MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Data-Driven MOR Methods for efficient simulation of Infrastructure Networks

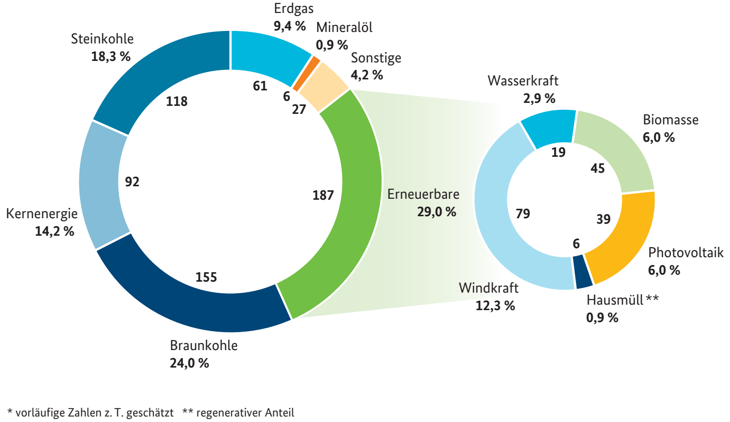
An overview

Peter Benner, Sara Grundel, Christian Himpe, Petar Mlinarić, Yue Qiu, Sarah Roggendorf, Maike Braukmüller

January 25, 2017

Electricity Production 2015

Data for Germany (TWh)



Source: AG Energiebilanzen, (August 2016)

Renewable Energies, a Trend

Renewable Energies

2000: 6%
2015: 29%
Goal of Germany:
2050: 60%-80%

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But ...

Consumption and Generation are not coordinated in time and space

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- Storage
- Transport

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Active Research Areas

- Batteries
- Energy Conversion Technologies
- Operation and Network Infrastructure

Simulation of Energy Networks

- Several **Large** Networks (Power, Gas, Heat)
- Specialised difficult components **(nonlinear, hyperbolic, ...)**
- PDEs, ODEs and Algebraic Constraints (PDAE)
- Switched Systems
- Coupled Systems (Power2Gas, Using of Heat from Conversion)
- ...

⇓

Powerful Simulation Tools are needed

Content

Content

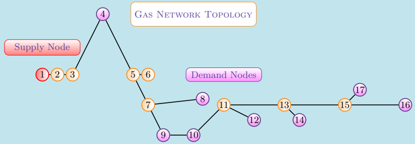
Network Modelling - Gas

- The network is modelled as a directed graph $\mathcal{G} = (\mathcal{A}, \mathcal{N})$,
- where the vertices are supply nodes $\mathcal{N}_+$, demand nodes $\mathcal{N}_-$ and interior nodes $\mathcal{N}_0$ (junctions),

$$\mathcal{N} = \mathcal{N}_+ \cup \mathcal{N}_- \cup \mathcal{N}_0.$$

- The edges can be **pipes**, compressors, valves, regulators, or other possible components of a realistic gas network.

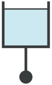
$$\mathcal{A} = \mathcal{A}_P \cup \mathcal{A}_C \cup \dots$$



supply pressures and demand fluxes are given

Equations - Node Elements

Supply nodes are gas sources with unlimited capacity. These are modeled by a given time dependent pressure function $p_{\text{set}}(t)$.



$$p = p_{\text{set}}(t)$$

A **demand node** has a given demand $q_{\text{set}} : I \longrightarrow \mathbb{R}_+$. Thus, the difference between the amount of gas flowing towards a node, and the amount of gas flowing away from the node has to be $q_{\text{set}}(t)$.

$$\sum_{i \in I_{in}} q_R^i - \sum_{i \in I_{out}} q_L^i = q_{\text{set}}(t)$$

An **interior node** is modelled as a demand node with $q_{\text{set}}(t) \equiv 0$.

