Modeling, simulation and control of multi-physical systems: A change of paradigm.

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Mathematics for key technologies

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Outline

Theses

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

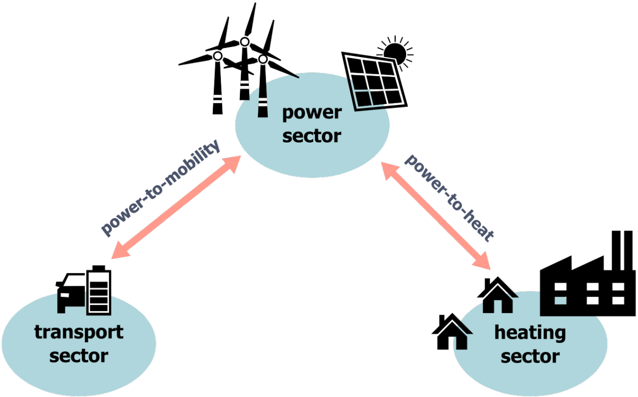


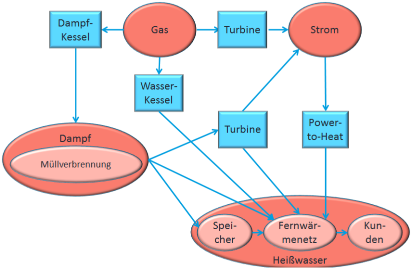
Figure: Sector coupling and the power-to-X concept

Heating sector

German Ministry of Education and Research (BMBF)

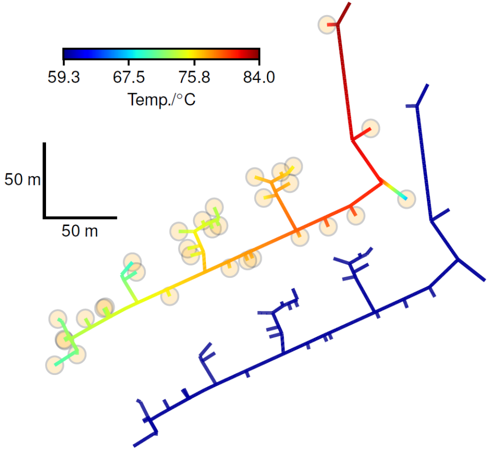
Energy efficiency via intelligent district heating networks (EiFer)

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: Simplified incompressible 1 D Euler equations.

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

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

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

- S.-A. Hauschild, N. Marheineke, V. Mehrmann, J. Mohring, A. Moses Badlyan, M. Rein, and M. Schmidt, Port-Hamiltonian modeling of disctrict heating networks, DAE Forum, 333-355, Springer Verlag, 2020.
- R. Krug, V. Mehrmann, and M. Schmidt, Nonlinear Optimization of District Heating Networks, Optimization and Engineering, Vol. 22, 783-819, 2021.
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- Collaborative Research Center CRC910. Stability exponents for *delay differential-algebraic equations in power networks*.
- DFG priority Programme 1984, Hybrid and multimodal energy systems. Project: Computational Strategies for Distributed Stability Control in Next-Generation Hybrid Energy Systems with Kai Strunz, EE, TU Berlin

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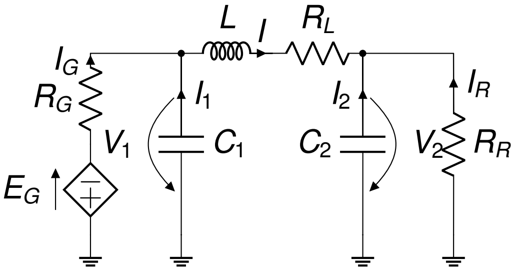
Toy example: power network

Let $R_G, R_L, R_R > 0$ be resistances, $L > 0$ inductor, $C_1, C_2 > 0$ capacitors and E_G controlled voltage source.
Basic model of a DC generator (E_G,R_G), connected to load (R_R) via transmission line.

$$
\begin{aligned}
L\dot{I} &= -R_L I + V_2 - V_1, \\
C_1 \dot{V}_1 &= I - I_G, \; C_2 \dot{V}_2 = -I - I_R, \\
0 &= -R_G I_G + V_1 + E_G, \; 0 = -R_R I_R + V_2.
\end{aligned}
$$



Other domains

- Gas transport CRC TRR 154
- Werner von Siemens Center Berlin. Electricity generation, gas turbine repair, additive manufacturing of turbine blades.
- Reactive flow control, new gas Turbine CRC 1029, until 2021.
- Poro-elastic networks.
- Multibody dynamics.
- Survey: V. M. and B. Unger, *Control of port-Hamiltonian differential-algebraic systems and applications*, http://arxiv.org/abs/2201.06590, 2022. Acta Numerica submitted.

