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FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
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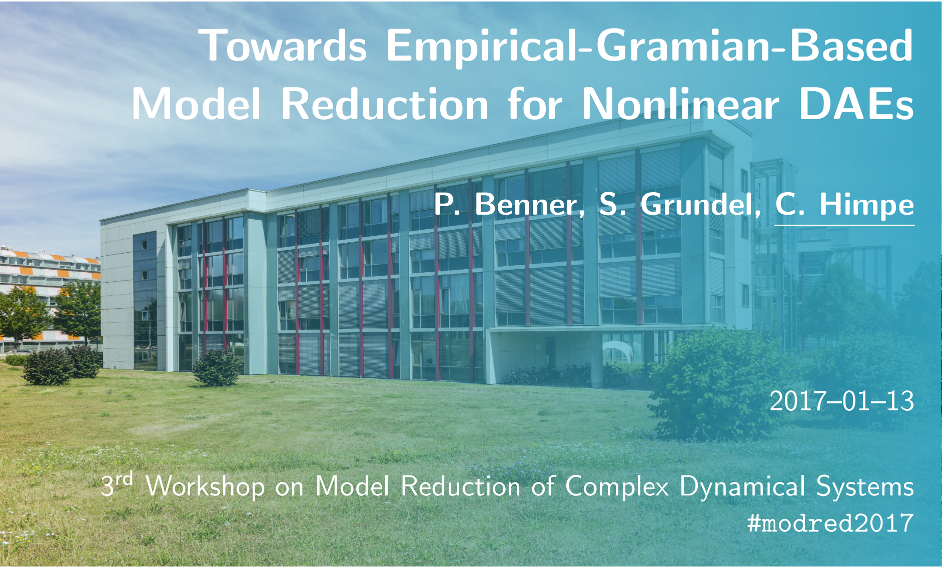
CSC COMPUTATIONAL METHODS IN
SYSTEMS AND CONTROL THEORY



Towards Empirical-Gramian-Based Model Reduction for Nonlinear DAEs

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3rd Workshop on Model Reduction of Complex Dynamical Systems
#modred2017

Aim

Model Reduction for:

- (Parametric)
- Nonlinear
- Descriptor

Input-Output Systems.

Motivation

Application:

- Scenario analysis
- for gas transportation networks
- to forecast and verify supply and demand balance.

Why Model Reduction?

- Enable or accelerate simulations (larger networks)
- in many-query settings
- such as uncertainty quantification.

MathEnergy Project

Cooperation Project Partners:

- Fraunhofer SCAI
- Fraunhofer ITWM
- **Max Planck Institute Magdeburg**
- Technische Universität Berlin
- Technische Universität Dortmund
- Humboldt Universität zu Berlin
- Friedrich-Alexander Universität Erlangen-Nürnberg
- PSI AG
- Venios GmbH

Funding:

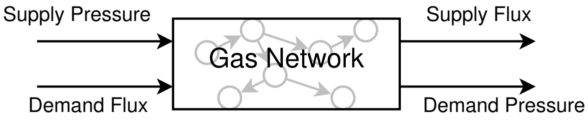
- German Federal Ministry for Economic Affairs and Energy (BMWi)

Outline

1. Gas network model
2. Model reduction
3. Preliminary results
4. Outlook

Gas Transport Network

Input-output model:



Input: supply pressure, demand mass flux

State: pressure & flux in network's **pipes**

Output: supply flux, demand pressure

Scenario analysis: simulating different

- supply pressure situations
- demand flux situations
- (parameter configurations)

1D (Simplified) Isothermal Euler Equations:

$$\frac{\partial p}{\partial t} = -\frac{\partial q}{\partial x}$$
$$\frac{\partial q}{\partial t} = -c^2 \frac{\partial p}{\partial x} - \frac{\lambda}{2D} \frac{q|q|}{p}$$

Variables:

$p(x, t)$ pressure

$q(x, t)$ (mass-)flux

Constants:

λ (approximate) friction coefficient

D pipe's diameter

c speed of sound in the transported gas

S. 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: 189–212, 2013.

Gas Pipeline Model (Semi-Discrete) [Grundel et al'14]