Equations - Pipe

pipe:	●————●	Hyperbolic PDE

$$\frac{\partial p}{\partial t}(x,t) + \frac{\rho_0 c^2}{a}\frac{\partial q}{\partial x}(x,t) = 0$$
$$\frac{\partial q}{\partial t}(x,t) + \frac{\partial}{\partial x}(f(p(x,t),q(x,t))) = g(p(x,t),q(x,t))$$

diameter d, cross-section $a = \frac{\pi}{4}d^2$ and length ℓ, time $t \in [t_0, T] := I \subset \mathbb{R}$ $x \in \Omega \subset \mathbb{R}$. mass flow $q\colon \Omega \times I \longrightarrow \mathbb{R}$ and the pressure $p\colon \Omega \times I \longrightarrow \mathbb{R}$.

$$f = \frac{a}{\rho_0}p(x,t) + \frac{\rho_0 c^2}{a}\frac{q(x,t)^2}{p(x,t)} \quad g = -\frac{\lambda\rho_0 c^2}{2da}\frac{q(x,t)|q(x,t)|}{p(x,t)} - \frac{ag}{\rho_0 c^2}p(x,t)\frac{\partial h(x)}{\partial x}$$

Equations - Valve, Regulator,...

valve:  Switch

$$\begin{aligned} p_L(t) = p_R(t),\ q_L(t) = q_R(t) \qquad & \text{if valve open} \\ q_L(t) = q_R(t) = 0 \qquad & \text{if valve closed} \end{aligned}$$

reguator:  nonsmooth

$$\begin{aligned} p_R(t) &= \max(p_L(t), p_C) \\ q_R(t) &= q_L(t) \end{aligned}$$

PDAE

Partial Differential Algebraic Equation

$$
\begin{aligned}
\partial_t p_i + \partial_x f_1(p_i, q_i) &= 0 \quad i \in \mathcal{A}_P \\
\partial_t q_i + \partial_x f_2(p_i, q_i) &= g(p_i, q_i) \quad i \in \mathcal{A}_P \\
(p_R)_i &= \max((p_L)_i, p_C) \quad i \in \mathcal{A}_R \\
(q_L)_i &= (q_R)_i \quad i \in \mathcal{A}_R \\
&\cdots\cdots \\
\sum_{i \in I_k} q_i(L_i) - \sum_{i \in O_k} q_i(0) &= 0 \quad k \in \mathcal{N}_0 \\
\sum_{i \in I_k} q_i(L_i) - \sum_{i \in O_k} q_i(0) &= q_{set}(t) \quad k \in \mathcal{N}_d \\
\rho_k(t) &= \rho_{set}(t) \quad k \in \mathcal{N}_s
\end{aligned}
$$

Challenges of (P)DAEs

- existence of solutions
- index concepts
- space discretization
- solver for the discretized PDAE (time integration)
- model order reduction (nonlinear, DAE, uncertain and parameterized)
- parameter optimization
- uncertainty quantification
- optimal control/ optimization

Content

First Step - Discretization

Discretization and Index

Details on the next slides

hyperbolic PDE

Finite Volume Type Methods

Port-Hamiltonian Structure

Preserve the structure in discretized scheme.

Index and Discretization

One Pipe Segment

$$\begin{aligned} \partial_t \rho + \partial_x q &= 0 \\ \partial_t q + a^2 \partial_x \rho + \partial_x \left(\frac{q^2}{\rho}\right) &= -\frac{\lambda(q)}{2D} \frac{q|q|}{\rho} \end{aligned}$$

Left end supply node with given pressure, right end demand node with given flux

Index and Discretization

$$
\begin{aligned}
\partial_t \rho_* + \frac{q_R - q_L}{L} &= 0, \\
\partial_t q_* + \frac{a^2}{L}(\rho_R - \rho_L) - \frac{\lambda(q_*)}{2D}\frac{q_*|q_*|}{\rho_*} &= 0, \\
\rho_L - \rho_{set}(t) &= 0, \\
q_R - q_{set}(t) &= 0
\end{aligned}
$$

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q_R - q_{set}(t) &= 0
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$\rho_* = \rho_L$ and $q_* = q_L$,

$$
\begin{aligned}
\partial_t \rho_{set} + \frac{q_{set} - q_L}{L} &= 0\\
\partial_t q_L + \frac{a^2}{L}(\rho_R - p_{set}) + f(q_L, p_{set}) &= 0
\end{aligned}
$$

This is a DAE

Index and Discretization

$$\begin{aligned}
\partial_t \rho_* + \frac{q_R - q_L}{L} &= 0, \\
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Purely algebraic equation

Index and Discretization

$$
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\partial_t \rho_* + \frac{q_R - q_L}{L} &= 0,\\
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\rho_L - \rho_{set}(t) &= 0,\\
q_R - q_{set}(t) &= 0
\end{aligned}
$$

$\rho_* = \rho_R$ and $q_* = q_L$.

$$
\begin{aligned}
\partial_t \rho_R + \frac{q_{set} - q_L}{L} &= 0\\
\partial_t q_L + \frac{a^2}{L}(\rho_R - \rho_{set}) + f(q_L, p_R) &= 0
\end{aligned}
$$

This is an ODE

Index of the system

Going from one pipe to the pipe network we assume continues solutions exist.