A Modelling 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,

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

Energy based network modeling

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

- P. C. Breedveld. *Modeling and Simulation of Dynamic Systems using Bond Graphs*, pages 128–173. EOLSS Publishers Co. Ltd./UNESCO, Oxford, UK, 2008.
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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 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.
- *Stability and passivity* analysis easy.
- 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.
- Systems are *easily extendable*: Open/closed systems.

Constrained Port-Hamiltonian systems

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

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

Definition (M./Morandin 2019)

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

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

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

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

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

Definition extends to weak solutions and infinite dimension.

Theorem (M./Morandin 2019)

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

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

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.

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.*

Autonomous form

Any pHDAE can be made autonomous without destroying the structure by setting

$$\begin{bmatrix} E & r \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \dot{x} \\ \dot{t} \end{bmatrix} = \begin{bmatrix} J-R & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} z \\ 0 \end{bmatrix} + \begin{bmatrix} B-P & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ 1 \end{bmatrix},$$

$$\begin{bmatrix} y \\ 0 \end{bmatrix} = \begin{bmatrix} B+P & 0 \\ 0 & 1 \end{bmatrix}^T \begin{bmatrix} z \\ 0 \end{bmatrix} + \begin{bmatrix} S-N & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u \\ 1 \end{bmatrix}.$$

Structure-preserving interconnection

Theorem

Consider two autonomous pHDAEs of the form

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

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 $Mu + Ny = 0$ for some $M, N \in \mathbb{R}^{k,m}$. Then interconneted system is pHDAE with Hamiltonian $\mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$.

Definition (E.g. Van der Schaft/Jeltsema 2014)

Let $\mathcal{F}$ be a linear space and $\mathcal{E} := \mathcal{F}^*$ its dual space. Let $<< \cdot, \cdot >>$ be the bilinear form on $\mathcal{F} \times \mathcal{E}$ defined as

$$<< (f_1, e_1), (f_2, e_2) >> := \langle e_1 \mid f_2 \rangle + \langle e_2 \mid f_1 \rangle,$$

where $\langle \cdot \mid \cdot \rangle$ denotes the duality pairing. A *Dirac structure* on $\mathcal{F} \times \mathcal{E}$ is then a linear subspace $\mathcal{D} \subseteq \mathcal{F} \times \mathcal{E}$, such that $\mathcal{D} = \mathcal{D}^{\perp\!\!\perp}$.

In finite dimensions, one only needs to prove $\dim \mathcal{D} = \dim \mathcal{F}$ and $\langle e \mid f \rangle = 0$ for all $(f, e) \in \mathcal{D}$.
If $(f, e) \in \mathcal{D}$, then f and e are called *flow* and *effort*, respectively.

Differential geometric viewpoint: A modulated Dirac structure over $\mathcal{X}$ is a subbundle of $T\mathcal{X} \oplus T^*\mathcal{X}$, the Whitney sum between the tangent and cotangent bundles of $\mathcal{X}$.

Definition (M./Morandin 2019)

Consider a state space $\mathcal{X}$ and a vector bundle $\mathcal{V}$ over $\mathcal{X}$ with fibers $\mathcal{V}_x$. A *Dirac structure* over $\mathcal{V}$ is a subbundle $\mathcal{D} \subseteq \mathcal{V} \oplus \mathcal{V}^*$ such that, for all $x \in \mathcal{X}$, $\mathcal{D}_x \subseteq \mathcal{V}_x \times \mathcal{V}_x^*$ is a linear Dirac structure.

Theorem (M./Morandin 2019)

Given autonomous pHDAE, define flow fiber $\mathcal{V}_x = \mathcal{F}_x^s \times \mathcal{F}_x^p \times \mathcal{F}_x^d$ *for all* $x \in \mathcal{X}$*, where* $\mathcal{F}_x^s := E(x)T_x\mathcal{X} \subseteq \mathbb{R}^\ell$ *is the storage flow,* $\mathcal{F}_x^p := \mathbb{R}^m$ *is the port flow, and* $\mathcal{F}_x^d := \mathbb{R}^{\ell+m}$ *is the dissipation flow fiber. Partition* $f = (f_s, f_p, f_d) \in \mathcal{V}$ *and* $e = (e_s, e_p, e_d) \in \mathcal{V}^*$*. Then the subbundle* $\mathcal{D} \subseteq \mathcal{V} \oplus \mathcal{V}^*$ *with*

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

is a Dirac structure over $\mathcal{V}$*. Furthermore, the system* $f_s - E(x)\dot{x}$*,* $e_s = z(x)$*,* $f_p = y$*,* $e_p = u$*,* $e_d = -W(x)f_d$*,* $(f, e) \in \mathcal{D}_x$ *is equivalent to the original pHDAE, and* $\langle e \,|\, f \rangle = 0$ *is the PBE.*

Geometric interpretation via mix of Lagrangian and Dirac structure Van der Schaft/Maschke 2018, 2020.

