Modelling, Simulation and Control in Key Technologies

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DFG Research Center MATHEON
Mathematics for key technologies

Overview

Wishes for a better future

Wouldn't it be nice, if

- our heating system makes our apartment nice and comfortable and a same time the energy resources are significantly reduced;
- our airplane flies through a turbulence and we don't notice;
- a high-speed train goes by our house and we don't hear it;
- the public transport system is always on time;
- our car makes less noise, uses less gas and produces less CO_2;
- our computers get faster every year and have more storage;
- fatal traffic accidents are avoided by automated help systems;
- . . ..

Theses

- Our engineers have built cars, airplanes, bridges, skyscrapers, chips, plants . . . for ages.
- Most engineers get away with the math from the first year.
- For the solution of differential equations, eigenvalue problems, optimization problems, there are wonderful commercial packages? **They always deliver good solutions.**
- If the problems become more complex then we just buy a bigger computer.
- **We don't really need mathematics** except as language for describing the models.
- **And the mathematicians don't really help, they spent their time looking for the zeroes of the Riemann Zeta-function.**
- **Optimization?** We just use genetic algorithms, they always find the optimal solution.

No technological development without modern mathematics! We need:

- Very good mathematical models, that represent the technological process well.
- Deep understanding of the models and the dynamics of the processes.
- Accurate and efficient algorithms to simulate the models/processes.
- Accurate and efficient methods to control and optimize the processes and products.

Overview

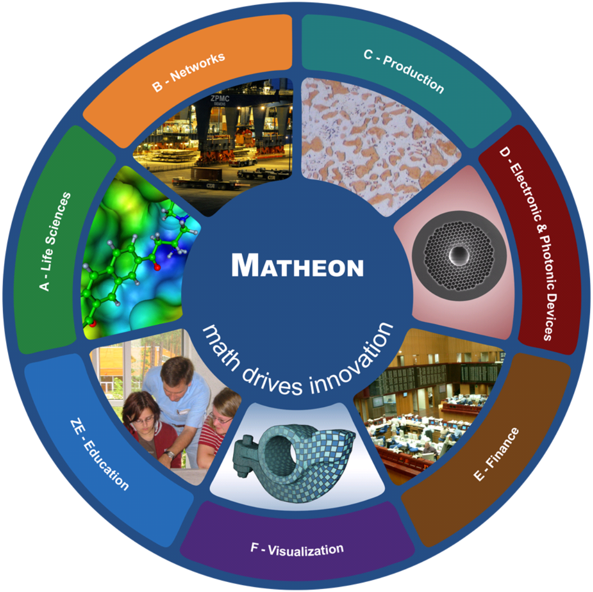
What is MATHEON?

- DFG Research center funded since June 2002.
- Mathematics for key technologies: Modelling, simulation, and optimization of real world processes.
- Participating institutions: TU Berlin, HU Berlin, FU Berlin, Weierstraß Institut (WIAS), Konrad Zuse Institut Berlin (ZIB).
- Funding volume, approx. 5.5 Mio Euro per year from DFG, 3 Mio per year from the research institutions and more than 7 Mio extra outside funding with about half from industry.
- Approx. 60 research projects.
- 45 math. professors.

- Modern key technologies become more and more complex.
- Innovation cycles become shorter.
- Flexible mathematical models are the prerequisite to master complexity, to act fast and to find smart solutions.
- To derive such models needs abstractions.
- The language of abstraction is mathematics.
- But mathematics is not only a language. It creates value.

Theoretical understanding, efficient algorithms, optimal solutions.

MATHEON application areas.