Theorem 1 [Grundel, Jansen, Hornung et al 2013]

The gas equation with midpoint discretization is a DAE of at most index 2. It has index 1 iff there is one supply node.

Theorem 2 [Jansen, Grundel 2015, Roggendorf 2015]

With an upwind type discretization the pure pipe network is an index 1 DAE (evaluate pressure on the right and flux on the left). There is an explicit decoupling to an ODE.

Theorem 3 [Braukmüller 2016]

Introducing interior discretization nodes on the pipe, the resulting DAE is still index 1.

The DAE

- without interior discretization points

Simple Gas Equation [Jansen, Grundel 2015]

$$\partial_t \rho_d = T_1 q_L + C_1 q_{set}$$
$$\partial_t q_L = T_2 \rho_d + C_2 \rho_{set} + F(q_L, \rho_d, \rho_{set}, q_{set})$$

Arbitrary Gas Equation [Roggendorf 2015]

$$\partial_t p = T_1(p) q_L + C_1(p) q_{set}$$
$$\partial_t q_L = F(q_L, p, p_{set}, q_{set})$$

The DAE

- with interior discretization points

Simplified Euler Equation [Braukmüller 2016]

$$\begin{aligned} \partial_t p_D &= f(p_N, p_D, p_{set}) \\ 0 &= g(p_N, p_D, p_{set}, q_{set}) \end{aligned}$$

- A simplification by Herty et al. is used to eliminate the flux.
- p_N is the pressure at the nodes.
- p_D is the pressure vector at all discretization points in all pipes.

Simulation - Time Integration

- Stiffness
- Hyperbolic nature
- Port Hamiltonian nature - Future

$$\dot{x} = Tx + f(x,t)$$

Explicit Time Integration fails

Simple IMEX scheme:

$$\frac{x_{n+1} - x_n}{h} = (1-\gamma)Tx_n + \gamma Tx_{n+1} + f(x_n, t),$$

for $\gamma \in [0,1]$ and time step h, which leads to the iteration

$$x_{n+1} = (1 - hT)^{-1}\left(x_n + hf(x_n)\right),$$

for $\gamma = 1$.

Linearization - An option?

$$\begin{aligned} \partial_t \rho_D &= T_1 q_L + C_1 q_{set} \\ \partial_t q_L &= T_2 \rho_d + C_2 \rho_{set} + F(q_L, \rho_d, \rho_{set}, q_{set}) \end{aligned}$$

Pick a **stationary solution** $\cdot^*$ and linearize the system to

$$\begin{aligned} \partial_t \rho_D &= T_1 q_L + C_1 q_{set} \\ \partial_t q_L &= T_2 \rho_d + C_2 \rho_{set} + J_{q_L} F(q_L^*, \rho_d^*, \rho_{set}^*, q_{set}^*) q_L + \dots \end{aligned}$$

How good is the linearized solution?
In what neighborhood is it a reasonable approximation?

Structure of Linearized System

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \begin{pmatrix} 0 & D_1\mathcal{A} \\ -D_2\mathcal{A}^T + D_3\mathcal{A}_R^T & -D_4 \end{pmatrix} \begin{pmatrix} p \\ q \end{pmatrix} + Bu$$

where the D_i are diagonal matrices given by

$$\begin{aligned} D_1 &> 0, \\ D_2 &> 0, \\ (D_3)_{kk} &= -\frac{a_k g}{RT_0}\frac{\Delta h_k}{L_k}\frac{1}{\left(z\left(\bar{p}_R^k\right)^2\right)} + \frac{\lambda_k RT_0 \bar{q}_L^k \left|\bar{q}_L^k\right|}{2d_k a_k \left(\bar{p}_R^k\right)^2}, \\ (D_4)_{kk} &= \frac{\lambda_k RT_0}{d_k a_k}\frac{z\left(\bar{p}_R^k\right)\left|\bar{q}_L^k\right|}{\bar{p}_R^k}. \end{aligned}$$

Stability of Linearized System

Theorem

The linear system is stable if $D_3 = 0$ and D_4 is positive definite.

