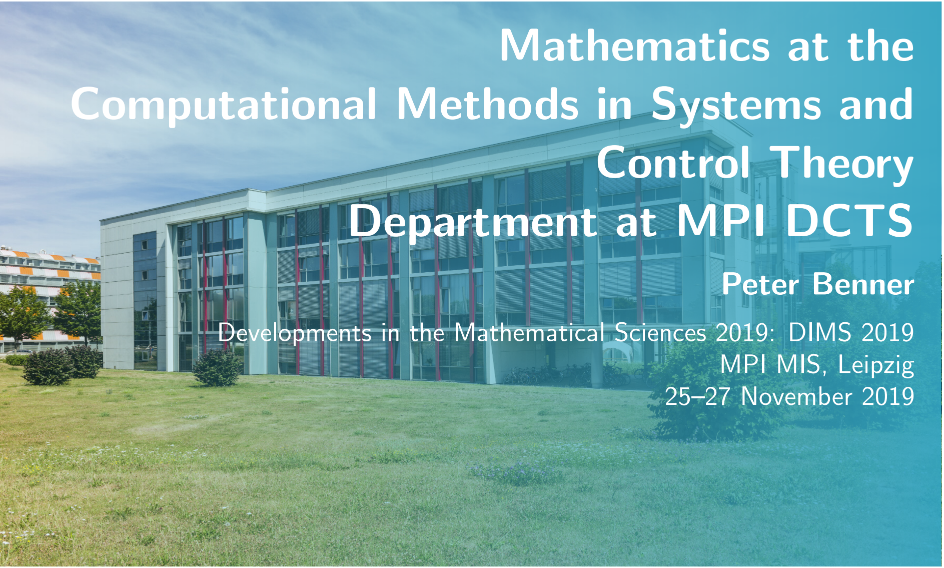
MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

CSC

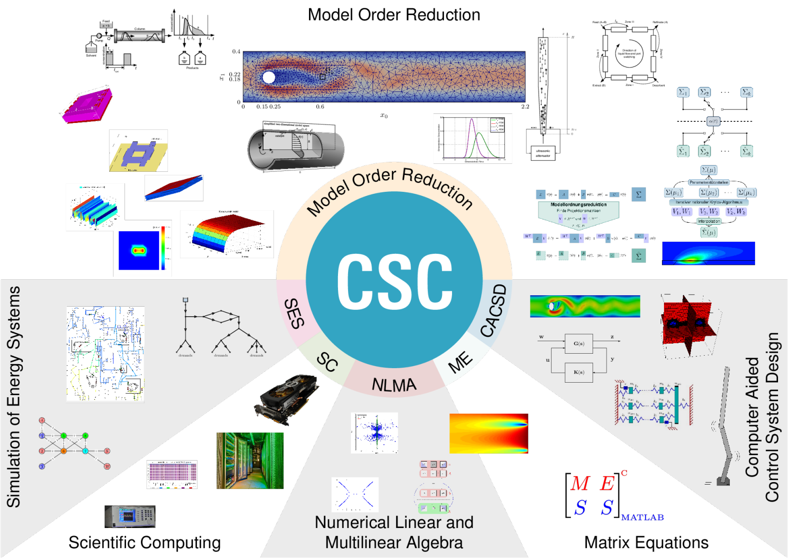


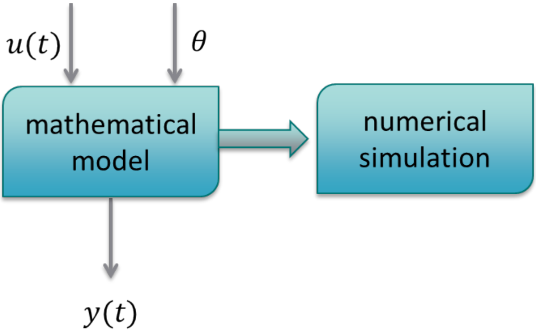
Mathematics at the Computational Methods in Systems and Control Theory Department at MPI DCTS

