Reduced order energy based modeling in energy transport networks

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Mathematics for key technologies

Outline

Theses

- Key technologies in industry require **M**odeling, **S**imulation, and **O**ptimization (MSO) of complex dynamical systems.
- Most real world systems are multi-physics systems, with different accuracies and scales in components.
- Modeling today becomes exceedingly automatized, linking subsystems together.
- Large sets of real time data are available and must be used in modeling and model assimilation.
- Modeling, analysis, numerics, control and optimization techniques should go hand in hand.
- Most real world (industrial) models are too complicated for optimization and control. **Model reduction is a key issue.**
- We need to be able to quantify errors and uncertainties in the reduction process.

What is model reduction?

... replace a big complicated (computational) model with a (much) smaller and simpler (but still accurate) one.

- Everybody does this. (It is also called **Science**)
- One wants to have the most simple model for a specific goal: analysis, simulation, optimization, or control.
- Ideally, reduced model should have good fidelity compared to reality, for the given MSO goal.

The MSO paradigm

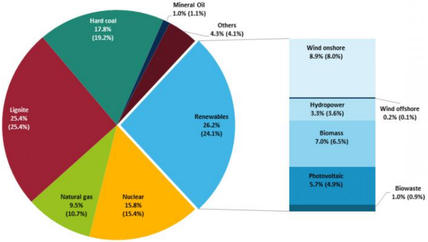
Modeling, simulation, optimization (MSO) of real system.

- Identify MSO goal (simulation, optimization, stabilization, ...)
- Build a model hierarchy. **Reduced models are just components in the hierarchy.**
- Analyze all sensitivities and errors (model, model reduction, discretization, solution of equations, roundoff in finite arithmetic.)
- **Adaptively choose model in the hierarchy, space-time discretization accuracy, and solver accuracy** depending on MSO goal and the required tolerance/uncertainty.

Outline

German energy transformation

The German government has decided to move out of nuclear energy and also to reduce CO_2 emissions drastically.



Share of energy sources in gross power production in 2014 (2013 values in parentheses)

Source: AG Energiebilanzen, 2015.

Scientific 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 simulation, optimization and control? Example in this talk: gas transport.

Outline

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

Planning, simulation, optimization, and operation of gas network.

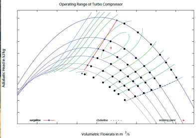
- HU Berlin
- TU Berlin
- Univ. Duisburg-Essen
- FA University Erlangen-Nürnberg
- TU Darmstadt
- Real industrial data (anonymized) from OGE.

Our project: Controlled coupling of hybrid network systems

Components of gas flow model

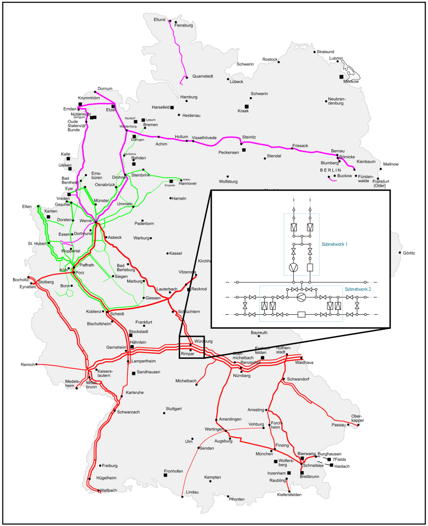
System of partial differential equations with algebraic constraints

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



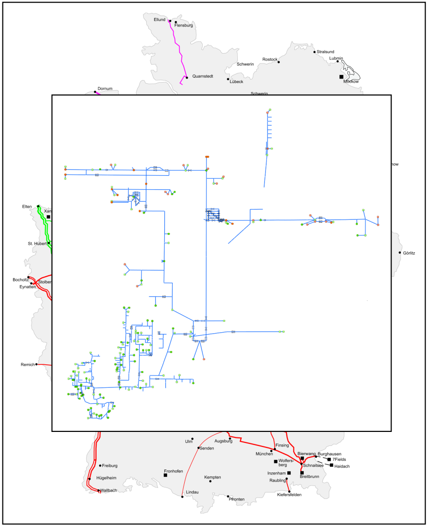
- Erratic demand and nomination of transport capacity.
- Can we use gas network as energy storage for hydrogen or methane produced from unused renewable energy. **Power to gas**.

