Energy Based Mathematical Modeling, Simulation, and Control of Real World Systems

Volker Mehrmann
Institute f. Mathematics
TU Berlin

Research Center MATHEON
Mathematics for key technologies

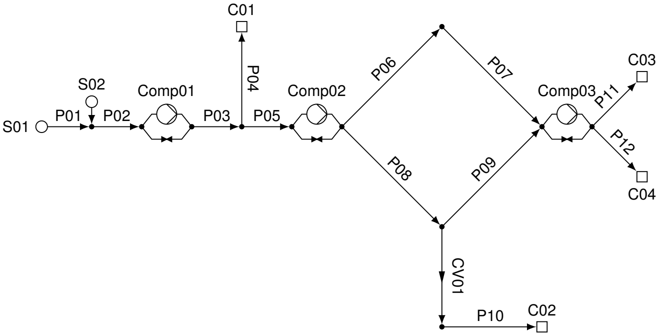
Outline

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

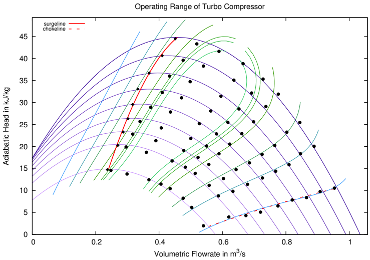
Planning, simulation, optimization, operation of gas networks.
Build a digital model (digital twin) that can handle all this.

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

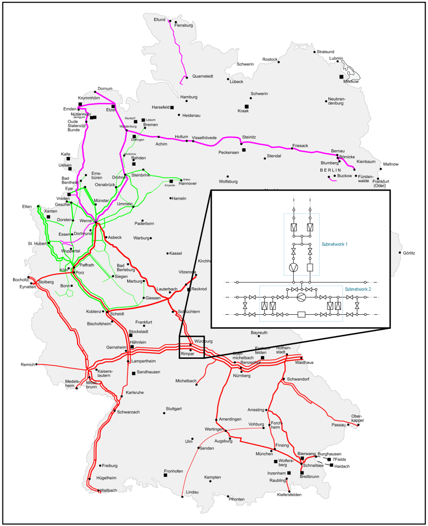
Network of partial differential equations with constraints.
Network elements: Sources S_i, pipes P_i, valves CV_i, compressors $Comp_i$, consumers C_i,



Data based surrogate and reduced order models.



Large network size



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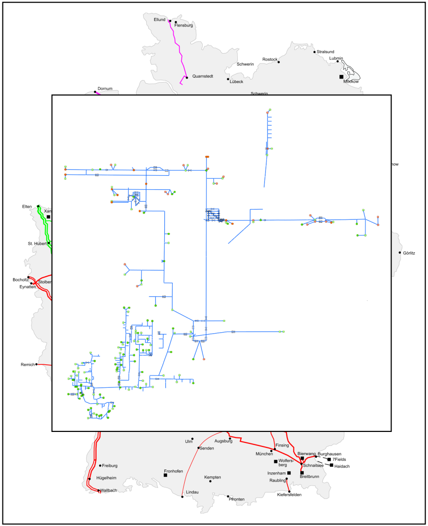

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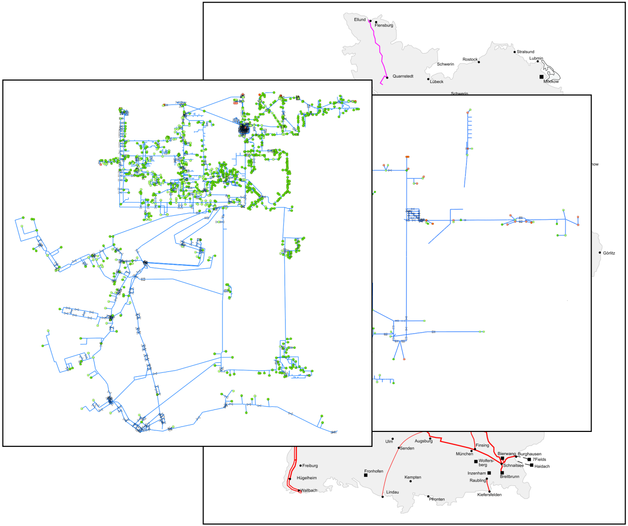