Peter Benner

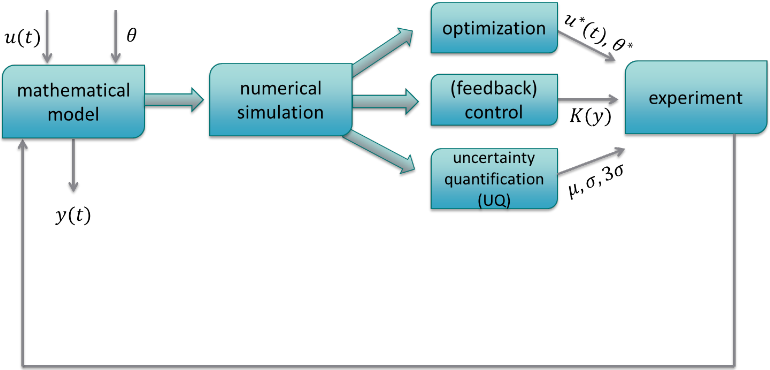
Developments in the Mathematical Sciences 2019: DIMS 2019
MPI MIS, Leipzig
25–27 November 2019

Research Areas / Teams

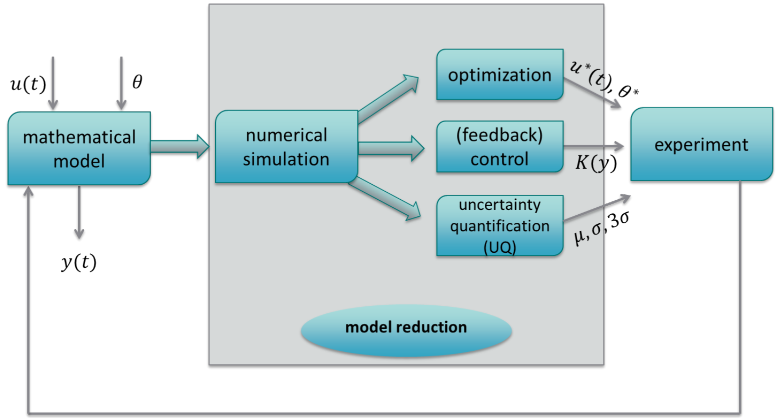




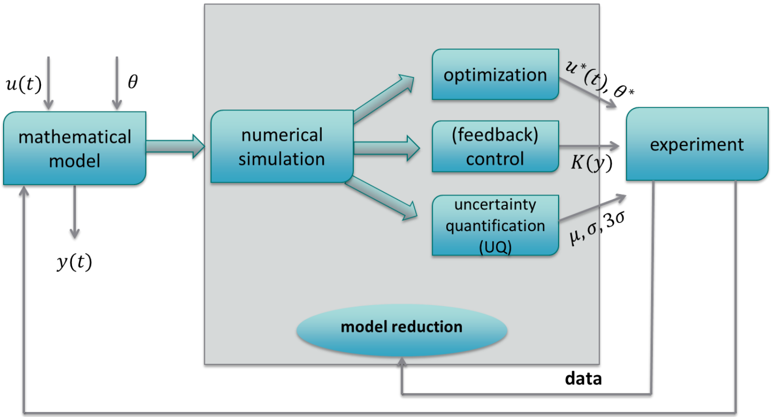
$u(t)$
θ
mathematical model
numerical simulation
$y(t)$



$u(t)$
θ
mathematical model
$y(t)$
numerical simulation
optimization
(feedback) control
uncertainty quantification (UQ)
$u^*(t), \theta^*$
$K(y)$
$\mu, \sigma, 3\sigma$
experiment



$u(t)$
θ
mathematical model
$y(t)$
numerical simulation
optimization
(feedback) control
uncertainty quantification (UQ)
$u^*(t), \theta^*$
$K(y)$
$\mu, \sigma, 3\sigma$
experiment
model reduction



$u(t)$
θ
mathematical model
$y(t)$
numerical simulation
optimization
(feedback) control
uncertainty quantification (UQ)
$u^*(t), \theta^*$
$K(y)$
$\mu, \sigma, 3\sigma$
experiment
model reduction
data

Curse of Dimensionality [Bellman 1957]

Increase in matrix size of discretized differential operator for $h \rightarrow \frac{h}{2}$ by factor 2^d.

