Data-Driven Model Reduction for Gas Network Digital Twins

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Model Reduction and Surrogate Modeling (MORE)

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Mathematics Münster
Cluster of Excellence

› Why Gas Networks?

Gas Transport is Complicated:

- Continent-spanning infrastructure
- Daily, reliable and safe delivery
- Cost and resource efficient transmission
- Weather-dependent consumption

Green Energy Transition:

- Volatile production: biogas, hydrogen
- Gas-fired power-plants
- Energy storage

→ **Many 24h forecast simulations!**

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Recent Events!

→ **Even more 24h forecast simulations!**

› Gas Pipeline

Friction-Dominated 1D Isothermal Euler Equations:

$$\frac{1}{T_0\, R_S\, z_0}\,\partial_t p = -\frac{1}{S}\,\partial_x q$$

$$\partial_t q = -S\,\partial_x p - \Big(\overbrace{\frac{S\,g\,h_x}{T_0\,R_S\,z_0}}^{\text{Gravity}} p + \overbrace{\frac{T_0\,R_S\,z_0 \lambda_0}{2\,d\,S}\,\frac{|q|\,q}{p}}^{\text{Friction}}\Big)$$

- Pressure: $p(x,t)$
- Mass-Flux: $q(x,t)$
- Pipe Incline: h_x
- Pipe Diameter: d
- Pipe Cross-Section: S
- Friction Factor: λ_0
- Compressibility Factor: z_0
- Temperature: $T_0 =: \theta_1$
- Specific Gas Constant: $R_S =: \theta_2$
- Gravity Acceleration: g

› Gas Network

Kirchhoff Laws:

1. The sum of mass-flux in- and outflows at every junction is zero:

$$\mathcal{A}\, q(t) = \mathcal{B}_d\, d_q(t)$$

2. The sum of pressure drops in every fundamental loop is zero.
   $\rightarrow$ Nodal pressures at in-flows equal to boundary function:

$$\mathcal{A}_0^\top\, p(t) + \mathcal{B}_s^\top\, s_p(t) = |\mathcal{A}_0^\top|\, p(t)$$

- Incidence Matrix: $\mathcal{A}$
- Reduced Incidence Matrix: $\mathcal{A}_0$
- Boundary Pressure Map: $\mathcal{B}_s$
- Boundary Mass-Flux Map: $\mathcal{B}_d$
- Pressure: $p(t)$
- Mass-Flux: $q(t)$
- Pressure Boundary: $s_p(t)$
- Mass-Flux Boundary: $d_q(t)$

› Input-Output System

Index Reduced Endpoint Discretization:

$$\overbrace{\begin{pmatrix} E_p(\theta) & 0 \\ 0 & E_q \end{pmatrix}}^{E} \overbrace{\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix}}^{\dot{x}} = \overbrace{\begin{pmatrix} 0 & A_{pq} \\ \hat{A}_{qp} & 0 \end{pmatrix}}^{A} \overbrace{\begin{pmatrix} p \\ q \end{pmatrix}}^{x} + \overbrace{\begin{pmatrix} 0 & B_{pd} \\ B_{qs} & 0 \end{pmatrix}}^{B} \overbrace{\begin{pmatrix} s_p \\ d_q \end{pmatrix}}^{u} + \overbrace{\begin{pmatrix} 0 \\ f_q(p, q, \theta) \end{pmatrix}}^{f}$$

$$\underbrace{\begin{pmatrix} s_q \\ d_p \end{pmatrix}}_{y} = \underbrace{\begin{pmatrix} 0 & C_{sq} \\ C_{dp} & 0 \end{pmatrix}}_{C} \underbrace{\begin{pmatrix} p \\ q \end{pmatrix}}_{x}$$

Input:

- Pressure @ supply: s_p
- Mass-flux @ demand: d_q

State:

- Pressure: p
- Mass-flux: q

Output:

- Mass-flux @ supply: s_q
- Pressure @ demand: d_p

› Digital Twin

Data Binding Definition for Digital Twins[1]:

