Disretization and model adaptivity for the simulation and optimization of Euler equations arising in gas transport and district heating.

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Mathematics for key technologies

Inria, Paris 08.06.22

Outline

Theses

- Modern key technologies require **M**odeling, **S**imulation, and **O**ptimization/control (MSO) of complex dynamical systems.
- Most real world systems are multi-physics systems, combining components from different physical domains, and with different accuracies and scales in the components.
- Modeling becomes exceedingly automatized, linking subsystems or numerical methods in a network fashion.
- Models of real world systems have to adapt to changes in the system during life time. **Digital Twins.**
- Modeling, analysis, numerics, control, optimization, data science techniques **should go hand in hand.**
- Most real world (industrial) models need **model reduction** for data assimilation, optimization and control.

An MSO Wish list !

- Want representations so that coupling of models works across different scales and physical domains.
- Want a representation that is close to the real physics for open and closed systems.
- Model class should have nice algebraic, geometric, and analytical properties.
- Models should be easy to analyze mathematically (existence, uniqueness, robustness, stability, uncertainty, errors etc).
- Invariance under local coordinate transformations (in space and time). Ideally local normal form.
- Model class should allow for easy (space-time) discretization and modelling error adaptation to user needs.
- Class should be good for simulation, control and optimization.

Outline

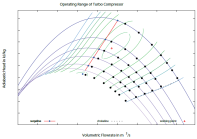
Collaborative Research Center Transregio
Modelling, simulation and optimization of Gas networks

- HU Berlin
- TU Berlin
- Univ. Duisburg-Essen
- FA University Erlangen-Nürnberg
- TU Darmstadt

Components of gas flow model

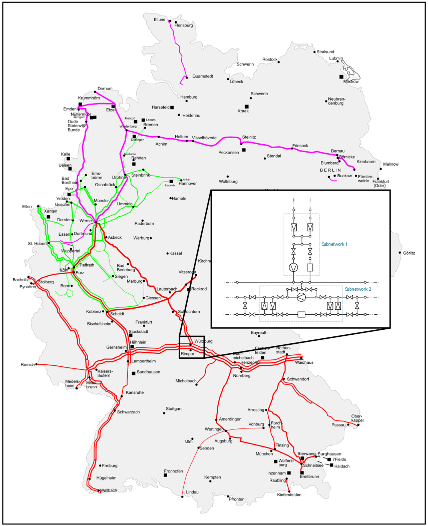
System of partial differential equations with algebraic constraints

- 1D Euler eqs (with temperature) to describe flow in pipes.
- Network model, flow balance equations (Kirchhoff's laws).
- Network elements: pipes, valves, compressors (controllers, coolers, heaters).
- Surrogate and reduced order models.



- Erratic demand and nomination of transport capacity.
- Can we use gas network as energy storage for hydrogen or methane produced from unused renewable energy.

Large network size



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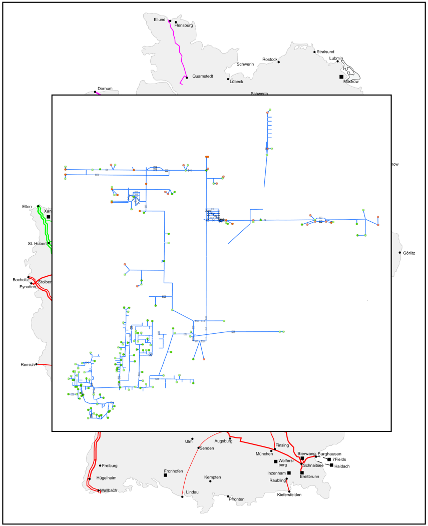