Spatial Finite Difference Discretization:

$$\frac{\partial}{\partial t}\frac{p_R + p_L}{2} = -\frac{q_R - q_L}{L}$$

$$\frac{\partial}{\partial t}\frac{q_R + q_L}{2} = -c^2\frac{p_R - p_L}{L} - \frac{\lambda}{4D}\frac{q_R + q_L|q_R + q_L|}{p_R + p_L}$$

Variables:

- $p_L(t)$ pressure at inlet
- $p_R(t)$ pressure at outlet
- $q_L(t)$ (mass-)flux at inlet
- $q_R(t)$ (mass-)flux at outlet

Constants:

- λ (approximate) friction coefficient
- D pipe's diameter
- c speed of sound in the transported gas
- L pipe's length

S. Grundel, 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: 183–205, 2014.

Network Representation by a Graph:

- Edges: correspond to pipelines
- Nodes: correspond to:
  - Junctions: connecting two pipelines
  - Supplies: inserting gas into the network
  - Demands: extracting gas from the network

Graph Encoding:

- N_e Number of edges
- N_0 Number of junctions
- N_S Number of supply nodes
- N_D Number of demand nodes

Junction and demand incidence matrix: $A_0 \in \{-1, 0, 1\}^{(N_0+N_D)\times N_e}$

Supply incidence matrix: $A_S \in \{0, 1\}^{N_S \times N_e}$

T.-P. Azeveda-Pericoulis and G. Jank. **Modelling Apspects of Describing a Gas Network Through a DAE System**. In Proceedings of the 3rd IFAC Symposium on System Structure and Control 40(20): 40–45, 2007.

Repetitive modeling:

$$\frac{\partial}{\partial t}\frac{p_R^k + p_L^k}{2} = -\frac{q_R^k - q_L^k}{L}$$

$$\frac{\partial}{\partial t}\frac{q_R^k + q_L^k}{2} = -c_k^2\frac{p_R^k - p_L^k}{L} - \frac{\lambda_k}{4D_k}\frac{q_R^k + q_L^k|q_R^k + q_L^k|}{p_R^k + p_L^k}$$

$$0 = \sum q_R^j - \sum q_L^j - d_i(t) \quad (1)$$

$$0 = p_L^i(t) - s_i(t) \quad (2)$$

Input functions:

$s_i(t)$ Supply pressure

$d_i(t)$ Demand flux

Balance Constraints:

- Kirchhoff's First Law: (1)
- Kirchhoff's Second Law: (2)

S. 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.

Matrix formulation:

$$
\begin{aligned}
|A_S|^\intercal \frac{\partial p_s}{\partial t} + |A_0|^\intercal \frac{\partial p_0}{\partial t} &= -L^{-1} \frac{q_R - q_L}{2} \\
\frac{\partial}{\partial t} \frac{q_R + q_L}{2} &= -\frac{c^2}{L} (A_S^\intercal p_s + A_0^\intercal p_0) - \frac{\lambda}{D} \frac{\frac{q_R - q_L}{2} \left| \frac{q_R - q_L}{2} \right|}{|A_S|^\intercal p_s + |A_0|^\intercal p_0} \\
0 &= A_0 q_R + |A_0| q_L - d(t) \\
0 &= p_s - s(t)
\end{aligned}
$$

- p_s supply pressure
- p_0 junction and demand pressure

Gas Network Properties

Input-Output Form:

$$
\begin{aligned}
E\dot{x}(t) &= f(x(t), u(t)) \\
y(t) &= Cx(t) \\
\det(E) &= 0
\end{aligned}
$$

- Hyperbolic (Transport terms)
- Nonlinear (Friction term)
- Hierarchical (Network description & physical description)
- Structured (Pressure & flux states)

Extensions:

- Gas compressibility
- Gravity
- Compressor stations

Analytic Index Reduction [Grundel et al'14]

Implicit ODE:

$$|A_0| L^{-1} |A_0|^\intercal \frac{\partial p_0}{\partial t} = A_0 \frac{q_R + q_L}{2} - d(t) - |A_0| L^{-1} |A_S|^\intercal \frac{\partial s}{\partial t}$$

$$\frac{\partial}{\partial t} \frac{q_R + q_L}{2} = -\frac{c^2}{L} A_0^\intercal p_0 + \frac{\frac{q_R+q_L}{2} \left| \frac{q_R+q_L}{2} \right|}{|A_S|^\intercal s(t) + |A_0|^\intercal p_0} - \frac{c^2}{L} A_S^\intercal s(t)$$