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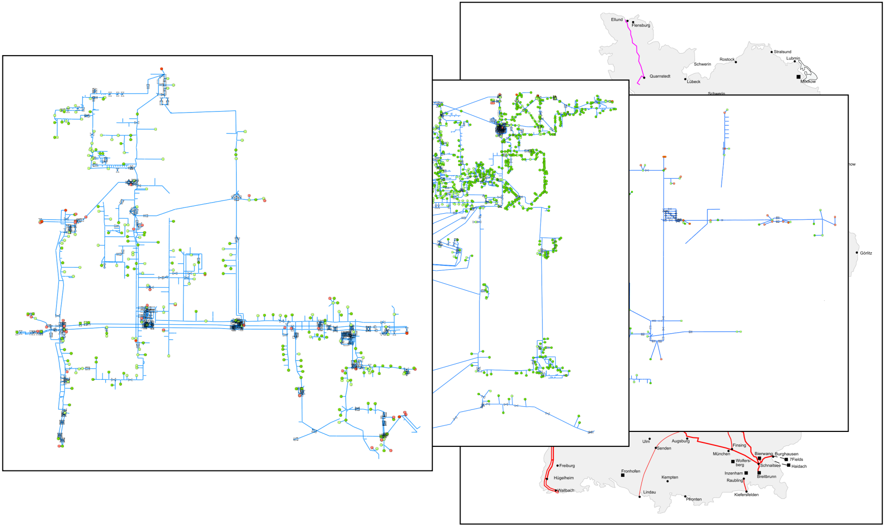


Mathematical model for flow

Typical model: Compressible 1D Euler equations.

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

Terms for pressure energy and dissipation work ignored.

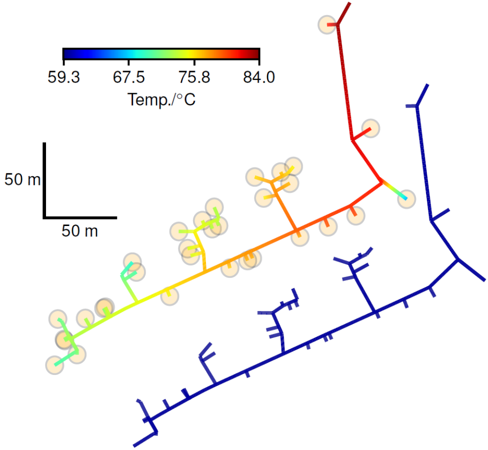
- **Variables:** density ρ, e internal energy, temperature T, velocity v, pressure p, h height, z compressibility factor.
- **Constants:** k_w heat transfer coefficient, λ friction coefficient, D diameter of pipe, T_w wall temperature , g gravitational force, R real gas constant. 3D model for hydrogen.

District heating networks

German Ministry of Education and Research (BMBF)

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

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



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

Typical Model: Incompressible 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.

- 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.

Our other research domains

Mathematical modeling, simulation, control, optimization:

- District heating networks.
- Electrical circuits.
- Power networks
- Electric generators.
- Manufacturing and repait of turbine blades.
- Reactive flow control, new gas turbine.
- Poro-elastic networks.
- Multibody dynamics.

A Modelling Wish list !

- Want a representation that is close to the real physics for open and closed systems.
- Want representations so that coupling of models works across different scales and physical domains.
- 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 forms.
- 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?

Energy based network modeling

- Use energy/power as 'lingua franca' of different physical systems (mechanical, hydraulic, electrical, chemical, thermal) and multi physics systems (electro mechanical, electro-chemical) connected as network via energy transfer.
- Split network into energy storage, energy dissipation components, control inputs and outputs, as well as interconnections and combine as network via a geometric 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 given by the model class of **(dissipative) port-Hamiltonian systems**.

Several different viewpoints.

Port-Hamiltonian systems

Classical nonlinear port-Hamiltonian (pH) ODE/PDE 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.

