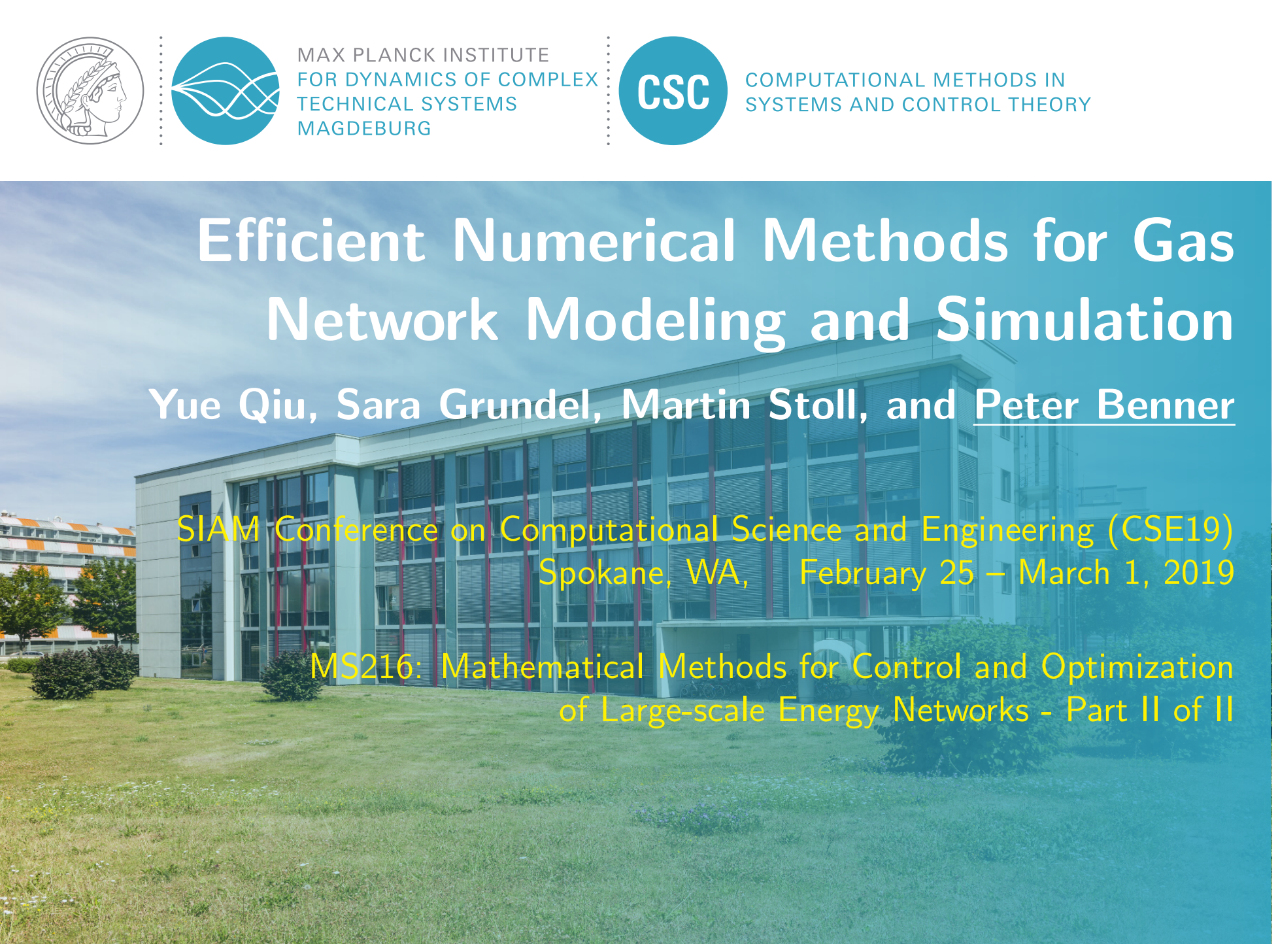


Efficient Numerical Methods for Gas Network Modeling and Simulation

Yue Qiu, Sara Grundel, Martin Stoll, and Peter Benner

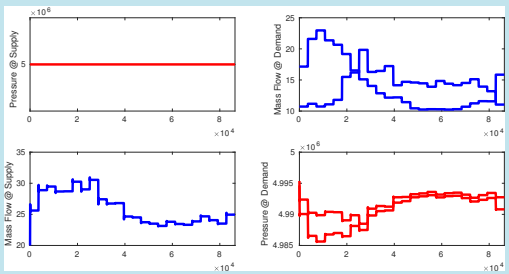
SIAM Conference on Computational Science and Engineering (CSE19)
Spokane, WA, February 25 – March 1, 2019

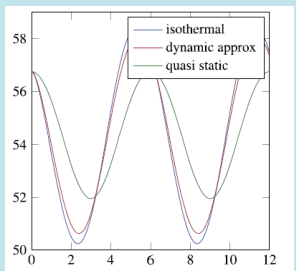
MS216: Mathematical Methods for Control and Optimization
of Large-scale Energy Networks - Part II of II