- Gas networks are very large!



Network size

- Gas networks are very large!



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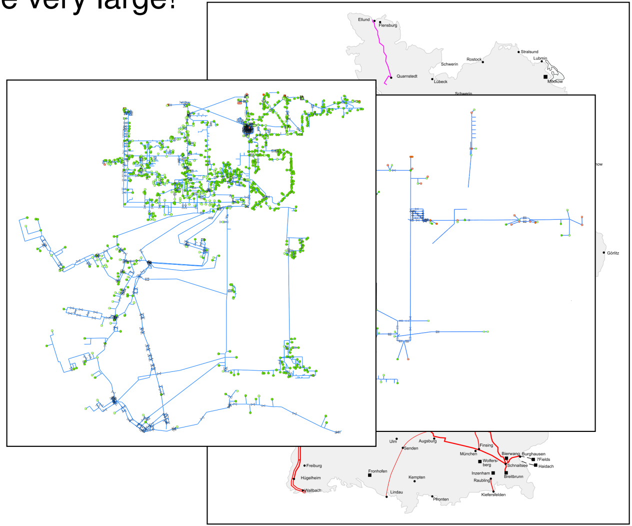

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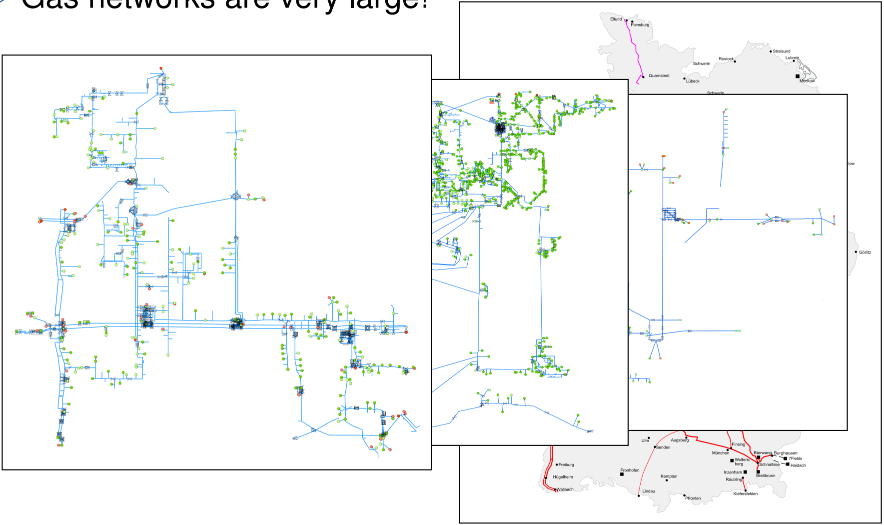


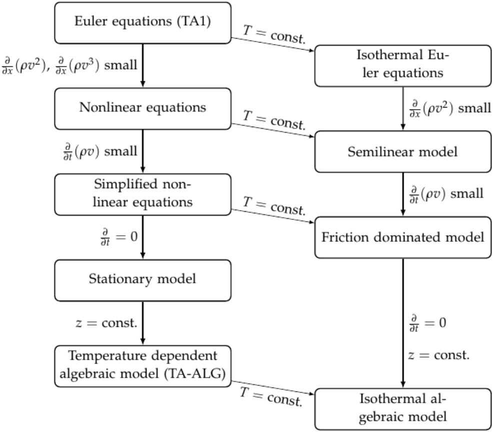
Flow model: 1D Euler equations

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

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

Variables/parameters:

- density ρ, k_w heat transfer coefficient,
- temperature T, wall temperature T_w,
- velocity v, g gravitational force,
- pressure p, λ friction coefficient,
- h' slope of pipe, D diameter of pipe,
- e internal energy, R gas constant of real gas.