Proof.

If μ is an eigenvalue of

$$\begin{pmatrix} 0 & D_1\mathcal{A} \\ -D_2\mathcal{A}^T + D_3\mathcal{A}_R^T & -D_4 \end{pmatrix}$$

and $\hat{x} = (\hat{x}_1^T, \hat{x}_2^T)^T$ is the corresponding eigenvector, then

$$\begin{aligned} \mu\hat{x}_1 &= D_1\mathcal{A}\hat{x}_2, && \text{(4a)} \\ \mu\hat{x}_2 &= -D_2\mathcal{A}^T\hat{x}_1 + D_3\mathcal{A}_R^T\hat{x}_1 - D_4\hat{x}_2. && \text{(4b)} \end{aligned}$$

□

Proof continued ...

Proof.

Multiplying (4a) by $\hat{x}_1^* D_1^{-1}$ and (4b) by $\hat{x}_2^* D_2^{-1}$ yields

$$\begin{aligned} \mu \hat{x}_1^* D_1^{-1} \hat{x}_1 &= \hat{x}_1^* \mathcal{A} \hat{x}_2, && \text{(5a)} \\ \mu \hat{x}_2^* D_2^{-1} \hat{x}_2 &= -\hat{x}_2^* \mathcal{A}^T \hat{x}_1 + \hat{x}_2^* D_2^{-1} D_3 A_R^T \hat{x}_1 - \hat{x}_2^* D_2^{-1} D_4 \hat{x}_2. && \text{(5b)} \end{aligned}$$

Now (5a) can be used to replace $\hat{x}_2^* \mathcal{A}^T \hat{x}_1$ in (5b), yielding

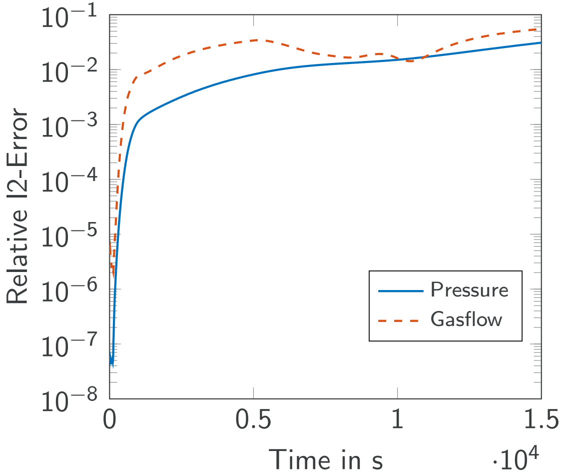
$$\mu \hat{x}_1^* D_1^{-1} \hat{x}_1 + \mu^* \hat{x}_2^* D_2^{-1} \hat{x}_2 = -\hat{x}_2^* D_2^{-1} D_4 \hat{x}_2 + \hat{x}_2^* D_2^{-1} D_3 \mathcal{A}_R^T \hat{x}_1.$$

Finally, taking the real part of the above equation leads to

$$\mathrm{Re}(\mu) \left(\hat{x}_1^* D_1^{-1} \hat{x}_1 + \hat{x}_2^* D_2^{-1} \hat{x}_2 \right) = -\hat{x}_2^* D_2^{-1} D_4 \hat{x}_2 + \mathrm{Re}(\hat{x}_2^* D_2^{-1} D_3 \mathcal{A}_R^T \hat{x}_1). \quad (6)$$

$\square$

Linear System - Performance



Content

Network MOR

Structure Preserving MOR on Networks [Trentelmann et al. 2014]