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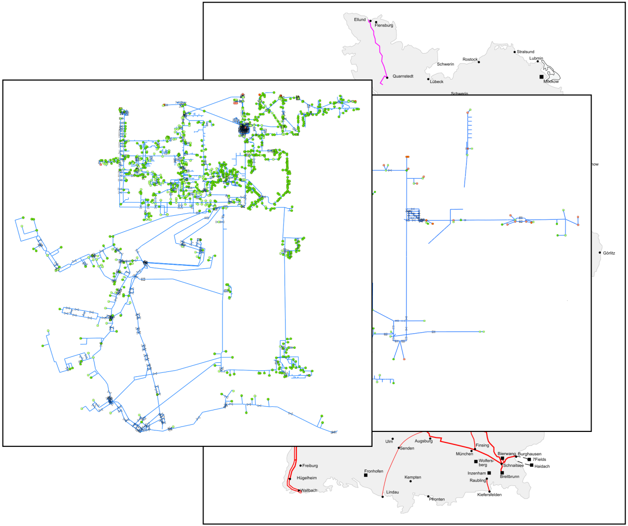
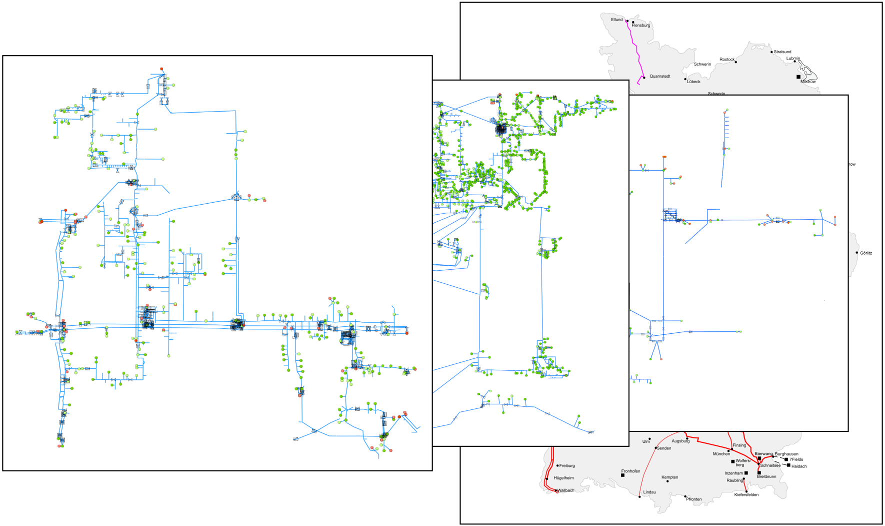


Large network size



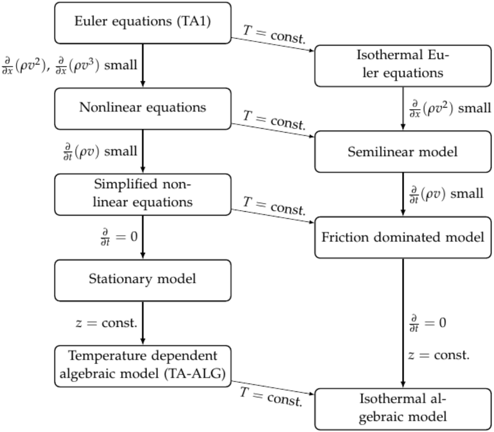
Model: Compressible Euler equations.

$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), \qquad \text{Mass conservation} \\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial}{\partial x}h, \ \text{Momentum balance} \\
0 &= \frac{\partial}{\partial t}\left(\rho(\frac{1}{2}v^2 + e)\right) + \frac{\partial}{\partial x}\left(\rho v(\frac{1}{2}v^2 + e) + pv\right) + \frac{4k_w}{D}(T - T_w), \\
& \qquad \text{Energy balance}
\end{aligned}
$$

with eq. for real gas $p = R\rho T z(p, T)$ init. and bound. cond.

- density ρ, k_w heat transfer coefficient,
- temperature T, wall temperature T_w,
- velocity v, g gravitational force,
- pressure p, λ friction coefficient,
- h height of pipe, D diameter of pipe,
- e internal energy, R gas constant of real gas.

Model hierarchy in a pipe



Every network element/node/edge modelled via a hierarchy, FE/FV/FD model, grid hierarchies, reduced, surrogate models.

