



MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG



COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Reduced-order Modelling and Simulation of Gas Transportation Networks

Peter Benner

Joint work with Sara Grundel and Christian Himpe

Trends in Mathematical Modelling, Simulation and
Optimisation: Theory and Applications

Virtual, 2–3 March 2021

Supported by:



Simulation of German energy transportation networks

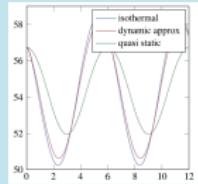
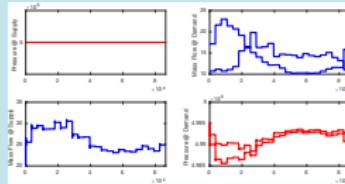
- Goals:

- hierarchical modeling of transport and distribution networks
- fast simulation on all levels
- real-time scenario analysis for network operators
- coupling of power and gas networks

- Results: New **discretization** and **model order reduction** methods for

- isothermal Euler equations on network graph
- with nonsmooth nonlinearity
- leading to coupled system of **differential-algebraic equations (DAEs)**
- with uncertain parameters

Implemented in **morgen** — Model Order Reduction of Gas and Energy Networks.



The German natural gas transportation network



Partners:

Fraunhofer SCAI
 Fraunhofer ITWM
 MPI Magdeburg
 TU Berlin
 HU Berlin
 TU Dortmund
 U Trier
 PSI AG

Funded by:





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Outline

We will do some gas network ...



We will do some gas network ...

- Modeling



We will do some gas network ...

- Modeling
- Model simplification



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- Model discretization



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- Model reduction



We will do some gas network ...

- Modeling
- Model simplification
- Model discretization
- Model reduction
- Simulation experiments



1. Introduction
2. Modeling
3. Model Order Reduction
4. Outlook, Summary, Details



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Introduction

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- Regulatory requirements, real-time (15min decision horizon) control.
- Employ modern developments in numerics and reduced-order modeling.
- It remains a challenge!



Some gas network properties:

- > 500,000km gas pipelines in Germany¹ (earth-moon < 400,000km).

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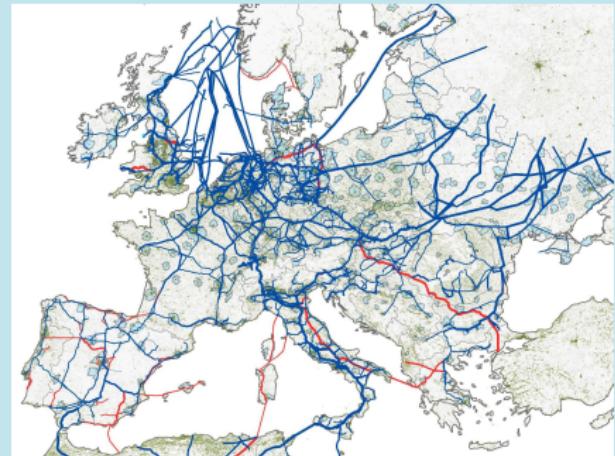
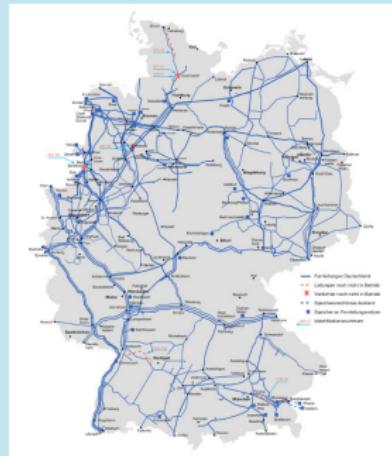
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Facts

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German gas transportation network . . . embedded into European network.





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- > 240,000,000m³ natural gas consumed per day.².

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- Planning horizon is 24h, operator decision horizon is 15min.

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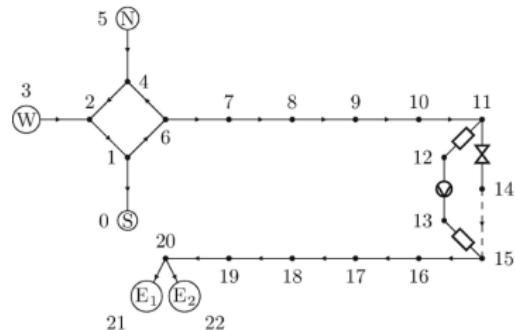
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Friction-dominated isothermal Euler equations for 1D pipes:

$$\frac{1}{\gamma_0 z_0} \partial_t p = -\frac{1}{S} \partial_x q$$

$$\partial_t q = -S \partial_x p - \left(\underbrace{\frac{S g \partial_x h}{\gamma_0 z_0} p}_{\text{Gravity}} + \underbrace{\frac{\gamma_0 z_0 \lambda_0}{2 d S} \frac{q |q|}{p}}_{\text{Friction}} \right)$$

