



MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG



COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY

Cross-Covariance-Based Model Reduction

P. Benner, S. Grundel, C. Himpe



Max Planck Institute Magdeburg
Computational Methods in System and Control Theory Group
Simulation of Energy Systems Team

MS28 – Model Reduction Methods for Simulation and (Optimal) Control
ENUMATH – European Conference on Numerical Mathematics

2017–09–26

Mathematically:

- Many-query large-scale nonlinear input-output system.
- Use data-driven nonlinear model reduction.
- Transfer concepts from linear systems.
- Reuse results from system theory,
- based on empirical balancing¹.

Practically:

- Repeated simulation of gas transportation networks.
- Transient behaviour on typical temporal resolutions.
- Test families of possible supply-demand scenarios.
- Uncertainty quantification for unsteady supply.
- Short-term dispatch forecasts.

¹C. H. **Combined State and Parameter Reduction for Nonlinear Systems with an Application in Neuroscience.** Westfälische Wilhelms Universität Münster, 2016.



MathEnergy:

 Mathematical Key Technologies for Evolving Energy Grids.

Partners:

 Fraunhofer SCAI

 Fraunhofer ITWM

 **Max Planck Institute Magdeburg** (Sub-Project: Model Reduction)

 Technische Universität Berlin

 Technische Universität Dortmund

 Humboldt Universität zu Berlin

 Friedrich-Alexander Universität Erlangen-Nürnberg

 PSI AG

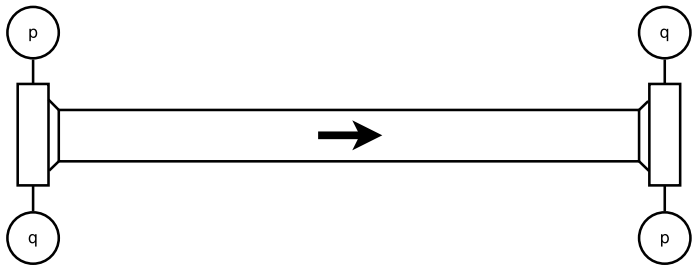
Funding:

 German Federal Ministry for Economic Affairs and Energy (BMWi)



Input:

- Pressure @ Inlet (Supply)
- Mass-Flux @ Outlet (Demand)



Output:

- Mass-Flux @ Inlet (Supply)
- Pressure @ Outlet (Demand)



1D Isothermal Euler Equation²:

$$\frac{1}{\gamma_0} \frac{\partial}{\partial t} p = - \left(\frac{z_0(p)^2}{z_0(p) - pz'_0(p)} \right) \frac{1}{S} \frac{\partial}{\partial x} q,$$

$$\frac{1}{S} \frac{\partial}{\partial t} q = - \frac{\partial}{\partial x} p \underbrace{- \frac{\gamma_0}{S^2} \frac{\partial}{\partial x} \frac{q^2 z_0(p)}{p}}_{\text{Inertia Term}} \underbrace{- \frac{g}{\gamma_0} \frac{p}{z_0(p)} \frac{\partial}{\partial x} h}_{\text{Gravity Term}} \underbrace{- \frac{\lambda(q)\gamma_0}{2DS^2} z_0(p) \frac{q|q|}{p}}_{\text{Friction Term}}$$

- Average pressure / mass-flux over pipe cross-section area.
- Conservation of momentum / mass
- Hyperbolic (coupled transport)
- Nonlinear (friction term)
- Additional nonlinearities (compressibility)

²S. Grundel, N. Hornung, B. Klaassen, P. Benner and T. Clees. **Computing Surrogates for Gas Network Simulation Using Model Order Reduction.** In: Surrogate-Based Modeling and Optimization, Applications in Engineering: 189–212, 2013.



