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# Gas Networks, Brain Networks, and Model Reduction

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SimTech Seminar on Model Reduction
and Data Techniques for Surrogate Modelling

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living.knowledge

MM Mathematics Münster Cluster of Excellence

MaRDI

# › Outline

- **Common Theme:**
  Projection-Based Model Reduction
- **Gas Networks:**
  Parametric Model Order Reduction
- **Brain Networks:**
  Combined State and Parameter Reduction
- **Common Approach:**
  Data-Driven Assembly of System-Theoretic Operators

# › Overarching Model

## Parametric Nonlinear Input-Output System:

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

- State: $x : \mathbb{R} \to \mathbb{R}^N$
- Input: $u : \mathbb{R} \to \mathbb{R}^M$
- Output: $y : \mathbb{R} \to \mathbb{R}^Q$
- Parameter: $\theta \in \mathbb{R}^P$
- Dimension: $N \gg 1$
- System Matrix: $A \in \mathbb{R}^{N \times N}$
- Input Matrix: $B \in \mathbb{R}^{N \times M}$
- Output Matrix: $C \in \mathbb{R}^{Q \times N}$
- Mass Matrix Map: $E : \mathbb{R}^P \to \mathbb{R}^{N \times N}$
- Nonlinearity: $f : \mathbb{R}^N \times \mathbb{R}^P \to \mathbb{R}^N$

# › Gas Networks

Joint work with: **P. Benner** & **S. Grundel**

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

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

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

P. Benner, S. Grundel, C. Himpe, C. Huck, T. Streubel, C. Tischendorf: **Gas Network Benchmark Models**;
Applications of Differential-Algebraic Equations: Examples and Benchmarks: 171–197, 2018. doi:10.1007/11221_2018_5

C. Himpe, S. Grundel, P. Benner: **Next-Gen Gas Network Simulation**;
Progress in Industrial Mathematics: In Press, 2022. arxiv:2108.02651

# › Motivation

## 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 mixture tracking (!!!)
- Gas-fired power-plants
- Energy storage

# › Gas Pipeline

## Friction-Dominated 1D Isothermal Euler Equations in a Long Pipe:

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

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

- Pressure: $p(x,t)$
- Mass-Flux: $q(x,t)$
- Pipe Incline: $h_x$
- Pipe Diameter: $d$
- Pipe Cross-Section: $S$
- Friction Factor: $\lambda_0$
- 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-State-Output System

## Port-Hamiltonian (pH) 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: $d_p$

# › Parametric Model Order Reduction

**Goal:**

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

**Reducing and Reconstructing Projections:**

$$x_r(t) := V_r\, x(t) \;\; \to \;\; x(t) \approx U_r\, x_r(t)$$

**Reduced Order Model:**

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

**Note:** Projection-based model reduction for a hyperbolic system!

# › System-Theoretic Idea (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):**

$$W_C \overset{\text{rrSVD}}{=} U_C D_C U_C^\top, \qquad W_O \overset{\text{rrSVD}}{=} U_O D_O U_O^\top$$
$$\begin{bmatrix} (U_C D_C) & (U_O D_O) \end{bmatrix} \overset{\text{rrSVD}}{=} U\;D\;T, \quad V := U^\top$$

# › System-Theoretic Idea (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 (Refined):

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

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

# › System-Theoretic Idea (DSPMR-X)

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

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

**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 Computation

## 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 the pH system's local (repeated scalar) nonlinarity.

# › Some Remarks

- Choice of solver is fundamental for efficiency and reducibility!
- Step functions as generic training input due to hyperbolicity!
- Fast training ($1h$ training for $24h$ tests)!
- Dynamics only relative to steady-state!
- Structured reduction ( $p$ and $q$ separately) is essential!
- Centering of training trajectories is important!
- Galerkin methods preserve stability for this pH model class!
- DSPMR(-X) is a (input-output) Galerkin method!
- Dimension reduction by SVDs of covariances of simulations ...
  $\rightarrow$ **Unsupervised Learning of System Properties via Synthetic Data**

