Port-Hamiltonian systems: algebraic, geometric and operator theoretic representations

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Mathematics for key technologies

Outline

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?

Application domains

Mathematical modeling, simulation, control, optimization:

- Gas transport networks.
- District heating networks.
- Electrical circuits.
- Control of turbulent flow.
- Hydraulic systems.
- Magneto-hydrodynnamics.
- Power networks.
- Electric generators.
- Thermo-dynamics.
- Manufacturing and repair of turbine blades.
- Reactive flow control, new gas turbine.
- Poro-elastic networks.
- Structural dynamics.
- Multibody dynamics.
- . . ..

Outline

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

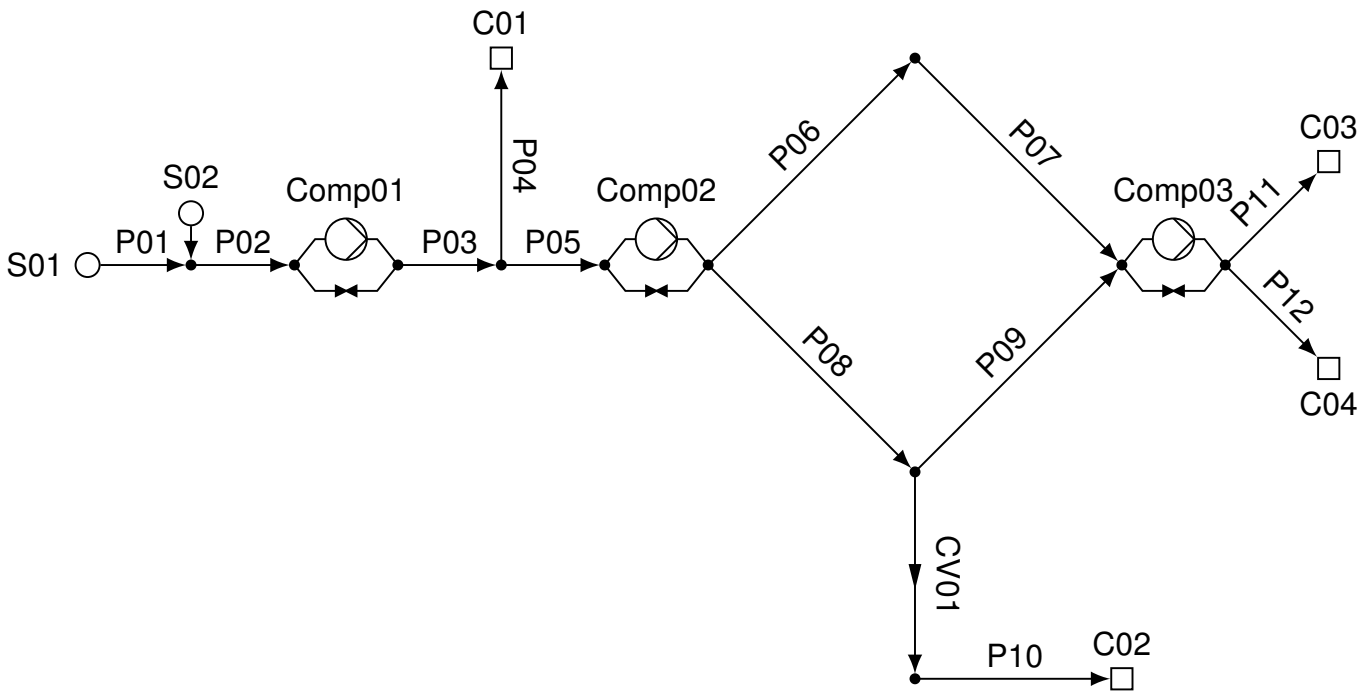
Planning, simulation, optimization, operation of gas networks.
Build a digital model (digital twin) that can handle all this.

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

Components of gas network model

Network of partial differential equations with constraints.