$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

Curse of Dimensionality [Bellman 1957]

Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.

$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

Low-rank techniques can beat the curse

Basic idea: consider $-\Delta u = f$ in $[\,0\,,\,1\,] \times [\,0\,,\,1\,] \subset \mathbb{R}^2$, uniformly discretized as

$$(I \otimes A + A \otimes I)\, x =: \mathcal{A}x = b \qquad \Longleftrightarrow \qquad AX + XA^T = B$$

with $x = \mathrm{vec}(X)$ and $b = \mathrm{vec}(B)$ with low-rank right hand side $B \approx b_1 b_2^T$.

Curse of Dimensionality [Bellman 1957]

Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.
$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

Low-rank techniques can beat the curse

Basic idea: consider $-\Delta u = f$ in $[\,0\,,\,1\,] \times [\,0\,,\,1\,] \subset \mathbb{R}^2$, uniformly discretized as

$$(I \otimes A + A \otimes I)\, x =: \mathcal{A}x = b \qquad \Longleftrightarrow \qquad AX + XA^T = B$$

with $x = \mathrm{vec}(X)$ and $b = \mathrm{vec}(B)$ with low-rank right hand side $B \approx b_1 b_2^T$.

Exploit low (numerical) rank $r \ll n$ of $\tilde{X} := VW^T \approx X$ due to properties of A, B, and in particular (approximate) separability $u(x,y) \approx v(x)w(y)$, $f(x,y) \approx g(x)h(y)$.

Curse of Dimensionality [BELLMAN 1957]

Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.

$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

Low-rank techniques can beat the curse

Basic idea: consider $-\Delta u = f$ in $[\,0\,,\,1\,] \times [\,0\,,\,1\,] \subset \mathbb{R}^2$, uniformly discretized as

$$(I \otimes A + A \otimes I)\,x =: \mathcal{A}x = b \qquad \Longleftrightarrow \qquad AX + XA^T = B$$

with $x = \mathrm{vec}(X)$ and $b = \mathrm{vec}(B)$ with low-rank right hand side $B \approx b_1 b_2^T$.

Exploit low (numerical) rank $r \ll n$ of $\tilde{X} := VW^T \approx X$ due to properties of A, B, and in particular (approximate) separability $u(x,y) \approx v(x)w(y)$, $f(x,y) \approx g(x)h(y)$.

Re-write solvers for linear systems in low-rank form, can prove (for certain problems)

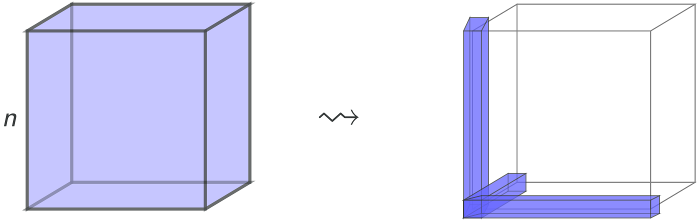
complexity $\mathcal{O}(rn)$ rather than $\mathcal{O}(n^2)$!

P. Benner, T. Breiten (2013), Numerische Mathematik 124(3):441–470.

Curse of Dimensionality [Bellman 1957]

Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.
$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

From low-rank matrix approximations to low-rank tensors:



For d-dimensions and max. rank $r \ll n$: **complexity $\mathcal{O}(rdn)$ rather than $\mathcal{O}(n^d)$!**

Results by De Lathauwer, Grasedyck, Hackbusch, Kressner, Oseledets, Tyrtyshnikov, ...

