

Model reduction for port-Hamiltonian differential-algebraic systems

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Research Center MATHEON Mathematics for key technologies



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- Key technologies require Modeling, Simulation, and Optimization (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 in a network.
- 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. Digital Twins.
- 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, and in the MSO.

Examples from gas and heating networks.



Gas transport

District heating network A modeling wishlist Model reduction, surrogate models MOR for linear pHDAEs MOR approaches fpr pHDAEs Moment matching Tangential interpolation for pHDAEs Conclusion The new turbine



SFB TRR 154

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

TRR 154

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

Goal: Gas flow simulation and optimization using a network based model hierarchy (digital twin).

Deal with erratic demand and nomination of transport capacity, use gas network as storage for hydrogen, methane produced from unused renewable energy, etc.



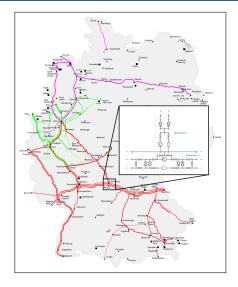
System of partial differential equations with algebraic constraints

- ID-3D compressible 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).
- Surrogate and reduced order models.

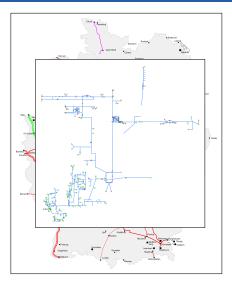


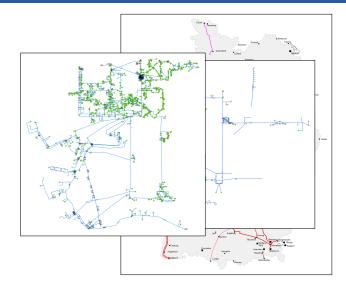




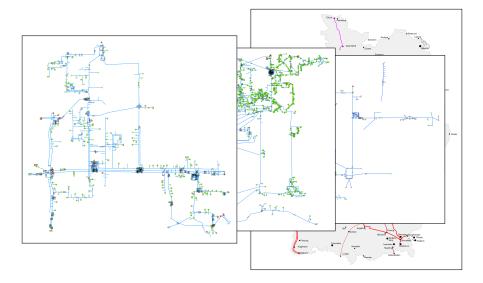














Pipe flow, classical formulation

Compressible Euler equations.

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

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

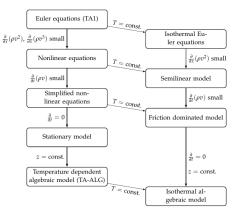
$$0 = \frac{\partial}{\partial t} \left(\rho(\frac{1}{2}v^2 + e)\right) + \frac{\partial}{\partial x} \left(\rho v(\frac{1}{2}v^2 + e) + \rho v\right) + \frac{4k_w}{D} (T - T_w),$$

Energy balance

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

- ▷ density ρ , k_w heat transfer coefficient,
- ▷ temperature T, wall temperature T_w ,
- ▷ velocity v, g gravitational force,
- \triangleright pressure p, λ friction coefficient,
- \triangleright *h* height of pipe, *D* diameter of pipe,
- ▷ e internal energy, R gas constant of real gas.





Every element/node/edge in the network is modelled via a model hierarchy, including surrogate models. This allows adaptivity in space-time-model via error estimates.

Domschke, Hiller, Lang, Tischendorf. Modellierung von Gasnetzwerken: Eine Übersicht, Preprint SFBTRR 154, 2017.





Gas transport

District heating network

A modeling wishlist Model reduction, surrogate models MOR for linear pHDAEs MOR approaches fpr pHDAEs Moment matching Tangential interpolation for pHDAEs Conclusion The new turbine



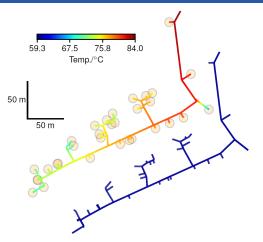
German Ministry of Education and Research (BMBF) Energy efficiency via intelligent district heating networks (EiFer)

- TU Berlin
- Univ. Trier
- Fraunhofer ITWM Kaiserslautern
- Stadtwerke Ludwigshafen.

Goal: Build a model hierarchy for heating network of different levels including surrogate models. Coupling of heat, electric, waste incineration, and gas.

Heating network





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



Hot water flow, classical formulation

Simplified incompressible Euler equations.

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

together with incompressibility condition.

