Port-Hamiltonian modeling, simulation, and optimization for coupled multi-physics and multi-scale systems

Volker Mehrmann
Institut für Mathematik
Technische Universität Berlin

Research Center MATHEON
Mathematics for key technologies
Motivation

Application: Gas transport networks
Energy based modeling
Gas transport pHDAE
Power networks
PHDAE formulation of generalized Kuramoto
Other physical domains
Conclusion
The German government has decided to move out of nuclear energy and also to reduce $CO_2$ emissions drastically. This leads to large scientific and technological challenges.

- The security of energy supply has to be guaranteed.
- Different energy sectors have to be coupled, e.g. green and fossil energy. Power-to-gas, gas-to-power, etc.
- Different components of energy networks have very different modeling accuracy.
- Different energy sectors live on very different (time) scales.
- Renewables require to deal with increased randomness and decentralization. Energy customers become ‘prosumers’.
- Dynamical rather than stationary approaches are needed.

How can we deal with these challenges in modeling, simulation, optimization and control? (MSO)
Figure: Major lines of power and gas grid in Europe.
The MSO paradigm

Modeling, simulation, and optimization (MSO) of real multiphysics system.

- Create a model hierarchy of different modeling accuracy for every component.
- Choose representations of the models so that the coupling of different physical domains works across many scales.
- Define the goal (simulation, optimization, stabilization, ...)
- Analyze all errors (model, data, discretization, solution of equations, even roundoff in finite arithmetic.)
- **Adaptively choose model in the hierarchy, space-time discretization accuracy, and solver accuracy** depending on goal and the required tolerance.
- Use a network approach via port-Hamiltonian systems.
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2. Application: Gas transport networks
   - Energy based modeling
   - Gas transport pHDAE
   - Power networks
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   - Other physical domains
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Collaborative Research Center Transregio Modelling, simulation and optimization of Gas networks

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

Project: Controlled coupling of hybrid network systems
Components of gas flow model

System of partial differential equations with algebraic constraints

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

- Erratic demand and nomination of transport capacity.
- Using gas network as storage for hydrogen, methane produced from unused renewable energy.

Goal: Gas flow simulation, control and optimization using a model hierarchy.
Gas networks are very large!
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Gas networks are very large!
Gas flow: Euler equations

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) = 0, \\
\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (p + \rho v^2) = -\frac{\lambda}{2D} \rho v |v| - g \rho h', \\
\frac{\partial}{\partial t} \left( \rho \left( \frac{1}{2} v^2 + e \right) \right) + \frac{\partial}{\partial x} \left( \rho v \left( \frac{1}{2} v^2 + e \right) + pv \right) = -\frac{k_w}{D} (T - T_w),
\]

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

- density \( \rho \), \( k_w \) heat transfer coefficient,
- temperature \( T \), wall temperature \( T_w \),
- velocity \( v \), gravitational force,
- pressure \( p \), friction coefficient,
- \( h' \) slope of pipe, \( D \) diameter of pipe,
- \( e \) internal energy, \( R \) gas constant of real gas.
Full model hierarchy for gas flow.

Constant temperature $\rightarrow$ the isothermal Euler equations. 

Model $M1$:

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

$$\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (p + \rho v^2) = -\frac{\lambda}{2D} \rho v |v| - g \rho h',$$

together with the state equation for real gases

$$p = \rho (1 + \alpha p) RT.$$
If \( v \) is small, neglect the term \( \frac{\partial}{\partial x} (\rho v^2) \rightarrow \) semilinear model

Model \( M2: \)

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) &= 0, \\
\frac{\partial}{\partial t} (\rho v) + \frac{\partial p}{\partial x} &= -\frac{\lambda}{2D} \rho v |v| - g \rho h',
\end{align*}
\]
Discretization using an implicit box scheme Wendroff 1960. For the scalar balance law

\[ u_t + f(u)_x = g(u), \]

with initial conditions \( u(x, 0) = u_0(x) \), the box scheme is

\[
\frac{u_{j-1}^{n+1} + u_j^{n+1}}{2} = \frac{u_{j-1}^n + u_j^n}{2} - \frac{\Delta t}{\Delta x} (f_j^{n+1} - f_{j-1}^{n+1}) + \Delta t \frac{g_{j-1}^{n+1} + g_j^{n+1}}{2}.
\]