- Pressure: $p(x, t)$
- Mass-flux: $q(x, t)$
- Height: $h(x)$
- Temperature: T_0
- Diameter: d
- Cross-section: S
- Roughness: k
- Gas Const.: R_S
- Gas state: $\gamma_0(T_0, R_S)$
- Compress.: $z_0(T_0, p)$
- Friction: $\lambda_0(k, d)$
- Grav. accel.: g



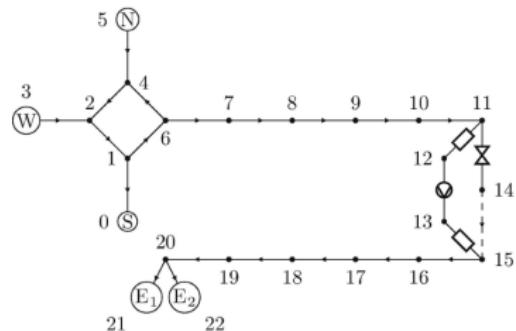
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Graph $(\mathcal{N}, \mathcal{E})$ incidence matrix \mathcal{A} :

$$\mathcal{A}_{ij} = \begin{cases} -1 & \mathcal{E}_j \text{ connects from } \mathcal{N}_i, \\ 0 & \mathcal{E}_j \text{ connects not } \mathcal{N}_i, \\ 1 & \mathcal{E}_j \text{ connects to } \mathcal{N}_i. \end{cases}$$



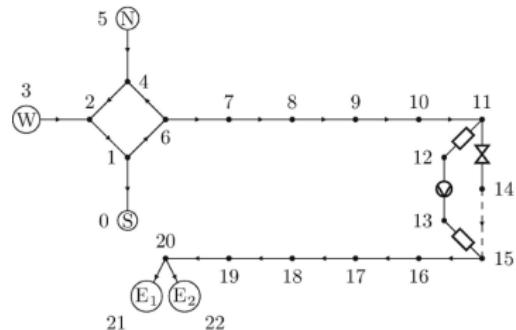
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Kirchhoff's laws:

- ① The net mass-flux at every node is zero.
- ② The sum of directed pressure drops in every loop is zero.



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Vectorized PDAE gas network model:

$$D_d \partial_t p^* = D_q \partial_x q,$$

$$\partial_t q^* = D_p \partial_x p - \left(D_g p^* + D_f \frac{q^* |q^*|}{p^*} \right),$$

$$\mathcal{A}_0 q^* = \mathcal{B}_d d_q,$$

$$\mathcal{A}_0^\top p^* = \mathcal{B}_s s_p,$$

- p^* is the pressure at a t.b.d. pipe location.
- q^* is the mass-flux at a t.b.d. pipe location.
- D_* are diagonal matrices.
- \mathcal{A}_0 is the incidence matrix without supply node rows.
- \mathcal{B}_s is the incidence matrix of supply node rows.
- \mathcal{B}_d is the incidence matrix of demand node columns.



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Simplification I: Index

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- Pipe midpoints:
 - (P)DAE tractability index bounded $\tau \leq 2$.
 - Given some weak topology constraints, PDAE becomes PDE [GRUNDEL ET AL, 2014].
 - Boundary values affect friction term.



S. Grundel, L. Jansen, N. Hornung, T. Clees, C. Tischendorf, P. Benner (2014). Model order reduction of differential algebraic equations arising from the simulation of gas transport networks. In: *Progress in Differential-Algebraic Equations*, 183–205, Springer, Cham. doi:10.1007/978-3-662-44926-4_9.



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- Pipe endpoints:
 - (P)DAE tractability index bounded $\tau < 2$.
 - Given some weak topology constraints, PDAE becomes PDE.
 - Less oscillatory behaviour.



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Simplification II: Model

Hidden assumptions in this model:



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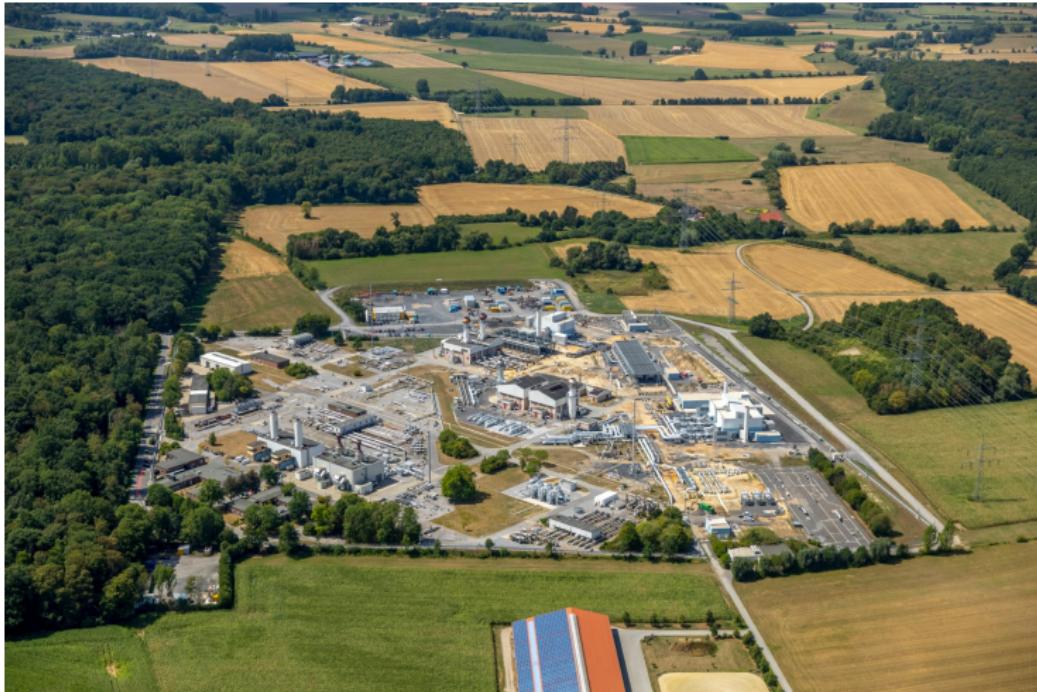
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- Only step function boundary values.



Natural gas compressor station in Werne, Germany, operated by Open Grid Europe.

Simplified edge-based compressor models:

- Energy-based:

$$q_{\text{out}} = q_{\text{in}}$$

$$p_{\text{out}} = p_{\text{in}} \left(\frac{P_{\max}}{p\gamma_0 z_0} \frac{\nu - 1}{\nu} + 1 \right)^{\frac{\nu}{\nu-1}}$$



T.W.K. Mak, P. Van Hentenryck, A. Zlotnik, R. Bent (2019). Dynamic compressor optimization in natural gas pipeline systems. *INFORMS Journal on Computing*, 31(1):1–26. doi:10.1287/ijoc.2018.0821.

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- Sub-divide too long pipes to set of unit-length pipes.



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- Consider: SSP optimality, stiff accuracy, passivity, efficiency.
- We recommend first order IMplicit-EXplicit method (i.e., combination of forward/backward Euler), providing often the best compromise between efficiency and accuracy, but other solvers are available in `morgen`, e.g. second-order IMEX (trapezoidal rule + SDIRK) with parametric Butcher tableau:

Explicit:			Implicit:		
0	0	0	λ	λ	0
1	1	0	$1 - \lambda$	$1 - 2\lambda$	λ
$\frac{1}{2}$			$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$

Parametric, Structured, Nonlinear, Non-Normal, Square:

$$\begin{aligned} \begin{bmatrix} E_p(\theta) & 0 \\ 0 & I_{N_q} \end{bmatrix} \begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} &= \begin{bmatrix} 0 & A_{pq} \\ A_{qp} & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} + \begin{bmatrix} 0 & B_{pd} \\ B_{qs} & 0 \end{bmatrix} \begin{bmatrix} s_p \\ d_q \end{bmatrix} + \begin{bmatrix} 0 \\ F_c + f_q(p, q, s_p, \theta) \end{bmatrix} \\ \begin{bmatrix} s_q \\ d_p \end{bmatrix} &= \begin{bmatrix} 0 & C_{sq} \\ C_{dp} & 0 \end{bmatrix} \begin{bmatrix} p \\ q \end{bmatrix} \\ \begin{bmatrix} p_0 \\ q_0 \end{bmatrix} &= \begin{bmatrix} \bar{p}(\bar{s}_p, \bar{d}_q) \\ \bar{q}(\bar{s}_p, \bar{d}_q) \end{bmatrix} \end{aligned}$$

Input:

- Pressure at supply: s_p
- Mass-Flux at demand: d_q

State:

- Pressure: p
- Mass-Flux: q

Output:

- Mass-Flux at supply: s_q
- Pressure at demand: d_p



Two-step steady state algorithm:

- 1a. Linear mass-flux steady-state: $A_{pq} \bar{q} = -B_{pd} \bar{d}_q$
- 1b. Linear pressure steady-state: $A_{qp} \bar{p} = -\left(B_{qs} \bar{s}_p + F_c \right)$
2. Corrected pressure steady-state: $A_{qp} p_{k+1} = -\left(B_{qs} \bar{s}_p + F_c + f_q(p_k, \bar{q}, \bar{s}_p, \theta) \right)$



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- If more accuracy is needed, iterate with 1st order IMEX solver.