Curse of Dimensionality [Bellman 1957]

Increase in matrix size of discretized differential operator for $h \to \frac{h}{2}$ by factor 2^d.
$\rightsquigarrow$ **Exponential Increase of Dimensionality**, called **Curse of Dimensionality** ($d > 3$).

Application to uncertain PDE Control / UQ — TU Chemnitz, MPI MIS, U Bath

Developed low-rank tensor-based iterative solvers for discrete optimality systems resulting from **PDE-constrained optimization under uncertainty (with $d \gg 3$ due to random parameters).**

Result: biggest problem solved so far has $\approx 10^{15}$ unknowns! (KKT system for unsteady incompressible Navier-Stokes control problem with uncertain viscosity).

Would require ≈ 10 **petabytes (PB)** $= 10,000$ **TB** to store the solution vector!

Using low-rank tensor techniques, we need less than 1 **GB** to solve the KKT system (using MATLAB) in less than one hour!

Note: *"The largest linear system solved on a supercomputer to date had 10^{13} unknowns."*
— according to U. Rüde, PACO 2017.

P. Benner, A. Onwunta, M. Stoll (2015), SIAM/ASA J. UQ 3(1):622-649
P. Benner, S. Dolgov, A. Onwunta, M. Stoll (2016), Comp. Meth. Appl. Mech. Engrg. 304:26–54
P. Benner, S. Dolgov, V. Khoromskaia, B.N. Khoromskij (2017), J. Comp. Phys. 334:221-239
P. Benner, Y. Qiu, M. Stoll (2018), SIAM/ASA J. UQ 6(2):965–989

From Quadratic-bilinear to Polynomial Systems

Imperial College, Virginia Tech, NUST

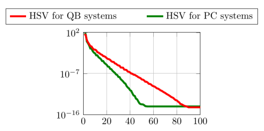
Recall:

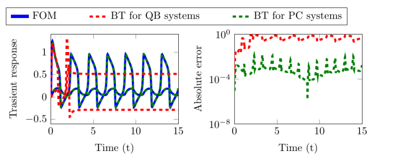
1. Many practically relevant (smooth) nonlinear systems can be re-written as quadratic or polynomial systems.
2. *System-theoretic (input-independent) methods* are superior to *POD/RB (input training-based) methods* for control applications.

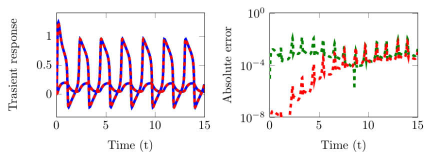
So far:

- Developed new methods for quadratic-bilinear systems.
- Adapted methods to various applications.

New: methods for polynomial systems.

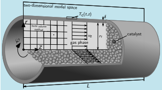




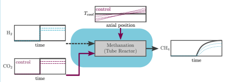


M.I. Ahmad, P. Benner, I.M. Jaimoukha (2016), IET Control Theory & Appl. 10(16):2010-2018
M.I. Ahmad, P. Benner, P. Goyal, J. Heiland (2017) ZAMM 97(10):1252-1267
P. Benner, P. Goyal, S. Gugercin (2018), SIAM J. Matrix Anal. Appl. 39(2):983–1032

Energy Conversion PSE



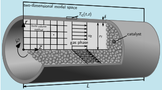
$$
\begin{aligned}
\frac{\partial \rho_\alpha}{\partial t} &= -\, v_z \frac{\partial \rho_\alpha}{\partial z} + \mathcal{D}_{r,\alpha}\left[\frac{\partial^2 \rho_\alpha}{\partial r^2} + \frac{1}{r}\frac{\partial \rho_\alpha}{\partial r}\right], \quad \alpha = 1\ldots 6 \ \text{(species)},\\
\frac{\partial T}{\partial t} &= -\, v_z \frac{\partial T}{\partial z} + \frac{\lambda_r}{\rho c_p}\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right],
\end{aligned}
$$