At every step, (under certain conditions) a unique solution exists, Kolb, Lang, and Bales 2010. Convergence of order 2 in space and order 1 in time. Space-Time-Adaptivity via step-size control and a posteriori error analysis.
When a stationary model is assumed, i.e., $\frac{\partial}{\partial t} = 0$, and $h' = 0$, two ODEs are obtained, which can be solved analytically. Model $M3$:

\[
\rho v = \text{const.},
\]

\[
p(x) = \sqrt{p_{in}^2 - \frac{\lambda c^2 x}{D}} \rho v |\rho v|.
\]

This algebraic model (Weymouth equation) is used in planning and often further approximated by piecewise linear model.

Further simplifications: Reduced order models (later).
Three level model hierarchy

- Isothermal Euler Equations (M1)
  \[ \frac{\partial}{\partial x} (\rho v^2) = 0 \]

- Semilinear Model (M2)
  \[ \frac{\partial}{\partial t} = 0, h' = 0 \]

- Algebraic Model (M3)

Figure: Model Hierarchy

Which model for which simulation/optimization goal?
Port-Hamiltonian formulation?
Can we use the hierarchy to control the errors?
Determine sensitivities in parameters, error estimates, distributions of uncertainties, when model is simplified, discretized, reduced, or subjected to data uncertainty.

- Sensitivity/error analysis has to be done with the simulation/optimization goal in mind.
- Carry out this analysis for the whole hierarchy, using analytic formulas or adjoint equations.
- Determine a posteriori error estimates $\eta_x$, $\eta_t$, $\eta_m$ in space, time, and model (or data uncertainty) to control computational cost.

Computational Cost Optimization

**MSO Goal: Simulation time minimization**

To optimize computational cost, choose cost function

\[ F(m, n_x, n_t) = C_m \cdot n_x^{\alpha_m} \cdot n_t^{\beta_m} \]

Tune (learn) constants \( C_m, \alpha_m, \) and \( \beta_m \) from simulations.
Minimization of CPU time

Search for a space-time-model error control which satisfies

\[ \sum_{j \in J_p} \left( \eta_{m,j} + \eta_{x,j} + \eta_{t,j} \right) \leq \text{tol} \]
\[
\left| J_p \right|
\]

- Included in the flow code ANACONDA (TU Darmstadt).
- Test case: Gas network of \( |J_p| = 12 \) pipelines.

- Achieved computing time reductions of 80%.

Minimize compressor costs subject to variable bounds, mass balance, compressor models. Classical switched nonlinear optimal control problem

Optimization code steers the accuracy, the discretization error, and chooses the model according to error estimates to obtain in each step a feasible solution.

Theorem

Suppose that the error estimator leads to a local error reduction for every arc in the pipe network and that every NLP is solved to local optimality. Then, the NLP solver terminates after a finite number of steps with an $\epsilon$-feasible solution with respect to a reference configuration.
Example: Compressor cost optimization

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

Intermediate summary, challenges

- Model hierarchy for gas networks.
- Space-time-model adaptivity.

Challenges

- Can we reduce the models further by model reduction?
- Can we use the same approach for power networks and coupled power/gas networks?
- How about the different time scales?
- What is the right framework for modeling?
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Energy based modeling

- Choose representations of models so that coupling of different physical domains works across many scales.
- Use energy as common quantity of different physical systems.
- We want a representation that is good for model coupling, that is good for discretization, and that is close to physics.
- A system theoretic way to deal with such energy based modeling is that of port-Hamiltonian systems.