- P. Domschke and B. Hiller and J. Lang and V. Mehrmann and R. Morandin and C. Tischendorf, *Gas Network Modeling: An Overview*, TRR 154 Preprint, 2021, https://opus4.kobv.de/opus4-trr154,
- R. Morandin PhD thesis in final stage 2022

Distributed heating

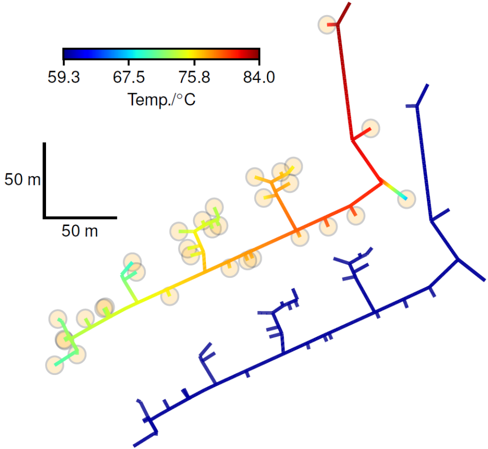
German Ministry of Education and Research (BMBF)

Energy efficiency via intelligent district heating networks (EiFer)

Coupling of heat, electric, waste incineration, and gas.

- TU Berlin
- Univ. Trier
- Fraunhofer ITWM Kaiserslautern
- Stadtwerke Ludwigshafen.

District Heating network



Simulated heat distribution in local district heating network: Technische Werke Ludwigshafen. Entry forward flow temperature 84C, backward flow temperature 60C.

Model equations

Model: Simplified incompressible 1 D Euler equations.

$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), && \text{Mass conservation,} \\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial}{\partial x}h, && \text{Momentum balance} \\
0 &= \frac{\partial}{\partial t}\left(\rho(\frac{1}{2}v^2 + e)\right) + \frac{\partial}{\partial x}(ev) + \frac{k_w}{D}(T - T_w) && \text{Energy balance}
\end{aligned}
$$

together with incompressibility condition for water. Terms for pressure energy and dissipation work have been ignored.

- velocity v, density ρ, k_w heat transfer coefficient,
- temperature T, wall temperature T_w, g gravitational force,
- λ friction coefficient, e internal energy, pressure p,
- h height of pipe, D diameter of pipe.

- S.-A. Hauschild, N. Marheineke, V. Mehrmann, J. Mohring, A. Moses Badlyan, M. Rein, and M. Schmidt, Port-Hamiltonian modeling of disctrict heating networks, DAE Forum, 333-355, Springer Verlag, 2020.
- R. Krug, V. Mehrmann, and M. Schmidt, Nonlinear Optimization of District Heating Networks, Optimization and Engineering, Vol. 22, 783-819, 2021.
- H. Dänschel, V. M., M. Roland, and M. Schmidt, *Adaptive Nonlinear Optimization of District Heating Networks Based on Model and Discretization Catalogs*, In preparation, next week, 2022.

Outline

Energy based network modeling

- Use energy/power as common quantity of different physical systems connected as network via energy transfer.
- Split components into energy storage, energy dissipation components, control inputs and outputs, as well as interconnections and combine via a Dirac structure.
- Allow every submodel to be a model hierarchy of fine or course, continuous or discretized, full or reduced models.
- A system theoretic way to realize this are **(dissipative) port-Hamiltonian differential-algebraic (pH DAE) systems**.