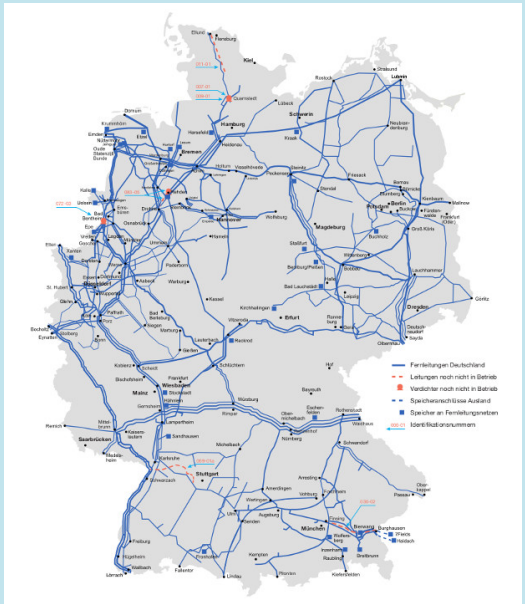
Simulation of coupled German energy transportation networks

- **Funding:** 6 million EUR for 2017–2021.
- **Goals:**
  - hierarchical modeling of transport and distribution networks
  - fast simulation on all levels
  - real-time scenario analysis for network operators
  - coupling of power and gas network
- **Results:** New **discretization** and **model order reduction** methods for
  - isothermal Euler equations on network graph
  - with nonsmooth nonlinearity
  - leading to coupled system of differential-algebraic equations (DAEs)
  - with uncertain parameters

  Implemented in **morgen** — **M**odel **O**rder **R**eduction of **G**as and **E**nergy **N**etworks.







The German natural gas transportation network

Math Energy

Partners:

Fraunhofer SCAI
Fraunhofer ITWM
TU Berlin
HU Berlin
TU Dortmund
U Trier
PSI AG
associated:
Venios GmbH
OGE

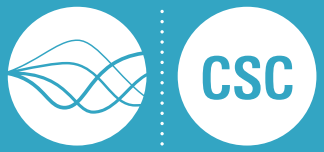
Funded by:

Federal Ministry for Economic Affairs and Energy

Motivation

- Change of load or operation condition in the gas network will lead to transient dynamics.
- Fast simulation of this transient process is necessary.
- Increasing need for accurate network dynamics requires finer discretization of the network.
- Resulting network model is represented by a system of nonlinear differential-algebraic equation (DAE).
- Network simulation needs computationally expensive solution of this large-scale nonlinear DAE system.

$\rightsquigarrow$ Efficient numerical algorithms to model and simulate network are necessary.



Outline

1. Pipeline Dynamics
2. Network Dynamics
3. Numerical Algorithms for Network Simulation
4. Numerical Experiments
5. Conclusions
6. Bibliography

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Pipeline Dynamics

Consider the 1D isothermal Euler equation in the spatial domain $[0,\ L]$

$$\begin{aligned}\frac{\partial}{\partial t}\rho &= -\frac{\partial}{\partial x}\varphi,\\ \frac{\partial}{\partial t}\varphi &= -\frac{\partial}{\partial x}p - \frac{\partial}{\partial x}(\rho v^2) - \rho g\frac{\partial}{\partial x}h - \frac{\tilde{\lambda}(\varphi)}{2d}\rho v|v|,\\ p &= \gamma(T_0)z(p,T_0)\rho.\end{aligned}$$

Here, ρ is the density (kg/m^3), φ is the flow rate (m^3/s), p represents the pressure (N/m^2).

Introducing the mass flow $q = \rho S v$, where S is the cross-section area, we get

$$\begin{aligned}&\text{Continuity} && \left\{\frac{\partial}{\partial t}p = -\frac{\gamma_0}{S}\frac{\partial}{\partial x}q,\right.\\ &\text{Momentum} && \left\{\frac{\partial}{\partial t}q = -S\frac{\partial}{\partial x}p \underbrace{-\frac{\gamma_0}{S}\frac{\partial}{\partial x}\frac{q^2}{p}}_{\text{Kinematic Term}} \underbrace{-S\frac{g}{\gamma_0}p\frac{\partial}{\partial x}h}_{\text{Gravity Term}} \underbrace{-\frac{\lambda(q)\gamma_0}{2dS}\frac{q|q|}{p}}_{\text{Friction Term}}.\right.\end{aligned}$$

Discretized Pipeline Model

Simplifications

Ignore the kinematic term as

$$\left|\frac{\gamma_0}{S^2}\frac{q^2}{p}\right| = \left|p\frac{v^2}{\gamma_0}\right| \ll |p|.$$

Furthermore, we assume that the pipe is at equal height ("equi-height" assumption). Therefore, we get

$$\begin{aligned}\frac{\partial}{\partial t}p &= -\frac{\gamma_0}{S}\frac{\partial}{\partial x}q,\\ \frac{\partial}{\partial t}q &= -S\frac{\partial}{\partial x}p - \frac{\lambda(q)\gamma_0}{2dS}\frac{q|q|}{p},\end{aligned} \tag{1}$$

with boundary conditions (BCs): $p(0,\ *) = p_s$ and $q(L,\ *) = q_d$.

Discretizing (1) using the finite volume method (FVM), we obtain the following system of nonlinear ODEs:

$$\begin{bmatrix} M_p & \\ & M_q \end{bmatrix}\begin{bmatrix}\partial_t p\\ \partial_t q\end{bmatrix} = \begin{bmatrix} 0 & K_{pq}\\ K_{qp} & 0\end{bmatrix}\begin{bmatrix}p\\ q\end{bmatrix} + \underbrace{\begin{bmatrix}B_q\\ 0\end{bmatrix}q_d}_{\text{right BCs}} + \underbrace{\begin{bmatrix}0\\ B_p\end{bmatrix}p_s}_{\text{left BCs}} + \underbrace{\begin{bmatrix}0\\ g(p,q)\end{bmatrix}}_{\text{nonlinear}}.$$

Non-constant height is not a problem, model structure stays the same, only K_{qp} changes.