- ...
Port-Hamiltonian systems

Classical port-Hamiltonian (pH) ODE/PDE systems

\[
\dot{x} = (J(x, t) - R(x, t)) \nabla_x \mathcal{H}(x) + (B(x, t) - P(x, t))u(t),
\]
\[
y(t) = (B(x, t) + P(x, t))^T \nabla_x \mathcal{H}(x) + (S(x, t) + N(x, t))u(t),
\]

- $\mathcal{H}(x)$ 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.
Port-Hamiltonian systems generalize Hamiltonian systems.

Conservation of energy replaced by dissipation inequality

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

Port-Hamiltonian systems are closed under power-conserving interconnection. Models can be coupled in modularized way.

Minimal constant coefficient pH systems are stable and passive.

Port-Hamiltonian 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 to incorporate multiphysics components: chemical reaction, thermodynamics, electrodynamics, mechanics, etc. Open/closed systems.

A linear variable coefficient (P)DAE of the form

\[
\begin{align*}
E\dot{x} &= [(J - R)Q - EK]x + (B - P)u, \\
y &= (B + P)^T Qx + (S + N)u,
\end{align*}
\]

with \( E, A, Q, R = R^T, K \in C^0(\mathbb{I}, \mathbb{R}^{n,n}), B, P \in C^0(\mathbb{I}, \mathbb{R}^{n,m}), \) \( S + N \in C^0(\mathbb{I}, \mathbb{R}^{m,m}) \) is called \textit{port-Hamiltonian DAE (pHDAE)} if:

i) \( \mathcal{L} := Q^T E \frac{d}{dt} - Q^T JQ - Q^T EK \) is skew-adjoint.

ii) \( Q^T E = E^T Q \) is bounded from below by a constant symmetric \( H_0 \).

iii) \( W := \begin{bmatrix}
Q^T R Q & Q^T P \\
P^T Q & S
\end{bmatrix} \geq 0, \ t \in \mathbb{I}. \)

Hamiltonian: \( \mathcal{H}(x) := \frac{1}{2} x^T Q^T E x : C^1(\mathbb{I}, \mathbb{R}^n) \to \mathbb{R} \).
Properties

- Nonlinear version available (not much analysis though).

- **Dissipation inequality** still holds.

- PH DAE systems closed under *power-conserving interconnection*. Models can be coupled in *modularized* way.

- PH DAE structure invariant under time varying basis changes.

- Canonical forms in constant and variable coefficient case.

- Port-Hamiltonian structure preserved under constraint preserving *Galerkin projection, model reduction*.

- Representation is very robust to structured perturbations.


Outline

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Figure: Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertices $\mathcal{V} = \{v_1, v_2, v_3, v_4\}$ and edges $\mathcal{E} = \{e_1, e_2, e_3\}$ defined by $e_1 = (v_1, v_2)$, $e_2 = (v_2, v_3)$, and $e_3 = (v_2, v_4)$.
Model on every edge $e \in \mathcal{E}$ the conservation of mass and the balance of momentum, $z = (p, q)$.

\[
a^e \partial_t p^e + \partial_z q^e = 0, \quad e \in \mathcal{E},
\]

\[
b^e \partial_t q^e + \partial_z p^e + d^e q^e = 0, \quad e \in \mathcal{E},
\]

where $p^e, q^e$ denote the pressure and mass flux, respectively.

Encode in $a^e(t, z), b^e(t, z) > 0$ physical properties of fluid and pipe, in $d^e(t, z) \geq 0$ damping due to friction, and introduce interior and exterior vertices $\mathcal{V}_0$ and $\mathcal{V}_\partial = \mathcal{V} \setminus \mathcal{V}_0$.

