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A Linear Cross Operator for Nonlinear Model Reduction

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Motivation

Network Connectivity in Neuroscience

- Infer connectivity between brain regions
- from functional neuroimaging data.
- For a large-scale network model
- with high-dimensional parameter-space
- modelling the brain connectivity,
- solve the inverse problem (many-query setting)

Overview

Nonlinear Input-Output System

Time-Invariant Parametric Nonlinear Control System:

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

Input:	$u : \mathbb{R} \to \mathbb{R}^M$	Parameter:	$\theta \in \mathbb{R}^P$
State:	$x : \mathbb{R} \to \mathbb{R}^N$	Vector Field:	$f : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^N$
Output:	$y : \mathbb{R} \to \mathbb{R}^Q$	Output Functional:	$g : \mathbb{R}^N \times \mathbb{R}^M \times \mathbb{R}^P \to \mathbb{R}^Q$

Combined State and Parameter Reduction

Reduced Order Model:

$$\dot{x}_r(t) = f_r(x_r(t), u(t), \theta_r)$$
$$y_r(t) = g_r(x_r(t), u(t), \theta_r)$$
$$x_r(0) = x_{r,0}$$

Reduced State:	$x_r : \mathbb{R} \to \mathbb{R}^{n \ll N}$
Reduced Parameter:	$\theta_r \in \mathbb{R}^{p \ll P}$
Reduced Vector Field:	$f_r : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^n$
Reduced Output Functional:	$g_r : \mathbb{R}^n \times \mathbb{R}^M \times \mathbb{R}^p \to \mathbb{R}^Q$
Model Reduction Error:	$\|y(\theta) - y_r(\theta_r)\| \ll 1$

Projection-Based Combined Reduction

Projection-Based Reduced Order Model:

$$\begin{aligned}
\dot{x}_r(t) &= Vf(Ux_r(t), u(t), \Pi\theta_r) \\
y_r(t) &= g(Ux_r(t), u(t), \Pi\theta_r) \\
x_r(0) &= Vx_0 \\
\theta_r &= \Lambda\theta
\end{aligned}$$

State Reduction:

- Trunc. proj. $U \in \mathbb{R}^{N \times n}$
- Trunc. proj. $V \in \mathbb{R}^{n \times N}$
- $VU = \mathbb{1}$

Parameter Reduction:

- Trunc. proj. $\Pi \in \mathbb{R}^{P \times p}$
- Trunc. proj. $\Lambda \in \mathbb{R}^{p \times P}$
- $\Lambda\Pi = \mathbb{1}$

Task: Determine U, V, Π, Λ

State-Space Reduction for Linear Systems

Linear Control System:

$$\dot{x}(t) = Ax(t) + Bu(t)$$
$$y(t) = Cx(t)$$
$$x(0) = x_0$$

Reduced Order Model:

$$\dot{x}_r(t) = A_r x_r(t) + B_r u(t)$$
$$y_r(t) = C_r x_r(t)$$
$$x_r(0) = x_{r,0}$$

Projection-Based Reduction:

$$\dot{x}_r(t) = (VAU)x_r(t) + (VB)u(t)$$
$$y_r(t) = (CU)x_r(t)$$
$$x_r(0) = Vx_0$$

Cross Gramian Matrix [Fernando & Nicholson'83, Laub et al.'83]

Controllability:

$$\mathcal{C}(u) := \int_{-\infty}^{0} \mathrm{e}^{-At} Bu(t)\mathrm{d}t$$

$$\mathcal{C} : \mathrm{L}_2^M \to \mathbb{R}^N$$

Observability:

$$\mathcal{O}(x_0)(t) := C\,\mathrm{e}^{At}\,x_0$$

$$\mathcal{O} : \mathbb{R}^N \to \mathrm{L}_2^Q$$

Hankel Operator (maps past inputs to future outputs):

$$H = \mathcal{O}\mathcal{C}$$

Cross Gramian (only applicable to square systems $M = Q$):

$$W_X := \mathcal{C}\mathcal{O} = \int_0^{\infty} \mathrm{e}^{At}\,BC\,\mathrm{e}^{At}\,\mathrm{d}t \Rightarrow \mathrm{tr}(W_X) = \mathrm{tr}(H)$$

Cross Gramian's Central Property:

$$CA^{-1}B = (CA^{-1}B)^{\intercal} \Rightarrow |\lambda_i(W_X)| = \sigma_i(H)$$

Non-Symmetric Cross Gramian [Moaveni & Khaki-Sedigh'06, H. & Ohlberger'15]

For the regular cross Gramian, the system ...

