

MAX PLANCK INSTITUTE FOR DYNAMICS OF COMPLEX TECHNICAL SYSTEMS MAGDEBURG



COMPUTATIONAL METHODS IN SYSTEMS AND CONTROL THEORY

Cultivating Cooperation in a Competitive Community P. Benner, J. Heiland, C. Himpe, J. Saak Max Planck Institute Magdeburg

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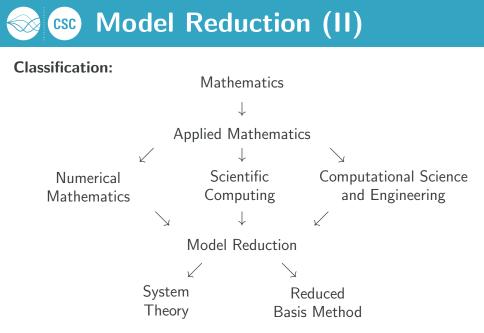
- Communities*
- Competition*
- Cooperation*
- Cultivation*

^{*} Exemplified by the field of Model Reduction.



What is Model Reduction?

- Model reduction or model order reduction
- determines algorithmically surrogates
- for high-dimensional differential equation models,
- i.e. originating from simulations or control problems,
- aiming to (significantly) reduce computational time,
- while preserving relevant properties of the original model.



System-Theoretic View:

Input-Output System:

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

Input
$$u : \mathbb{R} \to \mathbb{R}^M$$

State $x : \mathbb{R} \to \mathbb{R}^N$
Output $y : \mathbb{R} \to \mathbb{R}^Q$

Reduced Order Model:

$$\dot{x}_r(t) = f_r(t, x_r(t), u(t))$$
$$\tilde{y}(t) = g_r(t, x_r(t), u(t))$$

Reduced Basis View:

Semi-Discrete Parametric PDE:

$$\partial_t u_\mu(t) = -L_\mu(u_\mu(t))$$
$$y_\mu(t) = g_\mu(u_\mu(t))$$

- Parameter $\mu \in \mathcal{P}$
- Solution $u_{\mu} : \mathbb{R} \to V$
- Quantity of Interest $y_{\mu} : \mathbb{R} \to W$

Reduced Order Model:

$$\partial_t u_{\mu,n}(t) = -L_{\mu,n}(u_{\mu,n}(t))$$
$$\tilde{y}_{\mu}(t) = g_{\mu,n}(u_{\mu,n}(t))$$

Example: Transient Gas Network Simulations

- A gas network corresponds to a directed graph.
- Each edge represents a pipe, endowed with the Euler equations.
- Vertices introduce Kirchhoff-laws-type constraints.

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Isothermal (Simplified) Euler Equations for Gas Flow in a Pipe:

$$\partial_t p = \frac{R_S T_0 z}{S} \partial_x q$$

$$\partial_t q = -S \partial_x p - \frac{Sg}{R_S T_0 z} p \partial_x h - \frac{\lambda R_S T_0 z}{2DS} \frac{q|q}{p}$$

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Semi-Discrete (Index-Reduced) Gas Network Model:

$$\begin{pmatrix} \dot{p}_h \\ \dot{q}_h \end{pmatrix} = \begin{pmatrix} 0 & A_{pq} \\ A_{qp} & 0 \end{pmatrix} \begin{pmatrix} p_h \\ q_h \end{pmatrix} + \begin{pmatrix} 0 & B_d \\ B_s & 0 \end{pmatrix} \begin{pmatrix} p_s \\ q_d \end{pmatrix} + \begin{pmatrix} 0 \\ f_q(p_h, q_h, p_s, q_d) \end{pmatrix}$$

$$\begin{pmatrix} p_d \\ q_s \end{pmatrix} = \begin{pmatrix} C_d & 0 \\ 0 & C_s \end{pmatrix} \begin{pmatrix} p_h \\ q_h \end{pmatrix}$$

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Large-Scale System: $\dim(p_h(t)), \dim(q_h(t)) \gg 1$



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Inside Model Reduction:

- Backgrounds: Different (ST vs RBM)
- Problems: Similar (see previous slide)
- Approaches: Similar (ie "Projection")
- Language: Different (eg Input vs Parameter)
- Conferences: Exist (eg ModRed, MoRePaS)
- Journals: No, but: special issues, collections, standard outlets



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Takeaway: It's complicated.