Model conservation of mass and momentum at $v \in \mathcal{V}_0$ by

\[
\sum_{e \in \mathcal{E}(v)} n^e(v) q^e(v) = 0
\]

\[
p^e(v) = p^f(v), \quad e, f \in \mathcal{E}(v),
\]

where $\mathcal{E}(v) = \{ e : e = (v, \cdot) \text{ or } e = (\cdot, v) \}$ is the set of edges adjacent to $v$ and $n^e(v) = \mp 1$ (flow direction).
\[ p^e(v) = u_v, \quad v \in \mathcal{V}_\partial, \quad e \in \mathcal{E}(v) \]

\[ y_v = -n^e(v)q^e(v), \quad v \in \mathcal{V}_\partial, \quad e \in \mathcal{E}(v), \]

Initial conditions: \( p(0) = p_0, \quad q(0) = q_0 \) on \( \mathcal{E} \) for pressure and mass flux.

Quadratic Hamiltonian:

\[ \mathcal{H} = \frac{1}{2} \sum_{e \in \mathcal{E}} \int_e a^e |p^e|^2 + b^e |q^e|^2 \, dz. \]

Use this model for discretization and model reduction via Galerkin projection.
Discontinuous Galerkin discretization

Existence of unique solution for consistent initial conditions $p_0, q_0$ and sufficiently smooth inputs $(u_v)_{v \in \nu}$, in Egger/Kugler 2016. Mixed finite element space discretization leads to index two constant coefficient large scale pHDAE:

\[
E \dot{x} = (J - R)x + Bu, \\
y = B^T x, \\
x(0) = x^0,
\]

here $Q = I, S, N, P = 0$, $E = E^T$.

\[
E = \begin{bmatrix} M_1 & 0 & 0 \\ 0 & M_2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\
J = \begin{bmatrix} 0 & -G & 0 \\ G^T & 0 & N^T \\ 0 & -N & 0 \end{bmatrix}, \\
R = \begin{bmatrix} 0 & 0 & 0 \\ 0 & D & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\
B = \begin{bmatrix} 0 \\ \tilde{B}_2 \end{bmatrix}.
\]

The discretized Hamiltonian is given by

\[
\mathcal{H}(x) = \frac{1}{2} x^T E x = \frac{1}{2} (x_1^T M_1 x_1 + x_2^T M_2 x_2).
\]
Every Galerkin projection MOR method preserves the structure of pH systems. Replace

\[ \dot{x} = (J - R) \nabla_x H(x) + Bu, \quad y = B^T \nabla_x H(x) \]

by reduced system

\[ \dot{x}_r = (J_r - R_r) \nabla_{x_r} H_r(x_r) + B_r u, \quad y_r = B_r^T \nabla_{x_r} H_r(x_r) \]

with \( x \approx V_r x_r, \quad \nabla_x H(x) \approx W_r \nabla_{x_r} H_r(x_r) \), \( J_r = W_r^T J W_r \), \( R_r = W_r^T R W_r \), \( W_r^T V_r = I_r \), \( B_r = W_r^T B \).

If \( V_r \) and \( W_r \) are appropriate orthornormal bases, then the resulting system is again pH and all properties are preserved.


Extension to pHDAEs in an obvious way.
Galerkin MOR for gas flow

- Model reduction (projection spaces) via \textbf{moment matching}.
- Proof of Well-posedness, conservation of mass, dissipation inequality, and exponentially stability of steady states.
- Specially structured (modified) Krylov method to satisfy algebraic compatibility conditions.
- CS decomposition to guarantee Lagrangian structure in approximation.
- No reduction of constraints.
- Efficient construction of projection spaces $V_r$, $W_r$.
- Proof of a posteriori error bounds.

Splitting and CS decomposition

- Splitting of the projection matrix $W = [W_1; W_2; W_3]$ corresponding to the solution components $x = [x_1; x_2; x_3]$.
- Even if columns of $W$ are orthogonal, this is no longer true for the columns of $W_i$.
- Re-orthogonalization is required.
- Splitting very sensitive to numerical errors.
- Use cosine-sine (CS) decomposition,

$$
\begin{bmatrix}
W_1 \\
W_2
\end{bmatrix}
= 
\begin{bmatrix}
U_1 & 0 \\
0 & U_2
\end{bmatrix}
\begin{bmatrix}
C \\
S
\end{bmatrix}
X^T,
$$

with $U_1$, $U_2$, and $X$ orthogonal, and $C$, $S$ diagonal with entries $C_{ii}^2 + S_{ii}^2 = 1$. 
Pressure correction

With and without pressure correction via CS decomposition of the Galerkin-projection space.