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Recap:

From: Hyperbolic 2D PDAE

To: Non-normal, coupled, nonlinear, parametric ODE

Wish list:



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- Large-scale → Low-rank computable methods*



Split reduction operators

$$W = \begin{bmatrix} W_p \\ W_q \end{bmatrix} \in \mathbb{R}^{(N_p+N_q) \times r}$$

into structure-preserving reduction operator

$$\begin{bmatrix} W_p & \\ & W_q \end{bmatrix} \in \mathbb{R}^{(N_p+N_q) \times 2r},$$

where $W \in \{V, U\}$.



K. Kerns, A. Yang (1998). Preservation of passivity during RLC network reduction via split congruence transformations. *IEEE Trans. CAD Integr. Circuits Syst.* 17(7):582–591.

Model Reduction II: Structure Preservation

Split-congruence Transformations [KERNs/YANG 1998]

$$\begin{matrix} E_p \\ I_q \end{matrix} \begin{matrix} \dot{p} \\ \dot{q} \end{matrix} = \begin{matrix} A_{qp} \\ A_{qp} \end{matrix} \begin{matrix} p \\ q \end{matrix} + \begin{matrix} B_{qp} \\ B_{qp} \end{matrix} \begin{matrix} s_p \\ d_q \end{matrix} + \begin{matrix} f_q \\ f_q \end{matrix} \begin{matrix} p \\ q \end{matrix}$$

$$\begin{matrix} s_p \\ d_q \end{matrix} = \begin{matrix} C_q \\ C_p \end{matrix} \begin{matrix} p \\ q \end{matrix}$$

↓ Model Order Reduction

$$\begin{matrix} V_p \\ V_q \end{matrix} \begin{matrix} E_p \\ I_q \end{matrix} \begin{matrix} U_p \\ U_q \end{matrix} \begin{matrix} \dot{p} \\ \dot{q} \end{matrix} = \begin{matrix} V_p \\ V_q \end{matrix} \begin{matrix} A_{qp} \\ A_{qp} \end{matrix} \begin{matrix} U_p \\ U_q \end{matrix} \begin{matrix} p_r \\ q_r \end{matrix} + \begin{matrix} V_p \\ V_q \end{matrix} \begin{matrix} B_{qp} \\ B_{qp} \end{matrix} \begin{matrix} s_p \\ d_q \end{matrix} + \begin{matrix} V_p \\ V_q \end{matrix} \begin{matrix} f_q \\ U_p \end{matrix} \begin{matrix} p_r \\ U_q q_r \end{matrix}$$

$$\begin{matrix} s_p \\ d_q \end{matrix} = \begin{matrix} C_q \\ C_p \end{matrix} \begin{matrix} U_p \\ U_q \end{matrix} \begin{matrix} p_r \\ q_r \end{matrix}$$

↓ Reduced Order Model

$$\begin{matrix} E_r \\ I_r \end{matrix} \begin{matrix} \dot{p}_r \\ \dot{q}_r \end{matrix} = \begin{matrix} A_r \\ A_r \end{matrix} \begin{matrix} p_r \\ q_r \end{matrix} + \begin{matrix} B_r \\ B_r \end{matrix} \begin{matrix} s_p \\ d_q \end{matrix} + \begin{matrix} V_p \\ V_q \end{matrix} \begin{matrix} f_q \\ U_p \end{matrix} \begin{matrix} p_r \\ U_q q_r \end{matrix}$$

$$\begin{matrix} s_p \\ d_q \end{matrix} = \begin{matrix} C_r \\ C_r \end{matrix} \begin{matrix} p_r \\ q_r \end{matrix}$$



K. Kerns, A. Yang (1998). Preservation of passivity during RLC network reduction via split congruence transformations. *IEEE Trans. CAD Integr. Circuits Syst.* 17(7):582–591.



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Model Reduction III: Tested Methods

The tested model reduction methods:



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Model Reduction III: Tested Methods

The tested model reduction methods:

Structured POD, via: empirical reachability Gramian

All implemented via `emgr` software platform [HIMPE 2018].



The tested model reduction methods:

Structured POD, via: empirical reachability Gramian

Structured Dominant Subspaces, via:
empirical reachability & observability Gramian
empirical cross Gramian
empirical non-symmetric cross Gramian

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The tested model reduction methods:

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empirical reachability & observability Gramian
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empirical non-symmetric cross Gramian

Structured Balanced POD, via: empirical reachability & observability Gramian

All implemented via `emgr` software platform [HIMPE 2018].



The tested model reduction methods:

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Structured Dominant Subspaces, via:
empirical reachability & observability Gramian
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Structured Balanced POD, via: empirical reachability & observability Gramian

Structured Balanced Truncation, via:
empirical reachability & observability Gramian
empirical cross Gramian
empirical non-symmetric cross Gramian

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The tested model reduction methods:

Structured POD, via:	empirical reachability Gramian
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Structured Balanced POD, via:	empirical reachability & observability Gramian
Structured Balanced Truncation, via:	empirical reachability & observability Gramian empirical cross Gramian empirical non-symmetric cross Gramian
Structured Balanced Gains, via:	empirical reachability & observability Gramian empirical cross Gramian empirical non-symmetric cross Gramian

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Structured Balanced Gains, via:	empirical reachability & observability Gramian empirical cross Gramian empirical non-symmetric cross Gramian
Structured DMD Galerkin, via:	empirical reachability Gramian

All implemented via `emgr` software platform [HIMPE 2018].



