibniz University Hannover, and three of the institutions participating in MATHEON: the Humboldt University Berlin, the Weierstrass Institute, and the Zuse Institute. ForNe deals with capacity and topology planning for gas transport networks. In joint effort, we develop optimization-based methods for checking realizability of gas flow situations and work on techniques that provide cost-effective network expansion measures to increase freely allocable capacities.

Other cooperations along involved companies like Siemens, SAP, IBM, and federal authorities like the Bundesnetzagentur (the German office for the electricity and gas market).

The remainder of this chapter is organized as follows. In Section B4—1, we will give a formal definition of MINLPs, the class of mathematical optimization problems that we have studied. In Section B4—2, we will describe the design of a global MINLP solver and highlight our contributions to this field. Stochastic aspects of nonlinear optimization are covered by Section B4—3. In Section B4—4, modeling and simulation aspects for gas transport networks are discussed.

B4—1 Mixed-integer nonlinear programming

Nonlinear optimization problems containing both discrete and continuous variables are called *mixed-integer nonlinear programs* (MINLPs). Such problems arise in many fields, such as energy production and distribution, logistics, engineering design, manufacturing, and the chemical and biological sciences [23, 40, 43].

A general MINLP can be formulated as

$$\min\{f(x) : x \in X\} \tag{1a}$$

with

$$X := \{x \in [\underline{x}, \overline{x}] : Ax \le b,\ g(x) \le 0,\ x_i \in \mathbb{Z},\ i \in I\}, \tag{1b}$$

where $\underline{x}, \overline{x} \in \overline{\mathbb{R}}^n$ determine the *lower and upper bounds* on the variables ($\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$), the matrix $A \in \mathbb{R}^{m' \times n}$ and the vector $b \in \mathbb{R}^{m'}$ specify the *linear constraints*, $I \subseteq \{1, \dots, n\}$ denotes the set of variables with *integrality requirement*, $f : [\underline{x}, \overline{x}] \to \mathbb{R}$ is the *objective function*, and $g : [\underline{x}, \overline{x}] \to \mathbb{R}^m$ are the *constraint functions*. The set X is called *feasible set* of (1). The restriction to inequality constraints is only for notational simplicity. $f(x)$ and $g(x)$ are assumed to be at least continuous, but efficient solution algorithms often require continuous differentiability, sometimes also twice continuous differentiability. If $f(x)$ is linear and each $g_j(x)$ is a quadratic function ($g_j(x) = \langle x, Q_j x\rangle + \langle q_j, x\rangle + \bar{q}_j$ for some $Q_j \in \mathbb{R}^{n \times n}$, $q_j \in \mathbb{R}^n$, and $\bar{q}_j \in \mathbb{R}$), (1) is called a mixed-integer quadratically constrained program (MIQCP).

The combination of discrete decisions, nonlinearity, and possible nonconvexity of the nonlinear functions in MINLP merges the problems considered in the areas of mixed-integer linear programming, nonlinear programming, and global optimization into a single problem class. While linear and convex nonlinear programs are in theory solvable in polynomial time [31, 34] and very efficiently in practice [18, 39], nonconvexities as imposed by discrete variables or nonconvex nonlinear functions easily lead to problems that are NP-hard in theory and computationally demanding in practice. However, substantial progress has been made in the solvability of mixed-integer linear programs [19]. As a consequence, state-of-the-art MIP solvers are nowadays capable of solving a variety of MIP instances arising from real-world applications within reasonable time [35]. On the other hand, also global optimization has been a field of active research and development, see, e.g., the textbooks [23, 31, 43] and the survey papers [26, 38].

Since its beginning in the mid 1970's [5, 24], the integration of MIP and global optimization of NLPs and the development of new algorithms unique for MINLP has made a remarkable progress, see, e.g., the recent book [36] and the survey paper [6]. While the integration of nonlinear aspects into a MIP solver often accounts at first only for the easier case where the functions $f(x)$ and $g_j(x)$, $j = 1, \dots, m$, are assumed to be convex on $[\underline{x}, \overline{x}]$ [1, 20], discrete decision variables are integrated into a global optimization solver often by a simple extension of an already existing branch-and-bound algorithm. Then, the latter is gradually extended by more advanced MIP machinery (presolving, cutting planes, branching rules, ...). In MATHEON, we faced the much harder tasks of incorporating global optimization of nonconvex problems, discrete decision variables, and stochastic optimization techniques into a single framework which is based on constraint programming concepts, see Section B4—2.

Even though not competitive with MIP, yet, there exists nowadays a variety of general purpose software packages for the solution of medium-size nonconvex MINLPs, see [21, 44] for an overview.