- C. Beattie, V. M., H. Xu, and H. Zwart, *Linear port-Hamiltonian descriptor systems*. Math. Control Signals and Systems, 30:17, 2018.
- P. C. Breedveld. *Modeling and Simulation of Dynamic Systems using Bond Graphs*, pages 128–173. EOLSS Publishers Co. Ltd./UNESCO, Oxford, UK, 2008.
- B. Jacob and H. Zwart. *Linear port-Hamiltonian systems on infinite-dimensional spaces*. Operator Theory: Advances and Applications, 223. Birkhäuser/Springer Basel CH, 2012.
- V. M. and R. Morandin, Structure-preserving discretization for port-Hamiltonian descriptor systems. *Proceedings of the 58th IEEE Conference on Decision and Control (CDC)*, 9.-12.12.19, Nice, 2019. https://arxiv.org/abs/1903.10451
- A. J. van der Schaft, D. Jeltsema, Port-Hamiltonian systems: network modeling and control of nonlinear physical systems. In *Advanced Dynamics and Control of Structures and Machines*, CISM Courses and Lectures, Vol. 444. Springer Verlag, New York, N.Y., 2014.

Definition (M./Morandin 2019)

Let $\mathcal{X} \subseteq \mathbb{R}^m$ (state space), $\mathbb{I} \subseteq \mathbb{R}$ time interval, and $\mathcal{S} = \mathbb{I} \times \mathcal{X}$. Consider

$$\begin{aligned} E(t,x)\dot{x} + r(t,x) &= (J(t,x) - R(r,x))e(t,x) + (B(t,x) - P(t,x))u, \\ y &= (B(t,x) + P(t,x))^T e(t,x) + (S(t,x) - N(t,x))u, \end{aligned}$$

Hamiltonian $\mathcal{H} \in C^1(\mathcal{S},\mathbb{R})$, where $E \in C(\mathcal{S},\mathbb{R}^{\ell,n})$, $J, R \in C(\mathcal{S},\mathbb{R}^{n,n})$, $B, P \in C(\mathcal{S},\mathbb{R}^{\ell,m})$, $S = S^T$, $N = -N^T \in C(\mathcal{S},\mathbb{R}^{m,m})$ and $e, r \in C(\mathcal{S},\mathbb{R}^{\ell})$. The system is called *port-Hamiltonian DAE* if

$$\Gamma(t,x) = -\Gamma^T = \begin{bmatrix} J & B \\ -B^T & N \end{bmatrix}, \quad W(t,x) = W^T = \begin{bmatrix} R & P \\ P^T & S \end{bmatrix} \geq 0,$$

$$\frac{\partial \mathcal{H}}{\partial x}(t,x) = E^T(t,x)e(t,x), \quad \frac{\partial \mathcal{H}}{\partial t}(t,x) = e^T(t,x)r(t,x).$$

Definition extends to weak solutions and infinite dimension.

Why should this be the right approach?

- PH DAEs generalize *Hamiltonian/gradient flow systems*.
- *Conservation of energy* replaced by *dissipation inequality*

$$\mathcal{H}(x(t_1)) - \mathcal{H}(x(t_0)) \leq \int_{t_0}^{t_1} y(t)^T u(t)\, dt,$$

- PH DAE systems are closed under *power-conserving interconnection*. Modularized network based modeling.
- *Stability and passivity* analysis easy.
- PH DAE structure allows to preserve physical properties in *Galerkin projection, model reduction*.
- Physical properties encoded in *algebraic structure* of coefficients and in *geometric structure* associated with flow.
- Invariance under local/global diffeomorphisms.

Further properties

- Structure preserving time-discretization, so that time discrete system has dissipation inequality and power balance equation.
- Use non-uniqueness of representation to obtain robustness under perturbations.
- Local and global normal forms.
- Perturbation analysis, distance to instability, non-passivity, non-regularity.
- Different port-Hamiltonian PDE formulations, including terms that have been dropped due to model simplifications.