Model hierarchy for gas flow (by no means complete).

P. Domschke, B. Hiller, J. Lang, C. Tischendorf, Technical Report SFBTRR 154, (2017)

Constant temperature $\rightarrow$ the isothermal Euler equations.

Model $M1$:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) = 0,$$
$$\frac{\partial}{\partial t}(\rho v) + \frac{\partial}{\partial x}\left(p + \rho v^2\right) = -\frac{\lambda}{2D}\rho v\,|v| - g\rho h',$$

together with the state equation for real gases

$$p = \rho(1 + \alpha p)RT.$$

If v is small, neglect the term $\frac{\partial}{\partial x}\left(\rho v^2\right) \rightarrow$ semilinear model
Model $M2$:

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v) &= 0, \\
\frac{\partial}{\partial t}(\rho v) + \frac{\partial p}{\partial x} &= -\frac{\lambda}{2D}\rho v\,|v| - g\rho h',
\end{aligned}$$

Space-time-Discretization

Discretization using an implicit box scheme.
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

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

- At every step, a unique solution exists.
- Convergence of order 2 in space and order 1 in time.
- Space-Time-Adaptivity via step-size control and a posteriori error analysis.

Kolb, Lang, and Bales. An implicit box scheme for subsonic compressible flow with dissipative source term. Numer. Algorithms, 53(2-3):293Ű307, 2010. DOI: 10.1007/s11075-009-9287-y.2010

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 $M3$:

$$\begin{aligned} \rho v &= \text{const.}, \\ p(x) &= \sqrt{p_{\text{in}}^2 - \frac{\lambda c^2 x}{D} \rho v \, |\rho v|}. \end{aligned}$$

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

Simplification IV: Reduced order models (later).

see also: Christian Himpe, Parametric Model Reduction for Gas Flow Networks, MOREPAS 2018, Poster

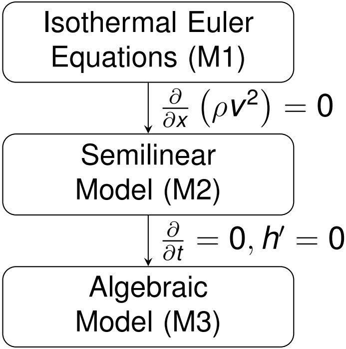


Figure: Model Hierarchy

Which model for which simulation/optimization goal?
Can we use the hierarchy to control the errors?

Sensitivities/error estimates

Determine sensitivities in parameters, error estimates, distributions of uncertainties, when model is simplified, discretized, reduced, or subjected to data uncertainty.

- The sensitivity/error analysis has to be done with the simulation/optimization goal in mind.
- We need to carry out this analysis for the whole hierarchy.
- Use analytic formulas or adjoint equations.
- Determine a posteriori error estimates η_x, η_t, η_m in space, time, and model (or data uncertainty) to control computational cost.

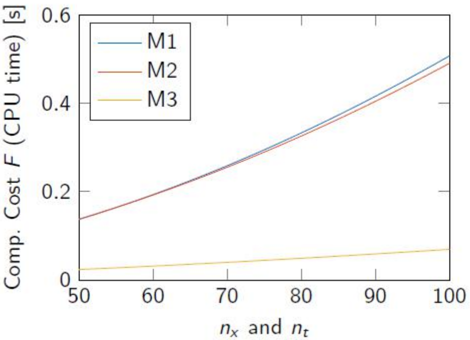
- Ern A., Vohralík, M. Polynomial-degree-robust a posteriori estimates in a unified setting for conforming, nonconforming, discontinuous Galerkin, and mixed discretizations. SIAM J. Numer. Anal. 53, 1058Ű1081, 2015.
- J.J. Stolwijk and V. M. *Error analysis and model adaptivity for flows in gas networks*. Anal. Stiintifice ale Univ. Ovidius Constanta. Seria Matematica, 2018.

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, α_m, and β_m from simulations.