B4—2 SCIP - a solver for MINLPs

Within the MATHEON project *Optimization of Gas Transport*, we have developed a general framework for solving the mixed-integer nonlinear programs arising in gas transport optimization. To this end, we have extended the framework SCIP [2, 4] that has originally been designed to solve mixed-integer linear programs with extensions to constraint programming (see, e.g., [13, 28, 29]) step by step to handle different kinds of nonlinearity.

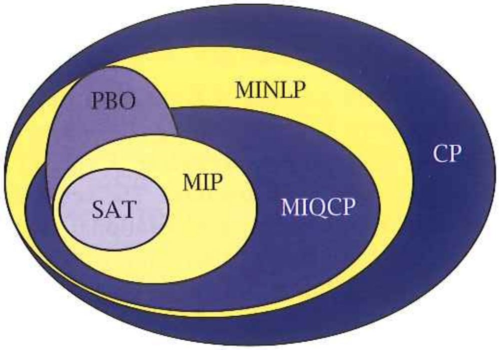

Figure 1. *Visualizing of the inclusions of the different problem space: constraint programs (CP), mixed-integer nonlinear programs (MINLP), mixed-integer quadratically constrained programs (MIQCP), pseudo Boolean optimization (PBO), mixed-integer programs (MIP), and satisfiability testing (SAT).*

First, we integrated algorithms for solving so-called pseudo-Boolean instances [14], i.e., optimization problems with constraint functions that are polynomials over 0-1 variables. As a next step, we extended our research towards mixed-integer quadratic problems, including nonconvexities [12, 16]. Finally, we made the SCIP framework capable of solving general nonconvex MINLPs to global optimality [44], incorporating powerful technologies from mixed-integer linear programming, global optimization of nonlinear programs, constraint satisfaction, and constraint programming. At the same time, we incorporated capabilities for stochastic programming, see Section B4—3. Figure 1 visualizes the relationship between different classes of mathematical optimization problems.

The most important elements of a branch-and-cut based MINLP solver are a fast and numerically stable LP solver, cutting plane separators, primal heuristics, presolving algorithms, and a suitable branching rule. A main focus of our project was to develop new strategies for primal heuristics and branching.

Often, in MIP and MINLP, problems do actually not need to be solved to proven optimality. A small gap to optimality might be sufficient, e.g., since the underlying data contains uncertainty by itself or the user is satisfied with a near-optimal solution because of limitations on the solution time. In both cases, primal heuristics can help to improve the performance significantly. Primal heuristics are algorithms that try to find feasible solutions of good quality within a reasonably short amount of time. Over time, primal heuristics have become a substantial ingredient of state-of-the-art MIP solvers [7]. In a recent publication, we present an overview of primal heuristics for MINLP [8].

Large neighborhood search (LNS) has been one focus of our research on primal heuristics. The main idea of LNS is to restrict the search for "good" solutions to a neighborhood of specific points – usually close to already known feasible solutions. This is typically done by defining a sub-MINLP of the original MINLP by fixing some variables to values from the reference solution, adding some very restrictive constraints or by modifying the objective to direct the search into a region with many feasible solutions.

We provided a generic way of generalizing LNS heuristics from MIP to MINLP [15], for the first time presenting nonlinear versions of Crossover and the DINS heuristic. Further, we introduced

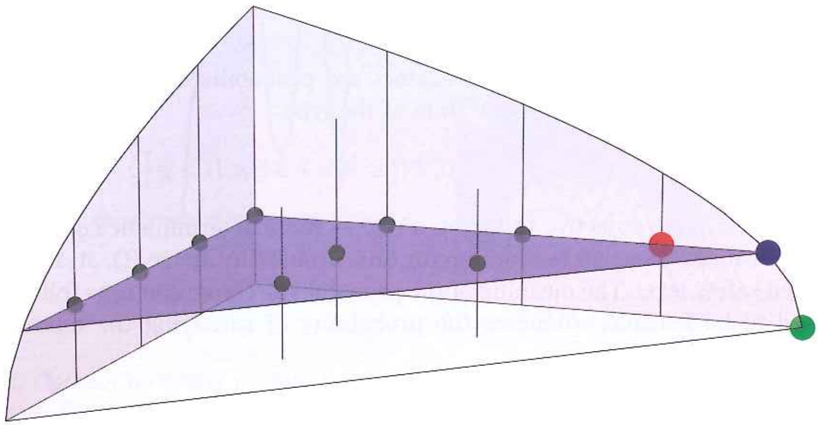

Figure 2. *A convex MIQCP and the Undercover sub-MIP induced by the NLP relaxation*

RENS [9], the *relaxation enforced neighborhood search*, a primal heuristic that uses a sub-MINLP to explore the set of feasible roundings of an optimal solution of a linear or nonlinear relaxation. We analyzed how the roundability is affected by different relaxations, the usage of cutting planes and the fractionality of the solution.