# › Tested Methods

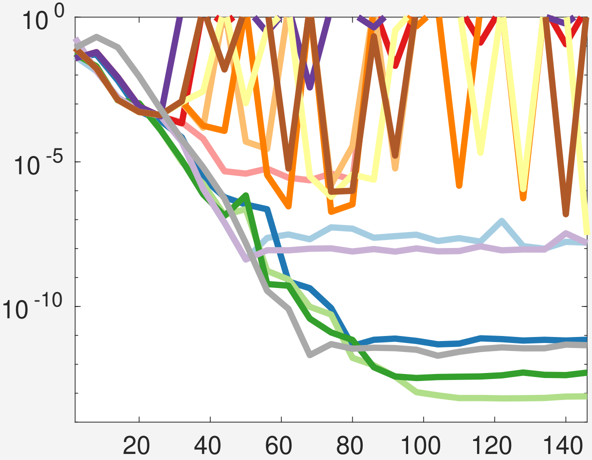
| Reductor | Properties |
|---|---|
| Structured Proper Orthogonal Decomposition (POD) | Reachability |
| Structured Empirical Dominant Subspaces (DSPMR) | Reachability & Observability |
| Structured Empirical Dominant Subspaces (DSPMR-X) | Minimality |
| Structured Empirical Dominant Subspaces (DSPMR-Z) | Average Minimality |
| Structured Balanced POD (BPOD) | Reachability & Observability |
| Structured Empirical Balanced Truncation (BT) | Reachability & Observability |
| Structured Empirical Balanced Truncation (BT-X) | Minimality |
| Structured Empirical Balanced Truncation (BT-Z) | Average Minimality |
| Structured Goal-Oriented POD (GOPOD) | Reachability |
| Structured Empirical Balanced Gains (BG) | Reachability & Observability |
| Structured Empirical Balanced Gains (BG-X) | Minimality |
| Structured Empirical Balanced Gains (BG-Z) | Average Minimality |
| Structured Dynamic Mode Decomposition Galerkin (DMDG) | Reachability |

# › Test Problems

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

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

# › Numerical Illustration (Yamal-Europe Pipeline)



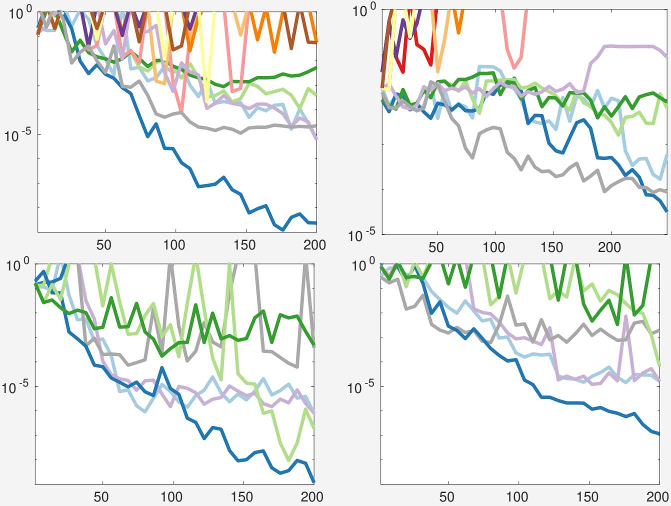

**MORscores:**

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

# › More Results

MORGEN

GasLib134




LotH67c

LotH67d

# › Conclusions

- Due to parametricity, hyperbolicity and nonlinearity:
  Balancing methods do not work well (unstable ROMs)
- Recommended ensemble:
  pH model, IMEX-1 solver, DSPMR reductor
- DMD-Galerkin works unreasonably well:
  This underestimated method needs more investigation
- Extends to:
  Water networks, district heating networks, and power networks
- Open-source MATLAB implementation:
  `morgen` – **M**odel **O**rder **R**eduction for **G**as and **E**nergy **N**etworks: `https://git.io/morgen`