- A (virtual) model relating to a real thing: $\boxed{\text{PT}} \mapsto \boxed{\text{DT}}$
- Data sets relating to the physical twin: $f_d(\boxed{\text{DT}}, 📊) \approx f_p(\boxed{\text{PT}}, 📊)$
- Adjustability of the model to data: $f_d^*(\boxed{\text{DT}}, 📊, 📄) = f_p(\boxed{\text{PT}}, 📊)$

Do We Have a Digital Twin? Yes:

- Mathematical model (based on physics)
- Network topology (i.a. of real networks)
- Scenario data (i.e. supply pressure, demand mass-flux, compressor settings)
- Model parameters (i.e. gas composition, temperature, pipe roughness)
- Adjustability (i.e. friction formula, compressibility formula, efficiency factor)

[1] L. Wright, S. Davidson: **How to tell the difference between a model and a digital twin**; Advanced Modeling and Simulation in Engineering Science 7: 13, 2020. `doi:10.1186/s40323-020-00147-4`

› Model Reduction

Situation:

- Quantities of Interest

Solution:

- System-Theoretic Methods

This image is a resource from Flaticon.com

› Model Reduction

Situation:

- Quantities of Interest
- Structured System

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Solution:

- System-Theoretic Methods
- Block-Diagonal Projections

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Situation:

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- Parametric System

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- Block-Diagonal Projections
- Accumulated Computation (of system-theoretic operators)

› Model Reduction

Situation:

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- Structured System
- Parametric System
- Nonlinear System

This image is a resource from Flaticon.com

Solution:

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- Block-Diagonal Projections
- Accumulated Computation (of system-theoretic operators)
- Data-Driven Computation (of system-theoretic operators)

› Model Reduction

Situation:

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- Nonlinear System
- Hyperbolic System

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Solution:

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- Step instead of Impulse Training

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- Step instead of Impulse Training

Which data-driven system-theoretic method works (best)?

› Model Reduction

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Which unsupervised learning method works (best)?

› Projection-Based Model Reduction

Goal:

$$n := \dim(x_r(t)) \ll \dim(x(t)) =: N \quad \text{s.t.} \quad \|y(\theta) - \tilde{y}(\theta)\| \ll 1$$

Global Structured Reducing and Reconstructing Projections:

$$x_r(t) := \underbrace{\begin{pmatrix} V_p & 0 \\ 0 & V_q \end{pmatrix}}_{V_r \in \mathbb{R}^{n \times N}} x(t) \quad \rightarrow \quad x(t) \approx \underbrace{\begin{pmatrix} U_p & 0 \\ 0 & U_q \end{pmatrix}}_{U_r \in \mathbb{R}^{N \times n}} x_r(t)$$

Projection-Based Reduced Order Model:

$$\begin{aligned} (V_r E(\theta) U_r)\, \dot{x}_r(t) &= (V_r A U_r)\, x_r(t) + (V_r B)\, u(t) + V_r\, f(U_r x_r(t), u(t), \theta) \\ \tilde{y}(t) &= (C U_r)\, x_r(t) \end{aligned}$$

› Tested Methods

Reductor	Type
Structured Proper Orthogonal Decomposition (POD)	Orthogonal
Structured Goal-Oriented POD	Orthogonal
Structured Empirical Dominant Subspaces (DSPMR)	Orthogonal
Structured Modified POD	Oblique
Structured Balanced POD	Bi-Orthogonal
Structured Empirical Balanced Truncation	Bi-Orthogonal
Structured Empirical Balanced Gains	Bi-Orthogonal
Structured Dynamic Mode Decomposition Galerkin	Orthogonal

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› DSPMR

Linear Time-Invariant System:

$$\dot{x}(t) = A\,x(t) + B\,u(t)$$
$$y(t) = C\,x(t)$$

Controllability and Observability:

$$W_C := \int_0^\infty (\mathrm{e}^{At}\,B)(\mathrm{e}^{At}\,B)^\top \,\mathrm{d}t, \qquad W_O := \int_0^\infty (\mathrm{e}^{A^\top t}\,C^\top)(\mathrm{e}^{A^\top t}\,C^\top)^\top \,\mathrm{d}t$$