Further results

- Structure preserving time-discretization, so that time discrete system has dissipation inequality and power balance equation and has a discretized Dirac structure. (Gauss Legendre collocation, or partitioned implicit Runge-Kutta methods)
- Use non-uniqueness to obtain robust representations under perturbations.
- Local and global normal forms.
- Perturbation analysis, distance to instability, non-passivity, non-regularity.
- Different port-Hamiltonian PDE formulations, including terms that have been dropped due to model simplifications.

Different approaches.

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

References:

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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.

Abstract port-Hamiltonian PDE formulation

$$\begin{aligned}\frac{\mathrm{d}z}{\mathrm{d}t} &= (\mathcal{J}(z) - \mathcal{R}(z))\,\frac{\delta\mathcal{E}(z)}{\delta z} + \mathcal{B}(z)u(z) \quad \text{in } \mathcal{D}_z^*,\\ y(z) &= \mathcal{B}^*(z)\frac{\delta\mathcal{E}(z)}{\delta z} \quad \text{in } \mathcal{D}_u^*,\end{aligned}$$

- $\mathcal{Z} = \{z \in \mathcal{D}_z \mid \rho \geq \delta,\ \delta > 0 \text{ a.e.}\} \subset \mathcal{D}_z = W^{1,3}((0,\ell);\mathbb{R}^3)$.
- For $z \in \mathcal{Z}$, $\mathcal{J}(z)[\cdot]$, $\mathcal{R}(z)[\cdot] : \mathcal{D}_z \to \mathcal{D}_z^*$ are linear continuous, $\mathcal{J}(z)$ is skew-adjoint, $\mathcal{R}(z)$ is self-adjoint semi-elliptic.
- The input is given by $u(z) \in \mathcal{D}_u = L^q(\{0,\ell\})$ with linear continuous $\mathcal{B}(z)[\cdot] : \mathcal{D}_u \to \mathcal{D}_z^*$, $\mathcal{D}_u^* = L^p(\{0,\ell\})$, $1/q + 1/p = 1$.
- The system theoretic output is denoted by $y(z)$.
- $\mathcal{E}(z)$ is the relative energy.

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pH PDE, hot water flow

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

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

We have to add node conditions, mixing conditions etc.

Variables $z = (\rho, M, e)^T$, $M = \rho v$, energy.

$$\mathcal{E}(z) = \mathcal{H}(z) - T_w \mathcal{S}(z) := \int_0^\ell \left(\frac{|M|^2}{2\rho} + e + \rho g h \right) \mathrm{d}x - T_w \int_0^\ell s(\rho, e) \, \mathrm{d}x.$$

where T_w is assumed to be constant. Introduce *ballistic free energy* $H(\rho, e) = e - T_w s(\rho, e)$, then functional $\mathcal{E}$ and its variational derivatives become

$$\begin{aligned} \mathcal{E}(z) &= \int_0^\ell \left(\frac{|M|^2}{2\rho} + H(\rho, e) + \rho g h \right) \mathrm{d}x \\ \frac{\delta \mathcal{E}(z)}{\delta z} &= \left(\frac{\delta \mathcal{E}(z)}{\delta \rho}, \frac{\delta \mathcal{E}(z)}{\delta M}, \frac{\delta \mathcal{E}(z)}{\delta e} \right)^T \\ &= \left(\left(-\frac{|M|^2}{2\rho^2} + \frac{\partial H}{\partial \rho} + g h \right), \frac{M}{\rho}, \frac{\partial H}{\partial e} \right)^T . \end{aligned}$$

