MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC
COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Compressed Gas Network Digital Twins

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KLAIM – Kaiserslautern Applied and Industrial Mathematics Days
Track: Multiscale Methods and Model Order Reduction
2021–10–13

Outline

The Gas Network Challenge

- More renewable energy $\rightarrow$ More volatility
- Gas-fired power plants $\rightarrow$ Fast reacting energy conversion
- Biogas and hydrogen $\rightarrow$ Convertible green energy
- Gas networks $\rightarrow$ Transport and store energy
- International infrastructure $\rightarrow$ Large-scale network
- Intraday interactions $\rightarrow$ Dynamic simulations
- Uncertainties $\rightarrow$ **Many day-ahead simulations, every day**

Applied math to the rescue![1]

[1] T. Clees, A. Baldin, P. Benner, S. Grundel, C. Himpe, B. Klaassen, F. Küsters, N. Marheineke, L. Nikitina, I. Nikitin, J. Pade, N. Stahl, C. Strohm, C. Tischendorf, A. Wirsen: **MathEnergy – Mathematical Key Technologies for Evolving Energy Grids**; in: Mathematical Modeling, Simulation and Optimization for Power Engineering and Management, Mathematics in Industry (34): 233–262, 2021. doi:10.1007/978-3-030-62732-4_11

Digital. Twin.

1. Digital twin (DT) $\Rightarrow$ Physical twin (PT)
2. Digital $\Rightarrow$ Machine-readable encoding
3. Twin $\Rightarrow$ Data-driven coupling

Classification

By Data Flow?[2]

- Digital Model: $\boxed{\text{PT}} \underset{\text{manual}}{\overset{\text{manual}}{\rightleftarrows}} \boxed{\text{DT}}$
- Digital Shadow: $\boxed{\text{PT}} \underset{\text{manual}}{\overset{\text{automatic}}{\rightleftarrows}} \boxed{\text{DT}}$
- Digital Twin: $\boxed{\text{PT}} \underset{\text{automatic}}{\overset{\text{automatic}}{\rightleftarrows}} \boxed{\text{DT}}$

By Data Binding?[3]

- 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: $f_d^*(\boxed{\text{DT}}, ,) = f_p(\boxed{\text{PT}},)$

[2] W. Kritzinger, M. Karner, G. Traar, J. Henjes, W. Sihn: **Digital Twin in manufacturing: A categorical literature review and classification**; IFAC PapersOnLine 51–11: 1016–1022, 2018. doi:10.1016/j.ifacol.2018.08.474

[3] 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

Gas Network Simulation

Type:

- Steady-state or dynamic simulation?
- Transport or distribution network?

$\rightarrow$ Transient gas transport network simulations.

Effect:

- Complexity due to nonlinearity!
- Large-scale due to hyperbolicity!

Gas Pipeline Model

Isothermal Euler Equations in a Long Pipe:

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

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

- Pressure $p(x,t)$
- Mass-Flux $q(x,t)$
- Pipe Incline h_x
- Pipe Diameter d
- Pipe Cross-Section S
- Gravity Acceleration g
- Friction Factor λ_0
- Compressibility Factor z_0
- Gas State $\gamma_0 = T_0 R_S$

Gas Network Model

Spatial Discretization and Index Reduction (Endpoint Discretization):

$$
\begin{aligned}
(\mathcal{A}_{0,R} D_p^{-1} d_0 \, \mathcal{A}_{0,R}^\intercal) \, \dot{p} &= -\mathcal{A}_0 \, q^L + \mathcal{B}_d \, d_q \\
D_q^{-1} \dot{q}^L &= \quad \mathcal{A}_0^\intercal \, p + \mathcal{B}_s^\intercal s_p - \left(D_g d_0 \, \mathcal{A}_{0,R}^\intercal \, p + D_q^{-1} D_f \frac{|q^L| \, q^L}{d_0 \mathcal{A}_{0,R}^\intercal \, p} \right)
\end{aligned}
$$