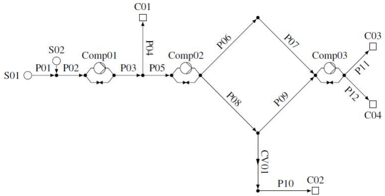


Minimization of CPU time

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

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

- Included in the flow code ANACONDA (TU Darmstadt).
- Test case: Gas network of $|\mathcal{J}_p| = 12$ pipelines.



- Achieved computing time reductions 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.

Minimization of compressor cost

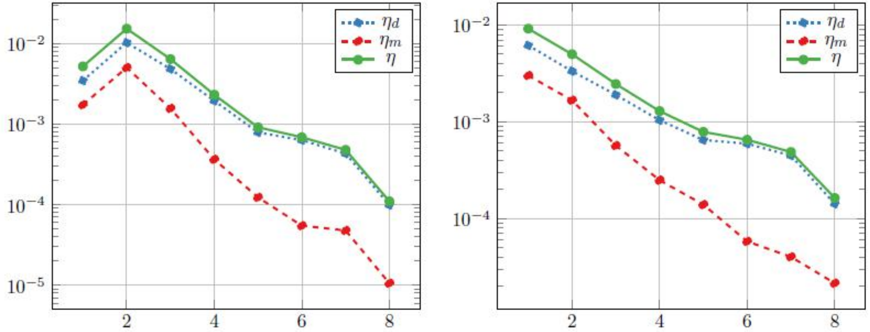
Minimize compressor costs subject to
variable bounds, mass balance, compressor models.
Classical switched nonlinear optimal control problem

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 ϵ-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.

▷ V. M., M. Schmidt, and J. Stolwijk, *Model and Discretization Error Adaptivity within Stationary Gas Transport Optimization*, http://arxiv.org/abs/1712.02745, 2017.

Further 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?
- Can we couple in a network based framework?
- What is the right framework for modeling?

Outline

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.
- Is there such a Jack of all trades?
- A system theoretic way to deal with such energy based modeling is that of **port-Hamiltonian systems**.

- P. C. Breedveld. *Modeling and Simulation of Dynamic Systems using Bond Graphs*, pages 128–173. EOLSS Publishers Co. Ltd./UNESCO, Oxford, UK, 2008.
- B. Jacob and H. Zwart. *Linear port-Hamiltonian systems on infinite-dimensional spaces*. Operator Theory: Advances and Applications, 223. Birkhäuser/Springer Basel CH, 2012.
- A. J. van der Schaft, D. Jeltsema, Port-Hamiltonian systems: network modeling and control of nonlinear physical systems. In *Advanced Dynamics and Control of Structures and Machines*, CISM Courses and Lectures, Vol. 444. Springer Verlag, New York, N.Y., 2004.
- A. J. van der Schaft, Port-Hamiltonian differential-algebraic systems. In *Surveys in Differential-Algebraic Equations I*, 173-226. Springer-Verlag, 2013. Port-Hamiltonian systems theory: An introductory overview.

Classical port-Hamiltonian (pH) ODE/PDE systems

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

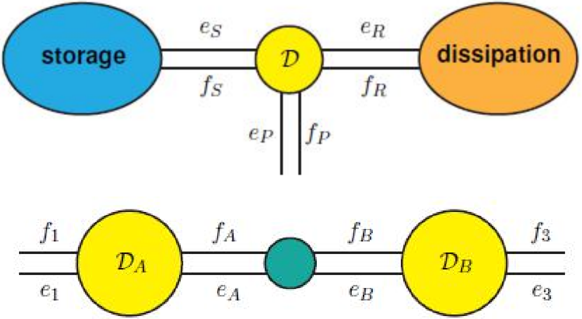
- $\mathcal{H}(x)$ is the *Hamiltonian*: it describes the distribution of internal energy among the energy storage elements;
- $J = -J^T$ describes the *energy flux* among energy storage elements within the system;
- $R = R^T \geq 0$ describes *energy dissipation/loss* in the system;
- $B \pm P$: *ports* 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.

Properties

- 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.



Can we add algebraic constraints, like e.g. Kirchhoff's laws

Definition (C. Beattie, V. M., H. Xu, H. Zwart 2017)

A linear variable coefficient (P)DAE of the form

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

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

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

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.

