Energy based modeling, simulation and control of multi-physics systems.

Volker Mehrmann
Institute f. Mathematics
TU Berlin

Research Center MATHEON
Mathematics for key technologies

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.**
- A new integrated MSO paradigm is needed.

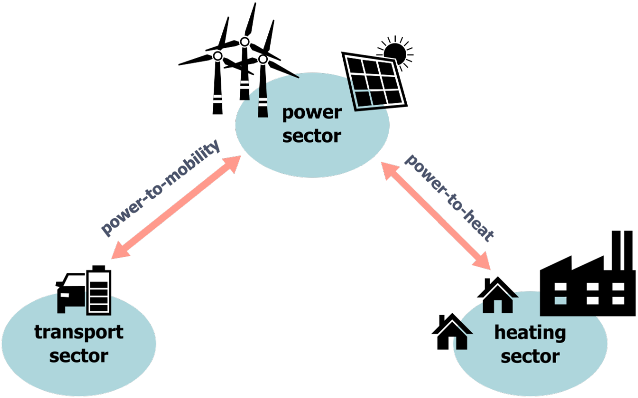


Figure: Sector coupling and the power-to-X concept

Challenges

- The security of energy supply has to be guaranteed.
- Energy conversion must be efficient.
- Different energy sectors have to be coupled.
- Different components of energy networks have very different modeling accuracy.
- Different energy sectors live on very different (time) scales.
- Deal with increased randomness and decentralization.
- Need dynamical rather than stationary approaches.

Build a mathematical model (**digital twin**) that deals with these challenges in mathematical simulation, optimization and control in real time?

A Modelling Wish list !

- Want representations so that coupling of models works across different scales and physical domains.
- Want a system theoretic 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,

Is there such a Jack of all trades, Eierlegende-Woll-Milch-Sau?

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

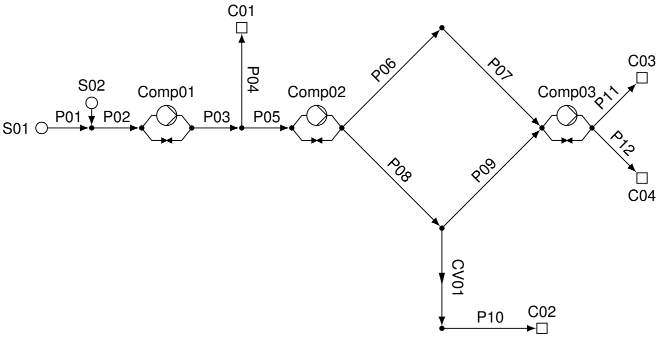
Planning, simulation, optimization, and operation of gas networks.
Construct a mathematical model that can handle all this.

- HU Berlin
- TU Berlin
- Univ. Duisburg-Essen
- FA University Erlangen-Nürnberg
- TU Darmstadt
- Real industrial data (anonymized) from OGE.

Network of partial differential equations with constraints.

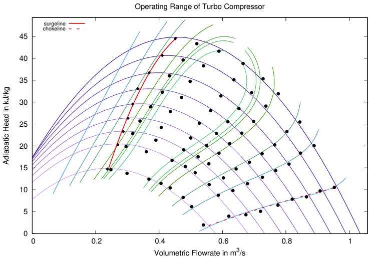
Euler eqs 1D (or 3D) with temperature to describe flow in pipes.

Network model, flow balance, network elements: Sources S_i, pipes P_i, valves CV_i, compressors $Comp_i$, consumers C_i,

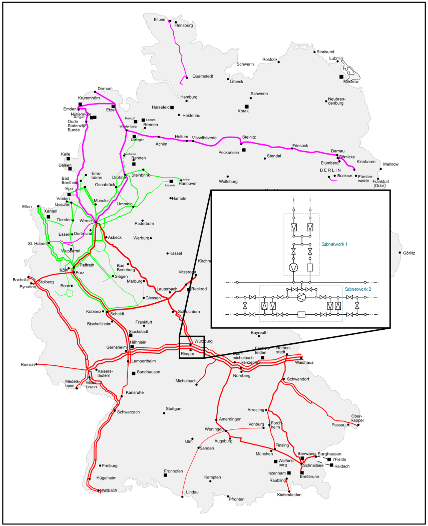


Components of gas flow model II

Data based surrogate and reduced order models.