- Incidence Matrix $\mathcal{A}_0$
- Outflow Incidence Matrix $\mathcal{A}_{0,R}$
- Pressure Boundary Operator $\mathcal{B}_s$
- Mass-Flux Boundary Operator $\mathcal{B}_d$
- Inflow Mass-Flux $q^L(t)$
- Outflow Pressure $p(t)$
- Boundary Pressure $s_p(t)$
- Boundary Mass-flux $d_q(t)$

Input-Output System

Quantities of Interest, Parametrization and Additive Compressors:

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

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

- Mass matrix E
- System matrix A
- Input matrix B
- Output matrix C
- Nonlinearity f

- Evolution $\dot{x}$
- State x
- Input u
- Output y
- Parameter θ

Input-State-Output Port-Hamiltonian System

Input-Output System:

$$
\begin{aligned}
E\dot{x}(t) &= Ax(t) + Bu(t) + f(x(t)) \\
y(t) &= Cx(t)
\end{aligned}
$$

Conditions:

- $E = E^\intercal \geq 0$
- $A = (J - R)Q$
  - $J = -J^\intercal$
  - $R = R^\intercal \geq 0$
  - $Q = Q^\intercal > 0$
- $B = (G - P)$
- $C = (G + P)^\intercal Q$
- f ?

Components:

- J Energy Flux
- R Energy Dissipation
- Q Energy Storage
- G Resistive Ports
- P Control Ports

Input-State-Output Port-Hamiltonian System

Input-Output System:

$$E\dot{x}(t) = (Ax(t) + f(x(t)) + Bu(t)$$
$$y(t) = Cx(t)$$

Conditions:

- $E = E^\intercal \geq 0$
- $A = JQ$
  - $J = -J^\intercal$
  - $Q = Q^\intercal > 0$
- $f(x(t)) = -R(x(t))Qx(t)$
  - $R(x(t)) = R(x(t))^\intercal \geq 0$
- $B = (G - P)$
- $C = (G + P)^\intercal Q$

Components:

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Input-State-Output Port-Hamiltonian System

Input-Output System:

$$\begin{aligned} E\dot{x}(t) &= (J - R(x(t))Qx(t) + (G - P)u(t) \\ y(t) &= (G + P)^\intercal Qx(t) \end{aligned}$$

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Components:

- J Energy Flux
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Do we have a digital twin?

- 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)

$\rightarrow$ Yes![4]

[4] Using the *data binding* definition.

Compression: Model Reduction

Goals:

- Faster simulations,
- via smaller state-space $(\dim(x_r) \ll \dim(x))$,
- but preserving input-output behavior $(\|\tilde{y} - y\| \ll 1)$.

Means:

- Input-output system $\rightarrow$ System-theoretic model reduction
- Parametric system $\rightarrow$ Robust model reduction
- Nonlinear system $\rightarrow$ Data-driven model reduction
- Coupled system $\rightarrow$ Structured model reduction
- Large-scale system $\rightarrow$ "Port-Hamiltonian model reduction"
- Hyperbolic system $\rightarrow$ Dominant subspace model reduction[5,6]?

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[5] P. Benner, C. Himpe: **Cross-Gramian-Based Dominant Subspaces**; Advances in Computational Mathematics 45(5): 2533–2553, 2019. doi:10.1007/s10444-019-09724-7

[6] S. Grundel, C. Himpe, J. Saak: **On Empirical System Gramians**; Proceedings in Applied Mathematics and Mechanics 19: e201900006, 2019. doi:10.1002/pamm.201900006

Projection-Based Model Reduction

Petrov-Galerkin Projection:

$$U \in \mathbb{R}^{N \times n}, V \in \mathbb{R}^{n \times N}, VU = I_n$$

Idea:

$$\dot{x} = f(x) \quad \underset{x \approx U x_r}{\overset{x_r := Vx}{\rightarrow}} \quad U\dot{x}_r = f(Ux_r) \quad \overset{VU = I_n}{\rightarrow} \quad \dot{x}_r = Vf(Ux_r)$$