![Graph 1](image1.png)

![Graph 2](image2.png)
Small network
Results for discretized model (blue) and reduced model (red) with dim. 2, 5, 10 and damping parameter $d = 0.1, 1, 5$ (top to bottom).
Consequences

- Continuous, discretized and reduced models close to physics.
- Conservation laws are included.
- Whole model hierarchy can be built in pHDAE form.
- A posteriori error estimates for DG discretization.
- Error estimates for model reduction the same as for discretization error.
- Reduced model can be added to model hierarchy.
Collaborative Research Center SFB 910, Control of self-organizing nonlinear systems: Theoretical methods and concepts of application with Theoretical Physics.


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

Incorporation in global/local optimization framework.

Coupling with gas and heat network in BMBF Project with N. Marheineke, J. Mohring, M. Schmidt, and industry.

Building the pHDAE model hierarchy. PhD students: Arbi Moses Badlyan, Riccardo Morandin
Each node (generators, loads, prosumers, etc) is modeled as an oscillator with phase angle $\theta$ and rotational speed $\omega = \dot{\theta}$.

The network is represented by an undirected, weighted graph $(V, E)$. The weight of the edges correspond to characteristics of the transmission lines (e.g. the admittance).

Assume: $\omega \approx \Omega$ operational speed.

Instantaneous power model

\[ m_j \dot{\theta}_j \ddot{\theta}_j = -d_j \dot{\theta}_j^2 - v_j l_j + P_j, \quad \text{for } 1 \leq j \leq n, \]

\[ L_{jk} \dot{i}_{jk} = -R_{jk} i_{jk} + v_j - v_k, \quad \text{for } (j, k) \in \mathcal{E}, \]

\[ 0 = -l_j + \sum_{k: (j, k) \in \mathcal{E}} i_{jk}, \quad \text{for } 1 \leq j \leq n. \]

- \( \theta_j \): phase angle of \( j \)
- \( i_{jk} \): current from \( j \) to \( k \)
- \( v_j \): voltage of \( j \) \((= |V_j| \cos \theta_j)\)
- \( l_j \): current leaving \( j \)
- \( P_j \): power balance in \( j \)
- \( m_j \): inertia of \( j \)
- \( d_j \): damping constant of \( j \)
- \( L_{jk} \): inductance in \((j, k)\)
- \( R_{jk} \): resistance in \((j, k)\)
Simplification I: Real power model

- Near steady-state (long time without disturbances);
- Transmission line resistance $R \approx 0$;
- Energy storage in inductors is ignored;
- Electrical ‘instantaneous’ power substituted by \textit{real power} (average over time).

This allows to ignore the electrical part for the dynamics.

$$m_j \ddot{\theta}_j = -d_j \dot{\theta}_j^2 + \sum_{k=1}^{n} g_{jk} \sin(\theta_k - \theta_j) + P_j, \quad \text{for} \ 1 \leq j \leq n,$$

$$g_{jk} = \frac{|V_j||V_k|}{2\Omega L_{jk}} \geq 0 \quad \text{for} \ (j, k) \in E, \quad \text{else} \ g_{jk} = 0.$$

Note that $G = G^T$. 
Simplification II, generalized Kuramoto model.
Using \( \dot{\theta}_j \approx \Omega \), one may consider the simplified system

\[
m_j \ddot{\theta}_j = -d_j \dot{\theta}_j + \sum_{k=1}^{n} \tilde{g}_{jk} \sin(\theta_k - \theta_j) + \tilde{P}_j, \quad \text{for } 1 \leq j \leq n.
\]

Simplification III, standard Kuramoto model with inertia

\[
m_j \ddot{\theta}_j = -d_j \dot{\theta}_j + K \sum_{k=1}^{n} \sin(\theta_k - \theta_j) + \Omega_j, \quad \text{for } 1 \leq j \leq n.
\]
Model hierarchy is currently being extended.
The complex order parameter

\[ r e^{i\phi} = \frac{1}{n} \sum_{j=1}^{n} e^{i\theta_j} \]

\( r(\theta_1, \ldots, \theta_n) \in [0, 1] \) measures synchronicity of the system.