- C. Beattie, V. M., H. Xu, and H. Zwart, *Linear port-Hamiltonian descriptor systems*. https://arxiv.org/pdf/1705.09081.pdf
- C. Beattie, V. Mehrmann, and P. Van Dooren, *Robust port-Hamiltonian representations of passive systems*. http://arxiv.org/abs/1801.05018
- N. Gillis, V. Mehrmann, and P. Sharma, *Computing nearest stable matrix pairs*. Numerical Linear Algebra with Applications, 2018. https://arxiv.org/pdf/1704.03184.pdf
- C. Mehl, V. M., and M. Wojtylak, *Linear algebra properties of dissipative Hamiltonian descriptor systems*. http://arxiv.org/abs/1801.02214
- L. Scholz, Condensed Forms for linear Port-Hamiltonian Descriptor Systems. Preprint 09-2017, Institut f. Mathematik, TU Berlin, 2017.

Outline

Model reduction for pH systems

Every Galerkin projection MOR method preserves the structure of pH systems Beattie/ Gugercin 2011. Replace

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

by reduced system

$$\dot{x}_r = (J_r - R_r)\nabla_{x_r} H_r(x_r) + B_r u, \; y_r = B^T \nabla_{x_r} H_r(x_r)$$

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

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.

Outline

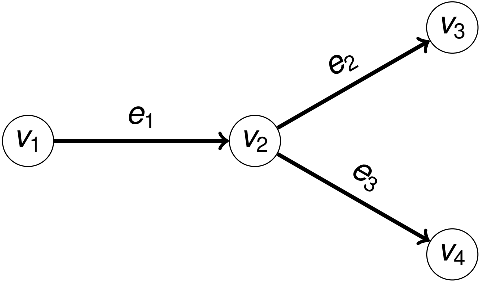


Figure: Graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertices $\mathcal{V} = \{v_1, v_2, v_3, v_4\}$ and edges $\mathcal{E} = \{e_1, e_2, e_3\}$ defined by $e_1 = (v_1, v_2)$, $e_2 = (v_2, v_3)$, and $e_3 = (v_2, v_4)$.

Gas transport pH-PDAE

- Model on every edge $e \in \mathcal{E}$ the conservation of mass and the balance of momentum, $z = (p, q)$.

$$\begin{aligned} a^e \partial_t p^e + \partial_z q^e &= 0, \qquad e \in \mathcal{E}, \\ b^e \partial_t q^e + \partial_z p^e + d^e q^e &= 0, \qquad e \in \mathcal{E}, \end{aligned}$$

  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

$$\begin{aligned} \sum_{e \in \mathcal{E}(v)} n^e(v) q^e(v) &= 0 \\ p^e(v) &= p^f(v), \qquad e, f \in \mathcal{E}(v), \end{aligned}$$

  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).

- Inputs: $p^e(v) = u_v, \quad v \in \mathcal{V}_\partial,\ e \in \mathcal{E}(v)$
- Output: the mass flux in and out of the network via the exterior vertices

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

- Initial conditions: $p(0) = p_0$, $q(0) = q_0$ 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 Galerkin projection.

Discontinuous Galerkin discretization

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

$$\begin{aligned} E\dot{x} &= (J-R)x + Bu, \\ y &= B^T x, \\ x(0) &= x^0, \end{aligned}$$

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

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

The discretized Hamiltonian is given by

$$\mathcal{H}(x) = \frac{1}{2} x^T E x = \frac{1}{2}(x_1^T M_1 x_1 + x_2^T M_2 x_2).$$

Consequences

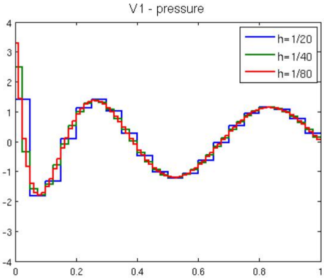
- Continuous and discretized models close to the real physics.
- Conservation laws are included.
- Model can be used for structure preserving model reduction via Galerkin projection.
- Whole model hierarchy can be built in pHDAE form.
- A posteriori error estimates for DG discretization.
- Error estimates for model reduction the same as for discretization error.
- Reduced model can be added to model hierarchy.