Use a Petrov-Galerkin projection with

$$V_r = P(\pi),$$
$$W_r = P(\pi)\left(P(\pi)^T P(\pi)\right)^{-1}.$$

Here $P(\pi)$ is the characteristic matrix of a partition π, e.g. for $\pi = \{\{1,2,3,4\},\{5,6\},\{7\},\{8\},\{9,10\}\}$ we have

$$P(\pi)^T = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}.$$

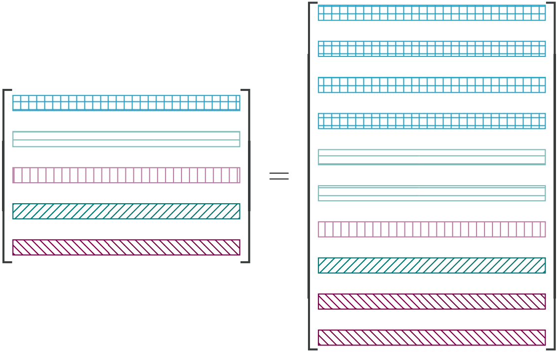
Clustering

Given a good projection V_r we want to find a partition π. such that

$$\operatorname{Im} V_r \approx \operatorname{Im} P(\pi).$$

We know that $\operatorname{Im} V_r = \operatorname{Im} P(\pi)$ if and only if $V_r = P(\pi)Z$ for a nonsingular Z.

$$P(\pi)Z = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$



,

How to find V_r?

V_r is the projection matrix such that any solution $x(t)$ of the full system is best approximated (or well approximated) by $V_r x_r(t)$ for an $x_r(t) \in \mathbb{R}^r$

$\Downarrow$

Classical MOR Methods.

Network MOR

Petar Mlinarić Thursday 11:00 Room: U1

Classical MOR

POD

- Nonlinear Method based on Snapshots.
- No Restriction on Model

Empirical Gramians

Christian Himpe Friday 10:30 Room: O100

$\mathcal{H}_2$ optimal MOR (IRKA)

- Linearized Model
- Adjusted to keep Block Diagonal Structure (Quasi-Optimal)

Singular Value Decay - Example

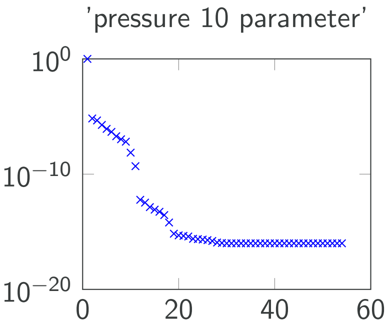
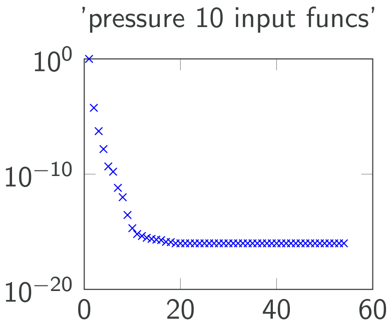


Figure : Singular values of the snapshot matrices.

Singular Value Decay - Example



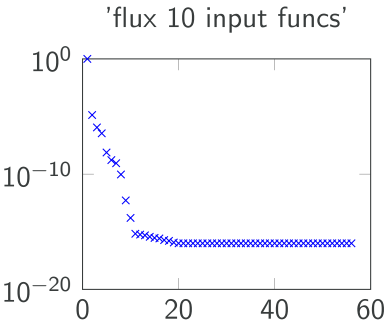


Figure : Singular values of the snapshot matrices.

MOR and IMEX

MOR and IMEX

If full model has the form

$$\dot{x} = Tx + f(x)$$

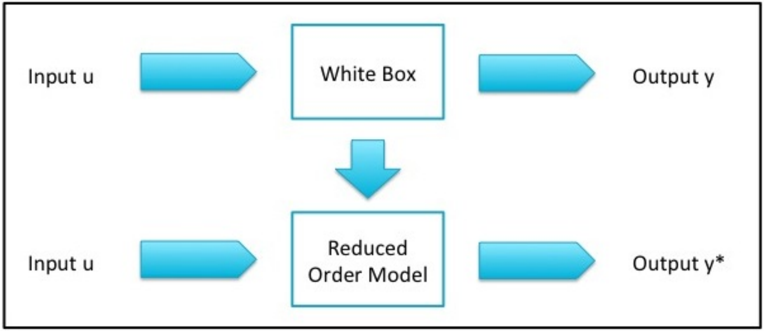
the reduced model will typically look like:

$$\dot{\hat{x}} = \hat{T}\hat{x} + \hat{f}(\hat{x})$$

This means we can use the same IMEX scheme.