Input-Output Form:

$$E\dot{x}(t) = f(x(t), u(t))$$
$$y(t) = Cx(t)$$
$$\det(E) \neq 0$$

General Model

Input-Output System:

$$E\dot{x}(t) = f(x(t), u(t))$$
$$y(t) = g(x(t), u(t))$$
$$x(0) = x_0$$

Input:	$u : \mathbb{R} \to \mathbb{R}^M$
State:	$x : \mathbb{R} \to \mathbb{R}^N$
Output:	$y : \mathbb{R} \to \mathbb{R}^Q$
Non-singular	$E \in \mathbb{R}^{N \times N}$
Vector field:	$f : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^N$
Output functional:	$g : \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}^Q$

Model Reduction

Reduced Order Model:

$$\begin{aligned} E_r \dot{x}_r(t) &= f_r(x_r(t), u(t)) \\ y_r(t) &= g_r(x_r(t), u(t)) \\ x_r(0) &= x_{r,0} \end{aligned}$$

Reduced state:	$x_r : \mathbb{R} \to \mathbb{R}^{n \ll N}$
Reduced output:	$y_r : \mathbb{R} \to \mathbb{R}^Q$
Model reduction error:	$\|y - y_r\| \ll 1$
Reduced matrix:	$E_r \in \mathbb{R}^{n \times n}$
Reduced vector field:	$f_r : \mathbb{R}^n \times \mathbb{R}^M \to \mathbb{R}^n$
Reduced output functional:	$g_r : \mathbb{R}^n \times \mathbb{R}^M \to \mathbb{R}^Q$

Projection-Based Reduced Order Model:

$$\begin{aligned} (V_1 E U_1)\dot{x}_r(t) &= V_1 f(U_1 x_r(t), u(t)) \\ y_r(t) &= g(U_1 x_r(t), u(t)) \\ x_r(0) &= V_1 x_0 \end{aligned}$$

Reconstructing truncated projection: $U_1 \in \mathbb{R}^{N \times n}$
Reducing truncated projection: $V_1 \in \mathbb{R}^{n \times N}$

Task: find U_1 and V_1.

Linear Time-Invariant System:

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

Cross Gramian (of a square system):

$$W_X := \int_0^\infty \mathrm{e}^{At}\, BC\, \mathrm{e}^{At}\, \mathrm{d}t \in \mathbb{R}^{N \times N}$$

Approximately balancing projection:

$$W_X \overset{\text{SVD}}{=} UDV \to \begin{cases} U = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \\ V = \begin{pmatrix} V_1 & V_2 \end{pmatrix}^\intercal \end{cases}$$

K.V. Fernando and H. Nicholson. **On the Structure of Balanced and Other Principal Representations of SISO Systems**. IEEE Transactions on Automatic Control 28(2): 228–231, 1983.
D.C. Sorensen and A.C. Antoulas. **The Sylvester equation and approximate balanced reduction**. Linear Algebra and its Applications 351–352: 671–700, 2002.

Empirical Linear Cross Gramian:

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

Empirical Cross Gramian:

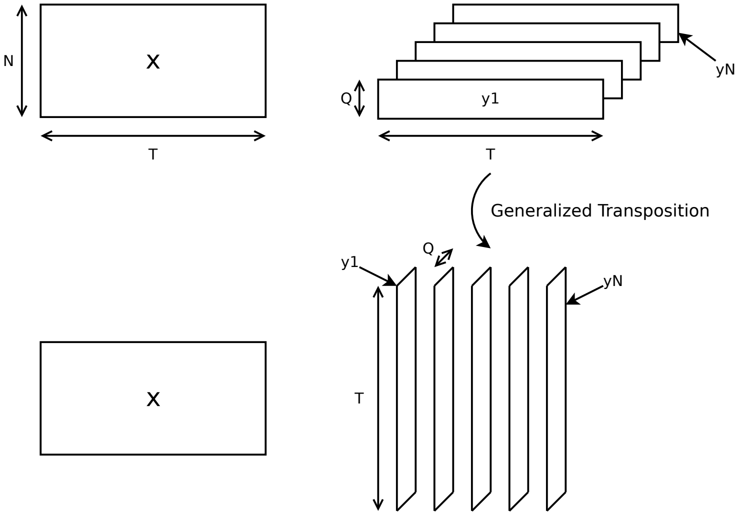
$$\widehat{W}_X := \frac{1}{|S_u||S_x|M} \sum_{k=1}^{|S_u|} \sum_{l=1}^{|S_x|} \sum_{m=1}^{M} \frac{1}{c_k d_l} \int_0^\infty \Psi^{klm}(t) \, \mathrm{d}t$$