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Spotlight: DMD-Galerkin

Plain Vanilla DMD:

$$X = [x_0 \ x_1 \ \dots \ x_T] \rightarrow \left\{ \begin{array}{l} X_0 := [x_0 \ x_1 \ \dots \ x_{T-1}] \\ X_1 := [x_1 \ x_2 \ \dots \ x_T] \end{array} \right\} \rightarrow X_1 \stackrel{!}{\approx} \mathcal{A}X_0 \Rightarrow \mathcal{A} \approx X_1 X_0^+$$



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...with centering⁴

$$X \rightarrow \bar{X} := [(x_0 - \bar{x}) \quad (x_1 - \bar{x}) \quad \dots \quad (x_T - \bar{x})]$$

⁴S.M. Hirsh, K.D. Harris, J.N. Kutz, B.W. Brunton. [Centering Data Improves the Dynamic Mode Decomposition](#). SIAM J. Appl. Dyn. Syst., 19(3): 1920–1955, 2020. doi:[10.1137/19M1289881](https://doi.org/10.1137/19M1289881)

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... used as Model reduction method: DMD-Galerkin⁵

$$\mathcal{A} \stackrel{\text{tSVD}}{=} U_1 D_1 V_1$$

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$$\mathcal{A} \stackrel{\text{tSVD}}{=} U_1 D_1 V_1$$

...can be computed via empirical Gramian (exact-DMD "kernel"):

$$W_R = \sum_m^M \kappa(\bar{X}_m, \bar{X}_m) \quad \begin{cases} \kappa_{\text{Linear}}(X, Y) := X Y^\top \\ \kappa_{\text{DMD}}(X, Y) := X_1 Y_0^+ \end{cases}$$

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→ (Centered) DMD-Galerkin via (Discrete) Empirical Reachability Gramian!

⁴ S.M. Hirsh, K.D. Harris, J.N. Kutz, B.W. Brunton. [Centering Data Improves the Dynamic Mode Decomposition](#). SIAM J. Appl. Dyn. Syst., 19(3): 1920–1955, 2020. doi:[10.1137/19M1289881](https://doi.org/10.1137/19M1289881)

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Disclaimer:



Disclaimer:

- First, what is the best linear subspace for model order reduction?



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Model Reduction IV: Hyper-Reduction

Disclaimer:

- First, what is the best linear subspace for model order reduction?
- What hyper-reduction should be used (DEIM, DMD, NL, etc.)?



Disclaimer:

- First, what is the best linear subspace for model order reduction?
- What hyper-reduction should be used (DEIM, DMD, NL, etc.)?
- How do model reduction and hyper-reduction interact?



Disclaimer:

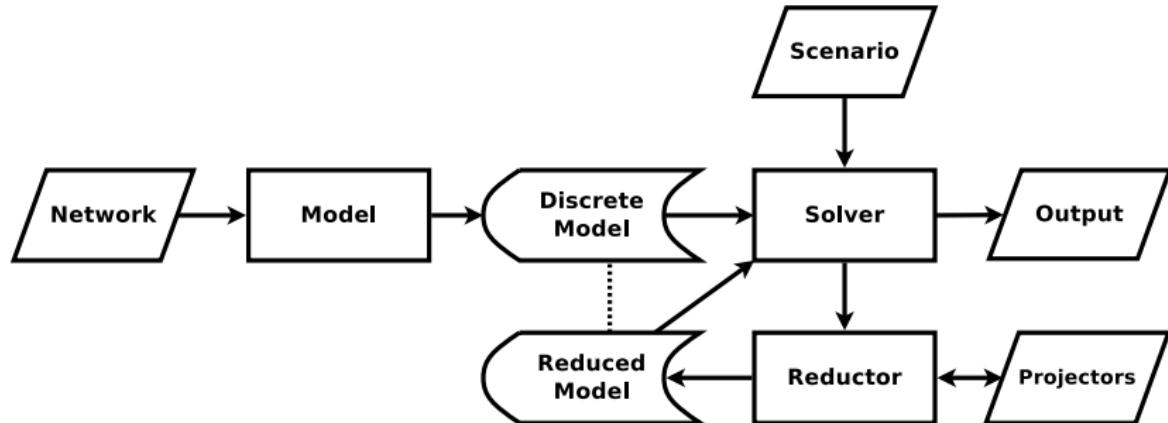
- First, what is the best linear subspace for model order reduction?
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- What hyper-reduction should be used (DEIM, DMD, NL, etc.)?
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- Is hyper-reduction avoidable due to repeated scalar nonlinearities?