The operators are assembled with respect to the (block-) structure of the state z.
Let $\varphi, \psi \in \mathcal{D}_z$ be block-structured $\varphi = (\varphi_\rho, \varphi_M, \varphi_e)^T$. Then

$$\mathcal{J}(z) = \begin{bmatrix} 0 & \mathcal{J}_{\rho,M}(z) & 0 \\ \mathcal{J}_{M,\rho}(z) & \mathcal{J}_{M,M}(z) & \mathcal{J}_{M,e}(z) \\ 0 & \mathcal{J}_{e,M}(z) & 0 \end{bmatrix},$$

is associated with the bilinear form

$$\begin{aligned} \langle \varphi, \mathcal{J}(z)\psi \rangle &= \langle \varphi_\rho, \mathcal{J}_{\rho,M}(z)\psi_M \rangle + \langle \varphi_M, \mathcal{J}_{M,\rho}(z)\psi_\rho \rangle + \langle \varphi_M, \mathcal{J}_{M,M}(z)\psi_M \rangle \\ &\quad + \langle \varphi_M, \mathcal{J}_{M,e}(z)\psi_e \rangle + \langle \varphi_e, \mathcal{J}_{e,M}(z)\psi_M \rangle \end{aligned}$$

$$\begin{aligned} \langle \varphi_\rho, \mathcal{J}_{\rho,M}(z)\psi_M \rangle &= \int_0^\ell \rho(\psi_M \partial_x)\varphi_\rho \,\mathrm{d}x, \\ \langle \varphi_M, \mathcal{J}_{M,M}(z)\psi_M \rangle &= \int_0^\ell M((\psi_M \partial_x)\varphi_M - (\varphi_M \partial_x)\psi_M) \,\mathrm{d}x, \\ \langle \varphi_e, \mathcal{J}_{e,M}(z)\psi_M \rangle &= \int_0^\ell e(\psi_M \partial_x)\varphi_e + (\psi_M \partial_x)(\varphi_e p) \,\mathrm{d}x \end{aligned}$$

The self-adjoint semi-elliptic operator $\mathcal{R}(z)$ has two parts corresponding to the friction in the pipe $\mathcal{R}^{\lambda}(z)$ and the temperature loss through the pipe walls $\mathcal{R}^{k_\mathrm{w}}(z)$.

$$\mathcal{R}(z) = \mathcal{R}^{\lambda}(z) + \mathcal{R}^{k_\mathrm{w}}(z) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \mathcal{R}^{\lambda}_{M,M}(z) & \mathcal{R}^{\lambda}_{M,e}(z) \\ 0 & \mathcal{R}^{\lambda}_{e,M}(z) & \mathcal{R}^{\lambda}_{e,e}(z) + \mathcal{R}^{k_\mathrm{w}}_{e,e}(z) \end{bmatrix},$$

associated with the bilinear form

$$\begin{aligned} \langle \varphi, \mathcal{R}(z)\psi \rangle &= \langle \varphi_M, \mathcal{R}^{\lambda}_{M,M}(z)\psi_M \rangle + \langle \varphi_M, \mathcal{R}^{\lambda}_{M,e}(z)\psi_e \rangle \\ &+ \langle \varphi_e, \mathcal{R}^{\lambda}_{e,M}(z)\psi_M \rangle + \langle \varphi_e, (\mathcal{R}^{\lambda}_{e,e}(z) + \mathcal{R}^{k_\mathrm{w}}_{e,e}(z))\psi_e \rangle \end{aligned}$$

$$\begin{aligned} \langle \varphi_M, \mathcal{R}^{\lambda}_{M,M}(z)\psi_M \rangle &= \int_0^\ell \varphi_M \left(\frac{\lambda}{2d} \frac{T}{\vartheta} \rho |v| \right) \psi_M \, \mathrm{d}x, \\ \langle \varphi_M, \mathcal{R}^{\lambda}_{M,e}(z)\psi_e \rangle &= \int_0^\ell -\varphi_M \left(\frac{\lambda}{2d} \frac{T}{\vartheta} \rho |v| v \right) \psi_e \, \mathrm{d}x, \\ \langle \varphi_e, (\mathcal{R}^{\lambda}_{e,e}(z) + \mathcal{R}^{k_\mathrm{w}}_{e,e}(z))\psi_e \rangle &= \int_0^\ell \varphi_e \left(\frac{\lambda}{2d} \frac{T}{\vartheta} \rho |v| v^2 + \frac{4k_\mathrm{w}}{d} T \right) \psi_e \, \mathrm{d}x. \end{aligned}$$