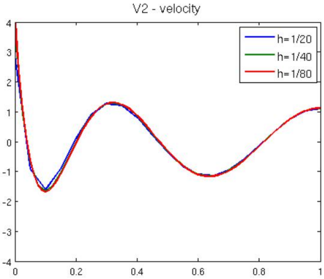
Galerkin MOR for gas flow

- Model reduction (projection spaces) via 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.

- 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, to appear 2018. http://arxiv.org/abs/1704.03206

Mesh Independence





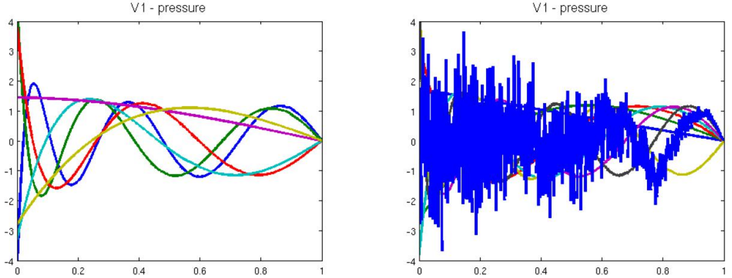
Basis functions for the pressure and velocity computed with space-discretized model on different meshes with mesh size $h = \frac{1}{20}, \frac{1}{40}$, and $\frac{1}{80}$.

Splitting and CS decomposition

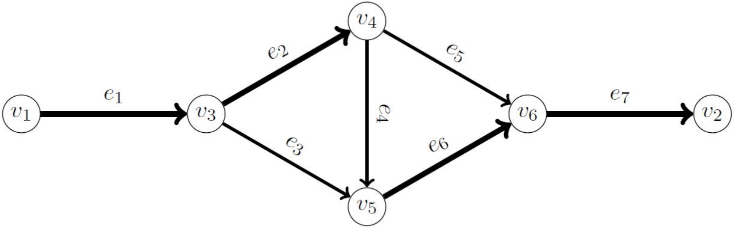
- Splitting of the projection matrix $W = [W_1; W_2; W_3]$ corresponding to the solution components $x = [x_1; x_2; x_3]$.
- Even if columns of W are orthogonal, this is no longer true for the columns of W_i.
- Re-orthogonalization is required.
- Splitting very sensitive to numerical errors.
- Use cosine-sine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

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

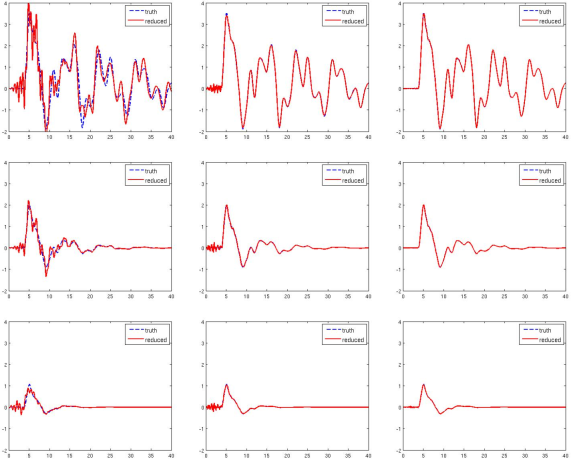
with U_1, U_2, and X orthogonal, and C, S diagonal with entries $C_{ii}^2 + S_{ii}^2 = 1$.



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

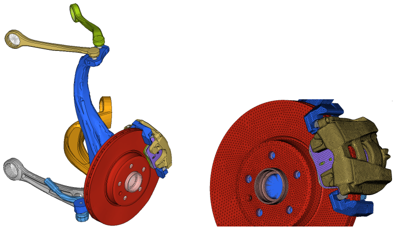

v_1
e_1
v_3
e_2
e_3
v_4
e_4
v_5
e_5
e_6
v_6
e_7
v_2

Paramamatric MOR



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).