Spatial Discretization and Index Reduction^{3,4}:

$$\begin{pmatrix} E_1 & 0 \\ 0 & \mathbb{1} \end{pmatrix} \begin{pmatrix} \dot{p}_h \\ \dot{q}_h \end{pmatrix} = \begin{pmatrix} 0 & A_1 \\ A_2 & 0 \end{pmatrix} \begin{pmatrix} p_h \\ q_h \end{pmatrix} + \begin{pmatrix} f_p(p_h, u_p) \\ f_q(p_h, q_h, u_p) \end{pmatrix} + \begin{pmatrix} 0 & B_1 \\ B_2 & 0 \end{pmatrix} \begin{pmatrix} u_p \\ u_q \end{pmatrix}$$
$$\begin{pmatrix} y_p \\ y_q \end{pmatrix} = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix} \begin{pmatrix} p_h \\ q_h \end{pmatrix}$$

- Descriptor system,
- Index-1 differential-algebraic equation (DAE).
- Analytic index reduction to index-0 \rightarrow implicit ODE.

³S. Grundel, L. Jansen, N. Hornung, T. Clees, C. Tischendorf and P. Benner. **Model Order Reduction of Differential Algebraic Equations Arising from the Simulation of Gas Transport Networks**. In: Progress in Differential-Algebraic Equations, Differential Equation Forum: 183–205, 2014.

⁴S. Grundel, N. Hornung and S. Roggendorf. **Numerical Aspects of Model Order Reduction for Gas Transportation Networks**. In: Simulation-Driven Modeling and Optimization: 1–28, 2016.

Abstract Input-Output System:

$$\begin{pmatrix} E_p \dot{p}_h \\ \dot{q}_h \end{pmatrix} = \begin{pmatrix} f_p(p_h, q_h, u_p, u_q) \\ f_q(p_h, q_h, u_p, u_q) \end{pmatrix}$$
$$\begin{pmatrix} y_p \\ y_q \end{pmatrix} = \begin{pmatrix} g_p(p_h) \\ g_q(q_h) \end{pmatrix}$$

- Supply pressure $u_p(t) := p(0, t)$
- Demand mass-flux $u_q(t) := q(L, t)$
- Demand pressure $y_p(t) := p(L, t)$
- Supply mass-flux $y_q(t) := q(0, t)$

Target:

1. Find reduced order model,
2. approximating input-output behaviour,
3. without linearization.

Actual:

- Coupling (Pressure / Mass-flux)
- Nonlinear (Friction / Compressibility)
- Hyperbolicity



Cross-Covariance:

$$X_C(\tau) := \int_0^{\infty} F(t)G^*(\tau + t) dt$$

- τ is the lag between F and G .
- Matrix of pair-wise shifted co-movement indices.
- Normalize to obtain cross-correlation.



State-Output Cross-Covariance with zero lag ($\tau \equiv 0$):

$$X_C = \int_0^\infty \underbrace{x(t; \tilde{u})}_F \underbrace{[y^\top(t; \tilde{x}_{0,1}), \dots, y^\top(t; \tilde{x}_{0,N})]}_{G^*} dt$$

- SISO System: $\dim(u(t)) = \dim(y(t)) = 1$
- $x(t; \tilde{u})$ perturbed input state trajectory
- $y(t; \tilde{x}_{0,i})$ perturbed i -th initial state output trajectory
- Input-to-state and state-to-output mappings
- identify input-output behaviour.



Linear SISO System:

$$\dot{x}(t) = Ax(t) + bu(t)$$

$$y(t) = cx(t)$$

State-Output cross-covariance with unit perturbation:

$$X_C(0) = \int_0^{\infty} (e^{At} b \mathbf{1})(c e^{At} \mathbf{1}) dt = \int_0^{\infty} (e^{At} b)(c e^{At}) dt$$

$$\Rightarrow AX_C + X_C A = -bc$$



Linear SISO System:

$$\dot{x}(t) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} x(t) + \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} u(t)$$
$$y(t) = \begin{pmatrix} 0 & 1 & 1 \end{pmatrix} x(t)$$

Associated Cross-Covariance Matrix:

$$X_C = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Interpretation:

- SISO: State-Output Co-Movement
- Square MIMO: Input-Average State-Output Co-Movement
- MIMO: Input-Output-Average State-Output Co-Movement

Nonlinear:

- Instead of a closed form (for the impulse response)
 - we have to use simulated or measured data.
- Approximate nonlinear cross-covariance by data-driven approach⁵.