Large network size



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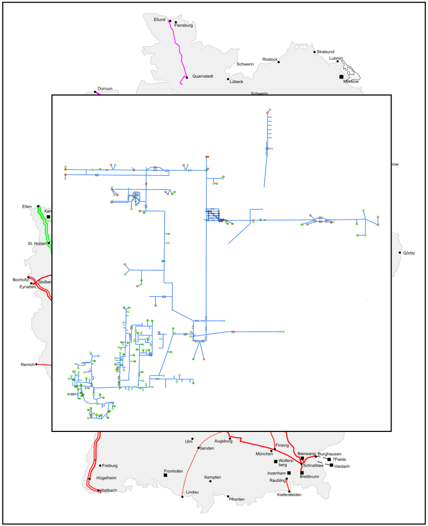
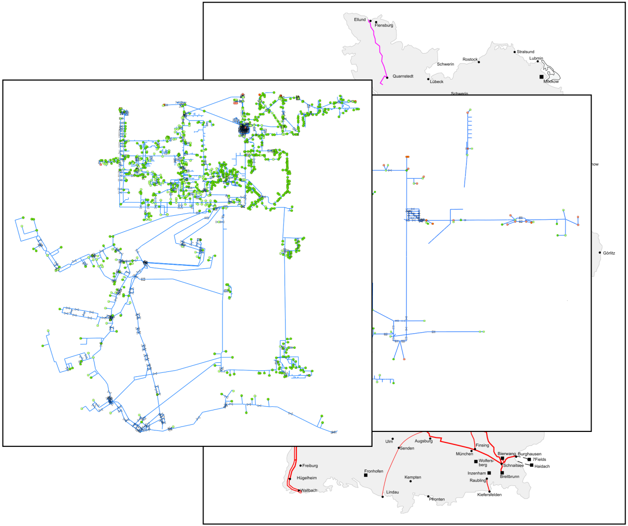
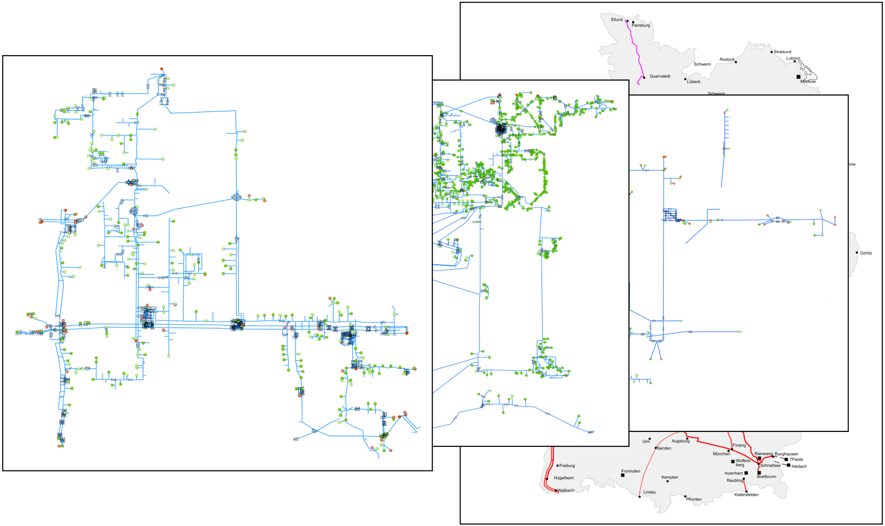


Large network size



Large network size



Model: Compressible 1D Euler equations.

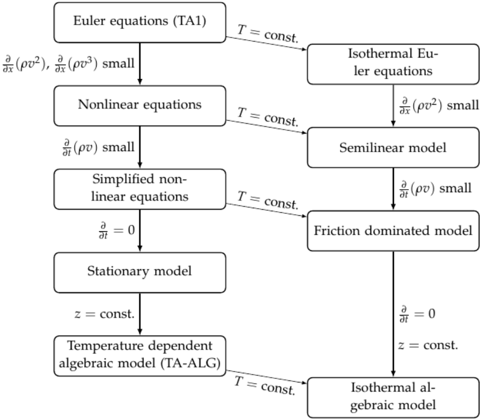
$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), && \text{Mass conservation} \\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial}{\partial x}h, && \text{Momentum balance}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

Energy balance

together with equations for real gas $p = R\rho T z(p, T)$.

terms for pressure energy and dissipation work terms ignored.