- B. Jacob and H. Zwart. *Linear port-Hamiltonian systems on infinite-dimensional spaces*. Operator Theory: Advances and Applications, 223. Birkhäuser/Springer Basel CH, 2012.
- 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, 2014.

Why should this be a good approach?

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

$$\mathcal{H}(x(t_1)) - \mathcal{H}(x(t_0)) \leq \int_{t_0}^{t_1} y(\tau)^T u(\tau)\, d\tau,$$ supplied energy

- Class of PH systems closed under *power-conserving interconnection*. Modularized network based modeling.
- *Stability and passivity* analysis easy ($\mathcal{H}$ Lyapunov fctn.)
- PH structure allows to preserve physical properties in *weak formulation, Galerkin projection, model reduction*.
- Physical properties encoded in *algebraic structure* of coefficients and in *geometric structure* of flow.

Add algebraic constraints, like Kirchhoff's laws, interface conditions, position constraints, conservation laws (pHDAEs).

- C. Beattie, V. M., H. Xu, and H. Zwart, *Linear port-Hamiltonian descriptor systems*. Math. Control Signals Systems, 2018.
- 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, Port-Hamiltonian differential-algebraic systems. In *Surveys in Differential-Algebraic Equations I*, 173-226. Springer-Verlag, 2013.

Definition: Nonlinear pHDAEs

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 $E \in C(\mathcal{S}, \mathbb{R}^{\ell,n})$, $J, R \in C(\mathcal{S}, \mathbb{R}^{n,n})$, $B, P \in C(\mathcal{S}, \mathbb{R}^{\ell,m})$, $S = S^T, N = -N^T \in C(\mathcal{S}, \mathbb{R}^{m,m})$, $e, r \in C(\mathcal{S}, \mathbb{R}^{\ell})$. System is called *port-Hamiltonian differential alg. eq. (pHDAE)* if

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

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

- 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
- R. Morandin, Modeling and Numerical Treatment of Port-Hamiltonian Descriptor Systems, PhD thesis, TU Berlin, 2023.

Power balance equation and dissipation inequality still hold.

Theorem (M./Morandin 2019)

Consider a pHDAE . Then the power balance equation (PBE)

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

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.

PHDAEs can be made autonomous without destroying structure.
Model class invariant under interconnection.

Theorem

Consider two autonomous pHDAEs of the form

$$\begin{aligned} E_i\dot{x}_i + r_i &= (J_i - R_i)e_i + (B_i - P_i)u_i, \\ y_i &= (B_i + P_i)^T e_i + (S_i - N_i)u_i, \end{aligned}$$

with Hamiltonians $\mathcal{H}_i$, for $i = 1, 2$, and assume that aggregated input $u = (u_1, u_2)$ and output $y = (y_1, y_2)$ satisfy interconnection relation $Mu + Ny = 0$ for some $M, N \in \mathbb{R}^{k,m}$. Then interconnected system is pHDAE with Hamiltonian $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$.

Transformation invariance

Theorem (M./Morandin 2019)

Consider a pHDAE and another state space $\tilde{\mathcal{X}} \subseteq \mathbb{R}^{\tilde{n}}$, let $\tilde{\mathcal{S}} := \mathbb{I} \times \tilde{\mathcal{X}}$, let $x = \varphi(t, \tilde{x}) \in \mathcal{C}^1(\tilde{\mathcal{S}}, \mathcal{X})$ local diffeomorphism (w.r.t. $\tilde{x}$) and $U \in \mathcal{C}(\tilde{\mathcal{S}}, \mathbb{R}^{\ell,\ell})$ pointwise invertible. Consider