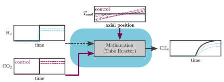
POD-DEIM for 2D reactor model

P. Benner, J. Bremer, L. Feng, P. Goyal, K. Sundmacher (2017), Comp. & Chem. Engrg. 106:777–783.

Energy Conversion — PSE



$$
\begin{aligned}
\frac{\partial \rho_\alpha}{\partial t} &= -v_z \frac{\partial \rho_\alpha}{\partial z} + \mathcal{D}_{r,\alpha}\left[\frac{\partial^2 \rho_\alpha}{\partial r^2} + \frac{1}{r}\frac{\partial \rho_\alpha}{\partial r}\right], \quad \alpha = 1\ldots 6 \ \text{(species)},\\
\frac{\partial T}{\partial t} &= -v_z \frac{\partial T}{\partial z} + \frac{\lambda_r}{\rho c_p}\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right],
\end{aligned}
$$



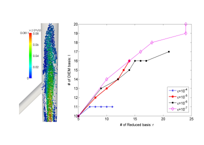
POD-DEIM for 2D reactor model

P. Benner, J. Bremer, L. Feng, P. Goyal, K. Sundmacher (2017), Comp. & Chem. Engrg. 106:777–783.

Crystallization — PCF, PSD

Adaptive POD-DEIM method for nonlinear population balance model.

$$
\begin{aligned}
A(x)\left.\frac{\partial n}{\partial t}\right|_{x,L,t} = & -\frac{\partial}{\partial x}\left(A(x)\, v_P(x,L,t)\, n(x,L,t)\right)\\
& + D\frac{\partial}{\partial x}\left(A(x)\left.\frac{\partial n}{\partial x}\right|_{x,L,t}\right)\\
& - A(x)\, G \left.\frac{\partial n}{\partial L}\right|_{x,L,t}\\
& + \dot{V}_{fr}\left(n_{fr}(L)\frac{\int_0^\infty n(x,l,t)\, l^3\, dl}{\int_0^\infty n_{fr}(l)\, l^3\, dl} - n(x,L,t)\right)\hat{\delta}(x - x_{fr})
\end{aligned}
$$

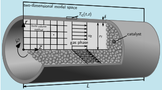


L. Feng, M. Mangold, P. Benner (2017), AIChE J 63(9):3832-3844.
M. Mangold, D. Khlopov, S. Palis, L. Feng, P. Benner, D. Binev, A. Seidel-Morgenstern (2015), J. Comp. Appl. Math. 289:253–266.

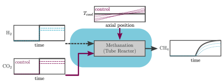
Selected Research Highlights

Model Reduction Applications

Energy Conversion — PSE



$$\frac{\partial \rho_\alpha}{\partial t} = -v_z \frac{\partial \rho_\alpha}{\partial z} + \mathcal{D}_{r,\alpha}\left[\frac{\partial^2 \rho_\alpha}{\partial r^2} + \frac{1}{r}\frac{\partial \rho_\alpha}{\partial r}\right], \quad \alpha = 1\ldots 6 \ \text{(species)},$$
$$\frac{\partial T}{\partial t} = -v_z \frac{\partial T}{\partial z} + \frac{\lambda_r}{\rho c_p}\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right],$$



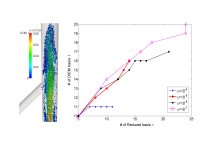
POD-DEIM for 2D reactor model

P. Benner, J. Bremer, L. Feng, P. Goyal, K. Sundmacher (2017), Comp. & Chem. Engrg. 106:777–783.

Crystallization — PCF, PSD

Adaptive POD-DEIM method for nonlinear population balance model.