Disclaimer:

- First, what is the best linear subspace for model order reduction?
 - What hyper-reduction should be used (DEIM, DMD, NL, etc.)?
 - How do model reduction and hyper-reduction interact?
 - How to recycle simulations (efficiently)?
 - Is hyper-reduction avoidable due to repeated scalar nonlinearities?
- No hyper-reduction implemented (yet).



Major modules:

- networks
- models
- solvers
- reductors
- tests

Minor modules:

- utils
- tools



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Workflow

Set-up



Set-up

- Short training, long testing



Set-up

- Short training, long testing
- Generic training scenario (constant input)



Set-up

- Short training, long testing
- Generic training scenario (constant input)
- Disjoint training and test parameters



Set-up

- Short training, long testing
- Generic training scenario (constant input)
- Disjoint training and test parameters
- Tested models: `ode_mid`, `ode_end`



Set-up

- Short training, long testing
- Generic training scenario (constant input)
- Disjoint training and test parameters
- Tested models: `ode_mid`, `ode_end`
- Tested solvers: `imex1`, `imex2`

Set-up

- Short training, long testing
- Generic training scenario (constant input)
- Disjoint training and test parameters
- Tested models: `ode_mid`, `ode_end`
- Tested solvers: `imex1`, `imex2`
 - `pod_r`
 - `eds_ro`, `eds_wx`, `eds_wz`
 - `bpod_ro`,
 - `ebt_ro`, `ebt_wx`, `ebt_wz`
 - `ebg_ro`, `ebg_wx`, `ebg_wz`
 - `dmd_r`,
- Tested reductors:

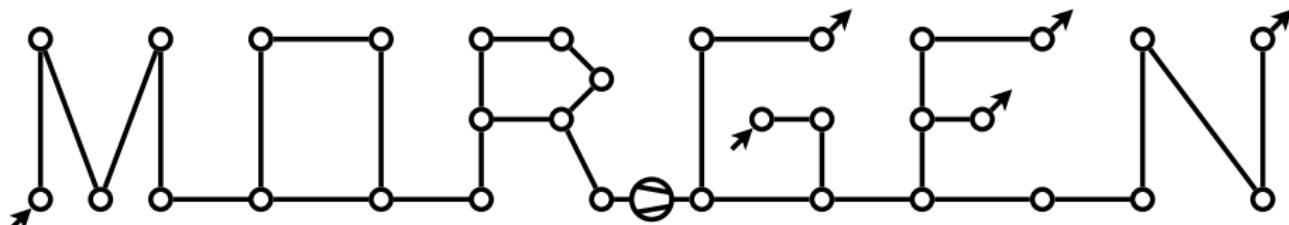
Set-up

- Short training, long testing
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- Disjoint training and test parameters
- Tested models: `ode_mid`, `ode_end`
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- Tested reductors:
- Heuristic $L_{i \in \{1,2,\infty\}} \otimes L_{j \in \{1,2,\infty\}}$ error norm computation

