





About emgr

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Computational Methods in Systems and Control Theory Group

Max Planck Institute Magdeburg

International Congress on Mathematical Software (ICMS 2020)

Session: "Accelerating Innovation Speed in Mathematics

by Trading Mathematical Research Data"

Supported by:





- 1. What is emgr (EMpirical GRamian Framework)?
- 2. Mathematical software as research data!



Applied mathematics



- Applied mathematics
 - Mathematical system theory
 - Modern system theory by Kalman (includes control theory)
 - Study of dynamical input-output systems



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 - Numerical linear algebra (matrix decompositions etc.)
 - Numerical analysis (differential equations etc.)



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 - Scientific computing
 - Efficient implementations
 - Parallelization



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Computational science and engineering

- Modeling and discretization of engineering applications
- Simulate, estimate, predict real-life behavior



Dynamical Input-Output System

General input-output system:

$$0 = f(t, x(t), u(t), \theta, D^{\alpha}x(t))$$
$$y(t) = g(t, x(t), u(t), \theta)$$



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Example: Linear time-invariant system

$$\dot{x}(t) = Ax(t) + Bu(t)$$
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Example: Gas network model

$$\begin{pmatrix} E_p & 0 \\ 0 & I \end{pmatrix} \begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} 0 & A_{pq} \\ A_{qp} & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} + \begin{pmatrix} 0 & B_d \\ B_s & 0 \end{pmatrix} \begin{pmatrix} s_p \\ d_q \end{pmatrix} + \begin{pmatrix} 0 \\ f_q(p, q, s_p) \end{pmatrix}$$

$$\begin{pmatrix} s_q \\ d_p \end{pmatrix} = \begin{pmatrix} 0 & C_q \\ C_p & 0 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix}$$



Core input-output system properties:

- Reachability (can the state be driven to any state by finite input?)
- Observability (can the state be decoded from outputs in finite time?)



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csc System Gramians

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$$W_R := \int_0^\infty \mathrm{e}^{At} B B^{\mathsf{T}} \, \mathrm{e}^{A^{\mathsf{T}} t} \, \mathrm{d}t$$



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$$W_R := \int_0^\infty e^{At} BB^{\mathsf{T}} e^{A^{\mathsf{T}}t} dt \quad \Leftrightarrow \quad AW_R + W_R A^{\mathsf{T}} = -BB^{\mathsf{T}}$$



Nonlinear system:

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Empirical Gramians

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csc Empirical Gramians

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- Use state trajectory data from (scaled) impulse responses.
- Impulse responses can also be computed for nonlinear systems!
- Observability can similarly be described by trajectory data.





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 - Parametric Model Order Reduction (pMOR)
 - Nonlinear Model Order Reduction (nMOR)
 - Combined state and parameter reduction (comred)



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CSC Model Reduction

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System dimensions:

- $x: \mathbb{R}_{>0} \to \mathbb{R}^N$
- $A \in \mathbb{R}^{N \times N}$
- $u: \mathbb{R}_{>0} \to \mathbb{R}^M$
- $B \in \mathbb{R}^{N \times M}$
- $y: \mathbb{R}_{>0} \to \mathbb{R}^Q$
- $\quad \blacksquare \ C \in \mathbb{R}^{Q \times N}$



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$$N = \dim(x(t)) \gg 1$$

$$M = \dim(u(t)) \ll \dim(x(t)) = N$$

$$Q = \dim(u(t)) \ll \dim(x(t)) = N$$



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$$x \cdot x > 0 \rightarrow x$$

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Projection-based model order reduction:

$$V: \mathbb{R}^N \to \mathbb{R}^n$$

$$x_r := Vx$$

$$\blacksquare$$
 $n \ll N$



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$$x \approx Ux_r$$

$$U:\mathbb{R}^n \to \mathbb{R}^N$$

$$x \approx Ux_n$$

$$\|y - \tilde{y}\|_? \ll 1$$



csc Model Reduction

Example: Linear time-invariant system

$$\dot{x}(t) = Ax(t) + Bu(t)$$
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System dimensions:

Projection-based model order reduction:

Reduced order model:

$$\dot{x}_r(t) = (V(A(Ux_r(t)))) + (V(Bu(t)))$$

$$\tilde{y}(t) = (C(Ux_r(t)))$$



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

$$\tilde{y}(t) = (CU)x_r(t)$$



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$$x \approx Ux_r$$

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Reduced order model:

$$\dot{x}_r(t) = A_r x_r(t) + B_r u(t)$$
$$\tilde{y}(t) = C_r x_r(t)$$



emgr — EMpirical GRamian Framework (Version: 5.8)

Initial release of

Empirical Gramians:

- Empirical Reachability Gramian
- Empirical Observability Gramian
- Empirical Linear Cross Gramian
- Empirical Cross Gramian
- Empirical Sensitivity Gramian
- Empirical Identifiability Gramian
- Empirical Joint Gramian

Features:

- Open-source Octave and MATLAB toolbox, with Python variant.
- Interfaces for: Solver, inner product kernels & low-rank computation.
- Configurable, vectorized and parallelizable.