Outline

pH PDE, gas flow

Port-Hamiltonian formulation of compressible Euler including pressure energy and dissipation work, as well as entropy (s) balance. A. Moses Badlyan 2019

$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), && \text{mass conservation}\\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial}{\partial x}h, && \text{momentum balance}\\
0 &= \frac{\partial e}{\partial t} + \frac{\partial}{\partial x}(ev)) + p\frac{\partial v}{\partial x} - \frac{\lambda}{2D}\rho v^2\,|v| + \frac{4k_w}{D}(T - T_w), && \text{energy bal.}\\
0 &= \frac{\partial s}{\partial t} + \frac{\partial}{\partial x}(sv)) - \frac{\lambda\,\rho}{2D\,T}v^2\,|v| + \frac{4k_w}{D}\frac{(T - T_w)}{T}, && \text{entropy balance}
\end{aligned}
$$

We have to add node conditions and boundary conditions. Kirchhoff's laws.

pH PDE, hot water flow

Port-Hamiltonian formulation of incompressible Euler including pressure energy and dissipation work, and entropy balance.

$$
\begin{aligned}
0 &= \rho \frac{\partial v}{\partial x}, \qquad \text{mass conservation} \\
0 &= \frac{\partial}{\partial t}(\rho v) + v^2 \frac{\partial \rho}{\partial x} + \frac{\partial p}{\partial x} + \frac{\lambda}{2D}\rho v\,|v| + g\rho \frac{\partial h}{\partial x}, \ \text{momentum balance} \\
0 &= \frac{\partial e}{\partial t} + v \frac{\partial e}{\partial x} - \frac{\lambda}{2D}\rho v^2\,|v| + \frac{4k_w}{D}\left(T - T_w\right), \ \text{energy balance} \\
0 &= \frac{\partial s}{\partial t} + v \frac{\partial s}{\partial x} - \frac{\lambda\,\rho}{2D\,T} v^2\,|v| + \frac{4k_w}{D}\frac{(T - T_w)}{T}, \ \text{entropy balance}
\end{aligned}
$$

We have to add node conditions, mixing conditions etc.

Space discretization

Structure preserving space discretization as in unstructured PDEs, typically easier than time discretization.
Use pH DAE weak formulations for finite element/finite volume approaches.
Galerkin preserves structure.

- ▷ A. M. Badlyan, B. Maschke, C. Beattie, and V. Mehrmann, Open physical systems: from GENERIC to port-Hamiltonian systems, Proceedings MTNS 2018. arxiv:1804.04064
- ▷ A. M. Badlyan, and C. Zimmer, Operator GENERIC formulation of thermodynamics of irreversible processes. Preprint TU Berlin, arxiv: 1807.09822, 2018.
- ▷ Egger, Energy stable Galerkin approximation of Hamiltonian and gradient systems, Numerische Mathematik, 2019.
- ▷ H. Egger and T. Kugler, Damped wave systems on networks: Exponential stability and uniform approximations. Numerische Mathematik, 138:839–867, 2018.
- ▷ H. Egger, T. Kugler, B. Liljegren-Sailer, N. Marheineke, and V.M., On structure preserving model reduction for damped wave propagation in transport networks, SIAM J. Scientific Computing, 40:A331–A365, 2018.
- ▷ A. Serhani, D. Matignon, and G. Haine. A partitioned finite element method for the structure-preserving discretization of damped infinite-dimensional port-Hamiltonian systems with boundary control. In F. Nielsen and F. Barbaresco, editors, Geometric Science of Information, pages 549–558. Springer, Cham, 2019.

- Most classical ODE/DAE methods do not preserve the energy or dissipation inequality.
- We need classes of integrators that do.
- Want integrators that lead to discrete-time pH systems.
- Preservation of constraints.

Idea: Use Dirac Structure and structure preserving methods
Gauss-Legrendre collocation methods (like implicit midpoint rule) are methods of choice and preserve quadratic Hamiltonians.

- E. Celedoni and E.H. Høiseth, *Energy-Preserving and Passivity-Consistent Numerical Discretization of Port-Hamiltonian Systems, arXiv:1706.08621v1*
- Kotyczka, Lefèvre, Discrete-Time Port-Hamiltonian Systems Based on Gauss-Legendre Collocation, IFAC-PapersOnLine 51, no. 3 (2018): 125–30.
- V. M. and R. Morandin, Structure-preserving discretization for port-Hamiltonian descriptor systems. *Proceedings of the 58th IEEE Conference on Decision and Control (CDC)*, 9.-12.12.19, Nice, 2019. https://arxiv.org/abs/1903.10451

Outline

- The 'ideal methods' are implicit methods and require the solution of (non)linear system.
- This is a large scale problem when the problem is a space discretized PDE.
- Does the pHD AE structure help?