(Partial) differential-algebraic equations (DAEs), descriptor systems, singular differential eqns are implicit systems of differential equations of the form

$$
\begin{aligned}
0 &= \mathcal{F}(t,\xi,u,\dot{\xi},p,\omega),\\
y_1 &= \mathcal{G}_1(t,\xi,u,p,\omega),\\
y_2 &= \mathcal{G}_2(t,\xi,u,p,\omega),
\end{aligned}
$$

with $F \in C^0(\mathbb{R}\times\mathbb{D}_\xi\times\mathbb{D}_u\times\mathbb{D}_{\dot{\xi}}\times\mathbb{D}_p\times\mathbb{D}_\omega,\mathbb{R}^\ell)$,
$G_i \in C^0(\mathbb{R}\times\mathbb{D}_\xi\times\mathbb{D}_u\times\mathbb{D}_p\times\mathbb{D}_\omega,\mathbb{R}^{p_i})$, $i=1,2$.

- $t\in\mathbb{I}\subset\mathbb{R}$ is the time,
- ξ denotes the state (finite or infinite dimensional), $\dot{\xi}=\frac{d}{dt}\xi$,
- u denotes control inputs, ω denotes uncertainties/disturbances,
- y_1 denotes controlled, y_2 measured outputs,
- p denotes parameters.

Overview

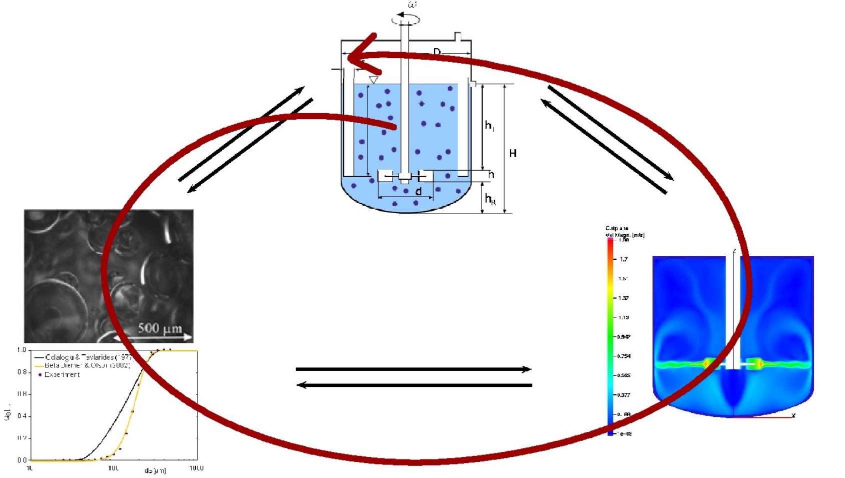
Modeling, simulation and software control of automatic gearboxes. Project with Daimler AG (Dissertation: Peter Hamann 2009) $\rightarrow$ film.

Technological Application

- Modeling of multi-physics model: multi-body system, elasticity, hydraulics, friction, ...
- Development of control methods for coupled system.
- Real time control of gearbox.

Goal: Decrease full consumption, improve switching
Large hybrid multi-physics control system (PDAE)

with M. Kraume (Chemical Eng., TU Berlin), M. Schäfer (Mech. Eng. TU Darmstadt)



Technological Application, Tasks

Chemical industry: pearl polymerization and extraction processes

- Modeling of coalescence and breakage in turbulent flow.
- Numerical methods for simulation of coupled system of population balance equations/fluid flow equations. $\rightarrow$ film.
- Development of optimal control methods for large scale coupled systems
- Model reduction and observer design.
- Feedback control of real configurations via stirrer speed.

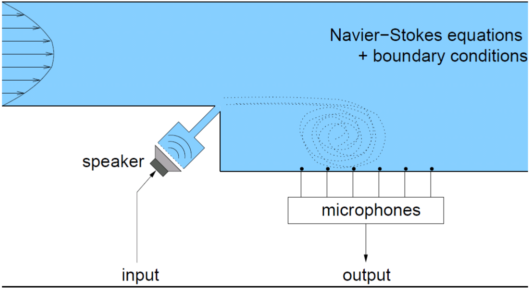
Goal: Achieve specified average drop diameter and small standard deviation for distribution by real time-control of stirrer-speed.