Terms for pressure energy and dissipation work ignored.

- ▷ density ρ , k_w heat transfer coefficient,
- \triangleright temperature *T*, wall temperature *T_w*,
- \triangleright velocity v, g gravitational force, pressure p,
- $\triangleright \lambda$ friction coefficient, *e* internal energy,
- \triangleright *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, http://arxiv.org/abs/1908.11226, submitted for publication, 2019.
- R. Krug, V. Mehrmann, and M. Schmidt, Nonlinear Optimization of District Heating Networks, Submitted for publication https://arxiv.org/abs/1910.06453 2019.





A modeling wishlist



- ▷ Want a modularized network based approach.
- 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.
- 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, German: Eierlegende-Woll-Milch-Sau?



- Use energy 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 network (Dirac structure).
- Allow every network node to be a model hierarchy of fine or coarse, 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.
- 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., 2014.



Port-Hamiltonian systems

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

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

- \triangleright x is the state, u input, y output.
- $\triangleright \mathcal{H}(x)$ is the *Hamiltonian*: it describes the distribution of internal energy among the energy storage elements;
- \triangleright $J = -J^T$ describes the *energy flux* among energy storage elements within the system;
- \triangleright $R = R^T \ge 0$ describes *energy dissipation/loss* in the system;
- \triangleright *B* ± *P*: *ports* where energy enters and exits the system;
- \triangleright 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

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

- PH systems are closed under *power-conserving interconnection*. Modularized network based modeling.
- 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.
 Can we add algebraic constraints, like Kirchhoff's laws, position constraints, conservation laws?
- C. Beattie, V. M., H. Xu, and H. Zwart, Linear port-Hamiltonian descriptor systems. Math. Control Signals and Systems, 30:17, 2018.
- A. J. van der Schaft, Port-Hamiltonian differential-algebraic systems. In Surveys in Differential-Algebraic Equations I, 173-226. Springer-Verlag, 2013.
- A. van der Schaft and B. Maschke, Generalized Port-Hamiltonian DAE Systems, Systems Control Letters 121, 31-37, 2018, 2018



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

$$E(t,x)\dot{x} + r(t,x) = (J(t,x) - R(r,x))z(t,x) + (B(t,x) - P(t,x))u,$$

$$y = (B(t,x) + P(t,x))^{T}z(t,x) + (S(t,x) - N(t,x))u,$$

with *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 $z, r \in C(\mathcal{S}, \mathbb{R}^{\ell})$. The system is called *port-Hamiltonian DAE* if

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

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



Dissipation inequality

$$\mathcal{H}(t_2, \boldsymbol{x}(t_2)) - \mathcal{H}(t_1, \boldsymbol{x}(t_1)) \leq \int_{t_1}^{t_2} \boldsymbol{y}(\tau)^T \boldsymbol{u}(\tau) \mathrm{d}\tau$$

- Definition extends to weak solutions and infinite dimension.
- Invariance under state-time diffeomorphisms.
- ▷ Stability, Hamiltonian is a Lyapunov function.
- Asymptotic stability, if no energy enters via input/output and dissipation inequality is strict.
- Structure invariant when making system autonomous.
- ▷ Structure invariant under power conserving interconnection.
- Structure invariant under constraint preserving Galerkin projection (FE Method, model reduction).
- Underlying Lagrangian structure, symplectic flow.





Abstract port-Hamiltonian PDE formulation

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

$$y(z) = \mathcal{B}^*(z) \frac{\delta \mathcal{E}(z)}{\delta z} \quad \text{in } \mathcal{D}_u^*,$$

$$\triangleright \ \mathcal{Z} = \{ z \in \mathcal{D}_z \mid \rho \geq \delta, \ \delta > 0 \text{ a.e.} \} \subset \mathcal{D}_z = W^{1,3}((0,\ell);\mathbb{R}^3).$$

- ▷ 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).
- $\triangleright \mathcal{E}(z)$ is the relative energy.
- Moses Badlyan, Maschke, Beattie, and V. M., Open physical systems: from GENERIC to port-Hamiltonian systems, Proceedings of MTNS, 2018.
- Moses Badlyan and Zimmer. Operator-GENERIC formulation of thermodynamics of irreversible processes. Preprint TU Berlin 2018.
- S.-A. Hauschild, N. Marheineke, V. Mehrmann, J. Mohring, A. Moses Badlyan, M. Rein, and M. Schmidt, Port-Hamiltonian modeling of disctrict heating networks, http://arxiv.org/abs/1908.11226, submitted for publication, 2019, a start of the start of th



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Port-Hamiltonian formulation of compressible Euler including pressure energy and dissipation work, as well as entropy balance. A. Moses Badlyan 2019

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

Add node conditions and boundary conditions. Kirchhoff's laws.