⁵ J. Hahn and T.F. Edgar. **Balancing Approach to Minimal Realization and Model Reduction of Stable Nonlinear Systems**. Industrial & Engineering Chemical Research, 41(9): 2204–2212, 2002.

Empirical Cross Covariance Matrix⁶ (square systems):

$$X_C := \sum_{m=1}^M \int_0^{\infty} \Psi^m(t) dt \in \mathbb{R}^{N \times N}$$

$$\Psi_{ij}^m(t) = (x_i^m(t) - \bar{x}_i^m)(y_m^j(t) - \bar{y}_m^j) \in \mathbb{R}$$

Empirical Cross Covariance Matrix⁷ (non-square systems):

$$X_c := \sum_{q=1}^Q \sum_{m=1}^M \int_0^{\infty} \Psi^m(t) dt \in \mathbb{R}^{N \times N}$$

$$\Psi_{ij}^m(t) = (x_i^m(t) - \bar{x}_i^m)(y_q^j(t) - \bar{y}_q^j) \in \mathbb{R}$$

⁶C. H. and M. Ohlberger. **Cross-Gramian Based Combined State and Parameter Reduction for Large-Scale Control Systems**. *Mathematical Problems in Engineering*, 2014:1–13, 2014.

⁷C. H. and M. Ohlberger. **A note on the cross Gramian for non-symmetric systems**. *System Science and Control Engineering*, 4(1): 199–208, 2016.



Reduced Order Input-Output (Descriptor) System:

$$\left. \begin{aligned} E\dot{x}(t) &= f(x(t), u(t)) \\ y(t) &= g(x(t), u(t)) \end{aligned} \right\} \xrightarrow{\text{MOR}} \left\{ \begin{aligned} E_r\dot{x}_r(t) &= f_r(x_r(t), u(t)) \\ \tilde{y}(t) &= g_r(x_r(t), u(t)) \end{aligned} \right.$$

- $u \mapsto x \mapsto y$
- $\dim(u(t)) \ll \dim(x(t))$
- $\dim(y(t)) \ll \dim(x(t))$
- $\dim(x_r(t)) \ll \dim(x(t))$
- $\|y - \tilde{y}\| \ll 1$

Projection-Based Reduced Order Model:

$$\begin{aligned}(V_1 E U_1) \dot{x}_r(t) &= V_1 f(U_1 x_r(t), u(t)) \\ \tilde{y}(t) &= g(U_1 x_r(t), u(t))\end{aligned}$$

- Approximation: $x_r := V_1 x(t) \rightarrow x(t) \approx U_1 x_r(t)$
- Reducing truncated projection: V_1
- Reconstructing truncated projection: U_1
- Bi-Orthogonality: $V_1 U_1 = \mathbb{1}$
- **Task:** Find U_1, V_1



Singular Value Decomposition:

$$X_C \stackrel{\text{SVD}}{=} U D V$$

Projections from Cross-Covariance based on D_{ii} :

- W.l.o.g. $\sigma_i = D_{ii}$ sorted descendingly.
- $U_{*(1\dots n)}$, $V_{(1\dots n)*}$ are left and right principal directions.
- Reconstructing projection: $U = (U_1 \ U_2)$
- Galerkin reducing projection: $V_1 = U_1^\top$
- Petrov-Galerkin reducing projection⁸: $V = (V_1 \ V_2)$

⁸D.C. Sorensen and A.C. Antoulas. **The Sylvester equation and approximate balanced reduction**. Linear Algebra and its Applications, 351–352: 671–700, 2002.