Example: Discretize $E\dot{x} = (J - R)x$ with implicit midpoint rule.

$$E(x_{i+1} - x_i) = \tau(J - R)(x_{i+1} + x_i)/2,$$

or equivalently

$$(E + \tau/2R - \tau/2J)x_{i+1} = (I + \tau/2(J - R))x_i$$

Matrix $E + \tau/2R - \tau/2J$ has pos. (semi)-def. symmetric part. Locally the pHDAE structure leads to such linear systems.

For linear systems of the form $(M+N)x = b$ with $M = M^T > 0$ $N = -N^T$ Widlund's method uses the symmetric part as preconditioner, and solves equivalent system

$$(I-K)x = \hat{b}, \quad \text{where} \quad K = M^{-1}N, \quad \hat{b} = M^{-1}b.$$

Here$K$ is M-normal i.e., $M^{-1}K^TM = -K$. This is necessary and sufficient for K to admit an optimal 3-term recurrence for generating an M-orthogonal basis of the Krylov subspace $\mathcal{K}_k(K, v)$ for each k and initial vector v.

Oblique projection method with Galerkin projection property:

$$x_k \in \mathcal{K}_k(K, \hat{b}) \quad \text{s.t.} \quad r_k = b - (M+N)x_k \perp \mathcal{K}_k(K, \hat{b}).$$

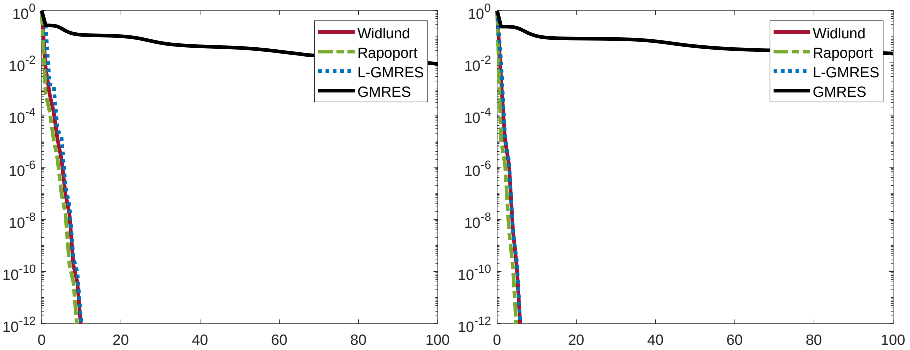
- C. Güdücü, J. Liesen, V. M., and D. Szyld, *On non-Hermitian positive (semi)definite linear algebraic systems arising from dissipative Hamiltonian DAEs*, http://arxiv.org/abs/2111.05616, SIAM J. Scientific Computing, 2022.
- M. Manguoğlu and V. M., A two-level iterative scheme for general sparse linear systems based on approximate skew-symmetrizers. Electronic Transactions Numerical Analysis, Vol. 54, 370–391, 2021.
- O. Widlund. A Lanczos method for a class of nonsymmetric systems of linear equations. *SIAM J. Numer. Anal.*, 15(4):801–812, 1978.

Example: Stokes flow

Method	*Time*	$\|Rel.Res.\|$	$\#Iter.$
Widlund	10.273	$6.794e-09$	10
GMRES	1672.294	$4.727e-02$	500

Stokes equation. Running times, relative residual norms at the final step, and total number of iterations for $\tau = 0.0001$.

Numerical example, convergence



Stokes flow. Relative residual norms with $\tau = 0.001$ and $\tau = 0.0001$ (left and right).
Run times differences drastic if step-size is decreased.

Outline

Model hierarchy and adaptivity

Use model hierarchy for adaptivity in space-time discretization, solver and model adaptivity for simulation and optimization. Find compromise between error tolerance/ computational speed.