The input is given as $u(z) \in \mathcal{D}_u$ by $u(z) = [M/\rho]|_0^\ell$ and the port operator $\mathcal{B}(z)[\cdot] : \mathcal{D}_u \to \mathcal{D}_z^\star$ via the pairing

$$\langle \varphi, \mathcal{B}(z)u(z)\rangle = -\left[(\varphi_\rho \rho + \varphi_M M + \varphi_e(e+p))\, u(z)\right]|_0^\ell ,$$

coming from the boundary terms via integration by parts.
With the adjoint operator $\mathcal{B}^*(z)[\cdot] : \mathcal{D}_z \to \mathcal{D}_u^*$, i.e., $\langle \varphi, \mathcal{B}(z)u(z)\rangle = \langle \mathcal{B}^*(z)\varphi, u(z)\rangle$, the system theoretic output is

$$y(z) = \mathcal{B}^*(z)\frac{\delta \mathcal{E}(z)}{\partial z} = -\left[\frac{|M|^2}{2\rho} + p + H(\rho, e) + \rho g h\right]\Bigg|_0^\ell .$$

The operators $\mathcal{J}$ and $\mathcal{R}$ satisfy non-interacting conditions

$$\mathcal{J}(z)\frac{\delta\mathcal{S}(z)}{\delta z} = 0, \qquad \mathcal{R}^{\lambda}(z)\frac{\delta\mathcal{H}(z)}{\delta z} = 0,$$

so flows of Hamiltonian and gradient system do not overlap.

- In the pH framework the choice of the state variables in the interplay with the energy functional is crucial for encoding the physical properties.
- Asymptotic simplifications (as limit to incompressibility) not straightforward, since they may change underlying structure.
- In compressible case (gas network) the ideal gas law implies

$$s(\rho, e) = \frac{R}{2}\rho \ln\left(c_{\mathrm{p}}\frac{e^3}{\rho^5}\right), \quad T(\rho, e) = \frac{2}{3R}\frac{e}{\rho}, \quad p(\rho, e) = \frac{2}{3}e,$$

with specific gas constant R and heat capacity c_{p}.

Outline

Replace state x in (operator) equation

$$E\dot{x} = (J - R)x + (B - P)u,\ y = (B + P)^T x + Du,\ D = S - N$$

by Galerkin projection $x \approx V_r x_r$ with finite (small) dimensional space V_r: projected (reduced) system

$$E_r \dot{x}_r = (J_r - R_r)x_r + (B_r - P_r)u,\ y_r = (B_r + P_r)^T x_r + Du,$$

$$E_r = V_r^T E V_r,\ J_r = V_r^T J V_r,\ R_r = V_r^T R V_r,\ B_r = V_r^T B,\ P_r = V_r^T P.$$

If V_r forms orthornormal basis, then resulting system is again a pHDAE and all properties are preserved.

- S. Chaturantabut, C. Beattie and S. Gugercin, Structure-Preserving Model Reduction for Nonlinear Port-Hamiltonian Systems, SIAM J. Scientific Computing, 2016,
- C. Beattie, S. Gugercin and V. M., *Structure-preserving Interpolatory Model Reduction for Port-Hamiltonian Differential-Algebraic Systems.* http://arxiv.org/abs/1910.05674. Festschrift for 70th birthday of A. Antoulas, 2021.
- 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 Journal Scientific Computing, Vol. 40, A331–A365, 2018.
- S. Hauschild, N. Marheineke and V. M., Model reduction techniques for linear constant coefficient port-Hamiltonian differential-algebraic systems, https://arxiv.org/abs/1901.10242, Control and Cybernetics, 2020.

Compute reduced order pHDAE

$$\begin{aligned} E_r \dot{x}_r &= (J_r - R_r)\, x_r + (B_r - P_r)\, u, \;\; x_r(t_0) = 0, \\ y_r &= (B_r + P_r)^T x_r + D_r\, u, \end{aligned}$$

such that $y_r(t)$ is good approximation to $y(t)$ over a wide range of $u(t)$. Let $H(s) = (B^T + P^T)(sE + R - J)^{-1}(B - P) + D$. Given right and left interpolation points $\{\sigma_1, \ldots, \sigma_r\}$, $\{\mu_1, \ldots, \mu_r\}$ with right and left tangent directions $\{k_1, \ldots, k_r\}$, $\{\ell_1, \ell_2, \ldots, \ell_r\}$, construct $H_r(s) = (B_r^T + P_r^T)(sE_r + R_r - J_r)^{-1}(B_r - P_r) + D_r$ such that

$$H(\sigma_i)k_i = H_r(\sigma_i)k_i \quad \text{and} \quad \ell_i^T H(\mu_i) = \ell_i^T H_r(\mu_i), \;\; \text{for} \;\; i = 1, 2, \ldots, r.$$