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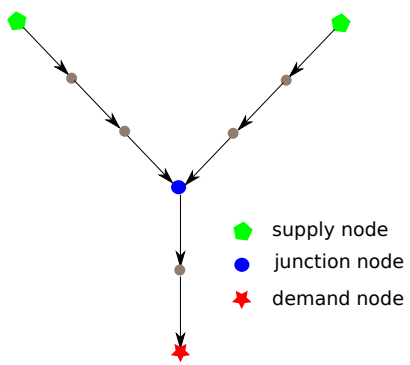
Network Structure



Example network

Passive network: network without active elements such as compressors, valves, etc. It is described by a directed graph

$$\mathcal{G} = (\mathcal{E},\ \mathcal{N}),$$

$\mathcal{E}$: the set of edges, i.e., the pipes in the gas network.
$\mathcal{N}$: the set of nodes, the union of supply nodes $\mathcal{N}_s$, demand nodes $\mathcal{N}_d$, and interior nodes $\mathcal{N}_0$.

Assembly of the pipeline model for each $e_i \in \mathcal{E}$ $\rightsquigarrow$ global network model. Insufficient boundary conditions (2 needed for each $e_i \in \mathcal{E}$) asks for algebraic constraints: coupling conditions for interior nodes

$$q_{\text{in}} = q_{\text{out}}, \quad \text{mass conservation},$$

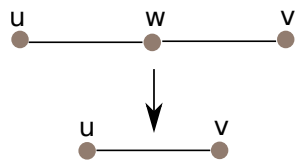
$$p^r_{\text{out}} = p^l_{\text{in}}, \quad \text{pressure at end of outflow pipe} = \text{pressure at connected inflow pipe},$$

need to be satisfied.

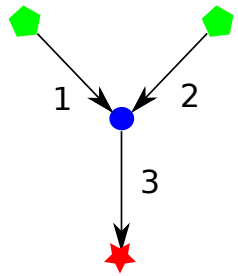
$$\#\text{algebraic constraints} = 2\#\mathcal{E} - \#\mathcal{N}_s - \#\mathcal{N}_d$$

Smoothing some interior nodes $\rightsquigarrow$ reducing number of algebraic constraints.

Topology-based Network Assembly



Smoothing node w



Smoothed network

Let the junction nodes $\mathcal{N}_j$ be nodes that connect at least three edges, and smooth the nodes $\mathcal{N}_o \backslash \mathcal{N}_j$, we obtain $\tilde{\mathcal{G}} = (\tilde{\mathcal{E}}, \tilde{\mathcal{N}})$ that has the same network topology.

Constraints reduction

After smoothing the interior nodes $\mathcal{N}_o \backslash \mathcal{N}_j$,

$$\#\text{algebraic constraints} = \#\tilde{\mathcal{E}} - \#\mathcal{N}_d.$$

For the example network:

- 2 constraints after reduction.
- 13 without reduction.

After network assembly, we get the following nonlinear DAE system:

$$\begin{bmatrix} \mathcal{M}_1 & & & & \\ & \mathcal{M}_2 & & & \\ & & \mathcal{M}_3 & 0 & 0 \end{bmatrix} \frac{\partial}{\partial t} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ q^1 \\ q^2 \end{bmatrix} = \begin{bmatrix} \mathcal{K}_1 & & & \mathcal{B}_q^1 & \\ & \mathcal{K}_2 & & & \mathcal{B}_q^2 \\ \bar{\mathcal{B}}_p^3 & & \mathcal{K}_3 & & \\ & & e_3 & 1 & 1 \\ e_1 & e_2 & & & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ q^1 \\ q^2 \end{bmatrix} + \begin{bmatrix} \mathcal{B}_p^1 & & \\ & \mathcal{B}_p^2 & \\ & & \end{bmatrix} \begin{bmatrix} p_s^1 \\ p_s^2 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ B_q^3 \\ 0 \\ 0 \end{bmatrix} q_d^3 + \mathcal{G}(*).$$

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Newton's Method

General network model has the following from,

$$\underbrace{\begin{bmatrix}\mathcal{M} & \\ & 0\end{bmatrix}}_{\mathbf{M}} \frac{\partial}{\partial t} \underbrace{\begin{bmatrix}u\\ q\end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix}\mathcal{K} & B_q\\ E & F\end{bmatrix}}_{\mathbf{K}} \begin{bmatrix}u\\ q\end{bmatrix} + \underbrace{\mathcal{B}_1 p_s + \mathcal{B}_2 q_d}_{d} + \mathcal{G}(u,q).$$

Applying implicit Euler method for temporal discretization, we have

$$\mathbf{F}(y^t) := (\mathbf{M} - \Delta t \mathbf{K})\mathbf{y}^t - \Delta t \mathcal{G}(\mathbf{y}^t) - \mathbf{M}\mathbf{y}^{t-1} - \Delta t \mathbf{d}^t = 0, \tag{2}$$

at time step t. Here, Δt is the time step size.

Algorithm 1 Newton's method

1: **procedure** NL_DAE(Δt, N_t, ε, max_it, $\mathbf{y}^0$) ▷ Solving (2) to simulate gas network
2: **for** $t = 1 : N_t$ **do** ▷ Outer iteration
3: $k = 1$
4: **while** $\|\mathbf{F}(\mathbf{y}_k^t)\| > \varepsilon$ && $k \leq$ max_it **do** ▷ Inner iteration
5: $\mathbf{y}_{k+1}^t = \mathbf{y}_k^t - \left(\frac{\partial \mathbf{F}}{\partial \mathbf{y}}|_{\mathbf{y}=\mathbf{y}_k^t}\right)^{-1} \mathbf{F}(\mathbf{y}_k^t), \qquad k \leftarrow k+1$
6: **end while**
7: $\mathbf{y}^t = \mathbf{y}_k^t$
8: **end for**
9: **end procedure**

Preconditioning

At each Newton (inner) iteration, need to solve linear system

$$\mathbf{F}(\mathbf{y}_k^t) + \partial_{\mathbf{y}}\mathbf{F}|_{\mathbf{y}=\mathbf{y}_k^t}(\mathbf{y} - \mathbf{y}_k^t) = 0, \tag{3}$$

Consider iterative solvers for (3), here, preconditioned Krylov methods.