Outline



- 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?

Model based approach

Interdisciplinary project with car manufacturers + SMEs
Supported by German Minist. of Economics via AIF foundation.
N. Hoffmann, TU Hamburg-Harburg, Mechanics, V.M. TU Berlin Mathematics, U. von Wagner, TU Berlin, Mechanics.

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. 

- N. Gräbner, V. M., S. Quraishi, C. Schröder, U. von Wagner, Numerical methods for parametric model reduction in the simulation of disc brake squeal *ZAMM*, Vol. 96, 1388Ű-1405, 2016.

FE model details

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

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

- 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.
- ω rotational speed of disk with reference velocity ω_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 $\dot{z} = (J - R_D)Qz - R_N Qz$, where

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

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

Instability and squeal arises only from indefinite perturbation term $R_N Qz$. 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 ω.
- 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 ω_i,

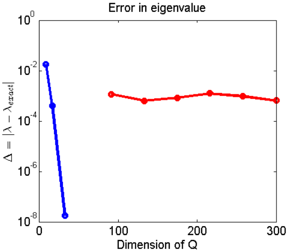
$$V = [V(\omega_1), V(\omega_2), V(\omega_3), \dots V(\omega_k)]$$

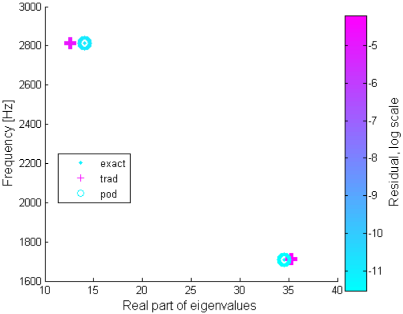
- Perform (partial) singular value decomposition (SVD) (cheap) $V = U\Sigma Z^H$

$$\tilde{V} \approx [\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_d] \begin{bmatrix} \sigma_1 & & & & \\ & \sigma_2 & & & \\ & & \sigma_3 & & \\ & & & \ddots & \\ & & & & \sigma_d \end{bmatrix} [\tilde{z}_1, \tilde{z}_2, \dots, \tilde{z}_d]^H$$

  by omitting singular values that are small.
- Choose $Q = [\tilde{u}_1, \tilde{u}_2, \dots, \tilde{u}_d]$ to project $P_\omega(\mu)$.
- Adapt sampling set.

Industrial model 1 million dof, Python and MATLAB implementation.





- ▷ Solution for every ω
  - Solution with 300 dimensional TRAD subspace $\sim$ 30 sec
  - Solution with 100 dimensional POD subspace $\sim$ 10 sec

DFG Priority program, SFB 910

- Collaborative Research Center SFB 910, Control of self-organizing nonlinear systems: Theoretical methods and concepts of application with Theoretical Physics.
  Project: Analysis and computation of stability exponents for delay differential-algebraic equations.
- 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

V. Mehrmann, R. Morandin, S. Olmi, and E. Schöll, *Qualitative Stability and Synchronicity Analysis of Power Network Models in Port-Hamiltonian form*, 2017. https://arXiv:1712.03160

Reactive flows/thermodynamics

- Navier-Stokes with reaction: R. Altmann und P. Schulze A port-Hamiltonian formulation of the Navier-Stokes equations for reactive flows *Systems Control Lett.*, Vol. 100, 2017, pp. 51-55.
- 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.
- Shifted POD for transport dominated problems: J. Reiss, P. Schulze, J. Sesterhenn, and V. M., The shifted proper orthogonal decomposition: A mode decomposition for multiple transport phenomena. *SIAM Journal Scientific Computing*, 2018. https://arXiv:1512.01985v2

Summary

- Goal oriented modeling, simulation, optimization.
- Energy based modeling for networks of multi-physics multi-scale problems.
- Model hierarchies of port-Hamiltonian DAE models.
- Structured model reduction.

Outlook

Many things To Do:

- Real time control, optimization.
- Further physical domains.
- Incorporate stochastics in models.
- Better time-discretization methods.
- Uncertainty quantification.
- ...

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