Dominant Subspace Projection Model Reduction (No Balancing):

$$W_C \overset{\text{rrSVD}}{=} U_C D_C U_C^\top, \qquad W_O \overset{\text{rrSVD}}{=} U_O D_O U_O^\top$$

$$\Big[(\|W_C\|_F^{-1} U_C D_C) \quad (\|W_O\|_F^{-1} U_O D_O)\Big] \overset{\text{rrSVD}}{=} U\;D\;T, \quad V := U^\top$$

› DSPMR-X

Square Linear Time-Invariant System ($M = Q$):

$$\dot{x}(t) = A\,x(t) + B\,u(t)$$
$$y(t) = C\,x(t)$$

Controllability • Observability = Minimality:

$$W_X := \int_0^\infty (\mathrm{e}^{At}\,B)(\mathrm{e}^{A^\top t}\,C^\top)^\top\,\mathrm{d}t$$

Dominant Subspace Projection Model Reduction (Cross Gramian):

$$W_X \overset{\text{rrSVD}}{=} U_X D_X T_X^\top$$
$$\begin{bmatrix} U_X & T_X \end{bmatrix} \overset{\text{rrSVD}}{=} U\;D\;T, \quad V := U^\top$$

› Data-Driven System Gramians

Empirical Gramians:

$$W_C = \int_0^\infty (\mathrm{e}^{At} B)(\mathrm{e}^{At} B)^\top \,\mathrm{d}t = \int_0^\infty x(t)x(t)^\top \,\mathrm{d}t \approx \Delta t X X^\top$$

$$W_O = \int_0^\infty (\mathrm{e}^{A^\top t} C^\top)(\mathrm{e}^{A^\top t} C^\top)^\top \,\mathrm{d}t = \int_0^\infty z(t)z(t)^\top \,\mathrm{d}t \approx \Delta t Z Z^\top$$

$$W_X = \int_0^\infty (\mathrm{e}^{At} B)(\mathrm{e}^{A^\top t} C^\top)^\top \,\mathrm{d}t = \int_0^\infty x(t)z(t)^\top \,\mathrm{d}t \approx \Delta t X Z^\top$$

- Applicable to nonlinear, parametric and unstable systems.
- However, nonlinear variant's complexity scales with state dimension (N).
- Linear variant's complexity scales with port dimensions ($M + Q$).
- An (approximate) adjoint system (z) is required.
- Possible due to local nonlinearity and port-Hamiltonian linearization.

› Lessons Learned

- Short training, long tests
- Choice of solver is fundamental
- Centering of training trajectories is important
- Orthogonal methods preserve stability for linearization
- Gain matching via extra feed-forward (D) of limited use

› Reusable Software

`morgen` (**M**odel **O**rder **R**eduction for **G**as and **E**nergy **N**etworks)

- **For engineers:** Test model reduction on your networks.
- **For mathematicians:** Test your model reduction on gas nets.
- **MATLAB & Octave** compatible
- **Open source** licensed
- **Version 1.2** upcoming

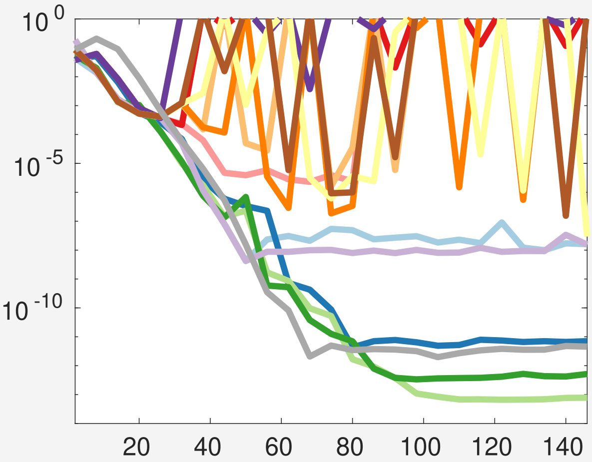
`https://git.io/morgen`

› Numerical Experiments

	Training	Test
Parameter Sampling	Sparse Grid	Uniformly Random
Input Function	Step	Scenario
Time Horizon	$1 - 12h$	$24h$