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



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,

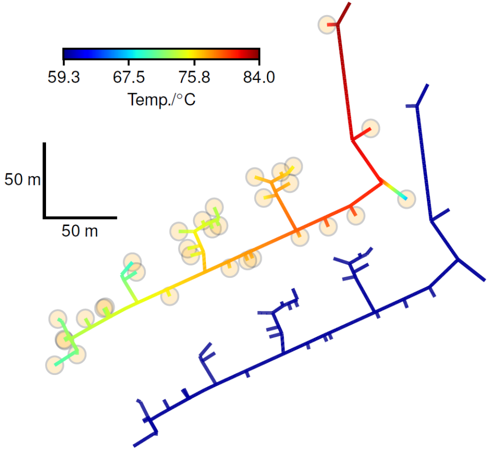
District heating network

German Ministry of Education and Research (BMBF)

Energy efficiency via intelligent district heating networks (EiFer)
Coupling of district heating network, hot water via electric, gas heating, waste incineration.

- TU Berlin
- Univ. Trier
- Fraunhofer ITWM Kaiserslautern
- Technische Werke (cityworks) 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: 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 ignored.

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

- 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.

Other applications in the TU Berlin group

- Power networks
- Werner von Siemens Center Berlin. Electricity generation, gas turbine repair, additive manufacturing of turbine blades.
- Reactive flow control, new gas turbine, CRC 1029.
- Poro-elastic networks.
- Multibody dynamics.

- R. Altmann, V. M., and B. Unger. Port-Hamiltonian formulations of poroelastic network models. http://arxiv.org/abs/2012.01949. *Mathematical and Computer Modelling Of Dynamical Systems*, Vol. 27, 429–452, 2021.
- R. Altmann und P. Schulze A port-Hamiltonian formulation of the Navier-Stokes equations for reactive flows Systems Control Lett., Vol. 100, 2017, pp. 51-55.
- A. M. Badlyan, B. Maschke, C. Beattie, and V. M., Open physical systems: from GENERIC to port-Hamiltonian systems, Proceedings of MTNS, 2018.
- A. Moses Badlyan and C. Zimmer. Operator-GENERIC formulation of thermodynamics of irreversible processes. Preprint TU Berlin 2018.
- K. Cherifi, V. M., P. Schulze, *Simulations in a Digital Twin of an Electrical Machine*. http://arxiv.org/abs/2207.02171, 2022.
- Survey: V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2023. Acta Numerica.

Outline

New paradigm: Energy based 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/Lagrange 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 systems**.

- 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.
- Survey: V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2023. Acta Numerica.
- 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.

Classical nonlinear port-Hamiltonian (pH) ODE systems

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

- x is the state, u input, y output.
- $\mathcal{H}(x)$ is the *Hamiltonian*: it describes the distribution of internal energy among the energy storage elements;
- $J = -J^T$ describes the *energy flux* among energy storage elements within the system;
- $R = R^T \geq 0$ describes *energy dissipation/loss* in the system;
- $B \pm P$: *ports* where energy/power enters and exits the system;
- $S - N$, $S = S^T$, $N = -N^T$, direct *feed-through* input to output.
- In the infinite dimensional case J, R, B, P, S, N are operators that map into appropriate function spaces.

Why should this be a good approach?

- PH systems 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 systems are closed under *power-conserving interconnection*. Modularized network based modeling.
- Hamiltonian is Lyapunov function, *Stability and passivity* analysis.
- PH 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.

Constrained Port-Hamiltonian systems

Can we add algebraic constraints, like Kirchhoff's laws, position constraints, further conservation laws?

Define pH differential-algebraic equations to fulfill as many points on the wishlist as possible.

- C. Beattie, V. M., H. Xu, and H. Zwart, *Linear port-Hamiltonian descriptor systems*. Math. Control Signals and Systems, 30:17, 2018.
- C. Beattie, V. M., and P. Van Dooren, *Robust port-Hamiltonian representations of passive systems*. Automatica, 100, 182–186, 2019.
- 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
- V. Mehrmann and A.J. van der Schaft. *Differential-algebraic systems with dissipative Hamiltonian structure*. http://arxiv.org/abs/2208.02737, 2022
- A. J. van der Schaft, Port-Hamiltonian differential-algebraic systems. In *Surveys in Differential-Algebraic Equations I*, 173-226. Springer-Verlag, 2013.
- A. van der Schaft and B. Maschke, Generalized Port-Hamiltonian DAE Systems, Systems Control Letters 121, 31-37, 2018.
- V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2023. Acta Numerica.

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

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

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

Def. extends to weak solutions and operators in infinite dimension.