Network elements: Sources S_i, pipes P_i, valves CV_i, compressors $Comp_i$, consumers C_i,



Mathematical model for pipe flow

Compressible 1D Euler equations,

$$0 = \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v), \qquad \text{Mass conservation}$$

$$0 = \frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}(p + \rho v^2) + \frac{\lambda}{2D}\rho v\,|v| + g\rho\frac{\partial}{\partial x}h, \qquad \text{Momentum balance}$$

$$0 = \frac{\partial}{\partial t}\left(\rho(\frac{1}{2}v^2 + e)\right) + \frac{\partial}{\partial x}\left(\rho v(\frac{1}{2}v^2 + e) + pv\right) + \frac{4k_w}{D}(T - T_w),$$

Energy balance

$$p = \rho R T z(p, T), \qquad \text{Real gas equation}$$

Terms for pressure energy and dissipation work omitted.

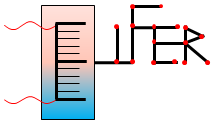
- **Variables:** density ρ, e internal energy, temperature T, velocity v, pressure p, h height, z compressibility factor.
- **Constants:** k_w heat transfer coeff., λ friction coeff., D diameter, T_w wall temperature , g gravitation constant, R real gas constant.

- 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

German Ministry of Education and Research (BMBF)

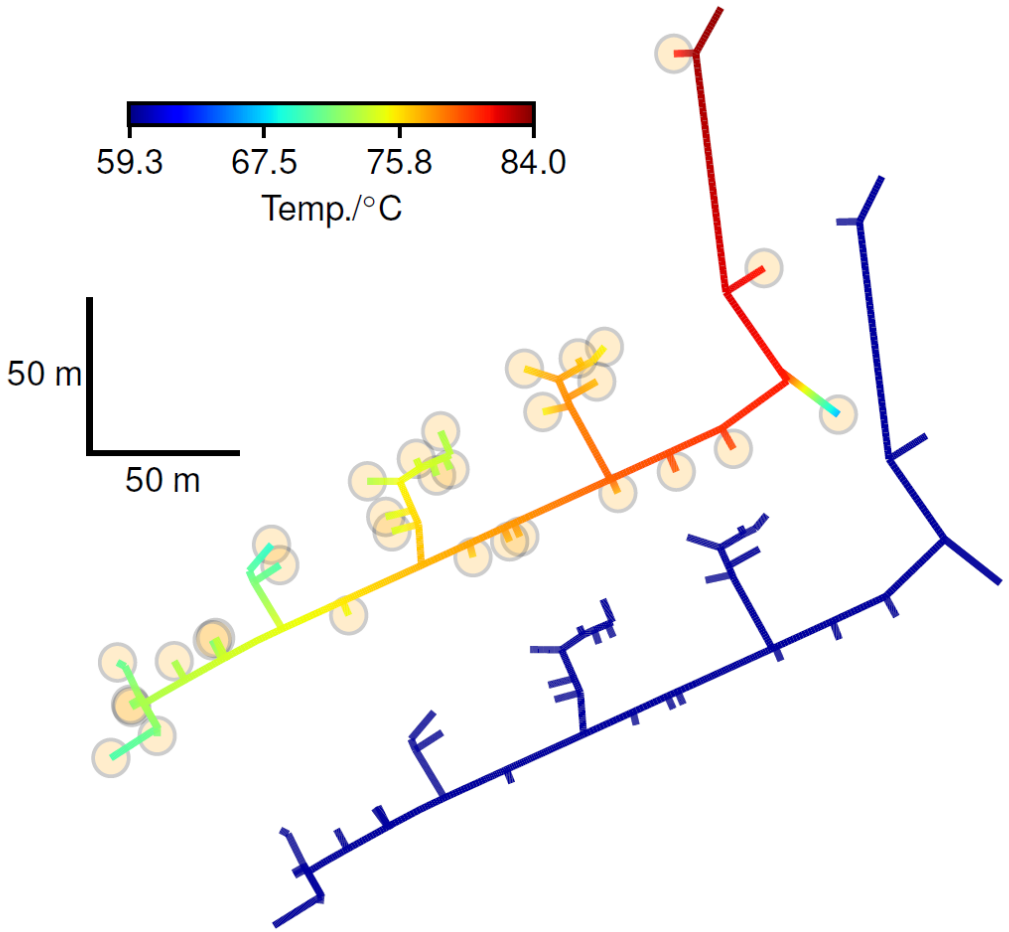
Energy efficiency via intelligent district heating networks (EiFer)



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 for pipe flow

Model: Simplified incompressible 1 D Euler equations.