Mathematical system components

- Navier Stokes equation (flow field)
- Population balance equation (drop size distribution).
- One or two way coupling.
- Initial and boundary conditions.

Space discretization leads to an extremely large control system of nonlinear DAEs.

Project in Sfb 557 Control of complex shear flows, with F. Tröltzsch, M. Schmidt



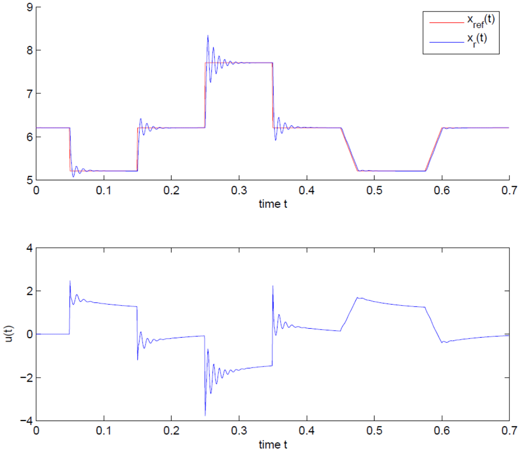
Technological Application, Tasks

Control of detached turbulent flow on airline wing

- Test case (backward step to compare experiment/numerics.)
- modeling of turbulent flow.
- Development of control methods for large scale coupled systems.
- Model reduction and observer design.
- Optimal feedback control of real configurations via blowing and sucking of air in wing.

Ultimate goal: Force detached flow back to wing.

Movement of recirculation bubble following reference curve.



Classical applications of (P)DAE modeling.

- Electronic circuit simulation (Kirchhoff's laws).
- Simulation and control of mechanical multi-body systems (position or velocity constraints).
- Flow simulation and flow control (mass conservation).
- Metabolic networks (balance equations).
- Simulation and control of systems from chemical engineering (mass balances).
- Simulation and control of traffic systems (mass conservation).
- …

Why (P)DAEs?

(P)DAEs provide a unified framework for the analysis, simulation and control of (coupled) dynamical systems (continuous and discrete time).

- **Automatic modeling leads to DAEs.** (Constraints at interfaces).
- Conservation laws lead to DAEs. (Conservation of mass, energy, momentum).
- Coupling of solvers leads to DAEs (discrete time).
- Control problems are DAEs (behavior).

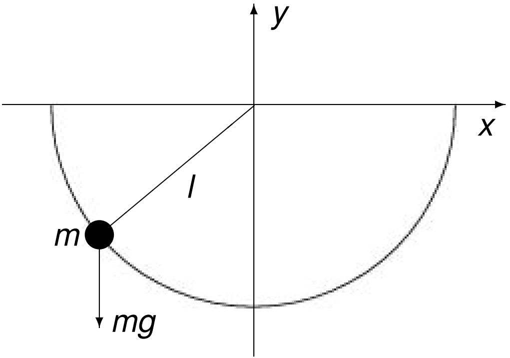


Figure: A mechanical multibody system

DAE modeling

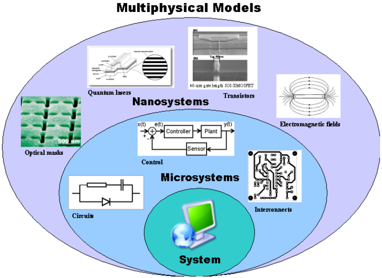
- Mass point with mass m in Cartesian coordinates (x, y) moves under influence of gravity in a distance l around the origin.
- Kinetic energy $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2)$
- potential energy $U = mgy$, where g is the gravity constant,
- Constraint equation $x^2 + y^2 - l^2 = 0$,
- Lagrange function $L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) - mgy - \lambda(x^2 + y^2 - l^2)$
- Equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q} = 0$$

  for the variables $q = x, y, \lambda$, i. e.,
- DAE model:

$$\begin{aligned} m\ddot{x} + 2x\lambda &= 0, \\ m\ddot{y} + 2y\lambda + mg &= 0, \\ x^2 + y^2 - l^2 &= 0. \end{aligned}$$

DAE modeling is standard in multi-physics systems.