Theorem (M./Morandin 2019)

For a pHDAE, the power balance equation (PBE)

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(t, x(t)) = -\begin{bmatrix} e \\ u \end{bmatrix}^T W \begin{bmatrix} e \\ u \end{bmatrix} + y^T u$$

holds along any solution x, for any input u. In particular, the dissipation inequality

$$\mathcal{H}(t_2, x(t_2)) - \mathcal{H}(t_1, x(t_1)) \leq \int_{t_1}^{t_2} y(\tau)^T u(\tau)\mathrm{d}\tau$$

holds.

pHDAE properties

- Power conserving interconnection preserves structure.
- Structure invariant under local and global space-time dependent diffeomorphisms.
- pHDAE system can be made autonomous w/o destroying structure.
- Qualitative stability and passivity results.
- Use non-uniqueness of representation to obtain robustness.
- Local and global normal forms.
- Galerkin projection, reduced basis, model reduction.
- Perturbation analysis, distance to instability, non-passivity.

- 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
- V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2023. Acta Numerica.

Different approaches

- Operator pH DAE modeling.
- Differential geometric: Gradient flow, GENERIC.
- Formal Dirac structures.
- Structured PDE systems with input and outputs.

References:

- R. Altmann und P. Schulze A port-Hamiltonian formulation of the Navier-Stokes equations for reactive flows Systems Control Lett., Vol. 100, 2017, pp. 51-55.
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- M. Hütter and B. Svendsen, Quasi-linear versus potential-based formulations of force-flux relations and the generic for irreversible processes: comparisons and examples. Continuum Mechanics and Thermodynamics, 25, 803–816, 2013.
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- H. Yoshimura and J Marsden. Dirac structures in Lagrangian mechanics part i: Implicit Lagrangian systems. Journal of Geometry and Physics, 57, 133–156, 2006.

How to deal with boundary conditions?

- Take a system theoretic approach.
- Distinguish between boundary condition for interconnection and those for control, and simulation.
- Choose boundary conditions according to application.

Examples: gas or hot water flow

- Wall temperature boundary conditions can be classical b.c. for simulation and optimization of network or coupling conditions when coupling with environment.
- Inflow and outflow boundary conditions are controls, or used for coupling, or classical boundary conditions for simulation.

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

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

Add node conditions and boundary conditions. Kirchhoff's laws.

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

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

We have to add node conditions, mixing conditions etc.

Outline

Structure preserving space discretization with Galerkin approaches as in unstructured PDEs.

Space discretization easier than time discretization.

Use pH DAE weak formulations for FEM/finite volume approaches. Galerkin preserves structure.

- ▷ A. M. Badlyan, B. Maschke, C. Beattie, and V. M., 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.
- ▷ H. Egger, Energy stable Galerkin approximation of Hamiltonian and gradient systems, Numerische Mathematik, 143, 85–106, 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.

Time integrators

- 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' for DAEs are implicit methods and require the solution of (non)linear system in each time-step.
- This is a large scale problem when the problem is a space discretized PDE.
- Does the pHDAE 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, pHDAE structure always 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., $M^{-1}K^TM = -K$. Necessary and sufficient for K to admit optimal 3-term recurrence for Krylov subspace $\mathcal{K}_k(K, v) = \mathrm{span}\{v, Kv, K^2v, \ldots, K^{k-1}v\}$ for each k and v.

Oblique projection method with Galerkin projection property:

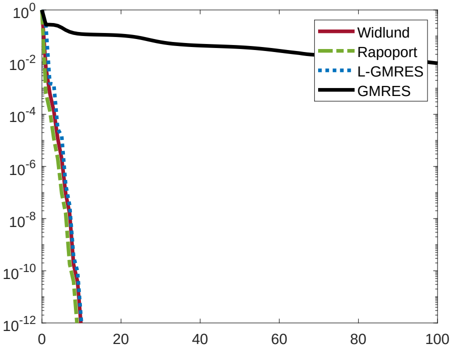
$$x_k \in \mathcal{K}_k(K, \hat{b}) \quad \text{s.t.} \quad r_k = b - (M+N)x_k \perp \mathcal{K}_k(K, \hat{b}).$$

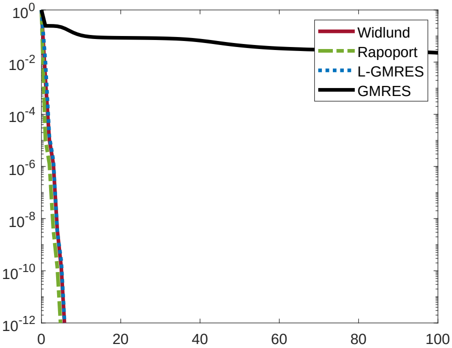
- C. Güdücü, J. Liesen, V. M., and D. Szyld, *On non-Hermitian positive (semi)definite linear algebraic systems arising from dissipative Hamiltonian DAEs*, http://arxiv.org/abs/2111.05616, SIAM J. Scientific Computing, 2022.
- M. Manguoğlu and V. M., A two-level iterative scheme for general sparse linear 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 $\tau = 0.0001$.