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

I/O are pressure, velocity, temperature at in- and outflow nodes.
plus initial/boundary conditions.

Terms for pressure energy and dissipation work omitted.

- 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.

Outline

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 via a geometric structure.
- Allow every submodel to be a model hierarchy of fine or course, continuous or discretized, full or reduced models.
- Consider system theoretic way via **(dissipative) port-Hamiltonian (pH)** 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.
- R. Morandin, Modeling and Numerical Treatment of Port-Hamiltonian Descriptor Systems, PhD thesis, January 2024.
- 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*, Vol. 444. Springer Verlag, New York, N.Y., 2014.
- Survey: V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, Acta Numerica, 2023.

Outline

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.
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Why should this be a good approach?

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

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

- 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.

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 $E \in C(\mathcal{S}, \mathbb{R}^{\ell,n})$, $J, R \in C(\mathcal{S}, \mathbb{R}^{n,n})$, $B, P \in C(\mathcal{S}, \mathbb{R}^{\ell,m})$, $S = S^T, N = -N^T \in C(\mathcal{S}, \mathbb{R}^{m,m})$, $e, r \in C(\mathcal{S}, \mathbb{R}^{\ell})$.
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.

Power balance equation and dissipation inequality still hold.

Theorem (M./Morandin 2019)

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

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

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 $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$.

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.

Robust Representations

Representation as pHDAE is not unique.

- The representation should work for parameters going to limiting situations.
- The representation should be good for numerics.
- For computations we need a good coordinate representation.
- The representation should be robust w.r.t modelling, data and numerical errors.
- The representation should be usable in digital twins (real time, data based model generation.)

Mass-spring-damper example I

Mass-spring-damper system

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} k & 0 \\ 0 & \frac{1}{m} \end{bmatrix} \begin{bmatrix} q \\ p \end{bmatrix},$$

with Hamiltonian $\mathcal{H}(q,p) = \frac{1}{2}kq^2 + \frac{p^2}{2m}$.
Express in position q and velocity $v := \frac{p}{m}$ as

$$\begin{bmatrix} \dot{q} \\ m\dot{v} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} kq \\ v \end{bmatrix}$$

with Hamiltonian $\mathcal{H}(q,v) = \frac{1}{2}kq^2 + \frac{1}{2}mv^2$. Then $m \to 0$ gives

$$\begin{bmatrix} \dot{q} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} kq \\ v \end{bmatrix},$$

Limit Hamiltonian $\mathcal{H}(q,v) = \frac{1}{2}kq^2$ not a function of v anymore.

Mass-spring-damper example II

Alternatively rewrite system in coordinates $F := kq$ and p as

$$\begin{bmatrix} \frac{1}{k}\dot{F} \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} F \\ \frac{p}{m} \end{bmatrix},$$

with Hamiltonian $\mathcal{H}(F,p) = \frac{1}{2k}F^2 + \frac{1}{2m}p^2$. Then $k \to \infty$ gives

$$\begin{bmatrix} 0 \\ \dot{p} \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} F \\ \frac{p}{m} \end{bmatrix},$$

with Hamiltonian $\mathcal{H}(F,p) = \frac{1}{2m}p^2$, not involving F.
Taking $m \to 0$ and $k \to \infty$, gives algebraic system

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -d \end{bmatrix} \begin{bmatrix} F \\ v \end{bmatrix},$$

with zero Hamiltonian, $v = 0$, $F = 0$, irrespective of damper.

Further freedom

The pHDAE representation is very flexible and allows further freedom in representations.