The Jacobian can be partitioned according to the DAE *(generalized saddle-point)* structure:

$$\partial_{\mathbf{y}}\mathbf{F} = \begin{bmatrix} D_{F_{11}} & D_{F_{12}} \\ D_{F_{21}} & D_{F_{22}} \end{bmatrix}.$$

Typical preconditioners are

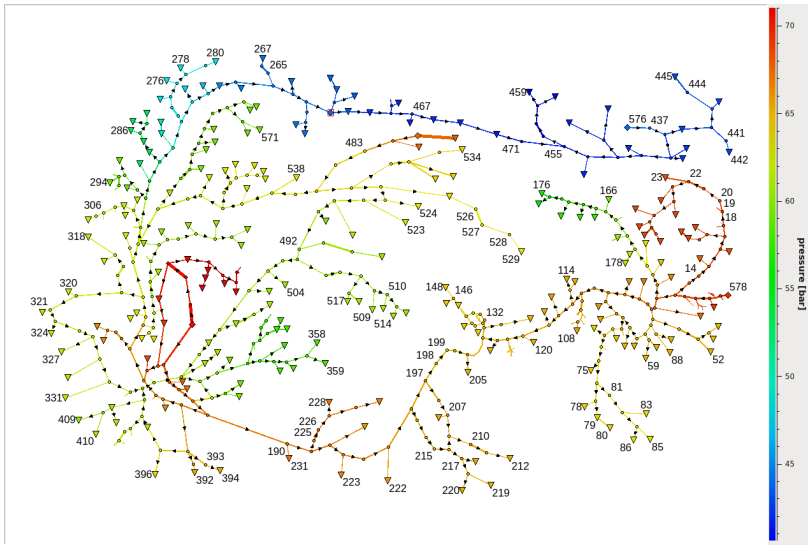
$$\mathcal{P}_1 = \begin{bmatrix} D_{F_{11}} & \\ & S \end{bmatrix}, \qquad \mathcal{P}_2 = \begin{bmatrix} D_{F_{11}} & \\ D_{F_{21}} & S \end{bmatrix},$$

where $S = D_{F_{22}} - D_{F_{21}} D_{F_{11}}^{-1} D_{F_{12}}$.

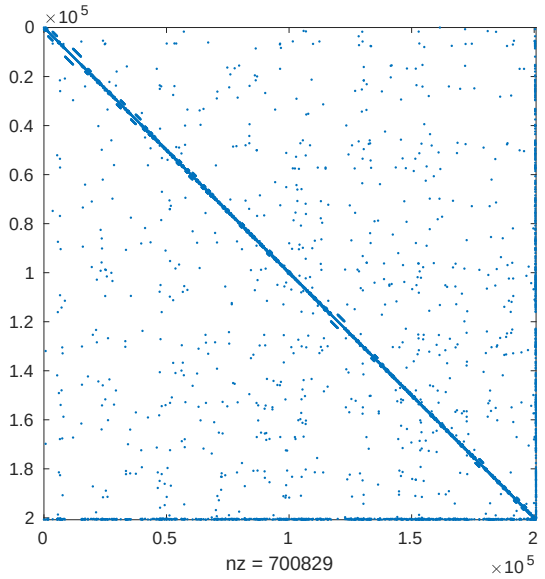
GMRES converges in 3 iterations with $\mathcal{P}_1$ and 2 iterations using $\mathcal{P}_2$.

Requirement: $D_{F_{11}}$ and S should be easy to approximate.

Graph Based Preconditioning



A large network example



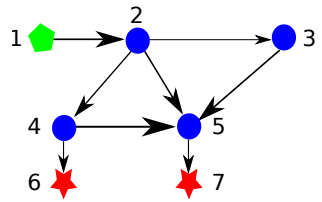
Sparsity pattern of $\partial_{\mathbf{y}}\mathbf{F}$

- The sparsity pattern of $\partial_{\mathbf{y}}\mathbf{F}$ is difficult to exploit for fast matrix computations.
- Keeping in mind that $\partial_{\mathbf{y}}\mathbf{F}$ originates from the network assembly, $\rightsquigarrow$ topology based reordering for fast computations.

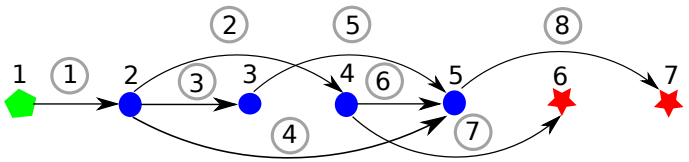
DF ordering [Qiu/Grundel/Stoll/B. 18]

The gas network is a directed acyclic graph (DAG), directions are away from supply nodes and towards demand nodes. We can order the edges in such a way that at every node all incoming edges have a lower order than all the outgoing edges, or it has no incoming edge. We call this a direction following (DF) ordering.