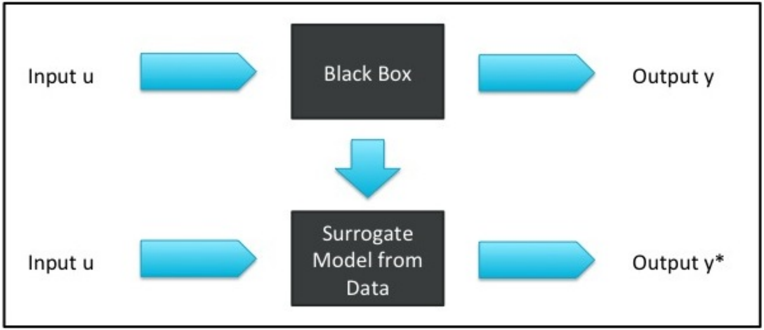
Content

White Box Model



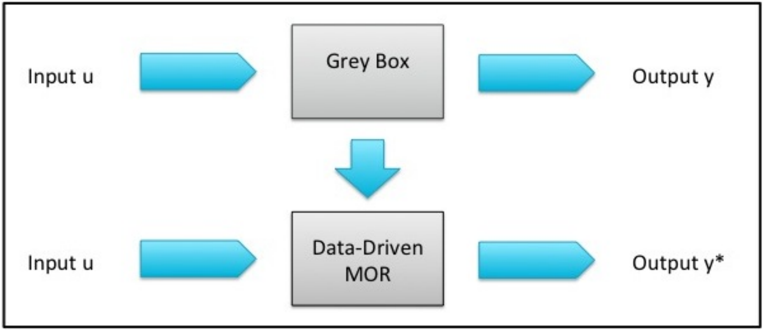
- Known Behaviour from Input to Output
- typically given by a PDE/ODE, MOR techniques can be used

Black Box



- We have Input/Output Data or we can produce Input/Output Data
- Surrogate Model by Interpolation (Radial Basis Functions,...)

Grey Box



- Approximate Model (e.g. parameters unknown, simplified model,...)
- Data-Driven MOR, Parameter Estimation, UQ, ...

Statistical inverse problem

We start with the *parameter-to-observable map (output map)* $g : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}^m$ defined as

$$Y = g(X, E)$$

where X, Y, E are random variables. Now Bayes' theorem is written as

$$\pi_{\text{post}} := \pi(x|y_{\text{obs}}) = \frac{\pi_{\text{prior}}(x)\pi(y_{\text{obs}}|x)}{\pi(y_{\text{obs}})} \propto \pi_{\text{prior}}(x)\pi(y_{\text{obs}}|x)$$

where we used the prior probability density function, the likelihood function, the data. We now assume

$$Y = AX + E.$$

and X and E are statistically independent

$$\pi_{\text{noise}}(e) = \pi_{\text{noise}}(y_{\text{obs}} - Ax).$$

and now Bayes' theorem can be written as

$$\pi_{\text{post}} \propto \pi_{\text{prior}}(x)\pi_{\text{noise}}(y_{\text{obs}} - Ax)$$

Bayesian inverse problem

Assuming that both probability density functions for X and E are Gaussian we can rewrite the PDFs and rewrite Bayes' theorem further to get

$$\pi_{\text{post}} \propto \exp\left(-\frac{1}{2}\|x - \bar{x}_{\text{prior}}\|^2_{\Gamma^{-1}_{\text{prior}}} - \frac{1}{2}\|y_{\text{obs}} - Ax - \bar{e}\|^2_{\Gamma^{-1}_{\text{noise}}}\right).$$

and the covariance matrix

$$\begin{aligned}\Gamma_{\text{post}} &= \left(A^T\Gamma^{-1}_{\text{noise}}A + \Gamma^{-1}_{\text{prior}}\right)^{-1} = \left(A^T\Gamma^{-1}_{\text{noise}}A + \Gamma^{-1}_{\text{prior}}\right)^{-1} \\ &= \Gamma^{1/2}_{\text{prior}}\left(\underbrace{\Gamma^{1/2}_{\text{prior}}A^T\Gamma^{-1}_{\text{noise}}A\Gamma^{1/2}_{\text{prior}}}_{\tilde{H}_{\mathrm{misfit}}} + I\right)^{-1}\Gamma^{1/2}_{\text{prior}}\end{aligned}$$

Low-Rank Approximation

We compute a low-rank approximation to the *prior-preconditioned Hessian* of $\tilde{H}_{\mathrm{misfit}} \in \mathbb{R}^{n,n}$

$$\tilde{H}_{\mathrm{misfit}} = \Gamma_{\text{prior}}^{1/2} A^T \Gamma_{\text{noise}}^{-1} A \Gamma_{\text{prior}}^{1/2} \approx V \Lambda V^T$$

where V and Λ represent the dominant eigenvectors and eigenvalues, respectively.