- Congruence transformations to deal with bad scaling.
- Adding algebraic equations that do not influence Hamiltonian.
- Removing algebraic equations that do not influence Hamiltonian.
- Index reduction for DAEs.
- Output feedback which does not make dissipaton matrix R indefinite.

Not clear what other freedom we have?

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. For computation and relation to DAE setting we need coordinate representations.

Theorem

A Lagrange structure $\mathcal{L} \subset \mathcal{X} \times \mathcal{X}^*$ can be (locally) represented as

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

for certain matrices $S, P \in \mathbb{R}^{n,n}$ satisfying $\operatorname{rank} \begin{bmatrix} P \\ S \end{bmatrix} = n$ 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 (local) kernel/image representation

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

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

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

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

Theorem

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

$$\mathcal{M} = \text{Image} \begin{bmatrix} N^\top \\ M^\top \end{bmatrix}$$

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.

Linear time invariant example

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

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

Detailed analysis in different representations.

- H. Gernandt, F. Haller, and T. Reis, T. A linear relation approach to port-Hamiltonian differential-algebraic equations. SIAM Journal on Matrix Analysis and Applications, 42(2), 1011-1044, 2021..
- V. M. 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. M.. *Linear port-Hamiltonian DAE systems revisited*. **System and Control Letters**, http://arxiv.org/abs/2211.06676, 2023.
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Outline

A linear system of the form

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t),\ x(0) = 0, \\ y(t) &= Cx(t) + Du(t), \end{aligned}$$

is passive if there exists a state-dependent storage function, $\mathcal{H}(x) \geq 0$, such that for any $t_1 > t_0 \in \mathbb{R}$ the dissipation inequality

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

holds. If for all $t_1 > t_0$, the dissipation inequality is strict then the system is called strictly passive.

Passivity for linear systems

- pHDAE systems are passive, $\mathcal{H}$ is a storage function.
- Every (minimal i.e. controllable and observable) strictly passive LTI system with coefficients $\mathcal{M} = \{\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D}\}$ can be transformed to pHDAE by computing solution $X > 0$ of the Kalman-Yacubovich-Popov (KYP) linear matrix inequality.

$$W(X, \mathcal{M}) := \begin{bmatrix} -\tilde{A}^T X - X\tilde{A} & \tilde{C}^T - X\tilde{B} \\ \tilde{C} - \tilde{B}^T X & \tilde{D}^T + \tilde{D} \end{bmatrix} \geq 0$$

The system with $E = X$, $J - R = XA$, $B = \frac{-C^T + X\tilde{B}}{2}$, $P = \frac{-C^T - X\tilde{B}}{2}$, $D = \tilde{D}$ is a pHDAE (implicit pHODE).

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Optimally robust pH representations

- Every pos. def. solution of KYP LMI gives a pHDAE representation.
- Use the freedom in the KYP LMI to find the solution X of the LMI that maximizes some optimality criteria e.g. distance to non-passivity or instability.

- Bankmann, V.M., Nesterov, and Van Dooren, Computation of the analytic center of the solution set of the linear matrix inequality arising in continuous- and discrete-time passivity analysis, *Vietnam J. Mathematics*, 2020.
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Many open problems

- Which measure to use for robustness of representation.
- Good solution methods for matrix inequality.
- Methods to optimize the distance to instability/nonpassivity.
- Pure data realizations.
- Reduced order modeling.

- C. Beattie, V. M., and H. Xu, *Port-Hamiltonian Realizations of Linear Time Invariant Systems*. http://arxiv.org/abs/2201.05355

Outline

pH PDE Modeling

Different approaches.

- Operator pH DAE modeling.
- Gradient flow, GENERIC.
- Formal geometric structures.

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Example: Gas flow

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

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

We have to add node conditions (interconnection) and boundary conditions (input/ouput) as well as constraints.

Outline

Space discretization

- Space discretization similar to unstructured PDEs e.g. Galerkin, Petrov/Galerkin.
- Exterior calculus approach.
- Hybrid approaches.

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

But boundary conditions have to be treated properly

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Boundary conditions, inputs/outputs

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.
For a new and very general setting see:

- R Morandin, Modeling and Numerical Treatment of Port-Hamiltonian Descriptor Systems, PhD thesis, January 2024.