Packages like MATLAB (SIMULINK, DYMOLA (MODELLICA) and SPICE like circuit simulators proceed as follows:

- ▷ Modularized modeling of uni-physics components.
- ▷ Network based connection of components.
- ▷ Identification of input and output parameters.
- ▷ Numerical simulation and control on full model.

Modeling becomes extremely convenient, but:

- Numerical simulation does not always work, instabilities and convergence problems occur (e.g. SIMULINK) !
- Solution may depend on derivatives of input functions.
- Consistent initialization is difficult.
- The discretized system may be unsolvable even if the DAE is solvable and vice versa.
- Numerical drift-off phenomenon.
- Model reduction is difficult.
- Classical control is difficult (non-proper transfer functions).

Black-box DAE modeling pushes all difficulties into the numerics. In general the methods cannot handle this!

We use derivative arrays (Campbell 1989).
We assume that derivatives of original functions are available or can be obtained via computer algebra or automatic differentiation.
Linear case: We put $E(t)\dot{x} = A(t)x + f(t)$ and its derivatives up to order μ into a large DAE

$$M_k(t)\dot{z}_k = N_k(t)z_k + g_k(t), \quad k \in \mathbb{N}_0$$

for $z_k = (x, \dot{x}, \ldots, x^{(k)})$.

$$M_2 = \begin{bmatrix} E & 0 & 0 \\ A - \dot{E} & E & 0 \\ \dot{A} - 2\ddot{E} & A - \dot{E} & E \end{bmatrix}, \; N_2 = \begin{bmatrix} A & 0 & 0 \\ \dot{A} & 0 & 0 \\ \ddot{A} & 0 & 0 \end{bmatrix}, \; z_2 = \begin{bmatrix} x \\ \dot{x} \\ \ddot{x} \end{bmatrix}.$$

Derivative arrays, nonlinear problems

Analogous approach for $F(t,x,\dot{x}) = 0$ yields derivative array:

$$0 = F_k(t,x,\dot{x},\ldots,x^{(k+1)}) = \begin{bmatrix} F(t,x,\dot{x}) \\ \frac{d}{dt}F(t,x,\dot{x}) \\ \ldots \\ \frac{d^k}{dt^k}F(t,x,\dot{x}) \end{bmatrix}.$$

We set

$$\begin{aligned} M_k(t,x,\dot{x},\ldots,x^{(k+1)}) &= F_{k;\dot{x},\ldots,x^{(k+1)}}(t,x,\dot{x},\ldots,x^{(k+1)}), \\ N_k(t,x,\dot{x},\ldots,x^{(k+1)}) &= -(F_{k;x}(t,x,\dot{x},\ldots,x^{(k+1)}),0,\ldots,0), \\ z_k &= (t,x,\dot{x},\ldots,x^{(k+1)}). \end{aligned}$$

Hypothesis: There exist integers μ, r, a, d, and v such that $\mathbf{L} = F_\mu^{-1}(\{0\}) \neq \emptyset$.
We have $\operatorname{rank} F_{\mu;t,x,\dot{x},\dots,x^{(\mu+1)}} = \operatorname{rank} F_{\mu;x,\dot{x},\dots,x^{(\mu+1)}} = r$, in a neighborhood of **L** such that there exists an equivalent system $\tilde{F}(z_\mu) = 0$ with a Jacobian of full row rank r. On **L** we have