Cross-Covariance Structure for Gas Transport:

$$X_C = \begin{pmatrix} X_{C,pp} & X_{C,pq} \\ X_{C,qp} & X_{C,qq} \end{pmatrix}$$

Structured Reduced Order Model⁹:

$$\begin{pmatrix} (V_p E_p U_p) \dot{p}_r \\ \dot{q}_r \end{pmatrix} = \begin{pmatrix} V_p f_p(\bar{p} + U_p p_r, \bar{q} + U_q x_q, u_p, u_q) \\ V_q f_q(\bar{p} + U_p p_r, \bar{q} + U_q q_r, u_p, u_q) \end{pmatrix}$$
$$\begin{pmatrix} \tilde{y}_p \\ \tilde{y}_q \end{pmatrix} = \begin{pmatrix} g_p(\bar{p} + U_p p_r) \\ g_q(\bar{q} + U_q q_r) \end{pmatrix}$$

- Pipe is a coupled square MIMO system: 2 inputs and 2 outputs.
- Center pressure and mass-flux around steady state \bar{p} , \bar{q} .
- Only Perturbation training!

⁹H. Sandberg and R.M. Murray. **Model reduction of interconnected linear systems**. Optimal Control Applications and Methods, 30(3): 225–245, 2009.

Modified pipeline test¹⁰:

- Length: 10 km
- Diameter: 1 m
- Inclination: 0 m
- Roughness: 0.1 mm
- Reynolds Number: 5000
- Time Horizon: 1 h
- Refinement: 500 segments

¹⁰M. Chaczykowski. **Sensitivity of pipeline gas flow model to the selection of the equation of state.** Chemical Research Engineering and Design, 87: 1596–1603, 2007.

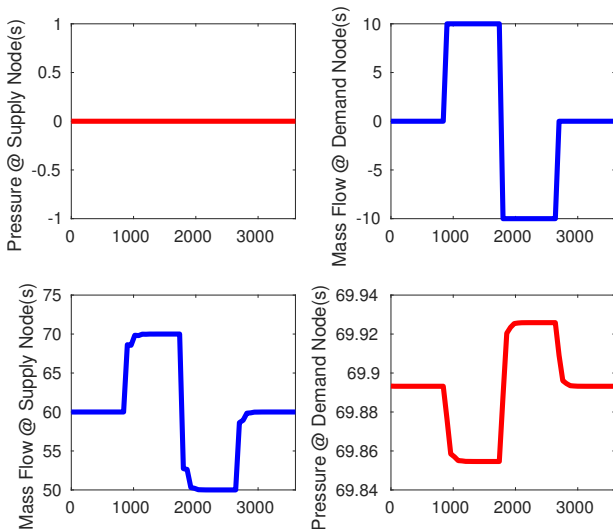


Figure: Supply pressure, demand mass-flux, supply mass-flux and demand pressure.



Empirical Gramians:

- Empirical Controllability Gramian
- Empirical Observability Gramian
- Empirical Linear Cross Gramian
- Empirical Cross Gramian*
- Empirical Sensitivity Gramian
- Empirical Identifiability Gramian
- Empirical Joint Gramian



Features:

- Interfaces for: Solver, inner product kernels & distributed memory
- Non-Symmetric option for all cross Gramians
- Compatible with OCTAVE and MATLAB
- Vectorized and parallelizable
- Open-source licensed
- Functional design