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.

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*

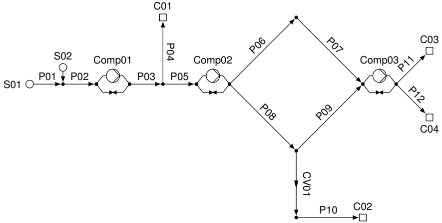
$$
\begin{aligned}
0 &= \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v),\\
0 &= \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial h}{\partial x},\\
p &= R\rho T z(p, T)
\end{aligned}
$$

  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.

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

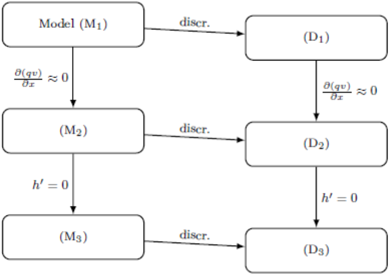


Non-adaptive simulation time is 4 hours using ANACONDA code.
Adapative method: computing time reduction of 80%.

- 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.

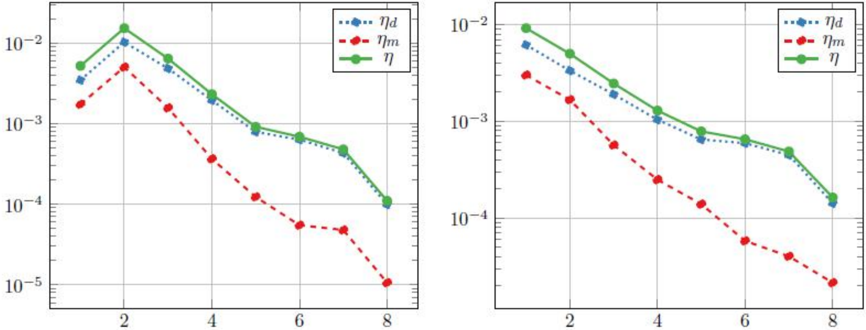
Adaptivity in nonlinear optimization

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.

Compressor cost optimization



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.

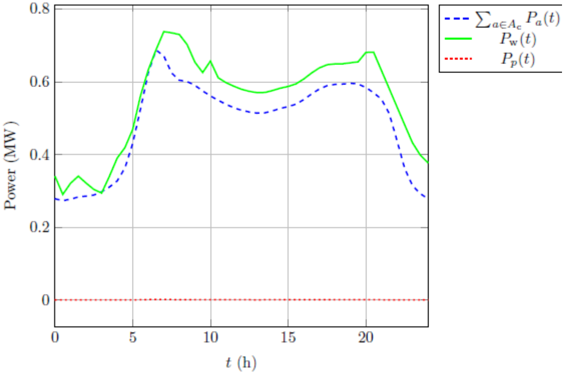
Optimization district heating network

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.

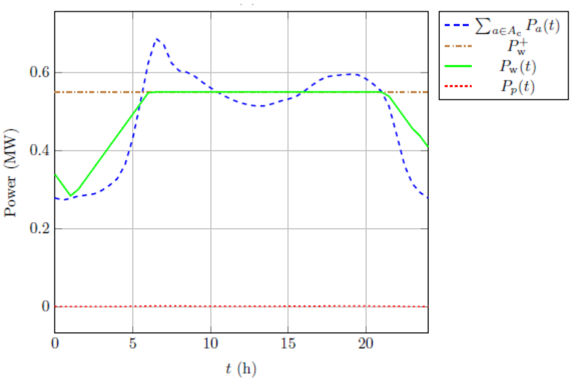
Optim. power consum. heat network



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.

Outline

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.

But there are many things to do

- Real time control, optimization.
- Other physical domains.
- Incorporate stochastics in models.
- pHDAE appropriate function Spaces.
- Error estimates.
- Preconditioning.
- Data based realization.
- Software.
- Digital twins
- ...

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for your attention
and my sponsors for their support

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- BMBF/industry project Eifer.

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