	Evaluation
Measure	Relative Output Error
Norm	$\| \cdot \|_{L_2 \otimes L_2}$
Ranking	MORscore

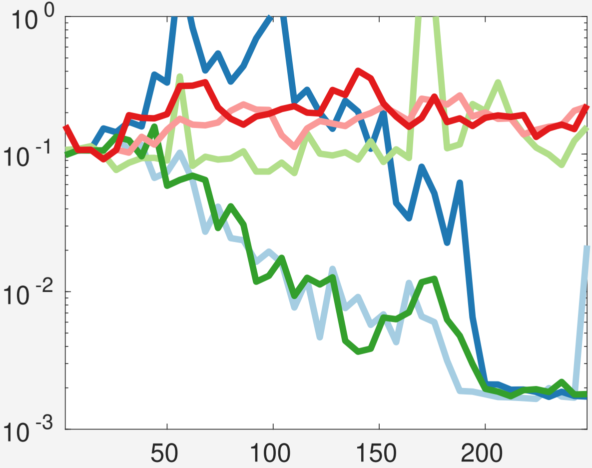
› Yamal-Europe Pipeline $(N \approx 1000)$



MORscores:

DSPMR-X	0.57
DSPMR-Z	0.56
DMDG	0.53
DSPMR	0.51
GOPOD	0.41
POD	0.40
BT-Z	0.15
BG-X	0.14
BPOD	0.14
BG-Z	0.11
BT-X	0.10
BT	0.03
BG	0.02

› Chinese Transport Network $(N \approx 11000)$



MORscores:

DSPMR	0.12
POD	0.12
GOPOD	0.07
DMDG	0.06
DSPMR-X	0.05
DSPMR-Z	0.04

› Conclusions

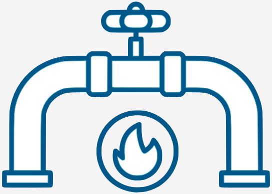
Recommended Ensemble:

- Model: **pH** (Port-Hamiltonian Endpoint Discretization)
- Application: **Gas** (Also: Water, District Heating, Power)
- Solver: **IMEX** (1st Order Implicit Explicit Time Stepper)
- Reductor: **DSPMR** (Dominant Subspace Projection Model Reduction)
- Software: **MORGEN** (Model Order Reduction for Gas and Energy Networks)

https://doi.org/gndbmv (Paper)

https://git.io/morgen (Code)

https://himpe.science (Slides)



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- *emgr:*
  C. Himpe: **emgr – EMpirical GRamian Framework Version 5.99**;
  arXiv [cs.CE]: 2209.03833, 2022.

› Game Over

Research Software:

- `emgr` – **EM**pirical **GR**amian Framework
  - `https://gramian.de` *(Contact: Me)*
- `hapod` – **H**ierarchical **A**pproximate **P**roper **O**rthogonal **D**ecomposition
  - `https://git.io/hapod` *(Contact: Stephan Rave)*
- `morgen` – **M**odel **O**rder **R**eduction for **G**as and **E**nergy **N**etworks
  - `https://git.io/morgen` *(Contact: Sara Grundel)*
- `AlgoData` – Numerical Algorithm Knowledge Graph
  - `https://algodata.mardi4nfdi.de` *(MaRDI)*

Me: `https://himpe.science`
`christian.himpe@wwu.de`

› Game Over

Research Software:

- emgr – **EM**pirical **GR**amian Framework *(10-year anniversary!)*
  - https://gramian.de *(Contact: Me)*
- hapod – **H**ierarchical **A**pproximate **P**roper **O**rthogonal **D**ecomposition
  - https://git.io/hapod *(Contact: Stephan Rave)*
- morgen – **M**odel **O**rder **R**eduction for **G**as and **E**nergy **N**etworks
  - https://git.io/morgen *(Contact: Sara Grundel)*
- AlgoData – Numerical Algorithm Knowledge Graph
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