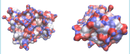
$$\begin{aligned} A(x)\left.\frac{\partial n}{\partial t}\right|_{x,L,t} = & -\frac{\partial}{\partial x}\left(A(x)\, v_P(x,L,t)\, n(x,L,t)\right) \\ & + D\frac{\partial}{\partial x}\left(A(x)\left.\frac{\partial n}{\partial x}\right|_{x,L,t}\right) \\ & - A(x)\, G \left.\frac{\partial n}{\partial L}\right|_{x,L,t} \\ & + \dot{V}_{fr}\left(n_{fr}(L)\frac{\int_0^\infty n(x,l,t)\, l^3\, dl}{\int_0^\infty n_{fr}(l)\, l^3\, dl} - n(x,L,t)\right)\hat{\delta}(x - x_{fr}) \end{aligned}$$



L. Feng, M. Mangold, P. Benner (2017), AIChE J 63(9):3832-3844.
M. Mangold, D. Khlopov, S. Palis, L. Feng, P. Benner, D. Binev, A. Seidel-Morgenstern (2015), J. Comp. Appl. Math. 289:253–266.

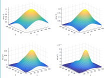
Molecular Simulation — MSD, MPI MIS

Combined POD-DEIM and range-separated tensor format for fast simulation of electrostatic potentials for molecules in solution.



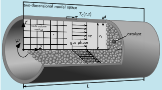
Poisson-Boltzmann equation

$$-\nabla \cdot (\epsilon(x)\nabla u(x)) + \bar{\kappa}^2(x)\sinh(u(x)) = \frac{4\pi e_c^2}{K_B T}\sum_{i=1}^{N_m} z_i \delta(x - x_i)$$

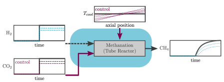


P. Benner, L. Feng, C. Kweyu, M. Stein (2017), arXiv:1705.08349

Energy Conversion — PSE



$$\frac{\partial \rho_\alpha}{\partial t} = -v_z \frac{\partial \rho_\alpha}{\partial z} + \mathcal{D}_{r,\alpha}\left[\frac{\partial^2 \rho_\alpha}{\partial r^2} + \frac{1}{r}\frac{\partial \rho_\alpha}{\partial r}\right], \quad \alpha = 1\ldots 6 \ \text{(species)},$$
$$\frac{\partial T}{\partial t} = -v_z \frac{\partial T}{\partial z} + \frac{\lambda_r}{\rho c_p}\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial T}{\partial r}\right],$$



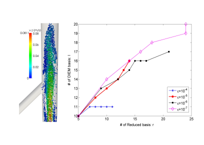
POD-DEIM for 2D reactor model

P. Benner, J. Bremer, L. Feng, P. Goyal, K. Sundmacher (2017), Comp. & Chem. Engrg. 106:777–783.

Crystallization — PCF, PSD

Adaptive POD-DEIM method for nonlinear population balance model.

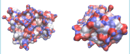
$$\begin{aligned} A(x)\left.\frac{\partial n}{\partial t}\right|_{x,L,t} = & -\frac{\partial}{\partial x}\left(A(x)\, v_P(x,L,t)\, n(x,L,t)\right) \\ & + D\frac{\partial}{\partial x}\left(A(x)\left.\frac{\partial n}{\partial x}\right|_{x,L,t}\right) \\ & - A(x)\, G \left.\frac{\partial n}{\partial L}\right|_{x,L,t} \\ & + \dot{V}_{fr}\left(n_{fr}(L)\frac{\int_0^\infty n(x,l,t)\, l^3\, dl}{\int_0^\infty n_{fr}(l)\, l^3\, dl} - n(x,L,t)\right)\hat{\delta}(x - x_{fr}) \end{aligned}$$



L. Feng, M. Mangold, P. Benner (2017), AIChE J 63(9):3832-3844.
M. Mangold, D. Khlopov, S. Palis, L. Feng, P. Benner, D. Binev, A. Seidel-Morgenstern (2015), J. Comp. Appl. Math. 289:253–266.