Time discretization

Idea: Use again Dirac Structure and structure preserving (symplectic) methods.

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

Dirac structure of discretization

Let $\mathcal{D}_x$ be the Dirac structure associated to the pHDAE and define Dirac structure of discretization as $\{\mathcal{D}_{x_i} : i = 1, \ldots, s\}$, i.e.,

$$\mathcal{D}_{x_i} = \left\{ (f^i, e^i) \in \mathcal{V}_{x_i} \times \mathcal{V}_{x_i}^* \;\middle|\; f^i + \begin{bmatrix} \Gamma(t_i, x_i) & I_{\ell+m} \\ -I_{\ell+m} & 0 \end{bmatrix} e^i = 0 \right\},$$

with $f^i = (f_s^i, y_i, f_r^i)$ and $e^i = (e_s^i, u_i, e_r^i)$.
Taking $(f^i, e^i) \in \mathcal{D}_{x_i}$, together with

$$\begin{aligned} x_f &= x_0 + h\sum_{i=1}^{s} \beta_i \dot{x}_i, \;\; x_i = x_0 + h\sum_{j=1}^{s} \alpha_{ij} \dot{x}_j, \\ f_s^i &= -E(x_i)\dot{x}_i, \;\; e_s^i = e(x_i), \;\; e_r^i = -W(x_i) f_r^i, \;\; u_i = u(x_i), \end{aligned}$$

the system is equivalent to applying a collocation method and computing the *discrete input* and *output* u_i, y_i, for $i = 1, \ldots, s$.

With $H(t) := \mathcal{H}(\tilde{x}(t))$ we get $H(t) - H(t_0) = \int_{t_0}^{t} \dot{H}(s)\mathrm{d}s$ and in collocation points, the Power Balance Equation is satisfied.

$$\begin{aligned} \dot{H}(t_i) &= \nabla\mathcal{H}(x_i)^T \dot{x}_i = e(x_i)^T E(x_i)\dot{x}_i = \\ &= -\langle e_s^i \mid f_s^i \rangle = \langle e_r^i \mid f_r^i \rangle + \langle y_i \mid u_i \rangle, i = 1, \ldots, s \end{aligned}$$

Apply collocation method of order p

$$H(t_f) - H(t_0) = \int_{t_0}^{t_f} \Big(\langle \tilde{e}_r(s) \mid \tilde{f}_r(s) \rangle + \langle \tilde{y}(s) \mid \tilde{u}(s) \rangle \Big) \mathrm{d}s + \mathcal{O}(h^{p+1}).$$

If the Runge-Kutta conditions satisfy $\beta_j \geq 0$ for $j = 1, \ldots, s$ then $h \sum_{j=1}^{s} \langle e_r^j \mid f_r^j \rangle \leq 0$, thus discrete system stays dissipative.
Exact if Hamiltonian is quadratic.

Outline

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.

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

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

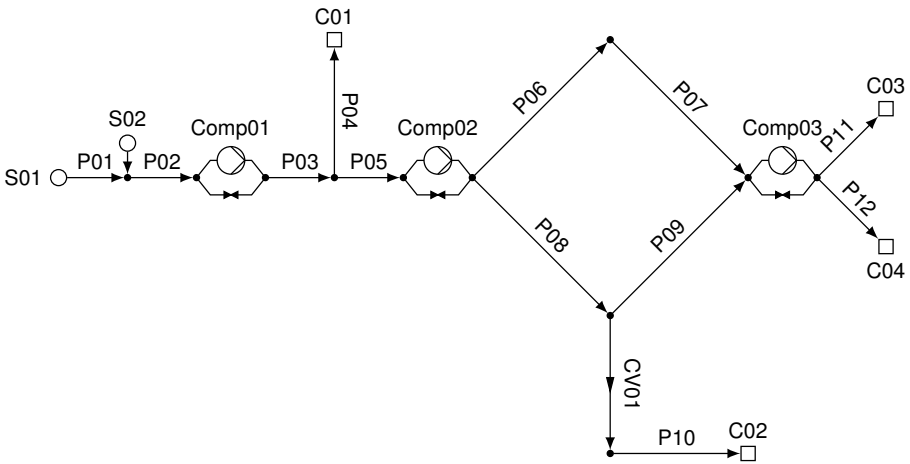
  together with boundary cond. and Kirchhoff's laws at nodes.