... has to be square,

... ideally is symmetric.

Cross Gramian Superposition ($B = \big(b_1 \dots b_M\big)$, $C = \big(c_1 \dots c_Q\big)^\intercal$):

$$W_X = \sum_{i=1}^{M=Q} \int_0^\infty \mathrm{e}^{At}\, b_i c_i \, \mathrm{e}^{At} \,\mathrm{d}t$$

Non-Symmetric Cross Gramian:

$$W_Z := \sum_{i=1}^{M} \sum_{j=1}^{Q} \int_0^\infty \mathrm{e}^{At}\, b_i c_j \, \mathrm{e}^{At} \,\mathrm{d}t$$

$$= \int_0^\infty \mathrm{e}^{At} \Big(\sum_{i=1}^{M} b_i\Big)\Big(\sum_{j=1}^{Q} c_j\Big) \mathrm{e}^{At} \,\mathrm{d}t$$

A Connection to Tangential Interpolation [H. & Ohlberger'15][1]

Tangential Interpolation (using directions: r^i and l^j):

$$V_1 := \bigoplus_i \mathcal{C}(s_i) r^i, \quad U_1 := \bigoplus_j l^j \mathcal{O}(s_j).$$

Frequency Domain Cross Gramian:

$$W_X = \mathcal{C}\mathcal{O} = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\imath\omega I - A)^{-1} BC (\imath\omega I - A)^{-1} \mathrm{d}\omega$$

Directed Cross Gramian:

$$W_{X,rl} := (\mathcal{C}r)(l\mathcal{O}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} (\imath\omega I - A)^{-1} BrlC (\imath\omega I - A)^{-1} \mathrm{d}\omega$$

$$= \int_0^{\infty} \mathrm{e}^{At} (Br)(lC) \, \mathrm{e}^{At} \, \mathrm{d}t$$

$$\rightarrow r_i = l_j = 1 \; \forall \, i, j \Rightarrow W_{X,rl} = W_Z$$

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[1] We thank the reviewers for motivating this property!

A Cross Operator [Fernando & Nicholson'83, Ionescu et al'11, Fujimoto & Scherpen'14]

The cross Gramian is generally non-symmetric and indefinite:

$$W_X \neq W_X^\intercal \not\succ 0$$

- Hence, it is **not** a Gramian matrix,
- except for state-space symmetric systems,
- but was introduced under this name.

W_X **is** an endomorphic linear cross operator:

$$W_X : \mathbb{R}^N \overset{\mathcal{O}}{\to} L_2^Q \overset{\mathcal{C}}{\to} \mathbb{R}^N$$

and maps an initial state to an output,
which serves as input that is mapped to a steady-state.

(Approximate) Balancing [Aldhaheri'91, Sorensen & Antoulas'02]

Balancing Transformation (for a symmetric system):

$$W_X \overset{EVD}{=} T \Lambda T^{-1}$$

Approximate Balancing Transformation:

$$W_X \overset{SVD}{=} UDV$$

State-Space Direct Truncation:

$$W_X \overset{\mathrm{SVD}}{=} UDV \rightarrow U = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \rightarrow V_1 := U_1^\intercal$$

Empirical Gramians [Moore'81, Lall et al'99]

Properties:

- Data-driven computation
- Applicable to nonlinear systems
- Consistent for linear systems
- Basic linear algebra operations
- Superior to plain linearization
- Quality depends on coverage of operating region
- Large dense matrices

Empirical Linear Cross Gramian [Fernando & Nicholson'85, Shaker'12, Baur et al.'16]

Empirical Linear Cross Gramian W_x:

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

- State trajectory $x(t)$ for impulse input $u(t) = \delta(t)$.
- Adjoint state trajectory $z(t)$ for impulse input $u(t) = \delta(t)$.