Reduced Order Model (ROM):

$$\begin{aligned} VE(U\dot{x}_r(t)) &= VA(Ux_r(t)) + VBu(t) + Vf(Ux_r(t)) \\ \tilde{y}(t) &= C(Ux_r(t)) \end{aligned}$$

Structured Projection → Structured ROM:

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}, V = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$$

Projection-Based Model Reduction

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Reduced Order Model (ROM):

$$\begin{aligned}(VEU)\dot{x}_r(t) &= (VAU)x_r(t) + (VB)u(t) + Vf(Ux_r(t)) \\ \tilde{y}(t) &= (CU)x_r(t)\end{aligned}$$

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Reduced Order Model (ROM):

$$\begin{aligned} E_r \dot{x}_r(t) &= A_r x_r(t) + B_r u(t) + Vf(Ux_r(t)) \\ \tilde{y}(t) &= C_r x_r(t) \end{aligned}$$

Structured Projection → Structured ROM:

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}, V = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$$

Projector Computation

Data-Driven Reachability:

$$W_R := \sum_{k=1}^{K} \sum_{m=1}^{N_s+N_d} \int_0^T X_m(t;\theta_k)\, X_m(t;\theta_k)^\intercal \, \mathrm{d}t$$

Data-Driven Observability (for nonlinear systems)**:**

$$W_O := \sum_{k=1}^{K} \int_0^T Y_{[1:N]}(t;\theta_k)^\intercal \, Y_{[1:N]}(t;\theta_k) \, \mathrm{d}t$$

$\rightarrow$ SVD of W_R (and W_O or W_R^*) then defines projectors.

Projector Computation

Data-Driven Reachability:

$$W_R := \sum_{k=1}^{K} \sum_{m=1}^{N_s+N_d} \int_0^T X_m(t;\theta_k)\, X_m(t;\theta_k)^\intercal \,\mathrm{d}t$$

Data-Driven Adjoint Reachability (= observability for port-Hamiltonian systems)**:**

$$W_R^* := \sum_{k=1}^{K} \sum_{m=1}^{N_s+N_d} \int_0^T Z_m(t;\theta_k)\, Z_m(t;\theta_k)^\intercal \,\mathrm{d}t$$

$\rightarrow$ SVD of W_R (and W_O or W_R^*) then defines projectors.

Tested Reductors

Reductor	Variants
Proper Orthogonal Decomposition (POD)	Reachability
Empirical Dominant Subspaces	Reachability & Observability
Empirical Dominant Subspaces	Minimality
Empirical Dominant Subspaces	Averaged Minimality
Balanced POD	Reachability & Observability
Empirical Balanced Truncation	Reachability & Observability
Empirical Balanced Truncation	Minimality
Empirical Balanced Truncation	Averaged Minimality
Goal-Oriented POD	Reachability
Empirical Balanced Gains	Reachability & Observability
Empirical Balanced Gains	Minimality
Empirical Balanced Gains	Averaged Minimality
Dynamic Mode Decomposition Galerkin	Reachability

Some Notes on Solvers

- Quality of the dynamic solution determines data-driven ROM quality.
- The initial condition for the dynamic problem is steady state solution.
- Steady-state problem is solved by iterated QR-based least-norm solver.
- Nonlinear system $\rightarrow$ explicit solver *vs.* Stiff system $\rightarrow$ implicit solver.

Tested Solvers	**Type**
`ode23s`	Adaptive 2nd Order Rosenbrock
IMEX1	1st Order Implicit-Explicit
IMEX2	2nd Order Implicit-Explicit Runge-Kutta
RK4	4th Order "Classic" Explicit Runge-Kutta
RK52	5-Stage, 2nd Order Hyperbolic Runge-Kutta
RK64	6-Stage, 4th Order Hyperbolic Runge-Kutta

Many-to-Many Benchmarking

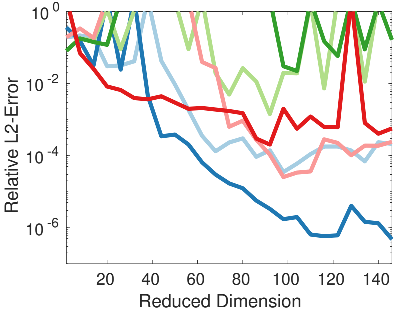
How to compare ... ?