- ▷ Determine sensitivities when moving in model hierarchy.
- ▷ Determine error estimates for time and space discretization.
- ▷ Choose cost functions or adaptation strategies.
- ▷ Use adaptivity to drive method for simulation and optimization.

System theoretic approach allows to jump between models in the hierarchy without changing the simulation, control, and optimization framework.

Example: 4-level-hierarchy gas transport

- Full model M_0 (truth (expensive)): *isothermal Euler equations*

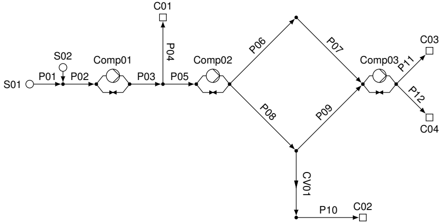
$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), \\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial h}{\partial x}, \\
p &= R\rho T z(p, T)
\end{aligned}
$$

  together with boundary cond. and Kirchhoff's laws at nodes.
- M_1: $\frac{\partial h}{\partial x} = 0$.
- M_2: Model M_1 and $\frac{\partial}{\partial x}(\rho v^2) = 0$.
- M_3: Model M_2 and stationary state.

- J.J. Stolwijk and V. M. *Error analysis and model adaptivity for flows in gas networks*. ANALELE STIINTIFICE ALE UNIVERSITATII OVIDIUS CONSTANTA. SERIA MATEMATICA, 2018.
- P. Domschke, A. Dua, J.J. Stolwijk, J. Lang, and V. Mehrmann, *Adaptive Refinement Strategies for the Simulation of Gas Flow in Networks using a Model Hierarchy*, Electronic Transactions Numerical Analysis, Vol. 48, 97–113, 2018.

For given tolerance *tol*, minimize computational cost.

$$\frac{\sum_{j\in\mathcal{J}_p}\left(\eta_{m,j}+\eta_{x,j}+\eta_{t,j}\right)}{|\mathcal{J}_p|}\leq \text{tol}$$

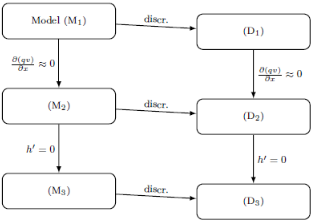


Non-adaptive simulation time is 4 hours using ANACONDA code.
Adapative method: computing time reduction of 80%.

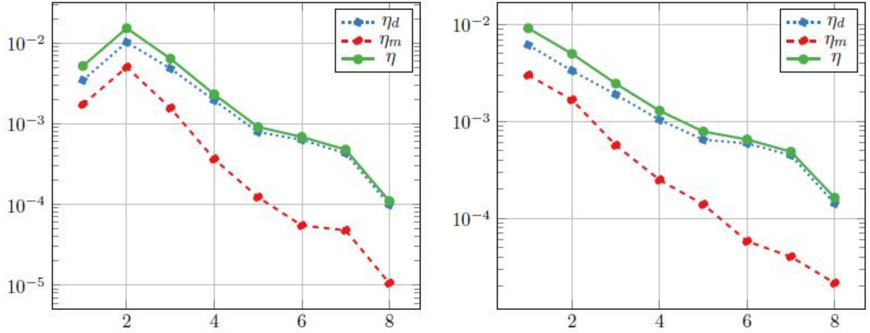
- P. Domschke, A. Dua, J.J. Stolwijk, J. Lang, and V. M., *Adaptive Refinement Strategies for the Simulation of Gas Flow in Networks using a Model Hierarchy*, Electronic Transactions Numerical Analysis, 2018.

Adaptivity in nonlinear optimization

Optimize compressor costs in stationary model of gas network.
Use hierarchy to get feasible sol. via space-model adaptivity.



Pipe model hierarchy based on the isothermal Euler equations.
Left: space contin. models, right: space discrete models.



Discretization, model, total error (*y*-axis) over course of optimization (*x*-axis). Left: GasLib-40, right: GasLib-135.