Interpolation conditions enforced via Petrov-Galerkin projection with

$$\begin{aligned} V_r &= \left[(\sigma_1 E + R - J)^{-1}(B - P)k_1, \;\; \cdots \; (\sigma_r E + R - J)^{-1}(B - P)k_r \right], \\ Z_r &= \left[(\sigma_1 E + R - J)^{-T}(B + P)\ell_1, \;\; \cdots \; (\sigma_1 E + R - J)^{-T}(B + P)\ell_r \right], \\ E_r &= Z_r^T E V_r, J_r = Z_r^T J V_r, R_r = Z_r^T R V_r, B_r = Z_r^T B, P_r = Z_r^T P, D_r = D. \end{aligned}$$

Difficulties

- The reduced quantities may no longer have the symmetry structure. Can be resolved by using a Galerkin projection, i.e., with $Z_r = V_r$. But then only half of the interpolation conditions hold.
- The polynomial parts of transfer functions may not match, leading to unbounded errors.
- We need to identify the constraints via a condensed form or directly from the structure of the equations.

- Beattie, Gugercin and V. M., *Structure-preserving Interpolatory Model Reduction for Port-Hamiltonian Differential-Algebraic Systems. Festschrift to honor the 70th birthday of A. Antoulas*, 2022. http://arxiv.org/abs/1910.05674.

Suppose we know the algebraic constraints explicitly and have the semi-explicit index one pHDAE structure

$$\begin{aligned} \begin{bmatrix} E_{11} & 0 \\ 0 & 0 \end{bmatrix} \dot{x}(t) &= \begin{bmatrix} J_{11} - R_{11} & J_{12} - R_{12} \\ -J_{12}^T - R_{12}^T & J_{22} - R_{22} \end{bmatrix} x(t) + \begin{bmatrix} B_1 - P_1 \\ B_2 - P_2 \end{bmatrix} u(t) \\ y(t) &= \begin{bmatrix} B_1^T + P_1^T & B_2^T + P_2^T \end{bmatrix} x(t) + Du(t). \end{aligned}$$

where $E_{11} = E_{11}^T > 0$ and $J_{22} - R_{22}$ is nonsingular.

Theorem (Beattie, Gugercin, V.M. 2019)

Consider semi-explicit index 1 *pHDAE, interpol. points* $\{\sigma_1, \sigma_2, \ldots, \sigma_r\}$ *and tangent dir.* $\{k_1, k_2, \ldots, k_r\}$. *Construct basis* $V_r = \begin{bmatrix} V_{r,1}^T & V_{r,2}^T \end{bmatrix}^T$ *as*
$V_r = \left[(\sigma_1 E + R - J)^{-1}(B - P)k_1, \;\cdots,\; (\sigma_r E + R - J)^{-1}(B - P)k_r\right]$
and set $K_r = \begin{bmatrix} k_1 & \cdots & k_r \end{bmatrix}$, $D_r = D - (B_2^T + P_2^T)(J_{22} - R_{22})^{-1}(B_2 - P_2)$.
Then transfer function $H_r(s)$ *of reduced model*

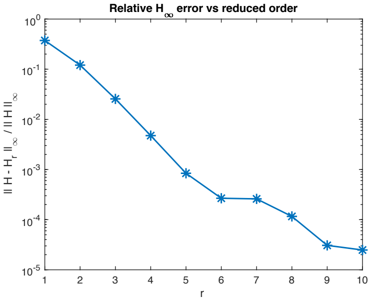
$$E_r \dot{x}_r(t) = (J_r - R_r)x_r(t) + (B_r - P_r)u(t), \; y_r(t) = (B_r + P_r)x_r(t) + D_r u(t)$$

with $E_r = V_{r,1}^T E_{11} V_{r,1}$, $J_r - R_r = V_r^T(J - R)V_r + K_r^T(D_r - D)K_r$,
$(B_r + P_r)^T = (B + P)V_r + (B_2^T + P_2^T)(J_{22} - R_{22})^{-1}(B_2 - P_2)K_r$,
matches polyn. part of $H(s)$ *and tangentially interpolates it. The reduced system is again a pHDAE if the reduced passivity matrix* $W_r = \begin{bmatrix} R_r & P_r \\ P_r^T & S_r \end{bmatrix}$ *is positive semidefinite.*

pHDAE formulation of incompressible Oseen equations,

$$\begin{array}{rclll} \partial_t v & = & -(a\cdot\nabla)v + \mu\Delta v - \nabla p + f & \text{in } \Omega\times(0,T], & v = 0, \\ 0 & = & -\text{div } v, & \text{in } \Omega\times(0,T], & v = v^0, \end{array}$$

with velocity v and pressure p, $\mu > 0$ is the viscosity, and $\Omega = (0,1)^2$. $f = b(x)u(t)$ is an externally body force.
FD/FEM discretization gives pHDAE with $n = 7399$, $n_v = 4900$, and $n_p = 2499$.