Better to use

\[ r^2 = \frac{1}{n^2} \sum_{j,k=1}^{n} \cos(\theta_k - \theta_j) \in [0, 1]. \]
The kinetic energy of the system is $\mathcal{K}(\dot{\theta}) = \frac{1}{2} \sum_{j=1}^{n} m_j \dot{\theta}_j^2$, so

$$\dot{\mathcal{K}} = \sum_{j=1}^{n} m_j \dot{\theta}_j \ddot{\theta}_j = \sum_{j=1}^{n} (-d_j \dot{\theta}_j^2 + \Omega_j \dot{\theta}_j) + \sum_{j,k=1}^{n} g_{jk} \dot{\theta}_j \sin(\theta_k - \theta_j).$$

To incorporate the network topology we define a new generalized order parameter

$$\xi = \xi_{b,c}(\theta) := \frac{1}{c} \sum_{j,k=1}^{n} g_{jk} \cos(\theta_k - \theta_j) + b$$

for $b, c \in \mathbb{R}$ chosen in optimal way.
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Write the generalized Kuramoto model as pH model

\[ E \dot{x} = (J(x) - R(x))Qx + Bu \]

with \( J = -J^T \), \( R = R^T \geq 0 \), \( Q^T E = E^T Q \) and \( \mathcal{H} = \frac{1}{2} x^T Q^T E x \).

We define \( x = (\omega, \rho, \sigma) = (\dot{\theta}, \cos \theta, \sin \theta) \) and \( u = \omega \). Thus,

\[
\begin{align*}
\sin(\theta_k - \theta_j) &= \rho_j \sigma_k - \sigma_j \rho_k, \\
\cos(\theta_k - \theta_j) &= \rho_j \sigma_k + \sigma_j \sigma_k,
\end{align*}
\]

\[
\left[ \sum_{k=1}^{n} g_{jk} \sin(\theta_k - \theta_j) \right]_{j=1,...,n} = D_\rho G_\sigma - D_\sigma G_\rho,
\]

with \( D_\rho = \text{diag}(\rho) \) and \( D_\sigma = \text{diag}(\sigma) \).
We can write the generalized Kuramoto model as

\[ M \dot{x} = -D \dot{x} - D_{\sigma} G \rho + D_{\rho} G \sigma + \Omega, \]
\[ \dot{\rho} = -D_{\sigma} \omega, \]
\[ \dot{\sigma} = D_{\rho} \omega, \]

that is equivalent to previous model with

\[ E = \text{diag}(M, I_n, I_n), \]
\[ Q = \text{diag}(I_n, -G, -G), \]
\[ J = \begin{bmatrix} 0 & D_{\sigma} & -D_{\rho} \\ -D_{\sigma} & 0 & 0 \\ D_{\rho} & 0 & 0 \end{bmatrix}, \]

The Hamiltonian has not changed.