Set-up

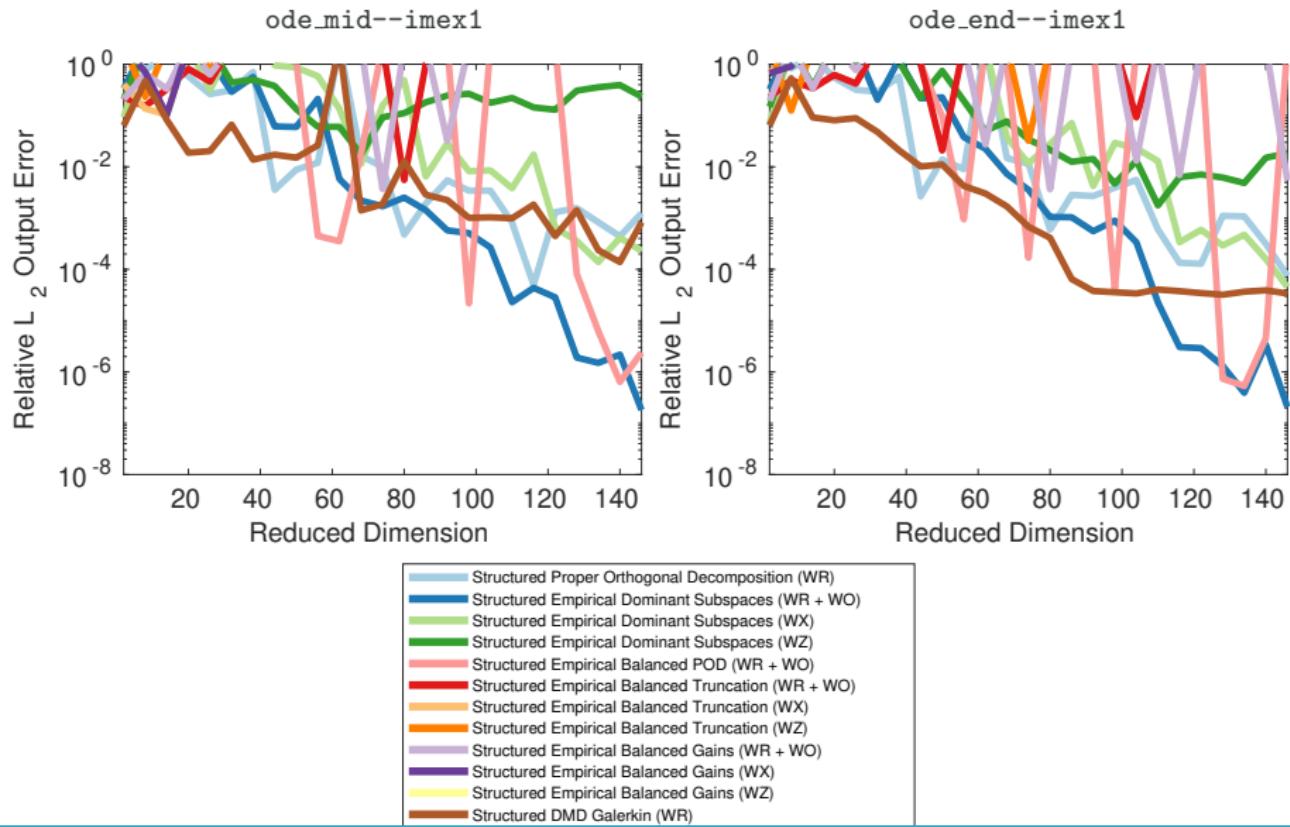
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- Tested reductors:
- Heuristic $L_{i \in \{1,2,\infty\}} \otimes L_{j \in \{1,2,\infty\}}$ error norm computation
- Compare MORscore⁶

⁶ C. Himpe (2020). Comparing (empirical-Gramian-based) model order reduction algorithms. arXiv [math.OC], arXiv:2002.12226.



- 2 Cycles
- 1 Compressor
- 2 Supply nodes
- 4 Demand nodes
- Pipe length [20, 60]km
- Time resolution 60s
- Temperature: [0, 15]°C
- Gas constant: [500, 600] $\frac{\text{J}}{\text{kg K}}$
- Schiffrinson friction factor
- AGA88 compressibility factor
- 900 States
- 6 Inputs & Outputs
- Training horizon: 1h
- Test horizon: 24h
- Perturbed steady-state training
- Standard load profiles testing

Experiment II: $L_2 \otimes L_2$ Model Reduction Error

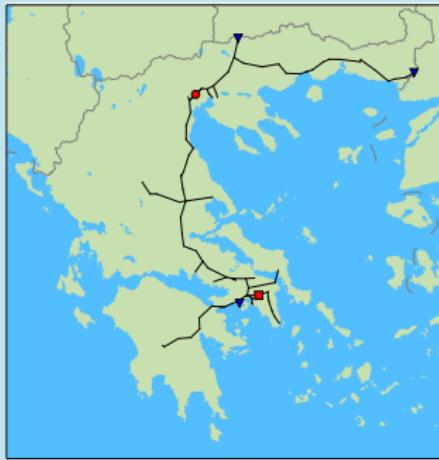


Experiment II: Evaluation

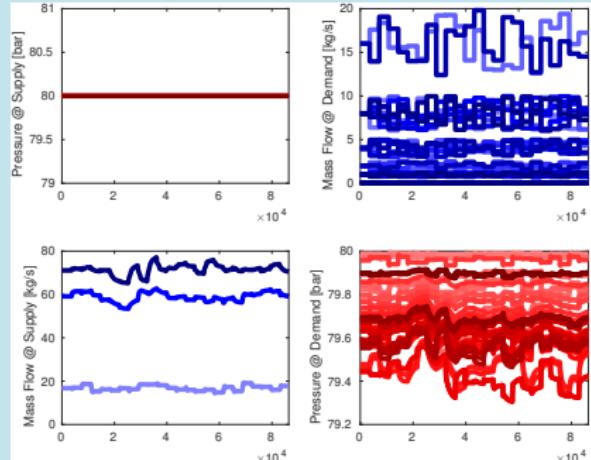
	ode_mid imex_1	ode_end imex_1	ode_mid imex_2	ode_end imex_2
pod_r	0.12	0.12	0.04	0.05
eds_ro	0.16	0.16	0.05	0.06
eds_wx	0.08	0.08	0.02	0.02
eds_wz	0.03	0.07	0.02	0.04
bpod_ro	0.07	0.07	0.02	0.02
ebt_ro	0.00	0.00	0.03	0.03
ebt_wx	0.00	0.00	0.00	0.00
ebt_wz	0.00	0.00	0.00	0.00
ebg_ro	0.00	0.01	0.02	0.02
ebg_wx	0.00	0.00	0.00	0.00
ebg_wz	0.00	0.00	0.00	0.00
dmd_r	0.14	0.18	0.03	0.04

MORSCORES $\mu(150, \epsilon_{\text{mach}(16)})$ in the $L_2 \otimes L_2$ norm for the “MORGEN” network.