Graph-based Preconditioning



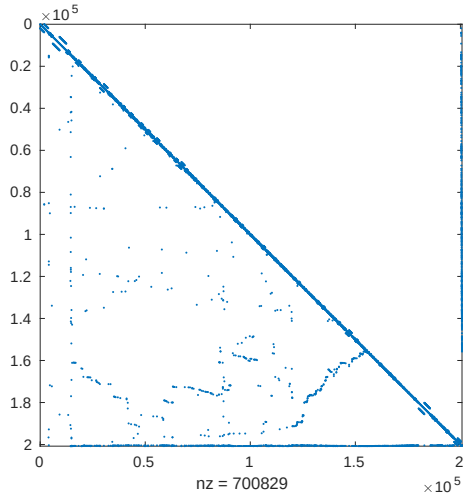
A network example



DF ordering of edges

Corollary [Qiu/Grundel/Stoll/B. 18]

After applying the DF ordering to the gas network, the $(1,1)$ block of the Jacobian matrix $\partial_{\mathbf{y}}\mathbf{F}$ has block lower-triangular structure.



$\partial_{\mathbf{y}}\mathbf{F}$ after DF ordering

Properties of block lower-triangular preconditioner

$$\mathcal{P}_2 = \begin{bmatrix} D_{F_{11}} & \\ D_{F_{21}} & S \end{bmatrix}.$$

- $D_{F_{11}}$ is block lower-triangular, $D_{F_{11}}^{-1}$ easy to compute.
- size of $S \ll$ size of $D_{F_{11}}$, therefore $S = D_{F_{22}} - D_{F_{21}} D_{F_{11}}^{-1} D_{F_{12}}$ can be computed directly.
- For the example, $D_{F_{11}}$ is $200,348 \times 200,348$, S is a 417×417 matrix.

Further Remarks

- Smoothed nodes are part of the virtual points used for network discretization.
- The direction of edges in the DAG is only used for the DF ordering. Real gas flow direction can be different, cf. numerical experiments.
- The DF ordering is not unique, we only need one.
- The size of the Schur complement is independent of the mesh size and only depends on the network structure.

Note that the Jacobian matrix $\partial_{\mathbf{y}}\mathbf{F}$ has two levels of indices: t for time and k for "Newton step", for each t and k computing a preconditioner $\mathcal{P}_2$ is still computational intensive.

$\rightsquigarrow$ compute only 1 $\mathcal{P}_2$ and apply it for all t and k.

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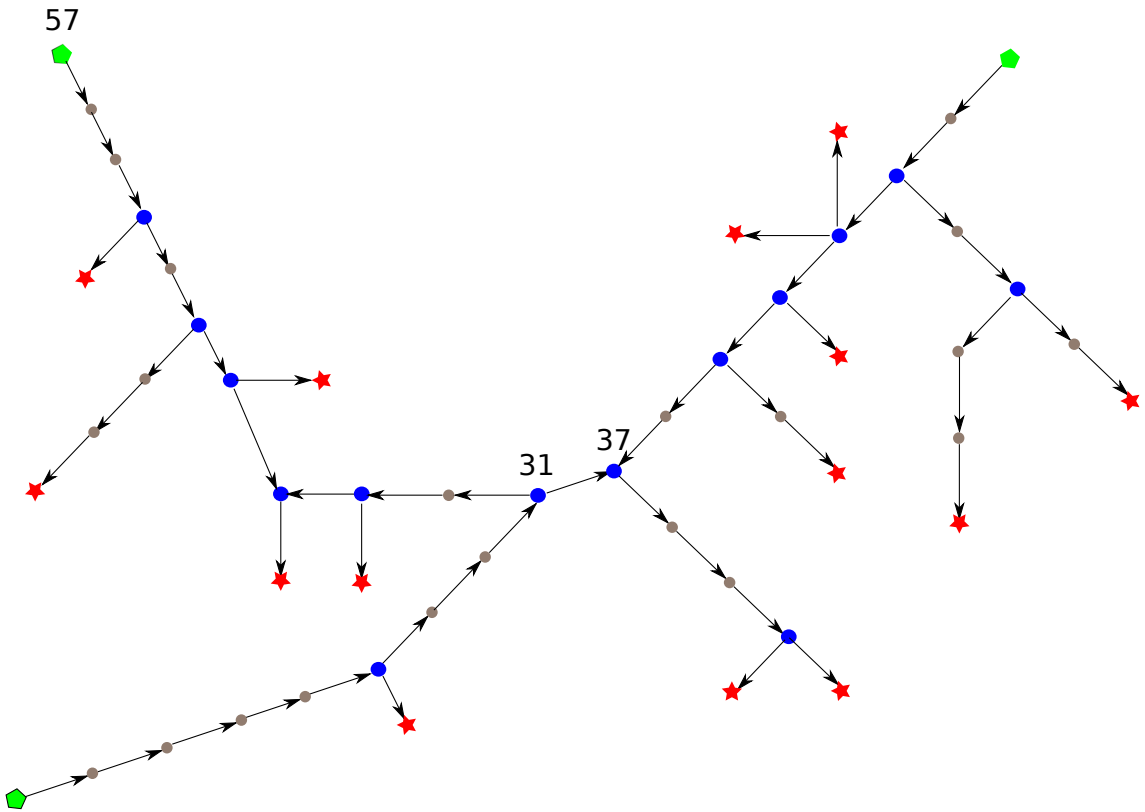
Real flow direction may differ from the DAG direction.