- 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.

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

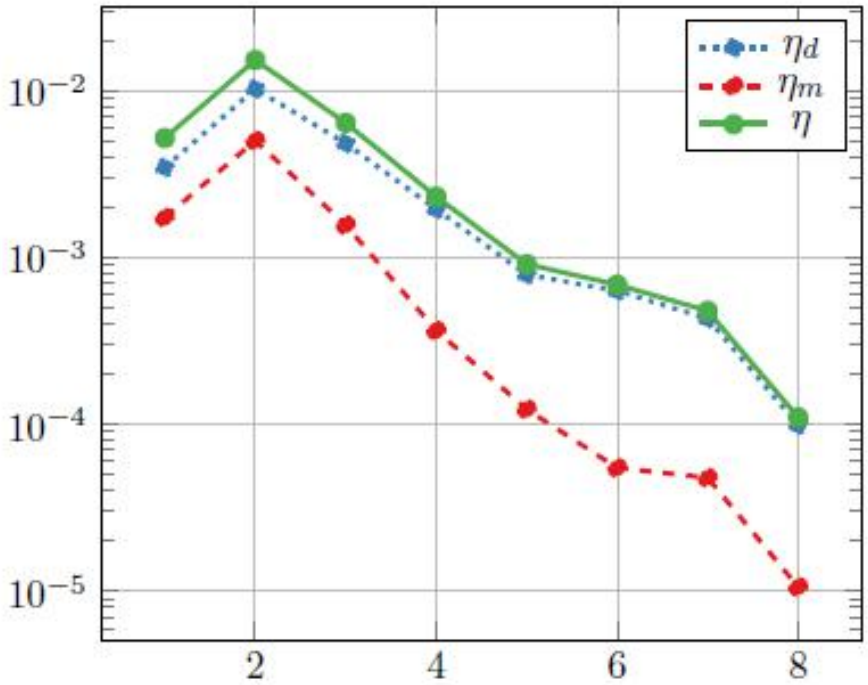


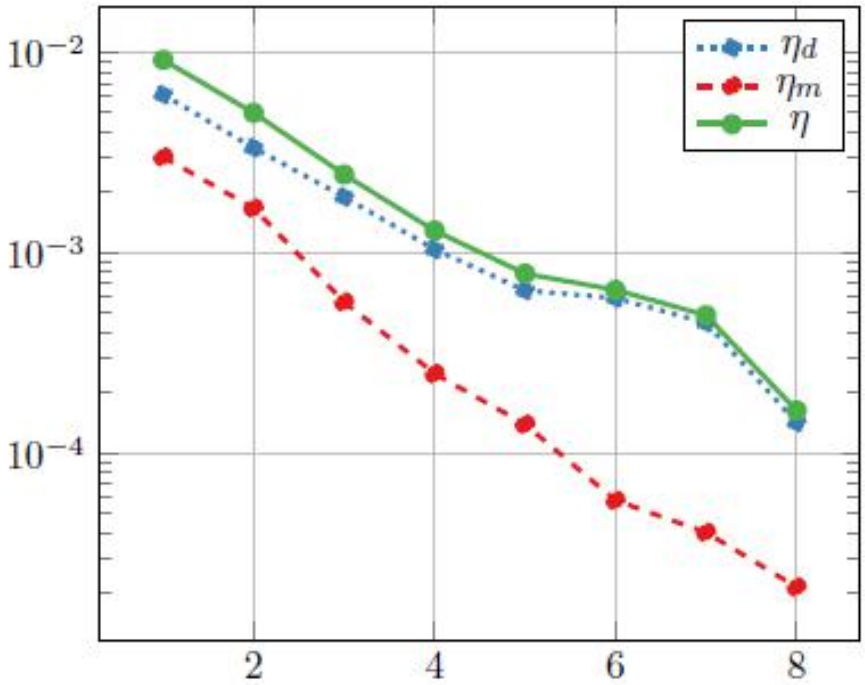
Non-adaptive simulation time is 4 hours using ANACONDA code.