$$\Psi_{ij}^{klm}(t) = \langle x_i^{km}(t) - \bar{x}_i^{km}, y_m^{lj}(t) - \bar{y}_m^{lj} \rangle$$

- Applicable to nonlinear (square) systems.
- For asymptotically stable systems: $\widehat{W}_X = W_X$
- Related to (balanced) POD and balanced truncation

S. Streif, R. Findeisen and E. Bullinger. **Relating Cross Gramians and Sensitivity Analysis in Systems Biology**. Theory of Networks and Systems 10.4: 437–442, 2006.
C. Himpe and M. Ohlberger. **Cross-Gramian Based Combined State and Parameter Reduction for Large-Scale Control Systems**. Mathematical Problems in Engineering 2014: 1–13, 2014.

Empirical Cross Gramian Assembly



Non-Symmetric Linear Cross Gramian:

$$W_Z = \int_0^\infty \mathrm{e}^{At} \Big(\sum_{i=1}^{M} B_{*,i} \Big) \Big(\sum_{j=1}^{Q} C_{j,*} \Big) \mathrm{e}^{At} \, \mathrm{d}t$$

Empirical Non-Symmetric Cross Gramian:

$$\widehat{W}_Z := \frac{1}{|S_u||S_x|M} \sum_{k=1}^{|S_u|} \sum_{l=1}^{|S_x|} \sum_{m=1}^{M} \sum_{q=1}^{Q} \frac{1}{c_k d_l} \int_0^\infty \Psi^{klmq}(t) \, \mathrm{d}t$$

$$\Psi_{ij}^{klmq}(t) = \langle x_i^{km}(t) - \bar{x}_i^{km}, y_q^{lj}(t) - \bar{y}_q^{lj} \rangle$$

- Applicable to systems with arbitrary input-output configurations,
- since a cross Gramian of a SISO system is effectively computed;
- in the linear case for the "averaged" system.

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

(Empirical) Cross Gramian Structure:

$$W_X = \begin{pmatrix} W_{X,pp} & W_{X,pq} \\ W_{X,qp} & W_{X,qq} \end{pmatrix}$$

Component-wise projections:

$$\left.\begin{aligned} W_{X,pp} &\overset{\text{SVD}}{=} U_p D_p V_p \to \begin{cases} U_p = \begin{pmatrix} U_{p,1} & U_{p,2} \end{pmatrix} \\ V_p = \begin{pmatrix} V_{p,1} & V_{p,2} \end{pmatrix}^\intercal \end{cases} \\ W_{X,qq} &\overset{\text{SVD}}{=} U_q D_q V_q \to \begin{cases} U_q = \begin{pmatrix} U_{q,1} & U_{q,2} \end{pmatrix} \\ V_q = \begin{pmatrix} V_{q,1} & V_{q,2} \end{pmatrix}^\intercal \end{cases} \end{aligned}\right\} \to \begin{cases} U_1 = \begin{pmatrix} U_{p,1} & 0 \\ 0 & U_{q,1} \end{pmatrix} \\ V_1 = \begin{pmatrix} V_{p,1} & 0 \\ 0 & V_{q,1} \end{pmatrix} \end{cases}$$

H.Sandberg and R.M. Murray. **Model reduction of interconnected linear systems**. Optimal Control Applications and Methods 30(3): 225–245, 2009.
A. Vandendorpe and P. Van Dooren **Model Reduction of Interconnected Systems**. In Model Order Reduction: Theory, Research Aspects and Applications: 305–321, 2008.