- Requires asymptotically stable linear systems.
- **Data-driven** computation.
- Usually not applicable to nonlinear systems,
- since an adjoint system is required.

Empirical Cross Gramian [Streif et al'06, H. & Ohlberger'14]

Empirical Cross Gramian:

$$\widehat{W_X} := \frac{1}{KLM} \sum_{k=1}^{K} \sum_{l=1}^{L} \sum_{m=1}^{M} \frac{1}{c_k d_l} \int_0^\infty \Psi^{klm}(t) \mathrm{d}t \in \mathbb{R}^{N \times N}$$

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

- State trajectory $x^{km}(t)$ for the impulse input $u(t) = c_k e_m \delta(t)$.
- Output trajectory $y^{lj}(t)$ for the initial state $x_0 = d_l e_j$.

- For asymptotically stable linear systems: $\widehat{W_X} = W_X$.
- Applicable to nonlinear systems.
- Extended to arbitrary input (empirical covariance matrix).
- Extended to an empircal non-symmetric cross Gramian.

Empirical Joint Gramian [Geffen et al'08, H. & Ohlberger'14]

Augmented system (treat parameters as constant states):

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

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

$$\begin{pmatrix} x(0) \\ \theta(0) \end{pmatrix} = \begin{pmatrix} x_0 \\ \theta_0 \end{pmatrix}$$

Joint Gramian (empirical cross Gramian of the augmented system):

$$W_J = \begin{pmatrix} W_X & W_m \\ 0 & 0 \end{pmatrix}$$

- Lower blocks are zero, as parameter-states are uncontrollable.
- Extended to an **empircal non-symmetric joint gramian**.

Empirical Cross-Identifiability Gramian [H. & Ohlberger'14]

Cross-Identifiability Gramian (Schur complement of symmetric part of W_J):

$$W_{\ddot{I}} = -\frac{1}{2} W_m^\intercal (W_X + W_X^\intercal)^{-1} W_m$$

- $W_{\ddot{I}}$ encodes the **observability** of parameters.
- Schur-complement can be approximated efficiently.

Parameter-Space Direct Truncation:

$$W_{\ddot{I}} \overset{\text{SVD}}{=} \Pi \Delta \Lambda \rightarrow \Pi = \begin{pmatrix} \Pi_1 & \Pi_2 \end{pmatrix} \rightarrow \Lambda_1 := \Pi_1^\intercal$$

Cross-Gramian-Based Combined Reduction

Compute Empirical Joint Gramian W_J.

State-Space Direct Truncation:

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

Parameter-Space Direct Truncation:

$$W_{\ddot{I}} \overset{\text{SVD}}{=} \Pi \Delta \Lambda \to \Pi = \begin{pmatrix} \Pi_1 & \Pi_2 \end{pmatrix} \to \Lambda_1 := \Pi_1^\intercal$$

Empirical-Cross-Gramian-Based Reduced Order Model:

$$\begin{aligned} \dot{x}_r(t) &= V_1 f(U_1 x_r(t), u(t), \Pi_1 \theta_r) \\ y_r(t) &= g(U_1 x_r(t), u(t), \Pi_1 \theta_r) \\ x_r(0) &= V_1 x_0 \\ \theta_r &= \Lambda_1 \theta \end{aligned}$$

Distributed Empirical Cross Gramian [H., Leibner and Rave'16]

Empirical Cross Gramian Partitioning:

$$\widehat{W}_X = \frac{1}{M}\Big[\sum_{m=1}^{M}\int_0^\infty \psi_1^m(t)\mathrm{d}t, \dots, \sum_{m=1}^{M}\int_0^\infty \psi_N^m(t)\mathrm{d}t\Big]$$

$$\psi_{i,j}^m(t) = (x_i^m(t) - \bar{x}_i)(y_m^j(t) - \bar{y}_m)$$

Hierarchical Approximate Proper Orthogonal Decomposition:

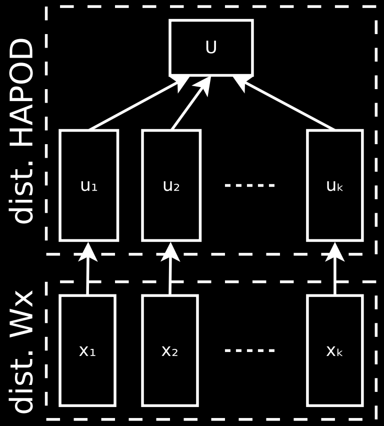
$$\mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon_{\mathcal{T}}](\alpha) = \mathrm{POD}(\mathcal{I}_\alpha, \varepsilon_{\mathcal{T}}(\alpha))$$

Special Case: Distributed HAPOD:

$$\mathrm{HAPOD}[\mathcal{S}, \mathcal{T}, D, \varepsilon_{\mathcal{T}}](\rho_{\mathcal{T}}) =$$

$$\mathrm{POD}\Big(\bigcup_{\beta \in \mathcal{L}_\mathsf{T}} \Big\{\sigma_n \cdot \varphi_n \,\Big|\, (\sigma_n, \varphi_n) \in \mathrm{POD}(D^{-1}(\beta))\Big\}, \varepsilon_{\mathcal{T}}(\rho_{\mathcal{T}})\Big)$$

Low Communication Computation



- Blocksize: $x_i \in \mathbb{R}^{N \times q_i},\ i = 1 \dots k$
- Partitioning: $\sum_{i=1}^{k} q_i = N$
- Currently: only fixed approximation error, not fixed rank.

emgr - Empirical Gramian Framework (Version: 4.0, 2016-06)

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, Kernel, Distributed Memory
- Non-Symmetric option for all cross Gramians
- Compatible with OCTAVE and MATLAB
- Vectorized and parallelizable
- Open-source licensed

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

Numerical Experiments[2]

Numerical Results:

1. Nonlinear Resistor Capacitor Cascade
2. Hyperbolic Network Model
3. fMRI & fNIRS Dynamic Causal Model
4. EEG & MEG Dynamic Causal Model

- Combined State and Parameter Reduction
- Joint Model Reduction Error Analysis

Joint State- and Parameter-Space Reduced Order Model Quality:

$$\|y(\theta) - y_r(\theta_r)\|_{L_2 \otimes L_2} = \sqrt{\int_\Theta \|y(\theta) - y_r(\theta_r)\|_{L_2}^2 \mathrm{d}\theta}$$

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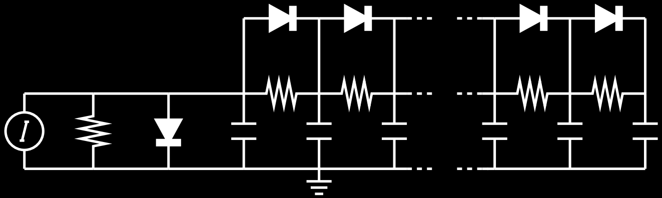
[2] Source code for the numerical experiments can be found at: doi:10.5281/zenodo.48122.

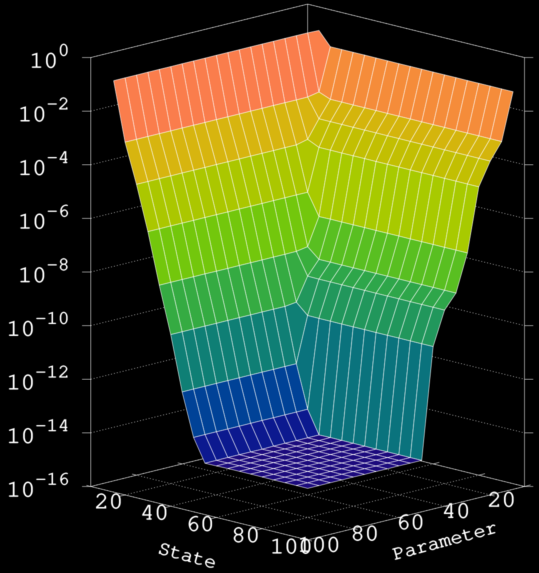
Nonlinear Benchmark System [Chen'99, Condon & Ivanov'04]