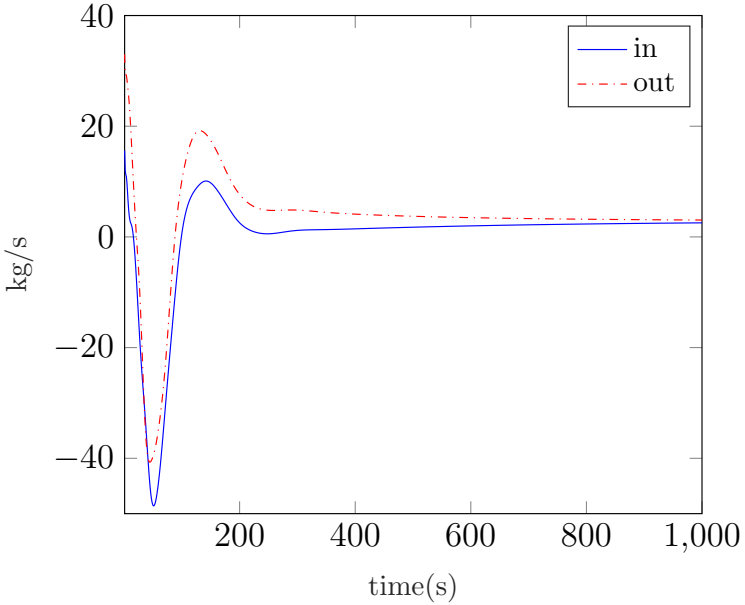


Network with 3 supply nodes, 14 demand nodes.

Numerical Experiments
Change of flow direction

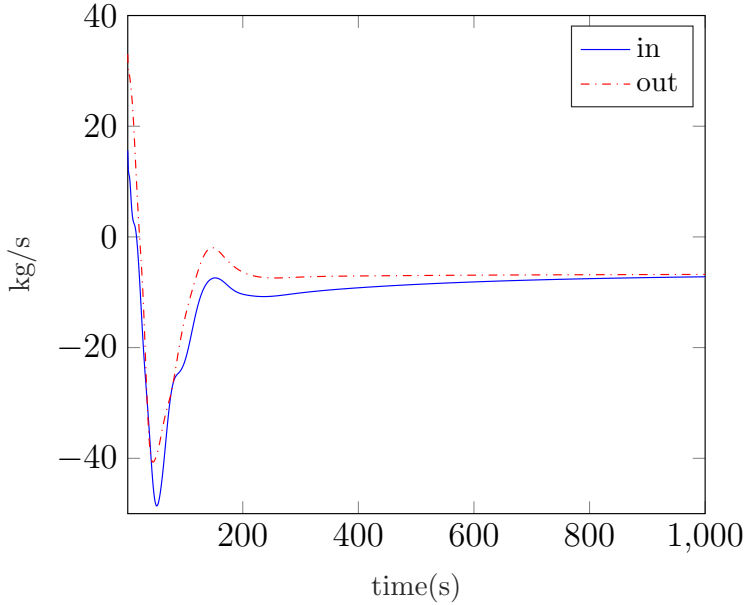
- Case 1: $p_s^{55} = 50.5\ bar$, $p_s^{56} = 50.5\ bar$, $p_s^{57} = 50.8\ bar$.
- Case 2: $p_s^{55} = 50.5\ bar$, $p_s^{56} = 50.5\ bar$, $p_s^{57} = 50.0\ bar$.

Case 1



mass flow at $31 \to 37$

Case 2

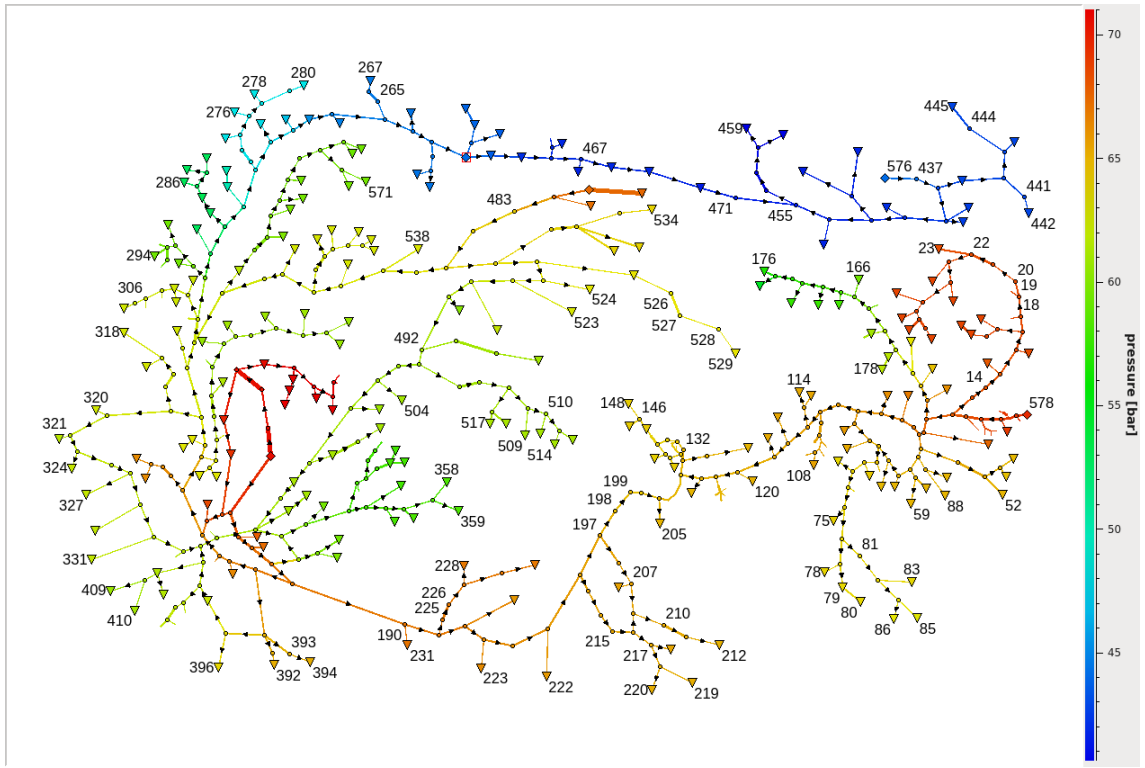


mass flow at $31 \to 37$

$\rightsquigarrow$ Mass flow imbalance induces pressure profile.