- 2 Models
- 6 Solvers
- 13 Reductors
- > 30 Networks

MORscore![7]

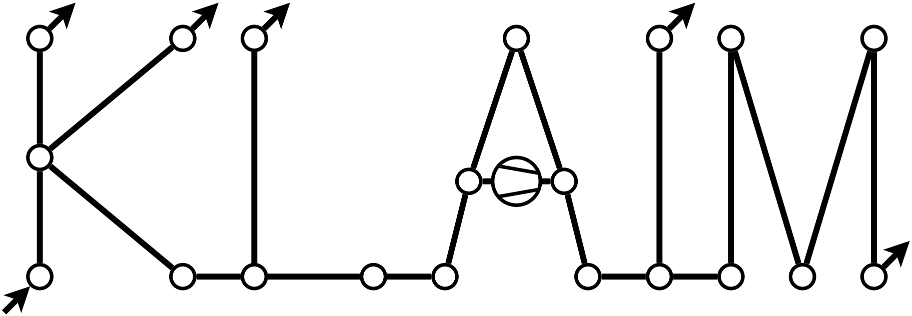
- Lowest attained error?
- Fastest error decay?
- Non-monotonic error decay?
- Sortable measure?

→ MORscore: Area above error graph.



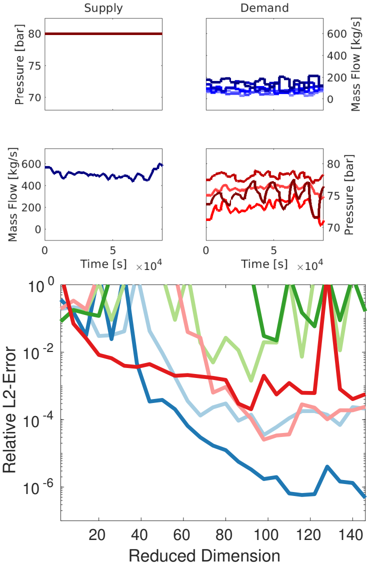
[7] C. Himpe: **Comparing (Empirical-Gramian-Based) Model Order Reduction Algorithms**; in: Model Reduction of Complex Dynamical Systems: 141–164, 2021. doi:10.1007/978-3-030-72983-7_7

Example: KLAIM Network

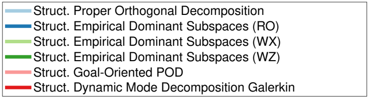


- Supply nodes: 1
- Demand nodes: 5
- Compressors: 1
- Solver: IMEX1
- Reductors: 6 (Galerkin-only)
- Boundary ports: 6
- State space: 1205
- Time horizon: $24h$
- Training*: Step inputs
- Scenario: Random demands

Numerical Results



Reductor	MORscore
Proper Orthogonal Decomposition	0.17
Empirical Dominant Subspaces (RO)	0.25
Empirical Dominant Subspaces (WX)	0.05
Empirical Dominant Subspaces (WZ)	0.01
Goal-Oriented POD	0.13
Dynamic Mode Decomposition Galerkin	0.16



Summary

After numerous tests with various networks we recommend:

- Model: Port-Hamiltonian Endpoint Discretization
- Solver: 1st Order Implicit-Explicit Time Stepper
- Reductor: Empirical Dominant Subspaces (Reachability-Observability)

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

https://git.io/morgen

C. Himpe, S. Grundel, P. Benner: **Model Order Reduction for Gas and Energy Networks**; Journal of Mathematics in Industry 11: 13, 2021.
doi:10.1186/s13362-021-00109-4