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

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

Add node conditions (Kirchhoff laws), mixing conditions etc.



PH PDE weak form

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

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

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

$$\mathcal{E}(z) = \int_{0}^{\ell} \left(\frac{|M|^{2}}{2\rho} + H(\rho, e) + \rho gh \right) dx$$

$$\frac{\delta \mathcal{E}(z)}{\delta z} = \left(\frac{\delta \mathcal{E}(z)}{\delta \rho}, \frac{\delta \mathcal{E}(z)}{\delta M}, \frac{\delta \mathcal{E}(z)}{\delta e} \right)^{T}$$

$$= \left(\left(-\frac{|M|^{2}}{2\rho^{2}} + \frac{\partial H}{\partial \rho} + gh \right), \frac{M}{\rho}, \frac{\partial H}{\partial e} \right)^{T}.$$



The ${\mathcal J}$ operator

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

$$\mathcal{J}(z) = \left[egin{array}{ccc} 0 & \mathcal{J}_{
ho, M}(z) & 0 \ \mathcal{J}_{M,
ho}(z) & \mathcal{J}_{M, M}(z) & \mathcal{J}_{M, e}(z) \ 0 & \mathcal{J}_{e, M}(z) & 0 \end{array}
ight],$$

is associated with the bilinear form

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

$$\begin{aligned} \langle \varphi_{\rho}, \mathcal{J}_{\rho,M}(z)\psi_{M} \rangle &= \int_{0}^{\ell} \rho(\psi_{M}\partial_{x})\varphi_{\rho} \, \mathrm{d}x, \\ \langle \varphi_{M}, \mathcal{J}_{M,M}(z)\psi_{M} \rangle &= \int_{0}^{\ell} M((\psi_{M}\partial_{x})\varphi_{M} - (\varphi_{M}\partial_{x})\psi_{M}) \, \mathrm{d}x, \\ \langle \varphi_{e}, \mathcal{J}_{e,M}(z)\psi_{M} \rangle &= \int_{0}^{\ell} e(\psi_{M}\partial_{x})\varphi_{e} + (\psi_{M}\partial_{x})(\varphi_{e}\rho) \, \mathrm{d}x \end{aligned}$$



The $\mathcal R$ operator

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 $\mathcal{R}^{k_w}(z)$.

$$\mathcal{R}(z) = \mathcal{R}^{\lambda}(z) + \mathcal{R}^{k_{w}}(z) = \left[egin{array}{ccc} 0 & 0 & 0 \ 0 & \mathcal{R}^{\lambda}_{M,M}(z) & \mathcal{R}^{\lambda}_{M,e}(z) \ 0 & \mathcal{R}^{\lambda}_{e,M}(z) & \mathcal{R}^{\lambda}_{e,e}(z) + \mathcal{R}^{k_{w}}_{e,e}(z) \end{array}
ight],$$

associated with the bilinear form

$$\begin{aligned} \langle \varphi, \mathcal{R}(\boldsymbol{z})\psi \rangle &= \langle \varphi_{\boldsymbol{M}}, \mathcal{R}^{\lambda}_{\boldsymbol{M},\boldsymbol{M}}(\boldsymbol{z})\psi_{\boldsymbol{M}} \rangle + \langle \varphi_{\boldsymbol{M}}, \mathcal{R}^{\lambda}_{\boldsymbol{M},\boldsymbol{e}}(\boldsymbol{z})\psi_{\boldsymbol{e}} \rangle \\ &+ \langle \varphi_{\boldsymbol{e}}, \mathcal{R}^{\lambda}_{\boldsymbol{e},\boldsymbol{M}}(\boldsymbol{z})\psi_{\boldsymbol{M}} \rangle + \langle \varphi_{\boldsymbol{e}}, (\mathcal{R}^{\lambda}_{\boldsymbol{e},\boldsymbol{e}}(\boldsymbol{z}) + \mathcal{R}^{k_{w}}_{\boldsymbol{e},\boldsymbol{e}}(\boldsymbol{z}))\psi_{\boldsymbol{e}} \rangle \end{aligned}$$