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

with $\tilde{E} = U^T(E \circ \varphi)\partial_{\tilde{x}}\varphi$, $\tilde{J} = U^T(J \circ \varphi)U$, $\tilde{R} = U^T(R \circ \varphi)U$, $\tilde{B} = U^T(B \circ \varphi)$, $\tilde{P} = U^T(P \circ \varphi)$, $\tilde{z} = U^{-1}(z \circ \varphi)$ and $\tilde{r} = U^T(r \circ \varphi + (E \circ \varphi)\partial_t\varphi)$, where $(F \circ \varphi)(t, \tilde{x}) = F(t, \varphi(t, \tilde{x}))$ for any $F \in \mathcal{C}(\mathcal{S}, \cdot)$, and let $\tilde{\mathcal{H}}(t, \tilde{x}) := (\mathcal{H} \circ \varphi)(t, \tilde{x})$. Then this is again pHDAE with Hamiltonian $\tilde{\mathcal{H}}$, and to any solution $(\tilde{x}, u, y)$ there corresponds a solution (x, u, y) of the original pHDAE with $x(t) = \varphi(t, \tilde{x}(t))$. Furthermore, if $\varphi(t, \cdot)$ is global diffeomorphism $t \in \mathbb{I}$, then the two systems are equivalent. Local normal forms can be constructed.

Outline

Let $\mathcal{F}$ be a linear space $\dim \mathcal{F} = n$ and $\mathcal{E} := \mathcal{F}^*$ its dual space. Define bilinear forms $\langle \cdot, \cdot \rangle_+$, $\langle \cdot, \cdot \rangle_-$ on $\mathcal{F} \times \mathcal{E}$

$$\begin{aligned} \langle (f_1, e_1), (f_2, e_2) \rangle_+ &:= \langle e_1 \mid f_2 \rangle + \langle e_2 \mid f_1 \rangle, \\ \langle (f_1, e_1), (f_2, e_2) \rangle_- &:= \langle e_1 \mid f_2 \rangle - \langle e_2 \mid f_1 \rangle, \end{aligned}$$

where $\langle \cdot \mid \cdot \rangle$ denotes the classical duality pairing.
A linear subspace $\mathcal{D} \subseteq \mathcal{F} \times \mathcal{E}$ is called *Dirac structure* if $\langle (f_1, e_1), (f_2, e_2) \rangle_+ = 0$ on $\mathcal{D}$ and $\mathcal{D}$ is maximal w.r.t. this property.
A linear subspace $\mathcal{L} \subseteq \mathcal{F} \times \mathcal{E}$ is called *Lagrange structure* if $\langle (f_1, e_1), (f_2, e_2) \rangle_- = 0$ on $\mathcal{L}$ and $\mathcal{L}$ is maximal w.r.t. this property.
A Lagrange structure is called *nonnegative* if the quadratic form associated with $\langle (f_1, e_1), (f_2, e_2) \rangle_+$ is nonnegative on $\mathcal{L}$.
A subspace $\mathcal{M} \subset \mathcal{X} \times \mathcal{X}^*$ is called *monotone* if $e^\top f \geq 0$ for all $(f, e) \in \mathcal{M}$, and *maximally monotone* if $\mathcal{M}$ is maximal w.r.t. this property.

- V. Mehrmann and A.J. van der Schaft. *Differential-algebraic systems with dissipative Hamiltonian structure*. **Mathematics of Control Signals and Systems**, https://doi.org/10.1007/s00498-023-00349-2, http://arxiv.org/abs/2208.02737, 2023.
- A.J. van der Schaft and V. Mehrmann. *Linear port-Hamiltonian DAE systems revisited*. **System and Control Letters**, http://arxiv.org/abs/2211.06676, 2023.

Abstract dissipative Hamiltonian DAEs

Consider a linear state space $\mathcal{X}$ with coordinates x, a maximally monotone subspace $\mathcal{M} \subset \mathcal{X} \times \mathcal{X}^*$, and a Lagrange structure $\mathcal{L} \subset \mathcal{X} \times \mathcal{X}^*$. A *dHDAE system* is a system $(\mathcal{X}, \mathcal{M}, \mathcal{L})$ satisfying

$$\{(\dot{x}, x) \mid \text{ there exists } e \in \mathcal{X}^* \text{ such that } (-\dot{x}, e) \in \mathcal{M}, (x, e) \in \mathcal{L}\}.$$

Generalization to pHDAEs *with external port variables*, by extending $\mathcal{M} \subset \mathcal{X} \times \mathcal{X}^*$ to a maximally monotone subspace $\mathcal{M}_e \subset \mathcal{X} \times \mathcal{X}^* \times \mathcal{F}_P \times \mathcal{F}_P^*$, with $\mathcal{F}_P \times \mathcal{F}_P^*$ space of port variables.