- SISO system
- Nonlinear resistors (Diodes)
- Parametrization of linear resistors
- Same state and parameter dimension $P = N$
- Benchmark in the **MORwiki**: http://modelreduction.org

$\rightarrow$ Empirical Joint Gramian

Nonlinear Benchmark System: $L_2 \otimes L_2$-Output Error



Hyperbolic Network Model [Quan et al.'01]

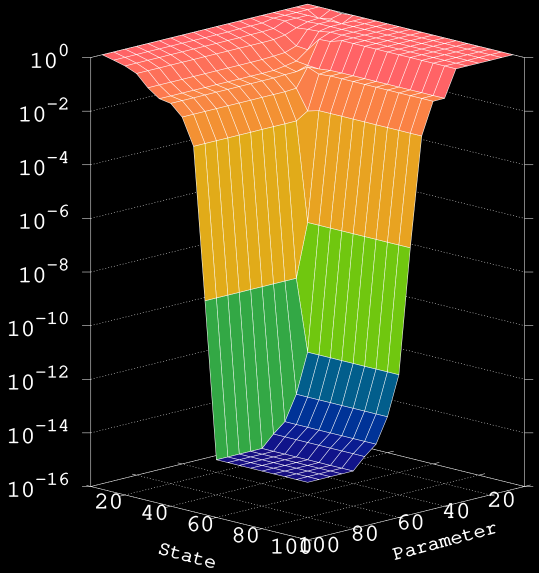
Hyperbolic Network Model:

$$\dot{x}(t) = A \tanh(K(\theta)x(t)) + Bu(t)$$
$$y(t) = Cx(t)$$

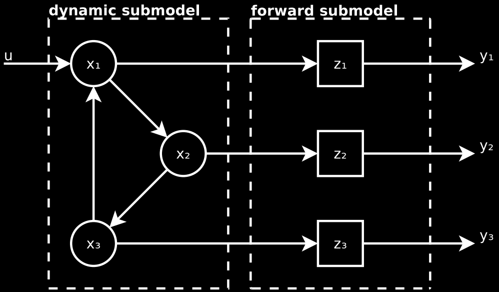
- SISO system
- Neural network model
- Weakly nonlinear
- Parameterized nonlinearity
- Same state and parameter dimension $P = N$

$\rightarrow$ Empirical Joint Gramian

Hyperbolic Network Model: $L_2 \otimes L_2$-Output Error



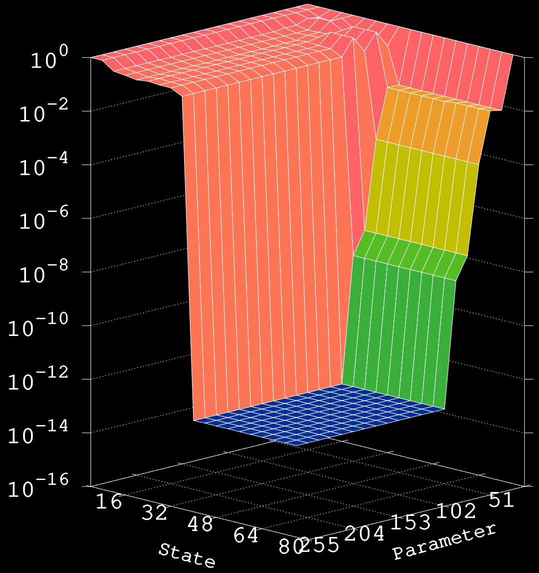
fMRI & fNIRS Dynamic Causal Model [Friston et al.'03, Kamrani et al.'12]



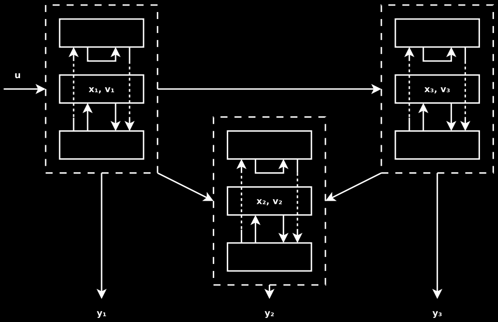
- SIMO System
- Two Component Model
- Linear Network Submodel
- Highly Nonlinear Observation Submodel
- Parametrization of Connectivity $P \sim N^2$