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

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

$$\langle arphi, \mathcal{B}(\boldsymbol{z}) \boldsymbol{u}(\boldsymbol{z})
angle = -\left[\left(arphi_{
ho}
ho + arphi_{M} \boldsymbol{M} + arphi_{oldsymbol{e}}(oldsymbol{e} + oldsymbol{p})
ight) \boldsymbol{u}(\boldsymbol{z})
ight] ig|_{oldsymbol{0}}^{\ell},$$

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

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





Model reduction, surrogate models



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- Replace fine phDAE model in network node by reduced or surrogate pHDAE model.
- ▷ Reduced order model or model from input/output data.
- ▷ Do not modify network coupling structure.
- Balance equations (Kirchhoff's laws) must still hold after reduction.
- Make sure that the physics is still reflected correctly after reduction, compressibility/incompressibility.
- ▷ Preserve other constraints (casimirs).
- ▷ Allow for space-time-model adaptation via tolerance control.



Model reduction state space

Replace semidiscretized (in space) system

$$F(t, x_h, \dot{x}_h, u_h) = 0, \quad x_h(t_0) = x_h^0$$

$$y_h(t) = c(x_h, u_h)$$

with $x_h \in \mathbb{R}^n$, $u_h \in \mathbb{R}^m$, and $y_h \in \mathbb{R}^p$, by a reduced model

$$F_r(t, x_r, \dot{x}_r, u_h) = 0, \quad x_r(t_0) = x_r^0$$

 $y_r(t) = c_r(x_r, u_h)$

with $x_r(t) \in \mathbb{R}^{n_r}$, $n_r \ll n$.

Goals

- ▷ Approximation error $||y y_r||$ small, global error bounds;
- Preservation of physics: stability, passivity, conservation laws;
- Stable and efficient method for model reduction.

Model reduction for ordinary pH systems

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

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

with $\nabla_x H(x) = Qx$ by reduced system

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

with $x \approx V_r x_r$, $Q_r x_r = W_r^T Q V_r x_r \approx W_r Q x$, $J_r = W_r^T J W_r$, $R_r = W_r^T R W_r$, $W_r^T V_r = I_r$, $B_r = W_r^T B$. If V_r and W_r are appropriate orthornormal bases, then the resulting system is again pH and all properties are preserved. Extension to pH/dH DAEs nontrivial

- Beattie and Gugercin. Structure-preserving model reduction for nonlinear port-Hamiltonian systems. In 50th IEEE Conference on Decision and Control and European Control Conference (CDC-ECC), 2011.
- Chaturantabut, Beattie and Gugercin, Structure-Preserving Model Reduction for Nonlinear Port-Hamiltonian Systems, SIAM J. Scientific Computing, 2016,
- Gugercin, Polyuga, Beattie and van der Schaft, Structure-Preserving Tangential Interpolation for Model Reduction of Port-Hamiltonian Systems, Automatica ,2012.





MOR for linear pHDAEs

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Linearization arround stationary solution.

Definition (C. Beattie, V. M., H. Xu, H. Zwart 2018)

A linear constant coefficient DAE of the form

$$E\dot{x} = [(J-R)Q]x + (B-P)u,$$

 $y = (B+P)^TQx + (S+N)u,$

with $E, Q \in \mathbb{R}^{\ell,n}$, $R = R^T, J \in \mathbb{R}^{n,n}$, $B, P \in \mathbb{R}^{n,m}$, $S + N \in \mathbb{R}^{m,m}$ is called *port-Hamiltonian DAE (pHDAE)* if

i)
$$Q^T E = E^T Q, Q^T J Q = -Q^T J^T Q$$

ii) $W := \begin{bmatrix} Q^T R Q & Q^T P \\ P^T Q & S \end{bmatrix} \ge 0.$

Quadratic Hamiltonian $\mathcal{H} = \frac{1}{2} x^T E^T Q x$

Model reduction for linear pHDAE systems

Replace

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

with reduced system

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

with
$$x \approx V_r x_r$$
, $E_r = W_r^T E V_r$, $Q_r = W_r^T Q V_r$, $J_r = W_r^T J W_r$,
 $R_r = W_r^T R W_r$, $B_r + P_r = W_r^T (B + P)$.

If V_r and W_r are appropriate orthornormal bases, then reduced system is again a pHDAE but constraints may not be preserved.