For abstract nonlinear version, use sub-bundle of $T\mathcal{X} \oplus T^*\mathcal{X}$, the Whitney sum between tangent and cotangent bundles of $\mathcal{X}$, that are locally described by the corresponding linear structures.

Outline

Theorem

Any Lagrange structure $\mathcal{L} \subset \mathcal{X} \times \mathcal{X}^*$ can be represented as

$$\mathcal{L} = \ker \begin{bmatrix} S^\top & -P^\top \end{bmatrix} = \mathrm{im} \begin{bmatrix} P \\ S \end{bmatrix} \subset \mathcal{X} \times \mathcal{X}^*,$$

for certain matrices $S, P \in \mathbb{R}^{n,n}$ satisfying $\mathrm{rank} \begin{bmatrix} P \\ S \end{bmatrix} = n$ as well as the generalized symmetry condition

$$S^\top P = P^\top S.$$

A Lagrange structure is nonnegative if and only if $S^\top P \geq 0$.
A quadratic Hamiltonian is defined by $\mathcal{H}(x) = \frac{1}{2} x^\top P^\top S x$.

Theorem

Using matrices $K, L \in \mathbb{R}^{n,n}$, any Dirac structure $\mathcal{D} \subset \mathcal{X} \times \mathcal{X}^*$ admits the kernel/image representation

$$\mathcal{D} = \ker \begin{bmatrix} K & L \end{bmatrix} = \mathrm{im} \begin{bmatrix} L^\top \\ K^\top \end{bmatrix} \subset \mathcal{X} \times \mathcal{X}^*,$$

with K, L satisfying $\mathrm{rank} \begin{bmatrix} K & L \end{bmatrix} = n$ and the generalized skew-symmetry condition

$$KL^\top + LK^\top = 0.$$

Conversely any such pair K, L defines a Dirac structure.

Theorem

Any maximally monotone structure $\mathcal{M} \subset \mathcal{X} \times \mathcal{X}^*$ *can be represented as*

$$\mathcal{M} = \operatorname{im} \begin{bmatrix} N^\top \\ M^\top \end{bmatrix}$$

for $M, N \in \mathbb{R}^{n,n}$ *satisfying* $\operatorname{rank} \begin{bmatrix} N & M \end{bmatrix} = n$ *and the* *semi-definiteness condition*

$$MN^\top + NM^\top \geq 0.$$

Conversely, any subspace defined by any such M, N *is a maximally monotone subspace.*

If in the maximally monotone subspace representation M is invertible, then the representation is equivalent to

$$E\dot{z} = (J - R)Qz, \ Q^\top E = E^\top Q, \ J = -J^\top, \ R = R^\top \geq 0.$$

- V. Mehrmann and A.J. van der Schaft. *Differential-algebraic systems with dissipative Hamiltonian structure*. **Mathematics of Control Signals and Systems**, https://doi.org/10.1007/s00498-023-00349-2, http://arxiv.org/abs/2208.02737, 2023.
- A.J. van der Schaft and V. Mehrmann. *Linear port-Hamiltonian DAE systems revisited*. **System and Control Letters**, http://arxiv.org/abs/2211.06676, 2023.
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Different approaches.

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

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- A. Moses Badlyan and C. Zimmer. Operator-GENERIC formulation of thermodynamics of irreversible processes. Preprint TU Berlin 2018.
- M. Grmela and H.Öttinger, Dynamics and thermodynamics of complex fluids. i. development of a general formalism. Physical Review E, 56 6620–6632, 1997.
- 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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Example: 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 (interconnection) and boundary conditions (input/ouput) as well as constraints.

There is no uniform way to treat boundary conditions.
One needs to proceed differently for analysis, PDE discretization, system and control.
Example: Gas flow.
Wall temperature boundary conditions in pipe network: Can be classical boundary conditions for PDE simulation and optimization of network or interconnection conditions when coupling with environment.
Inflow and outflow boundary conditions are controls and observations, or used for interconnection, or classical boundary conditions for simulation.