In [10], we developed Undercover, a primal heuristic for nonconvex mixed-integer nonlinear programs (MINLPs) that explores a mixed-integer linear subproblem (sub-MIP) of a given MINLP which is induced by the optimal solution of a vertex covering problem. An illustration of the Undercover idea can be seen in Figure 2. The lightly shaded region shows the solid corresponding to the NLP relaxation; the parallel lines show the mixed-integer set of the MINLP's feasible solutions. The darkly shaded area shows the polytope associated with the Undercover sub-MIP.

A minimum cover of an MINLP is an abstract structure that can be studied and employed beyond the contexts of primal heuristics. In [11], we extended the Undercover idea towards a branching strategy to subdivide a given MINLP into disjoint subproblems, which are not only smaller, but also "more linear" [11].

Hybrid branching [3] combines different branching rules (pseudocosts, inference values, VSIDS and conflict lengths) into a single variable selection criterion, thereby achieving a stable performance for very different kinds of optimization problems. Recently, we introduced *Cloud branching* [17], a framework for branching rules to exploit the knowledge of alternative relaxation solutions. We showed that a version of full strong branching that exploits the idea of cloud branching is about 30% faster than default full strong branching on a standard MIP test set with high dual degeneracy.

Having available a strong MIP core and state-of-the-art algorithms to solve nonconvex MINLP, the missing feature for handling energy optimization problems are the stochastic aspects of the underlying demand and supply. How such problems can be mathematically modeled and efficiently solved will be described in the next section.

B4—3 Stochastic aspects

A special class of nonlinear convex constraints are probabilistic constraints. We consider mixed-integer problems with such constraints of the type

$$\min\left\{f(x)\,|\,g(x) \le 0,\ \mathbb{P}(\underline{l} \le Ax + B\xi \le \bar{l}) \ge p\right\}. \tag{2}$$

Here, $f : \mathbb{R}^n \to \mathbb{R}$ is some objective function, $g : \mathbb{R}^n \to \mathbb{R}^m$ a deterministic constraint mapping, ξ some s-dimensional Gaussian random vector on a probability space $(\Omega, \mathcal{A}, \mathbb{P})$ and $p \in [0,1]$ some specified safety level. The meaning of the probabilistic constraint is as follows: a decision x is declared to be feasible, whenever the probability of satisfying the random inequality system

$$\underline{l}_i \le \sum_{j=1}^{n} A_{ij}x_j + \sum_{j=1}^{s} B_{ij}\,\xi_j \le \bar{l}_i \quad (i = 1,\dots,m)$$

is at least p. To solve such problems, we added a corresponding cutting plane separator to SCIP. The basic idea is to add linear inequalities to the problem formulation that separate the current solution x_{LP} from the linear relaxed problem without cutting off any part of the feasible set as defined by the nonlinear constraint. In this sense, the feasible set is approximated by linear constraints. To get a linear constraint that does not cut off the feasible set, it is necessary to calculate the gradient of the constraint mapping

$$F_\xi(x) := \mathbb{P}(\underline{l} \le Ax + B\xi \le \bar{l}), \quad \xi \sim \mathcal{N}(\mu, \Sigma).$$

One has to take into account, however, that the function F_ξ is not given by an explicit formula since the probability involved is defined by improper multivariate integrals. On the other hand, there exist efficient codes to approximate distribution functions of the multivariate normal distribution sufficiently well, see, e.g., [25]. Given the lack of explicit function values F_ξ, this is much less true for the gradients. On the other hand, approximating ∇F_ξ by finite differences is not practical since the inaccuracy of function values F_ξ will lead to highly unreliable estimations of $\partial_{x_i} F_\xi(x)$ when driving the finite differences step size to zero. Fortunately, for the case of the multivariate normal distribution, there exists an analytical relation between function values and gradients of the distribution function (cf. [45]). This means that no additional inaccuracy, beyond the one already present in the function values, is introduced when it comes to calculating gradients. In the employed supporting hyperplane approach this gradient is used to construct a linear constraint at a point very close to the feasible set. Such a point is obtained by bisecting the line between the aforementioned infeasible point x_{LP} and an a priori calculated point feasible w.r.t. the probability constraint. In this way a cutting plane separator is defined that allows SCIP to solve MINLPs with probabilistic constraints of type (2).