If Q = I use $W_r = V_r$ to keep E_r symmetric positive definite MOR must properly reflect the constraints. But they are not always known explicitely.



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

For a (regular) linear pHDAE there exists an orthogonal basis transformation \hat{V} such that in the new variable $\hat{x} = \begin{bmatrix} \hat{x}_1^T & \hat{x}_2^T & \hat{x}_3^T & \hat{x}_4^T & \hat{x}_5^T \end{bmatrix}^T = \hat{V}^T x$, the system has the form $y = \begin{bmatrix} (B_1 + P_1)^T & (B_2 + P_2)^T & B_3^T & B_4^T & B_5^T \end{bmatrix} \begin{bmatrix} x_1 \\ \hat{x}_2 \\ \hat{x}_3 \\ \hat{x}_4 \end{bmatrix} + (S + N)u,$

where $E_{11} > 0$, $R_{22} > 0$, J_{33} invertible and $\begin{bmatrix} J_{41} & J_{42} \end{bmatrix}$, B_4 , B_5 have full row rank.

First row dynamics, rows, 2, 3 index one equations, rows 4 and 5 are controllable index 2 and singular parts. Unfortunately not really computable for large scale problems.



Mixed finite element space discretization of acoustic wave in pipe flow leads to large scale pHDAE:

$$\Xi \dot{x} = (J - R)x + Bu, x(0) = x^{0},$$

 $y = B^{T}x,$

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

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

The discretized Hamiltonian is given by

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

 H. Egger and T. Kugler. Damped wave systems on networks: Exponential stability and uniform approximations. Numerische Mathematik, 138:839–867, 2018.

Similar structure in heating and other network based models.



Constraints: Gas example

Normal form: SVD $\tilde{N}^{T} = U_{N}^{T} \begin{bmatrix} 0 \\ \Sigma \end{bmatrix} V_{N}$. Transforming with $U = V = \text{diag}(I, U_{N}^{T}, V_{N}^{T})$ we obtain

 $\begin{bmatrix} M_1 & 0 & 0 & 0 \\ 0 & M_{2,2} & M_{2,3} & 0 \\ 0 & M_{2,3}^T & M_{3,3} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{x}_{2,2} \\ \dot{x}_{2,3} \\ \dot{\tilde{x}}_3 \end{bmatrix} + \begin{bmatrix} 0 & G_{1,2} & G_{1,3} & 0 \\ -G_{1,2}^T & D_{2,2} & D_{2,3} & 0 \\ -G_{1,3}^T & D_{2,3}^T & D_{3,3} & -\Sigma \\ 0 & 0 & \Sigma & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_{2,2} \\ x_{2,3} \\ \tilde{x}_3 \end{bmatrix} = \begin{bmatrix} 0 \\ B_2 \\ B_3 \\ 0 \end{bmatrix}$

Noncontrollable index two constraints $x_{2,3} = 0$. $x_1, x_{2,2}$ are solutions of the classical pH system

 $\begin{bmatrix} M_1 & 0 \\ 0 & M_{2,2} \end{bmatrix} \frac{d}{dt} \begin{bmatrix} x_1 \\ x_{2,2} \end{bmatrix} + \begin{bmatrix} 0 & G_{1,2} \\ -G_{1,2}^T & D_{2,2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_{2,2} \end{bmatrix} = \begin{bmatrix} 0 \\ B_{2,2} \end{bmatrix} u,$ with initial conditions $x_1(0) = x_1^0, x_{2,2}(0) = x_{2,2}^0.$

$$x_{3} = V_{N}^{T} \Sigma^{-1} (M_{2,3}^{T} \frac{d}{dt} x_{2,2} - G_{1,3}^{T} x_{1} + D_{2,3}^{T} x_{2,2} - B_{3,2} u),$$





MOR approaches fpr pHDAEs

Model reduction approaches for pHDAEs

- Moment matching (frequency domain)
- Interpolation methods (frequency domain)
- Balanced truncation methods. (frequency domain)
- Effort and flow based methods (time domain)
- POD (time domain)
- Reduced basis (time domain)

- Beattie, 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, 2020.
- Egger, Kugler, Liljegren-Sailer, 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. http://arxiv.org/abs/1704.03206
- Hauschild, Marheineke and V. M., Model reduction techniques for linear constant coefficient port-Hamiltonian differential-algebraic systems, https://arxiv.org/abs/1901.10242, 2019.