Outline

Space discretization

- Space discretization as in unstructured PDEs.
- Exterior calculus approach.
- Hybrid approaches.

Galerkin projection preserves pH structure, exterior calculus discretization preserves geometric structure.

But boundary conditions have to be treated properly

- D. Arnold, R.S. Falk and R. Winther, Finite element exterior calculus, homological techniques, and applications. Acta Numerica, 15, 2006.
- G. Awanou, M. Fabien, J. Guzman and A. Stern, Hybridization and postprocessing in finite element exterior calculus. Mathematics of Computation, 92, 2023,
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- 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.

Idea: Use geometric structure and structure preserving methods.

- Most classical ODE/DAE methods do not preserve the energy or dissipation inequality.
- Conflict between preserving Dirac structure and constraints.
- Want integrators that lead to discrete-time pH systems, i.e. preserve power balance equation (symplectic methods), as well as algebraic constraints (stiffly accurate methods).
- However: No implicit Runge-Kutta method is both stiffly accurate and symplectic.
- Way out: Use e.g. Gauss-Legrendre collocation (like implicit midpoint rule) for dynamics and stiffly accurate method for algebraic part, if these can be decoupled.

- 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.
- R. Morandin, PhD thesis, 2023.

- The space-time discretization methods require the solution of (non)linear systems.
- 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 linear system

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

Matrix $E + \tau/2R - \tau/2J$ has pos. (semi)-def. symmetric part.
Locally the pHDAE structure always lead to such linear systems.
Structure similar to saddle point problems.

Linear solvers

For systems $(M+N)x = b$ with $M = M^T > 0$, $N = -N^T$, Widlund's method uses symmetric part as preconditioner.

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

Leads to optimal 3-term recurrence to generate M-orthogonal basis of Krylov subspace $\mathcal{K}_k(K,v) = \mathrm{span}[v, Kv, \ldots, K^{k-1}v]$ for each k and initial vector v.

Oblique projection method with Galerkin projection property:

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

- M. Benzi, G. H. Golub, and J. Liesen, *Numerical solution of saddle point problems*, Acta Numerica, 14, 2005.
- 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. D. Rapoport, *A nonlinear Lanczos algorithm and the atationary Navier-Stokes wquation*, PhD thesis, Department of Mathematics, Courant Institute, New York University, 1978.
- O. Widlund. A Lanczos method for a class of nonsymmetric systems of linear equations. *SIAM J. Numer. Anal.*, 15, 1978.

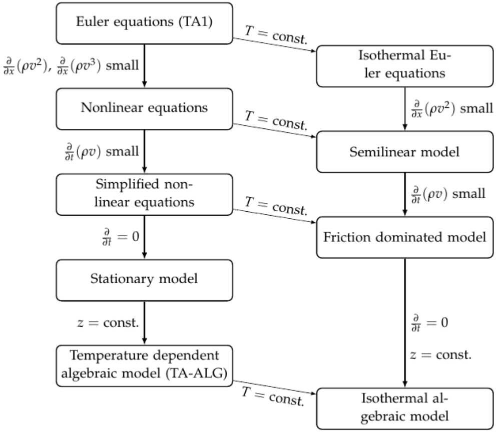
Example: Stokes flow

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

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

Outline

Model hierarchy in gas pipe



Every element/node/edge modelled via a hierarchy, PDE, 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,

Model hierarchy and adaptivity

Use model hierarchy for adaptivity in space-time discretization and model 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.

PHDAE approach allows jump between models in hierarchy without changing simulation, control, optimization framework.
Allows to solve control and optimization problems that otherwise could not be solved.

Example: 4-level-hierarchy gas transport

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

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

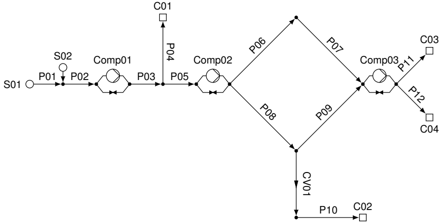
together with boundary cond. and Kirchhoff's laws at nodes.