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Techniques

- QR algorithm for all eigenvalues (expensive)
- Arnoldi/Lanczos techniques for parts of the spectrum (cheap)
- Utilizing tensor structure $\Longrightarrow$ Tensor-Arnoldi/Lanczos techniques for parts of the spectrum (no curse of dimensionality for high-dimensional problems)

Low-Rank Approximation

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- QR algorithm for all eigenvalues (expensive)
- Arnoldi/Lanczos techniques for parts of the spectrum (cheap)
- Utilizing tensor structure $\Longrightarrow$ Tensor-Arnoldi/Lanczos techniques for parts of the spectrum (no curse of dimensionality for high-dimensional problems)

Defines the relevant subspace for covariance information

Parametric MOR

Given a parametric Model

$$\dot{x} = f(x, p, u), \quad y = g(x, p).$$

PMOR creates a parametric ROM

$$\dot{\hat{x}} = \hat{f}(\hat{x}, p, u), \quad y = \hat{g}(\hat{x}, p)$$

Given observables y_{obs} one can do **parameter estimation** by many simulations of the fast reduced model.

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Given observables y_{obs} one can do **parameter estimation** by many simulations of the fast reduced model.

Reduced Model quick with a higher tolerance on the error.

Content

1. Introduction

2. Modelling - Gas

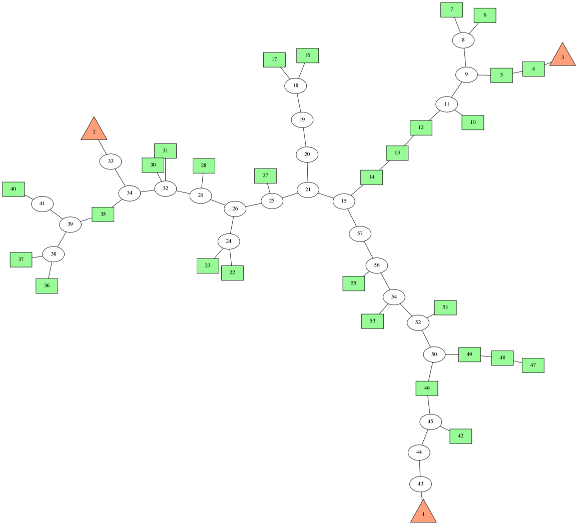
3. Simulation

4. MOR

5. Data

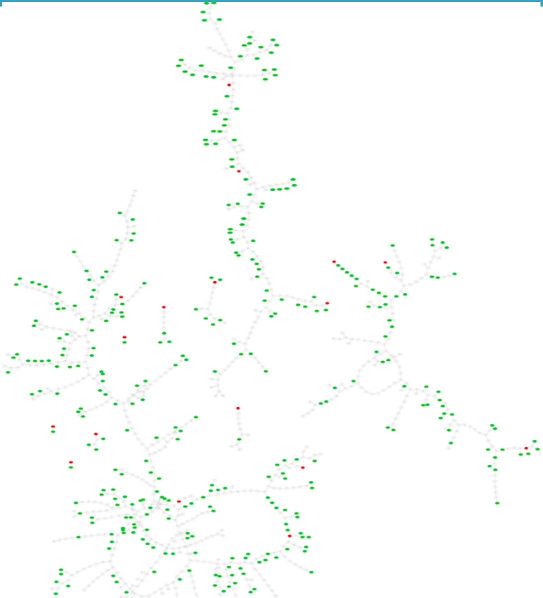
6. Numerics

Medium Size Model



- 57 Nodes
- 56 Pipes
- 28 Demand Nodes
- 1 Supply Nodes

Large Model

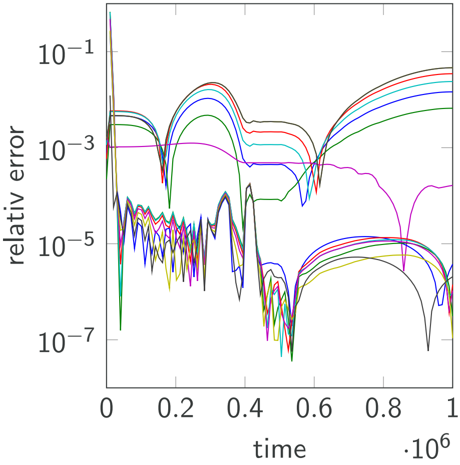


- 578 Nodes
- 586 Pipes
- 278 Demand Nodes
- 5 Supply Nodes

Medium Size Model

Proof of Concept

error plot



POD-DEIM

Modelling as Decoupled ODE

- Snapshots for varying parameters
- Snapshots for varying input functions

- Full Order: 110
- Reduced Order: 10
- Speedup: 500