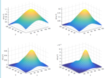
Molecular Simulation — MSD, MPI MIS

Combined POD-DEIM and range-separated tensor format for fast simulation of electrostatic potentials for molecules in solution.



Poisson-Boltzmann equation

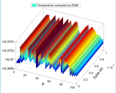
$$-\nabla\cdot(\epsilon(x)\nabla u(x)) + \bar{\kappa}^2(x)\sinh(u(x)) = \frac{4\pi e_c^2}{K_B T}\sum_{i=1}^{N_m} z_i \delta(x - x_i)$$

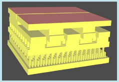


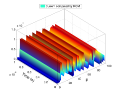
P. Benner, L. Feng, C. Kweyu, M. Stein (2017), arXiv:1705.08349

Nanoelectronics — Magwel NV

Index-aware moment-matching for **electro-thermal analysis** in nanoelectronics (EU project "nanoCOPS")





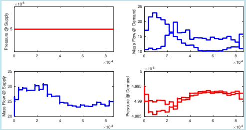


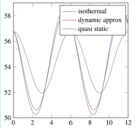
N. Banagaaya, P. Benner, L. Feng P. Meuris, W. Schoenmaker (2018), Appl. Math. Comp. 319:409–424

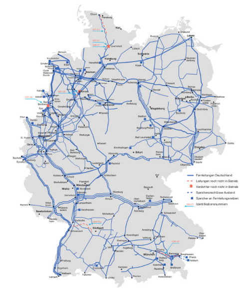
Simulation of coupled German energy transportation networks

- **Funding:** 6 million EUR for 2017–2021.
- **Goals:**
  - hierarchical modeling of transport and distribution networks
  - fast simulation on all levels
  - real-time scenario analysis for network operators
  - coupling of power and gas network
- **Results:** New **discretization** and **model order reduction** methods for
  - isothermal Euler equations on network graph
  - with nonsmooth nonlinearity
  - leading to coupled system of differential-algebraic equations (DAEs)
  - with uncertain parameters

Implemented in **morgen** — **M**odel **O**rder **R**eduction of **G**as and **E**nergy **N**etworks.







The German natural gas transportation network

Math Energy

Partners:

Fraunhofer SCAI
Fraunhofer ITWM
TU Berlin
HU Berlin
TU Dortmund
U Trier
PSI AG
associated:
Venios GmbH
OGE

Funded by:

Federal Ministry for Economic Affairs and Energy

Goals and Research Areas

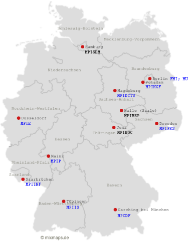
Funding: 5.8 million EUR from central MPG funds for 2017–2022.

Main goal: smart search of “materials configuration space” using big data techniques.

Research Areas:

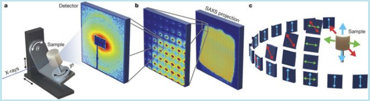
- Structure and plasticity of materials
- Data diagnostics in 3D imaging
- Discovering interpretable patterns, correlations, and causality
- Learning thermodynamic properties of materials
- Materials Encyclopedia

BiGmax MAX PLANCK RESEARCH NETWORK on big-data-driven materials science



CSC Contributions

- Co-chairing the network with M. Scheffler (FHI, Berlin)
- Implementation of fast methods for deep learning
- Image reconstruction from 6D SAXS data (with Fratzl group (MPI KG, Golm))



Outlook

- Smart use of available (simulation and experimental) data for Simulation, Optimization, Control, and Uncertainty Quantification (S-O-C-UQ).
- Nonlinear model order reduction, in particular nonsmooth, parametric DAE systems, using available data.
- Nonlinear controller and observer design based on “state-dependent Riccati equations”, extended Kalman filter.
- Further development, HPC implementation, and application of tensor techniques:
  - range-separated tensor format for multiparticle simulation
  - low-rank tensor techniques for uncertain control problems
  - tensor-based implementation of ML/AI algorithms