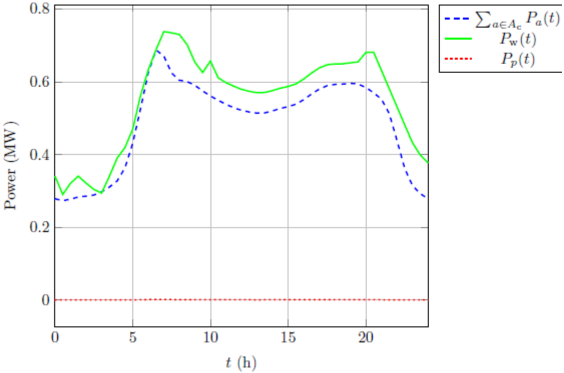
- V. M., M. Schmidt, and J. Stolwijk, *Model and Discretization Error Adaptivity within Stationary Gas Transport Optimization*, http://arxiv.org/abs/1712.02745, Vietnam J. Math. 2018.

Optimization district heating network

Optimization of energy cost while satisfying the heat demand of all consumers. Four level model hierarchy, stationary models, discretized with implicit midpoint rule.

- Construction of error measures.
- Adaptive algorithm applied to realistic networks.
- Convergence proof of adaptive algorithm to feasible solution.
- Can solve problems that no other solver could manage.

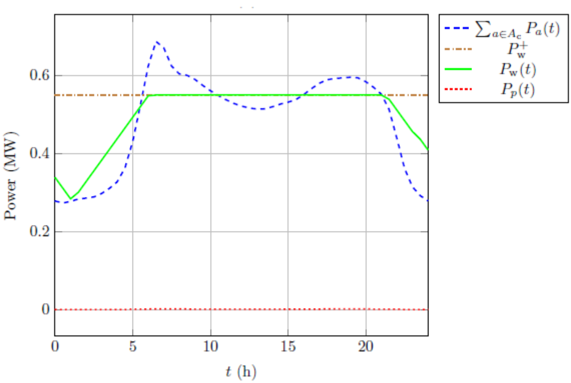
- R. Krug, V. M., M. Schmidt, Nonlinear Optimization of District Heating Networks, *Optimization and Engineering*, 1-37, 2020.
- H. Dänschel, V. Mehrmann, M. Roland, and M. Schmidt, *Adaptive Nonlinear Optimization of District Heating Networks Based on Model and Discretization Catalogs*, http://arxiv.org/abs/2201.11993, 2022.



Aggregated power consumption of households (dashed curve) without bound on power generated by waste incineration (solid curve) for district heating network.

▷ R. Krug, V. M., M. Schmidt, Nonlinear Optimization of District Heating Networks, *Optimization and Engineering*, 1-37, 2020.

Optimization of power consumption



Aggregated power consumption of households (dashed curve) with bound on power generated by waste incineration (solid curve) for distinct heating network.

- R. Krug, V. M., M. Schmidt, Nonlinear Optimization of District Heating Networks, *Optimization and Engineering*, 1-37, 2020.

What about our wish list?

- Want representations so that coupling of models works across different scales and physical domains.
- Want a representation that is close to the real physics for open and closed systems.
- Model class should have nice algebraic, geometric, and analytical properties.
- Models should be easy to analyze mathematically (existence, uniqueness, robustness, stability, uncertainty, errors etc).
- Invariance under local coordinate transformations (in space and time). Ideally local normal form.
- Model class should allow for easy (space-time) discretization and model reduction.
- Class should be good for simulation, control and optimization,

pH DAE systems are ideal, almost all wishes are fulfilled.

- Survey: V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2022. Acta Numerica submitted.

But there are many things to do

- Real time control, optimization.
- Other physical domains.
- Incorporate stochastics in models.
- Stability analysis.
- More error estimates.
- Preconditioning.
- Data based realization.
- Software.
- ...

Thank you very much
for your attention
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- DFG priority program 1984.
- BMBF/industry project Eifer.

Details: http://www.math.tu-berlin.de/?id=76888