Convergence of Newton-Krylov method

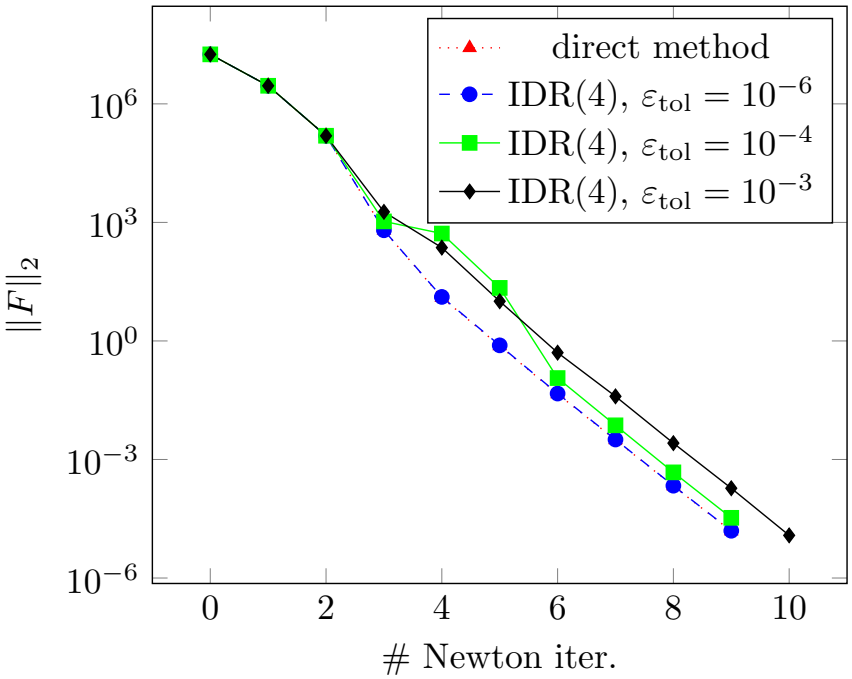
Large-scale network example.



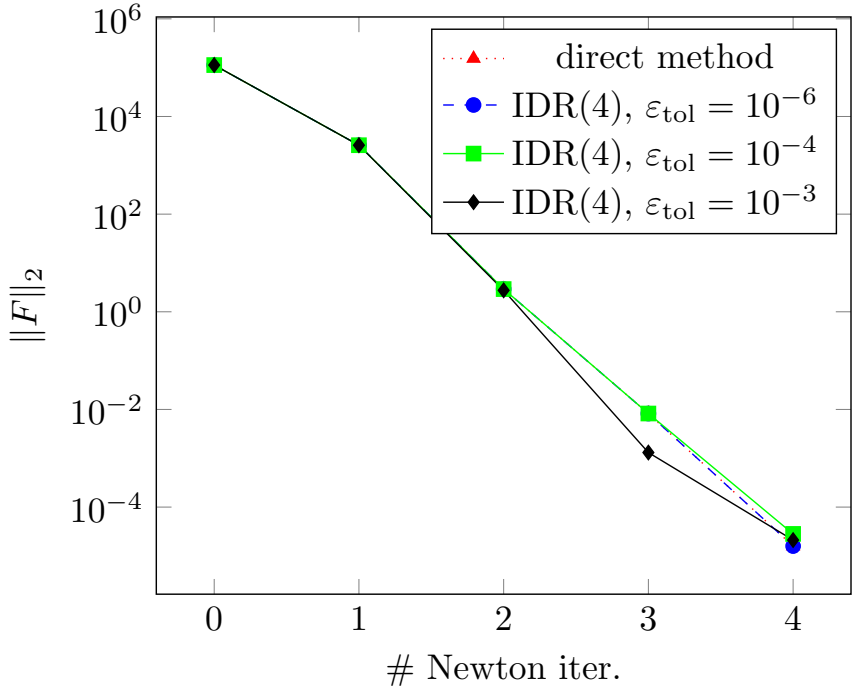
Network with 5 supply nodes, 278 demand nodes.

Convergence of Newton-Krylov method

FVM discretization with mesh size $h = 40$, $\Delta t = 1$. `backslash` in MATLAB as "direct method".



1st time step



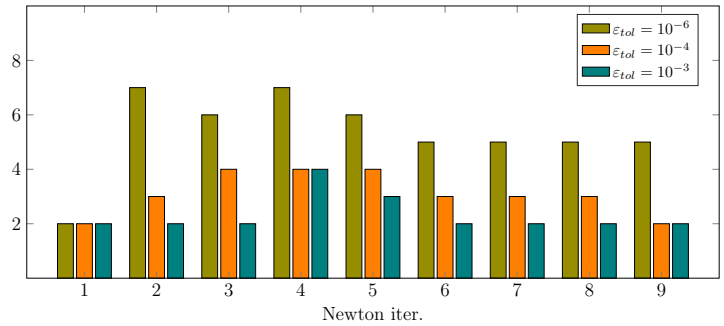
10th time step

Inexactness can further reduce the computational cost.