More info: https://gramian.de C.H. emgr - The Empirical Gramian Framework. Algorithms 11(7): 91, 2018. doi:c9hj

About emgr



Mathematical Software as Research Data

Through the lens of emgr



CSC Classes of Software

C. Himpe About emgr 11/18





CI Classes of Software

- Single-use software
 - Computational proofs
 - Numerical experiments
 - Visualization generators



csc Classes of Software

■ Single-use software

- Computational proofs
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- Visualization generators

Reusable software

- Few developers
- Few users (mostly developers)
- Continuous development



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Reusable software

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Sustainable software

- Many developers
- Many users (including non-developers)
- Sustained development





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Safety in numbers:

Project website / personal website / institute website



- Project website / personal website / institute website
- github project (https://github.com)



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- github project (https://github.com)
- Software Heritage archive (https://softwareheritage.org)



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- github project (https://github.com)
- Software Heritage archive (https://softwareheritage.org)
- Zenodo archive (https://zenodo.org)
- Internet Archive (https://archive.org)





Persistent Identifiers

Pinpointing state:

■ Website URL (Uniform Resource Locator)



CSC Persistent Identifiers

- Website URL (Uniform Resource Locator)
- github git tag / hash



CSC Persistent Identifiers

- Website URL (Uniform Resource Locator)
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- Software Heritage permalink



csc Persistent Identifiers

- Website URL (Uniform Resource Locator)
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- Software Heritage permalink
- Zenodo DOI (Digital Object Identifier)



csc Persistent Identifiers

- Website URL (Uniform Resource Locator)
- github git tag / hash
- Software Heritage permalink
- Zenodo DOI (Digital Object Identifier)
- Version (semantic version vs. calendar version)





■ Community (i.e. MORwiki, MoRePaS)



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- Subject (i.e *DSweb*, *Zenodo* communities)



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- Mathematics (ORMS, swMATH)
- Science (Researchgate, archives-ouvertes)
- Language (MATLAB File Exchange)



ALL CAPS:



Semantic Enrichment

ALL CAPS:

■ README (plain text minimal documentation)



CSC Semantic Enrichment

ALL CAPS:

- README (plain text minimal documentation)
- RUNME (working example)



CSC Semantic Enrichment

ALL CAPS:

- README (plain text minimal documentation)
- RUNME (working example)
- CODE (code meta-data, i.e.: https://github.com/gramian/code-ini)



A hard problem:



Software Peer Review

A hard problem:

■ Check Code initiative (https://codecheck.org.uk)



Software Peer Review

A hard problem:

- Check Code initiative (https://codecheck.org.uk)
- Journal of Open Source Software (https://joss.theoj.org)



csc Software Peer Review

A hard problem:

- Check Code initiative (https://codecheck.org.uk)
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- Test review
 - Developer defines and describes a test,
 - based on an analytically known solution,
 - or a solution computed by alternative means.
 - Reviewer evaluates test quality and result.



On Knowledge Sharing Beyond Classical Publications

Conservative values:



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- **Prefer** traditional publication
 - ightarrow document PDF & supplemental material zip archive
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 - → Jupyter Notebooks, Code Ocean



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 - → Jupyter Notebooks, Code Ocean
- Programming language longevity
 - \rightarrow FORTRAN, LISP, MATLAB
- Programming language readability
 - → MATLAB, MAPLE



Do you want to know more?

- Empirical Gramians: https://gramian.de
- Best Practices: https://doi.org/bsb2
- Sustainable Software: https://arxiv.org/abs/1909.09469
- Mathematical Software: https://doi.org/10.1016/C2013-0-11363-3

https://himpe.science

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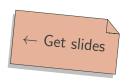
Supported by the German Federal Ministry for Economic Affairs and Energy, in the joint project: "MathEnergy – Mathematical Key Technologies for Evolving Energy Grids", sub-project: Model Order Reduction (Grant number: 0324019B).



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