1. $\operatorname{corank} F_{\mu;x,\dot{x},\dots,x^{(\mu+1)}} - \operatorname{corank} F_{\mu-1;x,\dot{x},\dots,x^{(\mu+1)}} = v$.
2. $\operatorname{corank} \tilde{F}_{x,\dot{x},\dots,x^{(\mu+1)}} = a$ and there exist smooth matrix functions Z_2 (left nullspace of M_μ) and T_2 (right nullspace of $\hat{A}_2 = \tilde{F}_x$) with $Z_2^T \tilde{F}_{x,\dot{x},\dots,x^{(\mu+1)}} = 0$ and $Z_2^T \hat{A}_2 T_2 = 0$.
3. $\operatorname{rank} F_{\dot{x}} T_2 = d, \quad d = \ell - a - v$, and there exists a smooth matrix function Z_1 with $\operatorname{rank} Z_1^T F_{\dot{x}} = d$.

Theorem (Kunkel/M. 2002)

The solution set **L** *forms a (smooth) manifold of dimension* $(\mu + 2)n + 1 - r$.
The DAE can locally be transformed (by application of the implicit function theorem) to a reduced DAE of the form

$$\begin{aligned} \dot{x}_1 &= G_1(t, x_1, x_3), && (d \text{ differential equations}), \\ x_2 &= G_2(t, x_1, x_3), && (a \text{ algebraic equations}), \\ 0 &= 0 && (v \text{ redundant equations}). \end{aligned}$$

The variables x_3 *represent undetermined components (controls).*

General numerical simulation procedure

- Consistent initial values are obtained by solving $F_\mu(t_0, x, \dot{x}, \dots, x^{(\mu+1)}) = 0$ at t_0 for the algebraic variable $(x, \dot{x}, \dots, x^{(\mu+1)})$.
- For the integration of the DAE, e.g. with `BDF` methods, the system

$$\begin{aligned} F_\mu(t_0 + h, x, \dot{x}, \dots, x^{(\mu+1)}) &= 0, \\ \tilde{Z}_1^T F(t_0 + h, x, D_h x) &= 0 \end{aligned}$$

  is solved for $(x, \dot{x}, \dots, x^{(\mu+1)})$.
- Here, $\tilde{Z}_1$ denotes a suitable approximation of Z_1 which projects onto the d differential equations at the desired solution, and

$$D_h x_i = \frac{1}{h} \sum_{l=0}^{k} \alpha_l x_{i-l},$$

  is the discretization by `BDF`.

Several productions codes are available.

- Production code GELDA Kunkel/M./Rath/Weickert 1998 (linear variable coefficients), uses BDF and Runge-Kutta discretization.
- Production code GENDA (nonlinear regular), Kunkel/M./Seufer 2002 based on BDF.
- Matlab code SOLVEDAE (nonlinear), Kunkel/Mehrmann/Seidel 2005.
- Special multi-body code GEOMS Steinbrecher 2006.
- Circuit codes, joint with NEC, Bächle, Ebert, 2006.

Acoustic field in car interior

Project with company SFE in Berlin 2007/2009.

- Computation of acoustic field for coupled system of car body and air.
- SFE has its own parameterized FEM model which allows geometry and topology changes. ($\rightarrow$ film)
- Frequent solution of linear systems and nonlinear eigenvalue problems (up to size $10,000,000$) is needed within optimization loop that changes geometry, topology, damping material, etc.
- Ultimate goal: Minimize noise in important regions in car interior.