More info: <http://gramian.de>

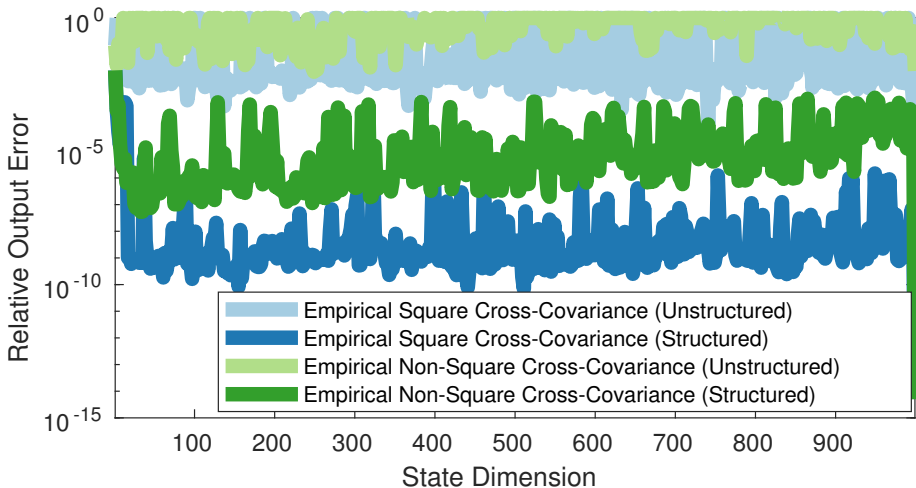


Figure: Relative L_2 model reduction error for the benchmark pipeline.

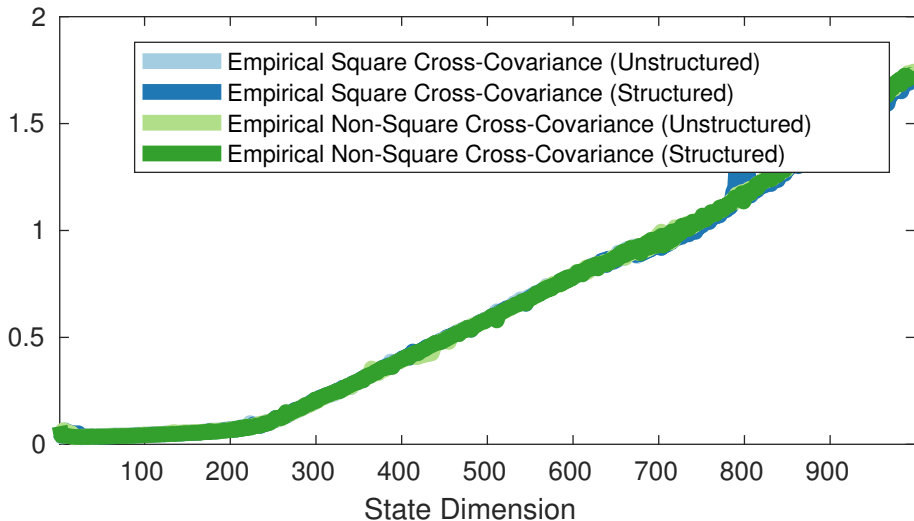


Figure: Relative computation time for the reduced order benchmark pipeline.



From Pipelines to Pipe Networks:

- Repetitive modelling¹¹.
- Conservation of mass in all nodes.
- Conservation of energy in all nodes.

Up Next:

- Large complex networks
- Include compressors
- Include valves
- Per-pipe parameters
- Power grid / gas net coupling

¹¹T.P. Azevedo-Perdicoúlis and G. Jank. **Modelling Aspects of Describing a Gas Network Through a DAE System.** IFAC Proceedings Volume, 40(20): 40–45, 2007.

- Gas Transport in Pipelines: Isothermal Euler equations.
- System-theoretic: Balancing controllability and observability.
- Nonlinear cross-covariance: Empirical cross Gramian matrix.

<http://mathenergy.de>

<http://himpe.science>

Acknowledgment:

Supported by the German Federal Ministry for Economic Affairs and Energy, in the joint project: “**MathEnergy** – Mathematical Key Technologies for Evolving Energy Grids”, sub-project: Model Order Reduction (Grant number: 0324019**B**).