Extension to nonlinear case

- Generate projection spaces via POD or shifted POD approaches in tranport dominant case.
- Combine with Empirical Interpolations Methods. (D)EIM.
- Incorporate information from physical system.
- Much to do, in particular if the system has many transports.

- Barrault, Maxime, et al. *An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations.* Comptes Rendus Mathematique 2004.
- Chaturantabut, Beattie, and Gugercin. Structure-preserving model reduction for nonlinear port-Hamiltonian systems. SIAM Journal Scientific Computing, 2016.
- Chaturantabut, Sorensen, Nonlinear Model Reduction via Discrete Empirical Interpolation, SIAM Journal Scientific Computing, 2010.
- Reiss, Schulze, Sesterhenn, and V.M. *The shifted proper orthogonal decomposition: A mode decomposition for multiple transport phenomena.* SIAM Journal Scientific Computing, 2018.

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

- 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.

Collocation methods for pHDAEs

Given input $u : \mathbb{I} \times \mathcal{X} \to \mathbb{R}^m$, interval $\mathbb{I} = [t_0, t_f]$ of length $h = t_f - t_0$, consistent initial condition x_0 at time t_0, we approximate the solution $x(t)$ with polynomial $\tilde{x}(t)$ of degree s, so that with $\tilde{x}(t_0) = x_0$, $\tilde{x}$ satisfies the pHDAE in s collocation points $t_i = t_0 + h\gamma_i$ with $\gamma_i \in [0, 1]$ for $i = 1, \dots, s$.
Let ℓ_i denote the i-th Lagrange interp. poly. with nodes $\gamma_1, \dots, \gamma_s$, i.e., $\ell_i(\tau) := \prod_{\substack{j=1 \\ j \neq i}}^{s} \frac{\tau - \gamma_j}{\gamma_i - \gamma_j}$. Then for certain $\dot{x}_i = \dot{\tilde{x}}(t_i)$,

$$
\begin{aligned}
\dot{\tilde{x}}(t_0 + \tau h) &= \sum_{i=1}^{s} \dot{x}_i \ell_i(\tau), \ \tilde{x}(t_0 + \tau h) = x_0 + h \sum_{j=1}^{s} \dot{x}_j \int_0^{\tau} \ell_j(\sigma) \mathrm{d}\sigma, \\
x_i &:= \tilde{x}(t_i) = x_0 + h \sum_{j=1}^{s} \alpha_{ij} \dot{x}_j, \ x_f := \tilde{x}(t_f) = x_0 + h \sum_{j=1}^{s} \beta_j \dot{x}_j,
\end{aligned}
$$

$\alpha_{ij} := \int_0^{\gamma_i} \ell_j(\sigma) \mathrm{d}\sigma$, $\beta_j := \int_0^1 \ell_j(\sigma) \mathrm{d}\sigma$, $i, j = 1 \dots s$ associated Runge-Kutta coefficients.

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 the collocation method and computing the *discrete input* and *output* u_i, y_i, for $i = 1, \ldots, s$.

Collocation flow and effort

Define the *collocation flows, efforts, input and output* as

$$\begin{aligned}
\tilde{f}_s(t_0 + h\tau) &= \sum_{i=1}^{s} f_s^i \ell_i(\tau), \quad \tilde{e}_s(t_0 + h\tau) = \sum_{i=1}^{s} e_s^i \ell_i(\tau), \\
\tilde{f}_r(t_0 + h\tau) &= \sum_{i=1}^{s} f_r^i \ell_i(\tau), \quad \tilde{e}_r(t_0 + h\tau) = \sum_{i=1}^{s} e_r^i \ell_i(\tau), \\
\tilde{y}(t_0 + h\tau) &= \sum_{i=1}^{s} y_i \ell_i(\tau), \quad \tilde{u}(t_0 + h\tau) = \sum_{i=1}^{s} u_i \ell_i(\tau).
\end{aligned}$$

Then, $(\tilde{f}_s, \tilde{y}, \tilde{f}_r; \tilde{e}_s, \tilde{u}, \tilde{e}_r) \in \mathcal{D}_{\tilde{x}}$ in all collocation points t_i.

▷ E. Hairer, C. Lubich and G. Wanner, *Structure-Preserving Algorithms for Ordinary Differential Equations*, Springer, Berlin, Germany: Springer-Verlag, 2006.