Then, we applied this solver to a simplified example of optimal power plant management (cf. [42]). To be precise, we consider a power management model consisting of a hydro plant coupled with a wind farm. Electricity produced by both components serve first to meet the local power demand of some area of interest and second to sell any surplus electricity on the market. We assume a known constant inflow of water to the hydro plant. We will also assume that the time profiles for the market price and for the demand are known for the considered short time period. In contrast, we do not neglect the randomness of the wind force, which can be highly fluctuating over the considered time frame. The wind farm, supported

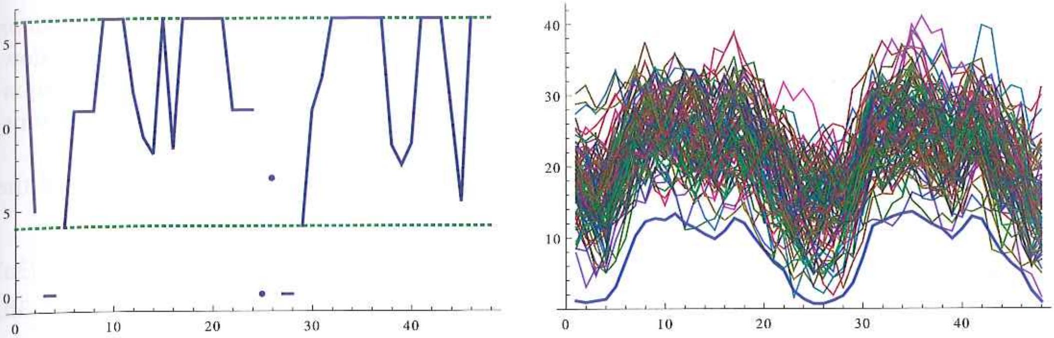

Figure 3. *Left: Optimal turbining profiles for the hydro reservoir, either switched off (zero level) or within operation limits (dotted lines), Right: energy supply (wind plus unsold hydro energy) for 100 simulated wind energy scenarios, demand profile: thick blue curve*

by a part of the hydro power generation, is supposed to meet the local demand of electricity. The remaining part of the hydro power generation is sold on the market for gaining maximum profit according to the given price signal. The hydro reservoir may be used to store water and, thereby, to better adapt the water release strategy to the time profiles of price and demand. In order to exclude production strategies which are optimal for the given time horizon but at the expense of future ones (e.g., maximum production within capacity limits), a so-called *end level constraint* is imposed for the final water level in the hydro reservoir. The decision variables of our problem are the profiles for hydro power generation over the considered time horizon used to support demand satisfaction or to sell electricity. The objective function is profit maximization. The constraints are simple bounds on the total water release, which is either zero or given by the positive operational limits of the turbine, the filling level of the hydro reservoir and demand satisfaction. The latter is a random constraint since it is met by the sum of a deterministic component of hydro energy and a stochastic component of wind energy. Moreover, to realize the water release constraints, binary decision variables are necessary. Now, the planning decision on optimal hydro power generation has to be taken a priori without knowing future realizations of the random parameter (wind force). Discretizing the time interval into 48 hour steps, the problem is solved using SCIP as described above. Figure 3 visualizes the optimal turbining profile and the energy demand satisfaction. The turbining profile shows connected parts in which turbines operate within their positive technical limits as well as disrupted parts due to shut down or switch on decisions. It can be seen in the right picture that most of the 100 plotted wind profile realizations satisfy the demand at every timestep. In fact the probabilistic constraint was setup such that 90% of all realizations are supposed to satisfy the demand through the whole time horizon. In this particular instance only six of the realizations violate the demand constraint at least once - and none of them more than twice.

B4—4 Numerical simulation aspects

The transient numerical simulation of gas transport networks aims at a prediction of the flow q and pressure values p in the network, supposed the pressure supplies and flow demands are given during the time period of interest. The Project *Stable Transient Modeling and Simulation of Flow Networks* addressed flow networks of different kinds: gas, water, current, blood flow. As each flow network, gas transport networks can be described by the mass flow balance equations in each node and the network element equations (pipe equations, valve model equations, compressor model equations, etc.) for each branch and node element, see [33].