Model and Reduction Summary

1. Assemble Semi-Discrete Model
   - Euler equations $\rightarrow$ pipe
   - Repetitive modeling $\rightarrow$ gas network
   - DAE model $\rightarrow$ implicit ODE model
2. Data-Driven Model Reduction
   - Simulate discrete state and output trajectories
   - Empirical Cross Gramian
     - Symmetric
     - Non-Symmetric
3. Reduced Order Model
   - Unstructured
   - Structured

Modular components:

- Networks
- Models
- Solvers
- Reductors

Features:

- Data-driven approach
- Functional design
- JSON encoded network data
- Compatible with OCTAVE and MATLAB
- Vectorized modules

Under Construction!

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:

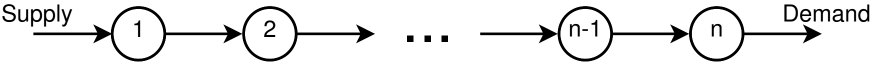
- Interfaces for: Solver, inner product kernels & distributed memory
- Non-Symmetric option for all cross Gramians
- Compatible with OCTAVE and MATLAB
- Vectorized and parallelizable
- Open-source licensed

More info: `http://gramian.de`

C. Himpe. **emgr - The empirical Gramian Framework**. Submitted, Preprint: arXiv (cs.MS): 1611.00675, 2016.

Numerical Experiment

Procedural Pipeline Model:



System Dimensions:

- $N_S = 1$
- $N_0 = 32$
- $N_D = 1$

Setup:

- Input-Output Model
- Implicit ODE model
- Impulse perturbation

Numerical Results: POD ROM

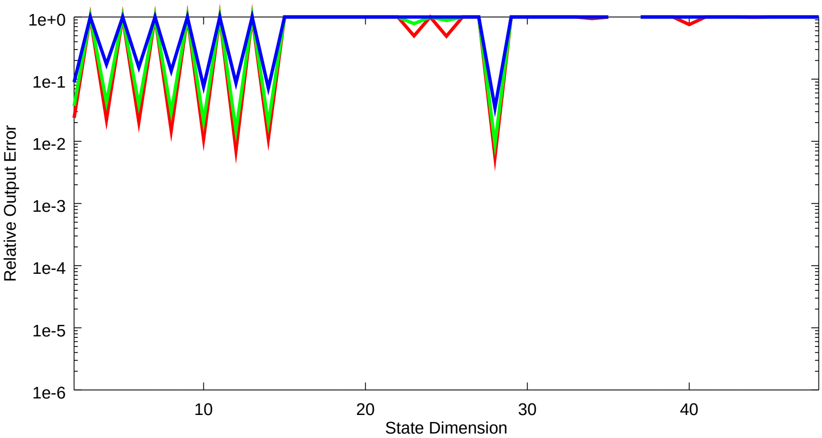


Figure: Relative L_1, L_2, L_∞ model reduction output error.

Numerical Results: W_X ROM

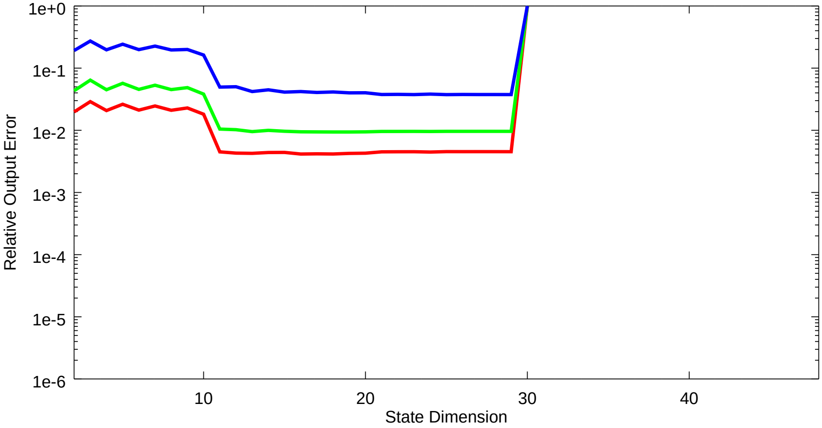


Figure: Relative L_1, L_2, L_∞ model reduction output error.