\[ \mathcal{H}(x) = \frac{1}{2} x^T Q^T E x = \frac{1}{2} \omega^T M \omega - \frac{1}{2} \rho^T G \rho - \frac{1}{2} \sigma^T G \sigma. \]
Make sure that the constraint $\rho_j^2 + \sigma_j^2 = 1$ holds numerically by adding equations

$$\rho_j^2 + \sigma_j^2 - \lambda_j = 0, \quad \text{for } j = 1, \ldots, n,$$

with $\lambda_1, \ldots, \lambda_n$ Lagrange multipliers. This leads to the pHDAE

$$\begin{bmatrix} E & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{x} \\ \dot{\lambda} \end{bmatrix} = \left( \begin{bmatrix} J & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} R & 0 \\ 0 & I \end{bmatrix} \right) \hat{Q} \begin{bmatrix} x \\ \lambda \end{bmatrix} + \begin{bmatrix} B \\ 0 \end{bmatrix} u$$

with

$$\hat{Q} = \begin{bmatrix} Q & 0 \\ 0 & 0 \\ 0 & D_\rho & D_\sigma & -I \end{bmatrix}$$
Simulations on the Italian power grid network.

- Connected graph \((\mathcal{V}, \mathcal{E})\) consisting of \(n = 127\) nodes and \(e = 171\) edges;

- We set \(g_{jk} = \begin{cases} 
10 & \text{if } (j, k) \in \mathcal{E}, \\
0 & \text{else}
\end{cases}\) for \(j \neq k\), and \(g_{jj} = -\sum_{k \neq j} g_{jk}\) for \(j = 1, \ldots, n\);

- We set all inertia constants \(m_j = m = 6\) and damping constants \(d_j = d = 1\);

- We choose randomly 34 nodes as generators \((\Omega_j = \Omega_{\text{gen}} = 2.7353)\) and all other nodes as consumers \((\Omega_j = \Omega_{\text{load}} = -1)\).
Example: implicit midpoint rule (IMP).

Lemma

Given PH system with $E$ invertible or pHDAE of differentiation index one, then the IMP with step size $h$ yields

$$
\mathcal{H}^{\ell+1} - \mathcal{H}^{\ell} = -\frac{h}{4} (x^{\ell+1} + x^\ell)^T Q^T R Q (x^{\ell+1} + x^\ell) \leq 0.
$$

In particular, if $R = 0$ the Hamiltonian is preserved.

Since $\rho_j^2 + \sigma_j^2$ is the Hamiltonian of a pH subsystem without dissipation, we expect the constraint to be well preserved.

In general: We need new classes of pHDAE integrators:

- P. Kotyczka, L. Lefevre, Discrete-time port-Hamiltonian systems based on Gauss-Legendre collocation. Proceedings of the 6th IFAC Workshop on Lagrangian and Hamiltonian Methods for Nonlinear Control, Valparaíso, Chile, May 1–4, 2018
Numerical solution for Lagrange multiplier $\mu$: Symplectic Euler (SE), Implicit Midpoint (IMP), Explicit Midpoint (EMP)). Orange and magenta, different convergence thresholds $10^{-6}$ and $10^{-12}$. 
Order parameters vs K

![Graph showing order parameters vs K](image_url)
Control of synchronization

(a)

(b)

(c)
Outline

1. Motivation
2. Application: Gas transport networks
   Energy based modeling
   Gas transport pHDAE
   Power networks
   PHDAE formulation of generalized Kuramoto
3. Other physical domains
4. Conclusion
Disc brake squeal is a frequent and annoying phenomenon (with cars, trains, bikes).

Important for customer satisfaction, even if not a safety risk.

Nonlinear effect that is hard to detect.

The car industry is trying for decades to improve this, by changing the designs of brake and disc.

Can we do this model based?
Interdisciplinary project with car manufacturers + SMEs
Supported by German Minist. of Economics via AIF foundation.

Goals:

▷ Develop model of brake system with all effects that may cause squeal. (Friction, circulatory, gyroscopic effects, etc).

▷ Simulate brake behavior for many different parameters (disk speed, material geometry parameters).

▷ Project on space assoc. with squealing evs.

▷ Optimization: Layout of shims.