▷ Kotyczka, Lefèvre, Discrete-Time Port-Hamiltonian Systems Based on Gauss-Legendre Collocation, IFAC-PapersOnLine 51, no. 3 (2018): 125–30.

Evolution of Hamiltonian

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.

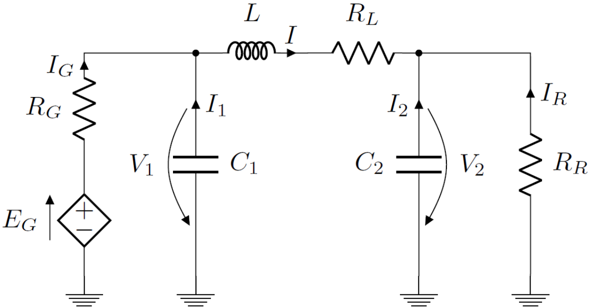
$$\begin{aligned} \dot{H}(t_i) &= \nabla \mathcal{H}(x_i)^T \dot{x}_i = e(x_i)^T E(x_i) \dot{x}_i = \\ &= -\langle e_s^i \mid f_s^i \rangle = \langle e_r^i \mid f_r^i \rangle + \langle y_i \mid u_i \rangle, i = 1, \ldots, s \end{aligned}$$

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.

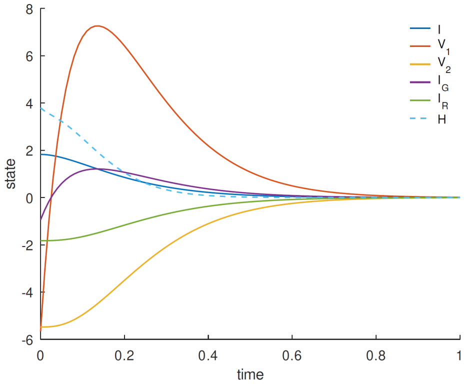
Toy example of DC power network:



The energy of the system is stored in the inductor and in the two capacitors, giving the Hamiltonian

$$\mathcal{H}(I, V_1, V_2) = \frac{1}{2}LI^2 + \frac{1}{2}C_1 V_1^2 + \frac{1}{2}C_2 V_2^2.$$

Choose $L = 2$, $C_1 = 0.01$, $C_2 = 0.02$, $R_L = 0.1$, $R_G = 6$, $R_R = 3$.



Implicit midpoint rule, (Gauss-Legendre) $s = 1$ stages, order $p = 2$ for ODEs and semi-explicit DAEs of index 1.

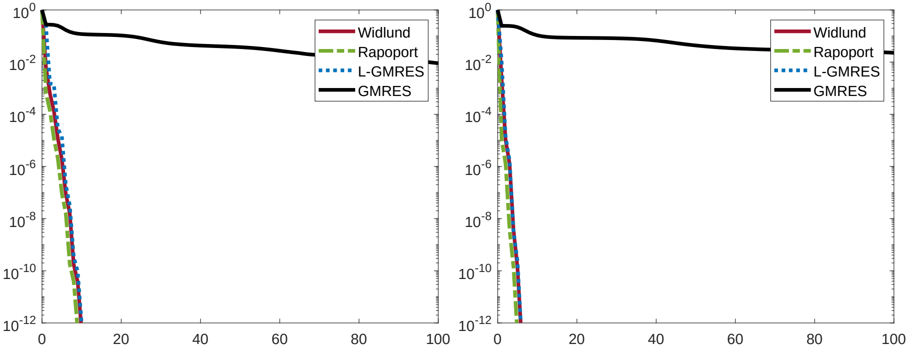
After discretization with implicit Gauss-Legendre, linear systems have positive (semi)-definite symmetric part.
For $(M+N)x = b$ with $M = M^T > 0$ $N = -N^T$ use symmetric part as preconditioner, and solve the equivalent system

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

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

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

- O. Widlund. A Lanczos method for a class of nonsymmetric systems of linear equations. *SIAM J. Numer. Anal.*, 15(4):801–812, 1978.
- M. Manguoğlu and V. Mehrmann, A two-level iterative scheme for general sparse linear systems based on approximate skew-symmetrizers. http://arxiv.org/abs/2009.06954, Electronic Transactions Numerical Analysis, Vol. 54, 370-–391, 2021.
- 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, 2021.



Stokes equation. Relative residual norms with $\tau = 0.001$ and $\tau = 0.0001$ (left and right).

Run times differences drastic if step-size is decreased.

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.
- Stability analysis.
- Function Spaces.
- Error estimates.
- Preconditioning.
- Data based realization.
- Uncertainty quantification.
- Software.
- Digital twins
- . . .

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