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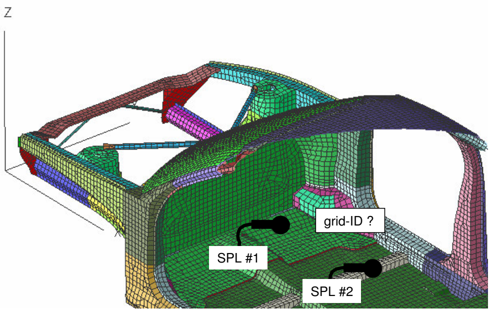
SFE AKUSMOD

FE Model: SPL for two microphone positions



SFE GmbH, Berlin
CEO: Hans Zimmer
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http://www.sfe-berlin.de

Frequency response: Linear system

Solve $P(\omega, \alpha)u(\omega, \alpha) = f(\omega, \alpha)$, where

$$P(\omega, \alpha) := -\omega^2 \begin{bmatrix} M_s & 0 \\ 0 & M_f \end{bmatrix} + \imath\omega \begin{bmatrix} D_s & D_{as}^T \\ D_{as} & D_f \end{bmatrix} + \begin{bmatrix} K_s(\omega) & 0 \\ 0 & K_f \end{bmatrix},$$

is complex symmetric of dimension up to $10,000,000$,

- M_s, M_f, K_f are real symm. pos. semidef. mass/stiffness matrices of structure and air, M_s is singular and diagonal, M_f is sparse. M_s is a factor $1000 - 10000$ larger than M_f.
- $K_s(\omega) = K_s(\omega)^T = K_1(\omega) + \imath K_2$.
- D_s is a real damping matrix, D_f is complex symmetric.
- D_{as} is real coupling matrix between structure and air.
- All or part of the matrices depend on geometry, topology and material parameters.

Detailed tasks of project

- Solve for a given set of parameters α_i, $i = 1, 2, \dots,$ the linear system $P(\omega)u(\omega, \alpha_i) = f(\omega, \alpha_i)$, for $\omega = 0, \dots,\ 1000hz$ in small frequency steps.
- The parameters α_i are determined in a manual or automatic optimization process, i.e. α_i and α_{i+1} are typically close.
- Parallelization in multi-processor multi-core environment.
- Often many right hand sides (load vectors) $f(\omega)$.
- Accuracy goal: Relative residual 10^{-6}.

Difficulties and challenges

- Problems are badly scaled and get increasingly ill-conditioned when ω grows.
- For some parameter constellations the system becomes exactly singular with inconsistent right hand side.
- Direct solution methods work only out-of-core.
- Blocks of matrices are changed with α.
- No multilevel or adaptive grid refinement is available, methods must be matrix based.

Eigenvalue problem

Consider nonlinear eigenvalue problem $P(\lambda, \alpha)x(\alpha) = 0$, where

$$P(\lambda, \alpha) := \lambda^2 \begin{bmatrix} M_s & 0 \\ 0 & M_f \end{bmatrix} + \lambda \begin{bmatrix} D_s & D_{as}^T \\ D_{as} & D_f \end{bmatrix} + \begin{bmatrix} K_s(\lambda) & 0 \\ 0 & K_f \end{bmatrix},$$

is **complex symmetric** and has dimension up to $10,000,000$, and all coefficients depend on parameter vector α. Tasks:

- Compute all eigenvalues in a given region of $\mathbb{C}$ and associated eigenvectors.
- Project the problem into the subspace spanned by these eigenvectors (for given sets of parameters) (Model reduction).
- Solve the second order differential-algebraic system (DAE).
- Optimize the eigenfrequencies/acoustic field, w.r.t. the set of parameters.

Difficulties and challenges

- We need to improve convergence and preconditioning.
- We need better linearization techniques.
- We need better perturbation and error analysis.
- We need multiple grids.
- We need adaptivity in mesh refinement, eigenvalue computation and optimization.
- The methods have to run as parallel methods on modern multi-core machines.

Conclusions

- Industrial applications lead to hard mathematical problems.
- Simulation and control of PDAEs.
- Large scale nonlinear eigenvalue problems within optimization loop.
- The mathematical theory and algorithms are still far from the needs in reality.
- Commercially available codes are not satisfactory.
- Industry is not interested in and does not pay for the analysis, convergence proofs, etc.
- Industrial production code development is a challenge.

References and papers see: `http://www.matheon.de/`

Thank you very much
for your attention.