Restricting to pipes as branch elements, the gas network can be written as a system of the form [27]

$$A_R q_R(t) + A_L q_L(t) = d(t) \tag{3a}$$

$$\partial_t \rho(x,t) + \partial_x q(x,t) = 0 \tag{3b}$$

$$\partial_t q(x,t) + a^2 \partial_x \rho(x,t) = -\frac{\lambda}{2D} \frac{q(x,t)|q(x,t)|}{\rho(x,t)} \tag{3c}$$

$$q(x_L,t) = q_L(t), \quad \rho(x_L,t) = A_L^\top \rho(t) + A_{Ls}^\top s(t) \tag{3d}$$

$$q(x_R,t) = q_R(t), \quad \rho(x_R,t) = A_R^\top \rho(t) + A_{Rs}^\top s(t) \tag{3e}$$

with the flows $q(x,t)$ and densities $\rho(x,t)$ along the pipes as well as the demand flows $d(t)$ and the supply densities $s(t)$ at the nodes. The components of $d(t)$ that do not belong to a demand node equal zero. Each pipe is equipped with one direction and the convention that it directs from the left node x_L to the right node x_R. Correspondingly, $q_L(t)$ and $q_R(t)$ are the flows at the left and right nodes. The incidence matrices A_R and A_L describe the branch to node relation for right and left nodes. Finally, $\rho(t)$ are the densities of all non-supplying nodes.

The equation (3a) describes the flow balance equation at each node. The equations (3b) and (3c) represent the isothermal Euler equations for slow flows where the geodesic height differences are neglected and the gas equation is approximated by

$$p(x,t) = a^2 \rho(x,t)$$

with a constant sound velocity $a \sim 300\text{ms}^{-1}$, see, e.g., [22, 30, 41]. The equations (3d) and (3e) reflect the boundary conditions for each pipe.

Figure 4 visualizes the distributed transient simulation of a gas transport network described by (3a)–(3e). It bases on three input pillars. The first one comprises the element models, e.g., pipe equations or valve model equations. The second one reflects the network topology in form of netlists, and the third one describes the scenario variables as flow demands and pressure supplies. As a result one gets the pressure and left/right flow values at each node.

Addressing the aim to optimize the dispatching of gas networks, one has to run a large number of simulations with different parameters and scenarios. It demands to reduce the time effort for each simulation run. We developed two ways of acceleration. Instead of running the simulation of the original model equations with various parameter values, we developed a delta algorithm that computes efficiently the differences of solutions for model equations with different parameter values [32]. Secondly, it has been shown [27] that the system (3a)–(3e) can be transformed into a system of the form

$$u'(t) = f(u(t), v_1(t), v_2(t), t) \tag{4a}$$

$$v_1(t) = g(u(t), v_2(t), t) \tag{4b}$$

$$v_2(t) = Ms'(t) \tag{4c}$$

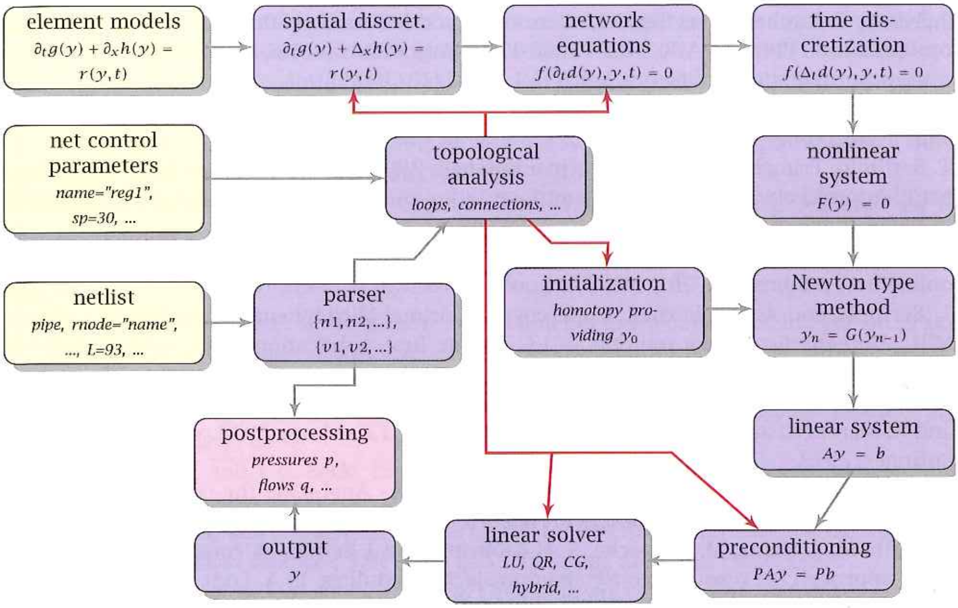

Figure 4. *Flow diagram for a distributed transient simulation of gas transport networks*

after a space discretization with just one linear finite element for each pipe. It has the advantage that the implicit structure of (3a)–(3e) is transformed into an explicit structure that can be solved more efficiently. Additionally, the explicit structure allows a direct application of POD methods resulting in efficient reduced order models, see [27].

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