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Moment matching

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Moment matching

Consider first a regular pHDAE system with transfer function

$$H(s) = B^{T}(sE + R - J)^{-1}B = R(s) + P(s)$$

with proper rational part R(s) and polynomial part P(s). Expansion of the transfer function of the system leads to

$$H(s) := B^{\top}(sE + R - J)^{-1}B = \sum_{l=0}^{\infty} m_l(s_0 - s)^l;$$

where s_0 is a given *shift parameter*.

The generalized moments $m_l = B^T d_l$ with vectors d_l can be derived by rational Krylov iteration (short recursion in energy inner product)

$$(s_0E+R-J)d_0=B,\,(s_0E+R-J)d_l=Ed_{l-1},\,r\geq 1.$$

Orthogonalize span{ d_0, \ldots, d_{r-1} } via Arnoldi-process to get V_r . Reduced model is a pHDAE and matches 2r - 1 moments but index and regularity may have changed. Difference $H(s) - H_r(s)$ may be unbounded.



Acoustic wave in pipe

$$E\dot{x} = (J-R)x + Bu, \ x(0) = x^{0},$$

$$y = B^{T}x$$

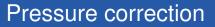
$$E = \begin{bmatrix} M_{1} & 0 & 0 \\ 0 & M_{2} & 0 \\ 0 & 0 & 0 \end{bmatrix}, J = \begin{bmatrix} 0 & -G & 0 \\ G^{T} & 0 & N^{T} \\ 0 & -N & 0 \end{bmatrix}, R = \begin{bmatrix} 0 & 0 & 0 \\ 0 & D & 0 \\ 0 & 0 & 0 \end{bmatrix}, B = \begin{bmatrix} 0 \\ \tilde{B}_{2} \\ 0 \end{bmatrix}$$

▷ Split projection matrix $V_r = [V_1; V_2; V_3]$ as $x = [x_1^T; x_2^T; x_3^T]$.

- ▷ Even if columns of V_r are orthogonal, this is no longer true for columns of V_i . Re-orthogonalization is required.
- ▷ Use cosine-sine (CS) decomposition for V_1 , V_2

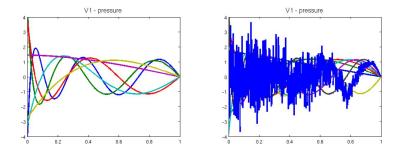
$$\begin{bmatrix} V_1 \\ V_2 \end{bmatrix} = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} C \\ S \end{bmatrix} X^{\top},$$

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



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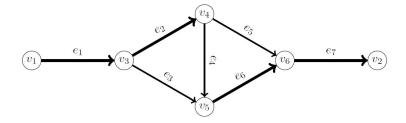


With and without pressure correction via CS decomposition of the Galerkin-projection space.

Small network

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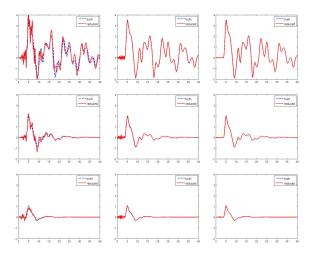




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Parametric MOR





Results for discretized (blue) and reduced model (red) with dim. 2, 5, 10 and damping parameter d = 0.1, 1, 5 (top to bottom).





Tangential interpolation for pHDAEs



Tangential interpolation

Compute reduced order pHDAE

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

such that $y_r(t)$ is good approximation to y(t) over a wide range of u(t). Let $H(s) = (B^T + P^T)(sE + R - J)^{-1}(B - P) + S + N$. 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 $H_r(s) = (B_r^T + P_r^T)(sE_r + R_r - J_r)^{-1}(B_r - P_r) + S_r + N_r$ such that $H(\sigma_i)k_i = H_r(\sigma_i)k_i$ and $\ell_i^T H(\mu_i) = \ell_i^T H_r(\mu_i)$, for $i = 1, 2, \ldots, r$.