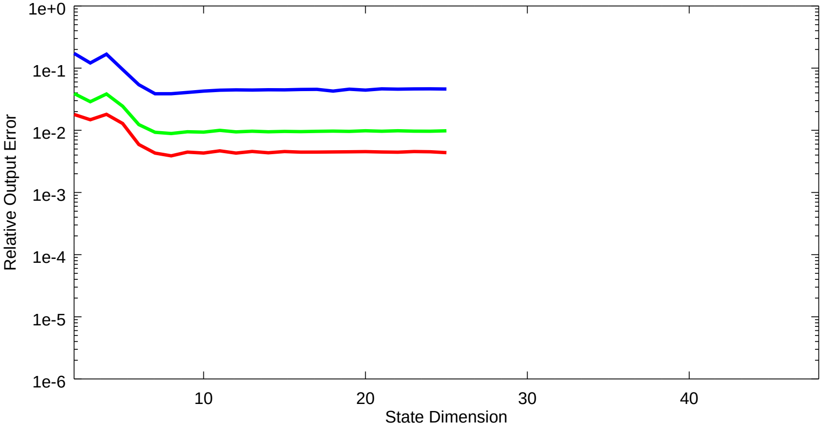


Figure: Relative L_1, L_2, L_∞ model reduction output error.

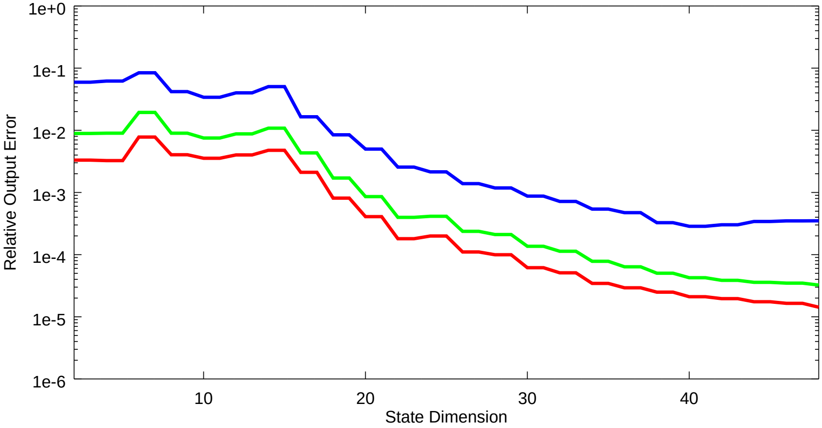


Figure: Relative L_1, L_2, L_∞ model reduction output error.

Numerical Results: W_Z^{pq} ROM

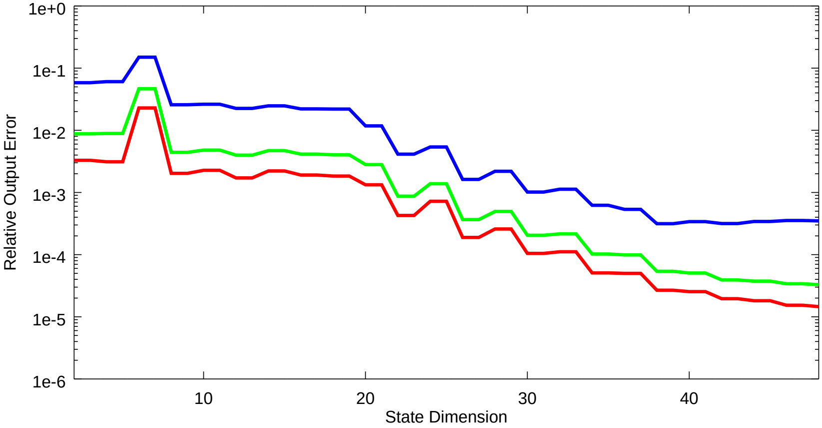


Figure: Relative L_1, L_2, L_∞ model reduction output error.

Outlook

- Compressors (linear / nonlinear)
- Valves (switched systems)
- Reservoirs
- **Hyperbolicity**
- DAE Decoupling
- Direct descriptor reduction

In Conclusion

Summary:

- Empirical-Cross-Gramian-Based model reduction
- for nonlinear (hyperbolic) DAE models
- of gas transport networks.

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