- 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.

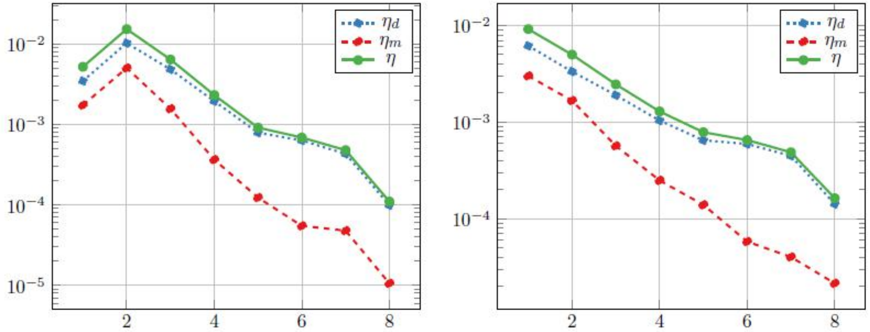
$$\frac{\sum_{j\in\mathcal{J}_p}\left(\eta_{m,j}+\eta_{x,j}+\eta_{t,j}\right)}{|\mathcal{J}_p|}\leq \text{tol}$$



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.

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.

▷ R. Krug, V. M., 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*, http://arxiv.org/abs/2201.11993, 2022.

Optimization district heating network

Minimize overall costs required to satisfy the heat demand of all the consumers. Objective function is given by the cost of pressure increase, waste incineration, and burning gas.
Constraints:

- pipe flow and thermal model, here stationary flow,
- mass conservation,
- pressure continuity,
- temperature mixing,
- depot constraints,
- consumer constraints, bounds.

Challenges

- Highly nonlinear and large-scale pHDAE-constrained mathematical program with complementarity constraints (MPCC).
- Change of flow direction at multiple junctions and cycles.
- Optimization of non-stationary case currently not possible.
- Solving for reasonably finely-discretized real world problem currently not possible.
- pHDAE model simplification not complete.
- Model reduction not complete. PhD Sarah Hauschild, Trier.

Simplifications: Stationary regime, constant density and velocity. Solve entropy equation in post-processing step.

Our approach: Space-model-adaptive optimization algorithm.

Table: Characteristics of the test networks.

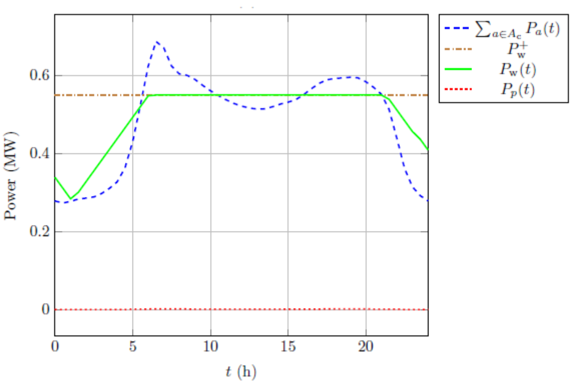
Network	# pipes	# depots	# consumers	pipe length (m)
AROMA	18	1	5	7262.4
STREET	162	1	32	7627.1

AROMA is an academic test network, whereas STREET is a part of an existing real-world district heating network.
None of the standard optimization solvers converges to a feasible point for both the AROMA and the STREET network.

Space-model-adaptive algorithm

- Algorithm works as expected and terminates after a finite number of iterations with locally optimal solution of required accuracy.
- We can solve realistic instances that have not been solvable before.
- Although we warm-start every with the solution of the previous one, we observe an increase of solution times due to the higher complexity of the successive models.
- Is accuracy worth the effort? The answer is a clear “Yes”.

Optimal 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 a representation that is close to the real physics for open and closed systems.
- Want representations so that coupling of models works across different scales and physical domains.
- 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,

With pHDAE systems most wishes are fulfilled.

But there are many things to do

- Real time control, optimization.
- Incorporate stochastics and delay in pHDAEs.
- Function Spaces.
- Error estimates.
- Data based realization.
- Software.
- Digital twins.
- ...

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