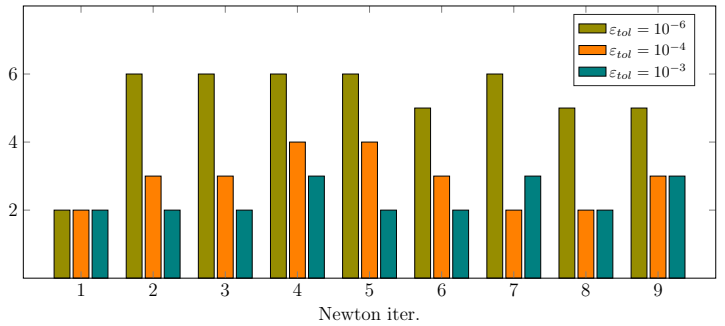
Preconditioner Performance

$\Delta t = 1$, Induced Dimension Reduction (IDR(s)) solver with different residual tolerance ε_{tol}.

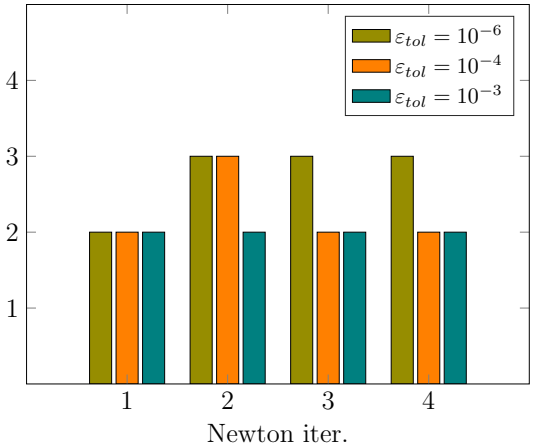
Number of IDR(4) iterations



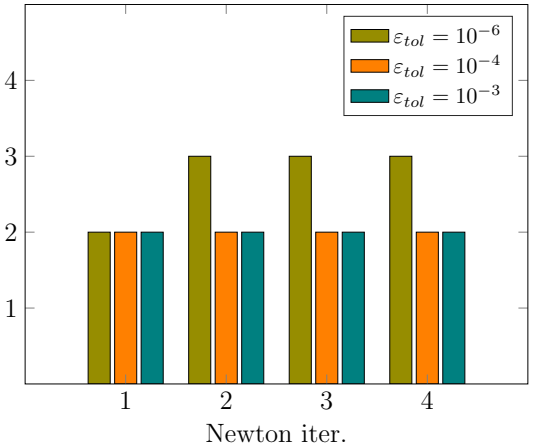
1st time step, $h = 40$



1st time step, $h = 50$



10th time step, $h = 40$



10th time step, $h = 50$

Computational time

$\Delta t = 1$, MATLAB implementation on a desktop with Intel(R) Core(TM)2 Quad CPU Q8400 at 2.66GHz, 8 GB memory and Linux 4.9.0-6-amd64 kernel.

Table: Computational time for the 1st Newton iteration, 1st time step

h	$\#\partial_{\mathbf{y}}\mathbf{F}$	S	IDR(4)	`backslash`
40	1.03e+05	3.85	0.25	0.13
20	2.01e+05	8.12	0.52	0.36
10	3.97e+05	17.84	1.06	1.18
5	7.91e+05	38.44	2.13	1054.62
2.5	1.58e+06	81.42	4.34	-

- S only needs to be computed once.
- Direct solver is called in each Newton iteration, and at each time step.

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Conclusions

- The concept of "smoothed network" reduces the number of algebraic constraints.
- For large-scale network simulation, direct solvers are not possible, while iterative solvers are needed.
- Network topology based preconditioning shows advantage over direct solvers.
- Numerical experiments show the efficiency of our method.
- Fast network simulation is also one of the building blocks of the network uncertainty quantification (UQ) problem.

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Bibliography

Y. Qiu, S. Grundel, M. Stoll, and P. Benner. Efficient Numerical Methods for Gas Network Modeling and Simulation, 2018. arXiv:1807.07142.

P. Benner, S. Grundel, C. Himpe, C. Huck, T. Streubel, and C. Tischendorf. Gas Network Benchmark Models, In: Differential-Algebraic Equations Forum, Springer International Publishing, 2018. doi:10.1007/11221_2018_5

P. Benner, M. Braukmüller, and S. Grundel. A Direct Index 1 DAE Model of Gas Networks. In: W. Keiper, A. Milde, S. Volkwein (eds.), Reduced-Order Modeling (ROM) for Simulation and Optimization, Springer International Publishing, 2018.

SFB Transregio 154: Mathematical Modeling, Simulation and Optimization using the Example of Gas Networks. https://trr154.fau.de/index.php/en/

Announcement

4th Workshop on Model Reduction of Complex Dynamical Systems - MODRED 2019 -

August 28th to 30th, 2019 in Graz

- Overview
- News
- Photos
- Scientific Program
- Participants
- Proceedings
- Location
- Social Activities
- Deadlines
- Abstracts
- Registration
- Accommodation
- Travel
- Useful links
- Contact

The conference starts Wednesday morning and ends on Friday. There will be **plenary talks** by a number of invited speakers. Moreover, there will be several **contributed talks** (20 minutes plus 5 minutes for questions and discussion).

Plenary Speakers

- Serkan Gugercin
- Bernard Haasdonk
- Dirk Hartmann (Siemens)
- Laura Iapichino
- J. Nathan Kutz

Contributed Talks

t.b.a.

Contact: modred2019@uni-graz.at

Last changed: 2018-06-19