A group of scientists individually proposing solutions for similar problems, and comparing among each other.



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Inside Model Reduction:

- Fastest (but: offline vs online?)
- Most accurate (but: what norm?)
- Most efficient (but: what measure?)
- Most features (ie applicability, optimality)
- Most elegant (...)



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Inside Model Reduction:

- Comparisons / rankings / progress (on universal benchmarks)
- Topical conferences (joint tracks, minisymposia)
- Accepted best practices and guidelines (under construction)
- Enforced rules (we are not there yet!)



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Takeaway: It's possible, but complicated.



Some scientists working on resolving roadblocks inside communities and between subcommunities.



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Inside Model Reduction:

- Agreement (too much overlap to ignore each others)
- Translate (joint publications, exchanges)
- Forum (we get to this)



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Takeaway: It's a lot of extra work.

So the research Data?

Research Data in Model Reduction:

- Model Reduction Algorithms
- Algorithm Implementations
- Algorithm Applicability Meta-Data
- Implementation Applicability Meta-Data
- Implementation Technical Properties
- Implementation Interface Specifications
- Benchmark Problems
- Benchmark Meta-Data
- Benchmark Environment
- Benchmark Results



- Lone wolfs
- Keeping secrets ("competitive advantage")
- Negligence (publish first)

¹J. Fehr, J. Heiland, C. Himpe and J. Saak. **Best Practices for Replicability, Reproducibility and Reusability of Computer-Based Experiments Exemplified by Model Reduction Software**. AIMS Mathematics (AIMS Math) 1(3): 261–281, 2016. https://doi.org/bsb2

Scientists 🐼 📾

Challenges:

- Lone wolfs
- Keeping secrets ("competitive advantage")
- Negligence (publish first)

Solutions:

- Meetings (PhD organized summer schools, ie RBSS / MORSS)
- Best practices¹
- Review practices (demand fair comparisons, and code)

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- Suprise endings
- Bit rot
- Method islands

²J. Fehr, C. Himpe, S. Rave, J. Saak. Sustainable Research Software Hand-Over. arXiv, cs.GL: 1909.09469, 2019. https://arxiv.org/abs/1909.09469



- Suprise endings
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Solutions:

- Start with requirement specification (aka Lastenheft)
- Sustainable project hand-over²
- Encourage exchange (seminars, summer schools, conferences)

²J. Fehr, C. Himpe, S. Rave, J. Saak. **Sustainable Research Software Hand-Over**. arXiv, cs.GL: 1909.09469, 2019. https://arxiv.org/abs/1909.09469



- Where to exchange?
- How to compare?
- How to obtain state-of-the-art?



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Solution:

A Wiki!

📚 👓 MORwiki – Model Order Reduction Wiki

MORwiki:

- https://modelreduction.org
- MediaWiki software
- Established 2013 (by MPI Magdeburg)
- Main sections:
 - Benchmarks: > 50 (plus variants)
 - Methods: 15 (plus variants)
 - Software: 15 (plus others)
- \bullet > 50 Authors (mostly single contributions though)
- Workshop calendar
- Publication list
- Textbook and review work overview



The Next Step: FAIR fair comparisons

- A unified framework to compare model reduction methods,
- and other numerical or general mathematical algorithms.
- Community defines benchmark data,
- and comparison norms.
- Groups and scientists compare their methods
- to others and state-of-the-art.
- Possibly even on the same hardware.



"Nobody will pay for this!"

³Letter-of-Intent: https://dfg.de/en/research_funding/programmes/nfdi/ absichtserklaerungen/2019/2019_ma_rdi.pdf

C. Himpe



"Nobody will pay for this!"

Well, maybe:

- NFDI (Nationale ForschungsDaten Initative)
- MaRDI Consortium (Mathematics)³
- Task Area 2 (Scientific Computing)
- Measure 3 (Benchmark Framework)

³Letter-of-Intent: https://dfg.de/en/research_funding/programmes/nfdi/ absichtserklaerungen/2019/2019_ma_rdi.pdf



- Cultivating \rightarrow **F**indable
- Cooperation → Accessible
- Competitive \rightarrow Interoperable
- $\blacksquare \mathsf{Communities} \to \mathbf{R}\mathsf{eusable}$

https://himpe.science

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