$\rightarrow$ Empirical (Non-Symmetric) Joint Gramian

fMRI & fNIRS Dynamic Causal Model: $L_2 \otimes L_2$-Output Error



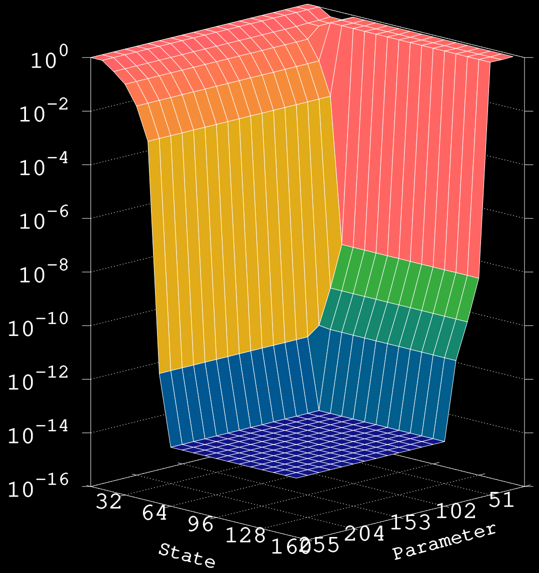
EEG & MEG Dynamic Causal Model [David et al.'06, Moran et al.'07]



- SIMO System
- Two Component Model
- Nonlinear Second-Order Network Submodel
- Linear Observation Submodel
- Parametrization of Connectivity $P \sim N^2$

$\rightarrow$ Empirical (Non-Symmetric) Joint Gramian

EEG & MEG Dynamic Causal Model: $L_2 \otimes L_2$-Output Error



Summary

Cross-Gramian-Based ...

- Combined Reduction
  - State-Space Direct Truncation
  - Parameter-Space Direct Truncation
- for Input-Output Systems
  - Non-Square
  - Nonlinear
- using the Empirical Joint Gramian
  - Empirical Cross Gramian
  - Empirical Cross-Identifiability Gramian
- on Distributed Memory Systems.

Outlook

Practically:

- Model reduction for
- energy supply networks
- modelled by nonlinear DAE systems (!)

Technically:

- Hyperreduction by EIM / DEIM
  [Melchior et al'14]
- Empirical Gramians for DAEs
  [Löffler & Marquardt'91, Hedengren & Edgar'05, Sun & Hahn'05]
- Time-Varying Systems by Averaging
  [Nilsson & Rantzer'09, H. & Ohlberger'14a]
- Kernel Methods using RKHS
  [Bouvrie & Hamzi'16]

References

- C. Himpe and T. Leibner and S. Rave. **Hierarchical Approximate Proper Orthogonal Decomposition**. In preparation, 2016.
- J. Fehr, J. Heiland, C. Himpe and J. Saak. **Best Practices for Replicability, Reproducibility and Reusability of Computer-Based Experiments Exemplified by Model Reduction Software**. Preprint, arXiv cs.MS:1607.01191, 2016.
- U. Baur, P. Benner, B. Haasdonk, C. Himpe, I. Martini and M. Ohlberger. **Comparison of methods for parametric model order reduction of instationary problems**. To appear in "Model Reduction and Approximation: Theory and Algorithms", 2016.
- C. Himpe and M. Ohlberger. **A Note on the Non-Symmetric Cross Gramian**. Preprint, arXiv math.OC:1501.05519, 2015.
- C. Himpe and M. Ohlberger. **The Empirical Cross Gramian for Parametrized Nonlinear Systems**. In Mathematical Modelling, vol 8, pages 727–728, 2015.
- 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.
- C. Himpe and M. Ohlberger. **Model Reduction for Complex Hyperbolic Networks**. In Proceedings of the ECC, pages 2739–2743, 2014.
- C. Himpe and M. Ohlberger. **A Unified Software Framework for Empirical Gramians**. Journal of Mathematics, 2013:1–6, 2013.