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.
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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.

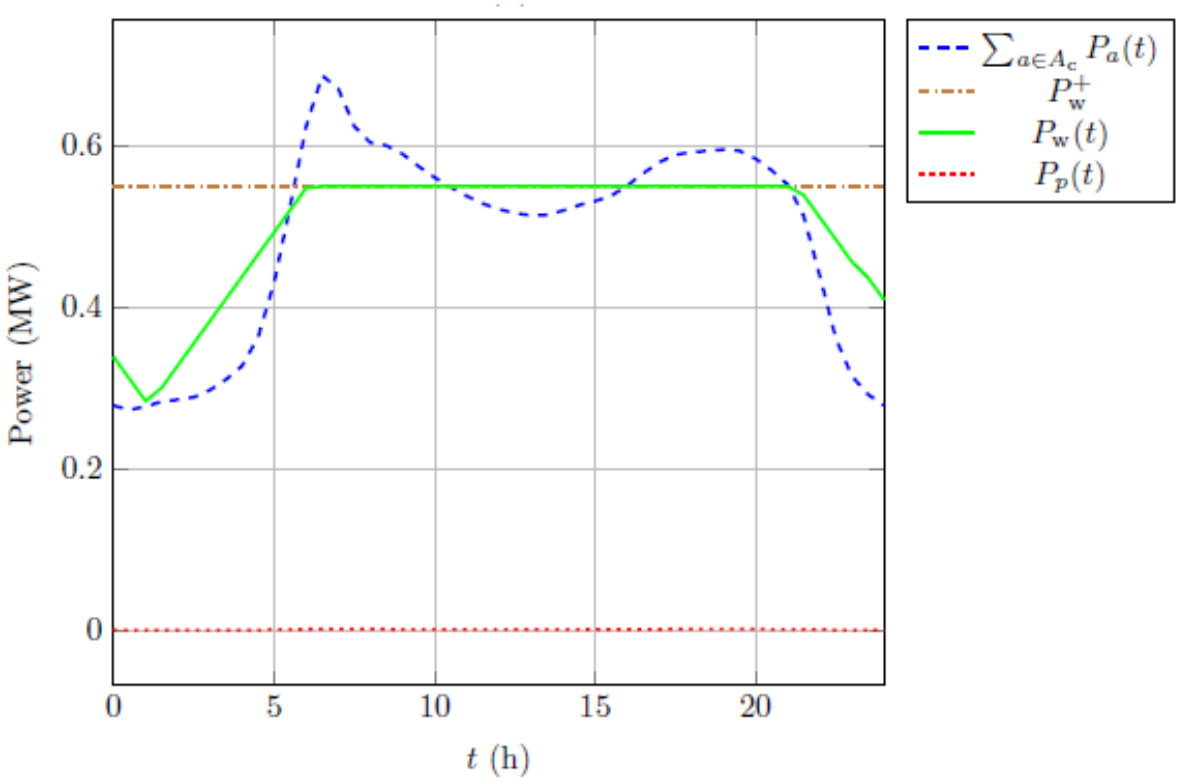
Network	# pipes	# depots	# consumers	pipe length (m)
AROMA	18	1	5	7262.4
STREET	162	1	32	7627.1

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.

Outline

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 almost all wishes are fulfilled.

Outlook

But there are many things to do

- Relation to other energy-based modeling approaches. (GENERIC, gradient flows)
- Real time control, optimization.
- Incorporate stochastics and delay in pHDAE models.
- Function Spaces.
- Error estimates.
- Preconditioning.
- Data based realization.
- Software.
- Digital twins
- . . .

Thank you very much
for your attention
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Details: http://www.math.tu-berlin.de/?id=76888