Large differential-algebraic equation (DAE) system dep. on parameters (here only disk speed displayed).

\[ M\ddot{q} + \left(C_1 + \frac{\omega_r}{\omega} C_R + \frac{\omega}{\omega_r} C_G\right)\dot{q} + \left(K_1 + K_R + \left(\frac{\omega}{\omega_r}\right)^2 K_G\right)q = f, \]

- \( q \) vector of FE coefficients.
- \( M \) symmetric, pos. semidef., singular matrix,
- \( C_1 \) symmetric matrix, material damping,
- \( C_G \) skew-symmetric matrix, gyroscopic effects,
- \( C_R \) symmetric matrix, friction induced damping, (phenomenological)
- \( K_1 \) symmetric stiffness matrix,
- \( K_R \) nonsymmetric matrix modeling circulatory effects,
- \( K_G \) symmetric geometric stiffness matrix.
- \( \omega \) rotational speed of disk with reference velocity \( \omega_r \).
FE model of disk brake (simplified $M, K > 0$)

$$M\ddot{q} + (D + G)\dot{q} + (K + N)q = f.$$ 

Rewrite as perturbed pHDAE system $\dot{z} = (J - R_D)Qz - R_NQz$, where

$$J := \begin{bmatrix} G & K + \frac{1}{2}N^H \\ -(K + \frac{1}{2}N^H) & 0 \end{bmatrix}, \quad Q := \begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix}^{-1},$$

$$R := R_D + R_N = \begin{bmatrix} D & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & \frac{1}{2}N \\ \frac{1}{2}N^T & 0 \end{bmatrix}.$$ 

Instability and squeal arises only from indefinite perturbation term $R_NQz$. Change the damping to avoid instability?

Perturbation $N$ is restricted (to FE nodes on pad).
Use spectral functions for Galerkin projection to get a reduced order model.

- Project QEP:
  \[ P_\omega(\lambda) v(\omega) = (\lambda^2 M + \lambda C(\omega) + K(\omega)) v(\omega) = 0 \]
  into small subspace spanned by \( Q \) independent of \( \omega \).

- Projected QEP

\[ \tilde{P}_\omega(\lambda) = Q^T P_\omega(\lambda) Q = \lambda^2 Q^T M Q + \lambda Q^T C(\omega) Q + Q^T K(\omega) Q \]

- How to choose \( Q \)?
  - Sufficiently good approximation of evs with pos. real part;
  - Ideally \( Q \) should contain good approximations to the desired evecs for all parameter values;
  - Construct \( Q \) in a reasonable amount of computing time.
Construct a measurement matrix \( V \in \mathbb{R}^{n,km} \) containing 'unstable' evecs for a set of parameters \( \omega_i \),

\[
V = [V(\omega_1), V(\omega_2), V(\omega_3), \ldots, V(\omega_k)]
\]

Perform (partial) singular value decomposition (SVD) (cheap)

\[
V = U \Sigma Z^H
\]

by omitting singular values that are small.

Choose \( Q = [\tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_d] \) to project \( P_\omega(\mu) \).

Adapt sampling set.
Results with new Galerkin method

Industrial model 1 million dof, Python and MATLAB implementation.

Solution for every $\omega$

- Solution with 300 dimensional TRAD subspace $\sim 30$ sec
- Solution with 100 dimensional POD subspace $\sim 10$ sec
Reacting flows/thermodynamics


- **Flows and Thermodynamics:** A. M. Badlyan, B. Maschke, C. Beattie, and V. M., Open physical systems: from GENERIC to port-Hamiltonian systems, Proceedings of MTNS, 2018.

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2 Application: Gas transport networks
3 Energy based modeling
4 Gas transport pHDAE
5 Power networks
6 PHDAE formulation of generalized Kuramoto
7 Other physical domains
8 Conclusion
Goal oriented modeling, simulation, optimization.
Model hierarchies.
Energy based modeling for networks of multi-physics multi-scale problems.
DAE formulation of PH systems.
Many things To Do:

- Other physical domains.
- Big Data handling.
- Real time control, optimization.
- Incorporate stochastics in models.
- Better time-discretization methods.
- Model reduction for all components.
- Uncertainty quantification.
- ...
Thank you very much for your attention and my sponsors for their support

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