Interpolation conditions enforced via Petrov-Galerkin projection with

$$V_r = \left[(\sigma_1 E + R - J)^{-1} (B - P) k_1, \cdots (\sigma_r E + R - J)^{-1} (B - P) k_r \right],$$

$$Z_r = \left[(\sigma_1 E + R - J)^{-T} (B + P) \ell_1, \cdots (\sigma_1 E + R - J)^{-T} (B + P) \ell_r \right],$$

$$E_r = Z_r^T E V_r, J_r = Z_r^T J V_r, R_r = Z_r^T R V_r, B_r = Z_r^T B, P_r = Z_r^T P, D_r = D,$$





- ▷ The reduced quantities may no longer have the structure. This can be resolved by using a Galerkin projection, i.e., with $Z_r = V_r$. But then only the right interpolation conditions hold.
- ▷ The polynomial parts of H(s) and $H_r(s)$ may not match, leading to unbounded errors.
- We need to identify the constraints via the normal 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. http://arxiv.org/abs/1910.05674, 2019.

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

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

where E_{11} and $J_{22} - R_{22}$ are nonsingular.



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

Consider a semi-explicit index one pHDAE structure, interpolation points { $\sigma_1, \sigma_2, ..., \sigma_r$ } and corresponding tangent directions { $k_1, k_2, ..., k_r$ }. Construct basis $V_r = \begin{bmatrix} V_{r,1}^T & V_{r,2}^T \end{bmatrix}^T$ as $\begin{bmatrix} (\sigma_1 E + R - J)^{-1}(B - P)k_1, ..., (\sigma_r E + R - J)^{-1}(B - P)k_r \end{bmatrix}$ 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 the transfer function $H_r(s)$ of the 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 polynomial 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.



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

Consider a semi-explicit index one pHDAE structure, with $B_2 - P_2 = 0$, interpolation points { $\sigma_1, \sigma_2, ..., \sigma_r$ } and corresponding tangent directions { $k_1, k_2, ..., k_r$ }. Construct basis $V_r = \begin{bmatrix} V_{r,1}^T & V_{r,2}^T \end{bmatrix}^T$ as $\begin{bmatrix} (\sigma_1 E + R - J)^{-1}(B - P)k_1, ..., (\sigma_r E + R - J)^{-1}(B - P)k_r \end{bmatrix}$

and set $K_r = \begin{bmatrix} k_1 & \cdots & k_r \end{bmatrix}$. Then the transfer function $H_r(s)$ of the reduced model

 $E_r \dot{x}_r(t) = (J_r - R_r) x_r(t) + (B_r - P_r) u(t), \ y_r(t) = (B_r + P_r) x_r(t) + Du(t)$ with $E_r = V_{r,1}^T E_{11} V_{r,1}, \ J_r - R_r = V_r^T (J - R) V_r, \ (B_r + P_r)^T = (B + P) V_r,$ is a phDAE, matches the polynomial part of H(s), and tangentially interpolates it.



Numerical example

Consider pHDAE formulation of incompressible Oseen equations,

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

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 discretization gives siso index-2 pHDAE with *n* = 7399, $n_v = 4900$, and $n_p = 2499$.

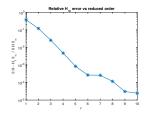


Figure: Model reduction error for Oseen example with IRKA as r varies



- Generate projection spaces via POD or shifted POD approaches in tranport dominant case.
- ▷ Combine with Empirical Interpolations Methods. (D)EIM.
- Incorporate as much as possible information from physical system.
- There is still much to do for the DAE case, 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.

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Conclusion

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- Energy based modeling for networks of multi-physics multi-scale problems.
- ▷ Model hierarchies of port-Hamiltonian DAE models.
- Structured model reduction.
- ▷ Tangential interpolation for pHDAEs.
- Moment matching for pHDAEs.
- Beattie, 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, 2020.
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- ▷ Real time control, optimization.
- Nonlinear pHDAEs.
- ▷ EIM, DEIM, POD, shifted POD.
- Application in Gas networks and heating networks.
- Application in new turbine development.
- Application in brake squeal.
- Application in digital twins.
- Data based methods.





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- ▷ DFG collaborative Research Centers 1029, 910, TRR154.
- BMBF/industry project Eifer

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





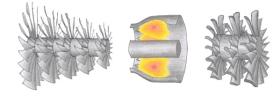
The new turbine

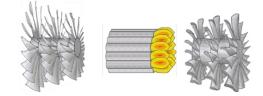
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A new turbine

Collaborative Research Center 1029 'TurbIn' at TU Berlin. Goal: Significant increase of efficiency of gas turbines via the interactive use of instationary effects of combustion and flow in gas turbines.







Can we use the same approach for the new turbine?