Large Model - IMEX

Timestep

- nonstiff solver have a step size of $\approx 0.01s$
- Matlabs ode23s has a step size of $\approx 1s$
- IMEX solver work with a step size of $\approx 1 - 100s$

Large Model - IMEX

Timestep

- nonstiff solver have a step size of $\approx 0.01s$
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Reduced Model

- seems to be even stiffer
- speedup from IMEX more significant ≈ 1000

Large Model - IMEX

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Speedup Large Model

≥ 1000

Large Model - IMEX

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Reduced Model

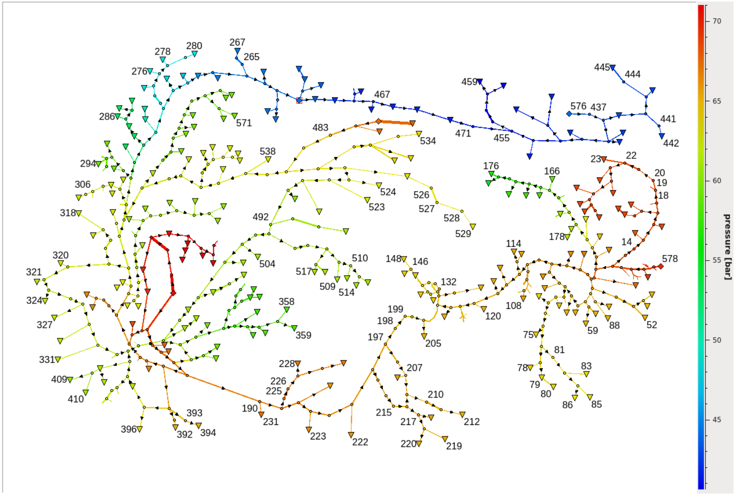
- seems to be even stiffer
- speedup from IMEX more significant ≈ 1000

Speedup Large Model

≥ 1000

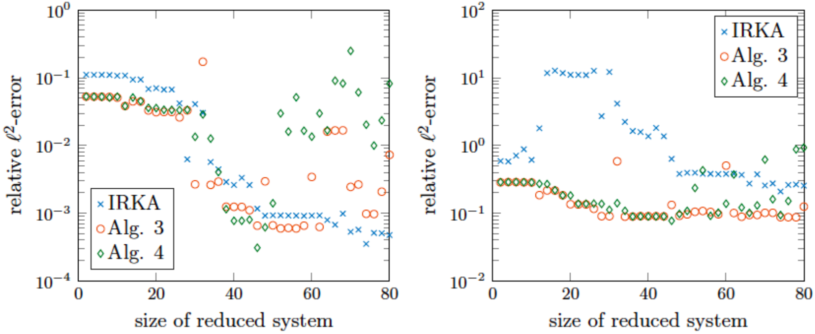
- Full System Size: 1159
- Reduced System Size: 10
- Error: 1%

Solution: Pressure Distribution



Linearized Model and IRKA

Figure 4.23: Network 2 ($n = 110$): Relative ℓ^2-error in the pressure component (left) and the mass flow component (right).



Alg. 3: enforce block structure after convergence
Alg. 4: block structure in each iteration step

Network MOR

- Clustering keeps sparsity
- DEIM is not needed

Network MOR

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structure-preserving

Network MOR

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structure-preserving

Preliminary results

- Medium Size Model
- Full Size: 57+88
- Reduced Size: 40
- Speedup: ≈ 10
- Error: $\approx 1\%$

Thank you for your attention.

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- Sara Grundel, Lennart Jansen, Nils Hornung, Tanja Clees, Caren Tischendorf, Peter Benner *Model order reduction of differential algebraic equations arising from the simulation of gas transport networks*. Springer, 2014
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