# › MORe Challenges

- **Realistic compressors:**
  $\rightarrow$ Non-smooth nonlinearites
- **Gas mixture:**
  $\rightarrow$ Additional transport equation for composition tracking
- **Valves:**
  $\rightarrow$ Switched systems
- **Many ports:**
  $\rightarrow$ Port reduction?
- **Hyper reduction:**
  $\rightarrow$ Heuristic combinatorial comparison necessary
- **Pipeline attrition:**
  $\rightarrow$ Large-scale parameter-space … …

# › Brain Networks

Joint work with: **M. Ohlberger**

C. Himpe: **Combined State and Parameter Reduction for Nonlinear Systems with an Application in Neuroscience**;
Sierke Verlag Göttingen, 2017. doi:10.14626/9783868448818

C. Himpe, M. Ohlberger: **A Note on the Cross Gramian for Non-Symmetric Systems**;
System Science and Control Engineering: 199–208, 2016. doi:10.1080/21642583.2016.1215273

C. Himpe, M. Ohlberger: **Cross-Gramian-Based Combined State and Parameter Reduction for Large-Scale Control Systems**;
Mathematical Problems in Engineering 2014: 843869, 2014. doi:10.1155/2014/843869

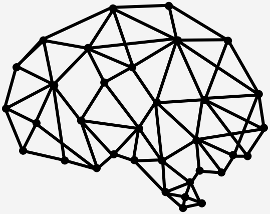
# › Motivation

**The Brain is Complicated:**

- A human brain consists of billions of neurons
- Myriad connections exists between neurons
- How does the brain work?
- How is information propagated between neuronal regions?

**Understanding Brain Connectivity:**

- Expensive experiments
- Complicated experimental set ups
- Indirect measurements
- (Bayesian) inverse problem



# › Single Region EEG / MEG Model

$$\tau_e \dot{v}_1 = x_1$$
$$\tau_e \dot{x}_1 = H_e \gamma_1 \bar{\sigma}_\kappa(v_4 - v_5) - 2x_1 - v_1$$
$$\tau_i \dot{v}_2 = x_2$$
$$\tau_i \dot{x}_2 = H_i \gamma_2 \bar{\sigma}_\kappa(v_1 - v_2) - 2x_2 - v_2$$

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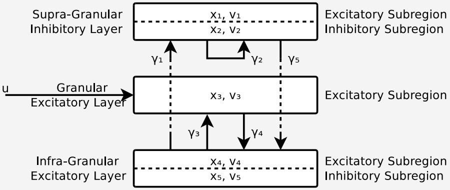
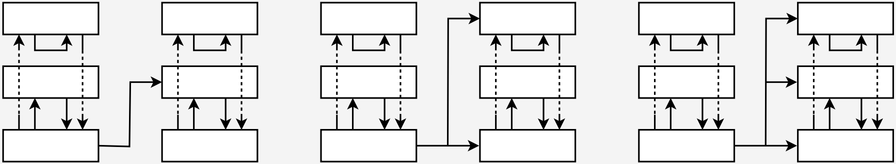
$$\tau_e \dot{v}_3 = x_3$$
$$\tau_e \dot{x}_3 = H_e \gamma_3 \bar{\sigma}_\kappa(v_4 - v_5) - 2x_3 - v_3 + H_e u$$

---

$$\tau_e \dot{v}_4 = x_4$$
$$\tau_e \dot{x}_4 = H_e \gamma_4 \bar{\sigma}_\kappa(v_3) - 2x_4 - v_4$$
$$\tau_i \dot{v}_5 = x_5$$
$$\tau_i \dot{x}_5 = H_i \gamma_5 \bar{\sigma}_\kappa(v_1 - v_2) - 2x_5 - v_5$$