- ▷ Flow is reactive and transport dominated.
- Fast moving shocks and reaction fronts.
- Highly nonlinear.
- ▷ All well-known MOR approaches fail to get a small model.
- ▷ We have to capture the transport (shocks) with few modes.
- ▷ Different physics represented in different modes.

Proper Orthogonal Decomposition (POD)

$$F(t, x, \dot{x}, u) = 0, \quad x(t_0) = x^0$$

 $y(t) = c(x)$

Consider snapshots for some control u (and or different initial conditions), i.e. determine

$$\mathcal{X} = \left[\begin{array}{ccc} x(t_1) & x(t_2) & \dots & x(t_N) \end{array} \right]$$

- ▷ Singular value decomposition: $\mathcal{X} = U_N \Sigma_N V_N^T \approx U_{n_r} \Sigma_{n_r} V_{n_r}^T$ with $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_N)$
- ▷ Truncate small singular values σ_i , $i = n_r, ..., N$, $n_r << n$
- Reduced system

$$F_r(t, U_{n_r}x_r, U_{n_r}\dot{x}_r, u) = U_{n_r}^T F(t, U_{n_r}x_r, U_{n_r}\dot{x}_r, u) = 0.$$



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Reactive compressible 3D-Navier-Stokes equations in pipe.

$$\begin{array}{rcl} \partial_t \rho + \partial_x (\rho \mathbf{v}) &=& \mathbf{0}, \\ \partial_t (\rho \mathbf{v}) + \partial_x (\rho \mathbf{v}^2 + \mathbf{p} + \tau) &=& \mathbf{0}, \\ \partial_t (\rho \mathbf{e}) + \partial_x (\rho \mathbf{e} \mathbf{v} + (\mathbf{p} + \tau) \mathbf{v} + \mathbf{\Phi}) &=& \mathbf{0}, \\ \partial_t (\rho \mathbf{y}_i) + \partial_x (\rho \mathbf{y}_i \mathbf{v} + \mathbf{j}_i) &=& \mathbf{M}_i \omega_i \end{array}$$

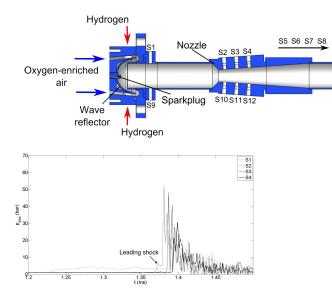
with density ρ , velocity v, pressure p, shear stress τ , specific total energy e, heat flux density Φ , mass fraction y_i , diffusion flux density j_i , molar masses M_i and molar rates of formation ω_i for species i = 1, ..., n. PH PDE formulation Altmann/Schulze 2017

R. Altmann and P. Schulze. A port-Hamiltonian formulation of the Navier-Stokes equations for reactive flows. Systems Control

Lett., Vol. 100, 2017, pp. 51-55.

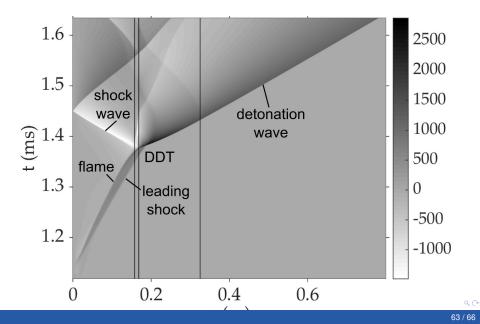


Measurements





Velocity profile





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New approach

- Identify amplitudes, phases and directions of waves from SVD spectrum.
- Separate them as contributions in the transport phenomenon and do POD on the remaining components.

Ansatz:

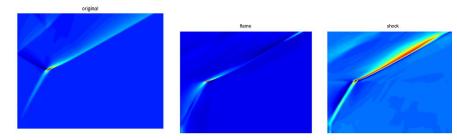
$$u(x,t) = \sum_{k=1}^{n} \sum_{i} \alpha_{i}^{k}(t) \phi_{i}^{k}(x - \Delta^{k}(t))$$

Perform Galerkin model assimilation with this ansatz.

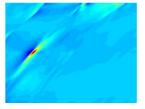
J. Reiss, P. Schulze, J. Sesterhenn, and V. Mehrmann, *The shifted proper orthogonal decomposition: A mode decomposition for multiple transport phenomena.* SIAM Journal Scientific Computing 2018. https://arXiv:1512.01985v2

Reduced velocity profile

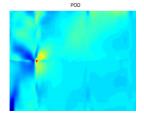




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