The Network

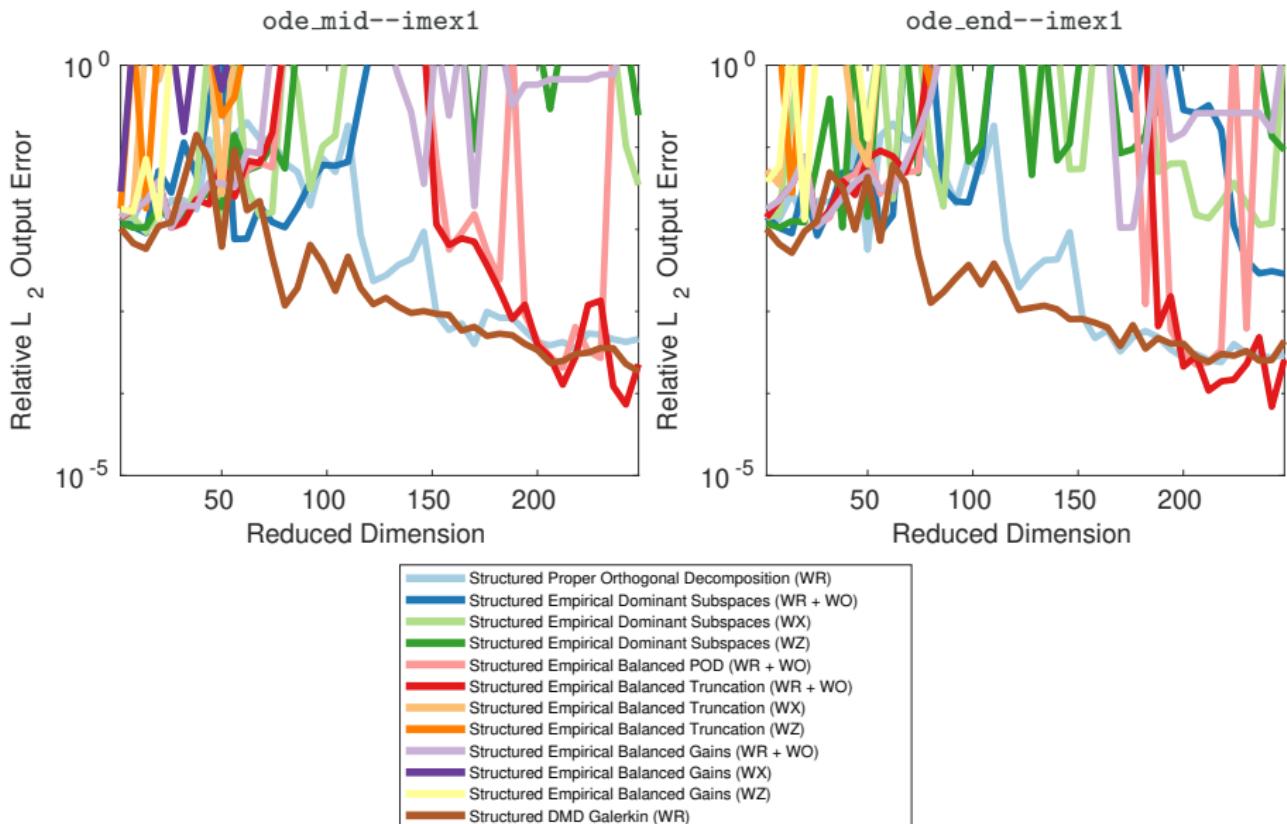


The Scenarios



- total length: 1412km
- steady-state, used as initial state:
 - pressure of 80bar at supply nodes and compressor;
 - demand mass-fluxes up to 16kg.
- 1 compressor
- 3886 states
- 48 inputs and outputs
- 20sec time steps

Experiment III: $L_2 \otimes L_2$ Model Reduction Error





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Outline

1. Introduction
2. Modeling
3. Model Order Reduction
4. Outlook, Summary, Details



Some open problems and future work:

- Port-Hamiltonian model
- Parametric pipe roughness
- Intraday switchable valves
- Minimal training horizon
- SciGRID_gas network
- OGE partDE network



Conclusions from computational experiments:

- Prefer the endpoint model.
- Prefer the first-order IMEX solver.
- Prefer Galerkin model reduction methods.

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The Software: morgen (Model Order Reduction for Gas and Energy Networks)

MATLAB code (Octave-compatible), under BSD 2-Clause License, available at:

doi:10.5281/zenodo.4288510