# › Multi-Region EEG / MEG Model




$$\begin{pmatrix} \tau_* \mathbb{1} & 0 \\ 0 & \tau_* \mathbb{1} \end{pmatrix} \begin{pmatrix} \dot{v} \\ \dot{x} \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & -2\,\mathbb{1} \end{pmatrix} \begin{pmatrix} v \\ x \end{pmatrix} + \begin{pmatrix} 0 \\ A_v \end{pmatrix} \bar{\sigma}_\kappa(A_\sigma v) + H_e(\delta_{8,1}^{10\times 1} \otimes B)u$$

$$y = \begin{pmatrix} 0 & 0 & 0 & L & -L & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} v \\ x \end{pmatrix}$$

# › Combined State and Parameter Reduction

**Goal:**

$$\dim(x_r(t)) \ll \dim(x(t)) \wedge \dim(\theta_r) \ll \dim(\theta) \quad \text{s.t.} \quad \|y(\theta) - \tilde{y}(\theta_r)\| \ll 1$$

**Reducing and Reconstructing Projections:**

$$\begin{aligned} x_r(t) &:= V_r x(t) \quad \rightarrow \quad x(t) \approx U_r x_r(t) \\ \theta_r &:= \Pi_r^\top \theta \quad \rightarrow \quad \theta \approx \Pi_r \theta_r \end{aligned}$$

**Reduced Order Model:**

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

# › System-Theoretic Idea

## Parametric Input-Output System:

$$\begin{aligned} \dot{x}(t) &= f(x(t), u(t), \theta) \\ y(t) &= g(x(t), u(t), \theta) \end{aligned}$$

## Augmenting System with Parameter-States:

$$\begin{bmatrix} \dot{x}(t) \\ \dot{\theta}(t) \end{bmatrix} = \begin{bmatrix} f(x(t), u(t), \theta) \\ 0 \end{bmatrix}$$

$$y(t) = g(x(t), u(t), \theta)$$

# › Data-Driven Computation

**Empirical Augmented Observability Gramian / Joint Gramian:**

$$\widetilde{W}_O = \begin{pmatrix} W_O & W_M \\ W_M^\top & W_A \end{pmatrix}, \qquad W_J := \widetilde{W}_X = \begin{pmatrix} W_X & W_M \\ 0 & 0 \end{pmatrix}$$

**Identifiability Gramian / Cross-Identifiability Gramian:**

$$W_I := W_A - W_M^\top W_O^+ W_M, \qquad W_{\ddot{I}} := -\frac{1}{2} W_M^\top (W_X + W_X^\top)^+ W_M$$

**Parameter Projection:**

$$W_I \overset{\text{SVD}}{=} \Pi \, \Sigma \, \Pi^T, \qquad W_{\ddot{I}} \overset{\text{SVD}}{=} \Pi \, \Sigma \, \Pi^T$$

# › Some Remarks

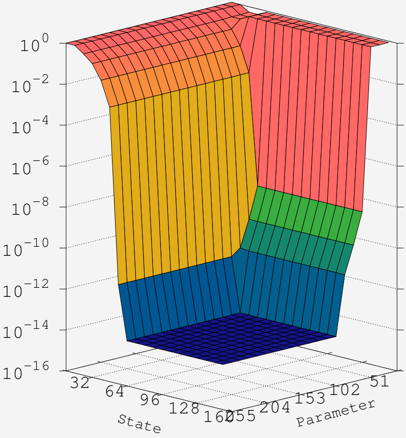
- Identifiability as parameter-state observability!
- Parameter projection always one-sided (Galerkin)!
- Impulse responses are basically Jacobians wrt parameters!
- Complexity scales with state plus parameter dimension $(N + P)$!
- Operating range of parameters is important!
- Related to Fisher information matrix.
- Related to active subspaces method.
- Related to Hessian in unconstrained optimization.
- Dimension reduction by SVDs of covariances of simulations ...
  $\rightarrow$ **Unsupervised Learning of System Properties via Synthetic Data**

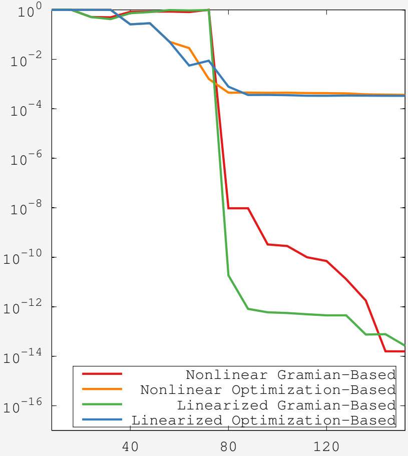
# › Test Problems

| | Training | Test |
|---|---|---|
| **Input Function** | Impulse | Experiment |
| **Parameter Sampling** | Sparse Grid | Uniformly Random |
| **Time Horizon** | $2s/20s$ | $2s/20s$ |

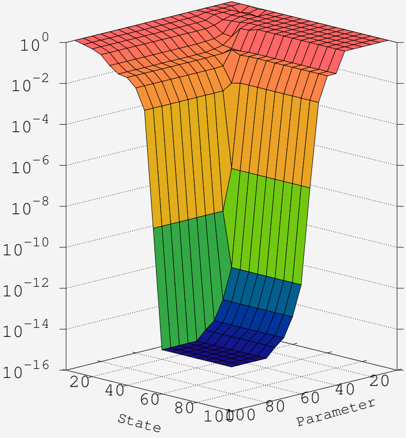
| | Evaluation |
|---|---|
| **Measure** | Relative Output Error |
| **Norm** | $\|\cdot\|_{L_2 \otimes L_2}$ |
| **Ranking** | Uniform Reduction |

# › Numerical Illustration (EEG/MEG)

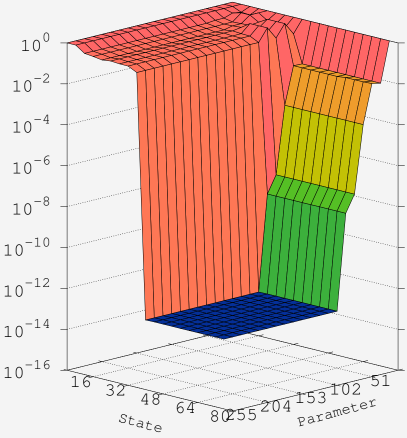


# › More Results




HNM




fMRI/fNIRS

# › Conclusions

- Cross-Gramian for non-square systems:
  Non-symmetric cross Gramian
- Parameter controllability is not needed:
  Parameter observability is sufficient and more efficient
- Gramian-based parameter reduction is feasible:
  The cross Gramian can encode parameter identifiability
- Underlying inference problem:
  Solvable over reduced parameter space
- Low-Rank (Cross-)Identifiability Gramian:
  Can be re-used in optimization as Hessian

# › MORe Challenges

- **Bilinear, quadratic extension:**
  → Even higher dimensional parameter spaces
- **Region variability:**
  → Additional non-connectivity parameters
- **fMRI / fNIRS BOLD:**
  → Severely nonlinear models

# › Lastly ...

- `emgr` – **EM**pirical **GR**amian Framework: `https://gramian.de`
- **H**ierarchical **A**pproximate **P**roper **O**rthogonal **D**ecomposition
- **Full Circle:** very nonlinear systems biology networks
  with high-dimensional parameter-spaces (U Potsdam)

# › Summary

- Parametric Model Order Reduction for *Gas Networks*
- Combined State and Parameter Reduction for *Brain Networks*
- One Data-Driven All-Purpose Tool: *Empirical Gramians*

https://himpe.science