Model reduction in the simulation, control and optimization of real world processes

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A consecutive effort of my students: Benner, Penzl, Stykel, Schmelter, Schmidt, Baur

Outline

$$\begin{tikzcd}
 & \textbf{Physical system} \arrow[dl] \arrow[dr] & \\
\textbf{Modelling} \arrow[d] & & \textbf{Modelling} \arrow[d] \\
\textbf{ODEs} \arrow[d] & & \textbf{PDEs} \arrow[ll, "\textit{semidiscr.}"'] \\
\textbf{Mod. reduction} \arrow[d] & & \\
\textbf{Reduced ODE} \arrow[rr] & & \textit{Sim., Control}
\end{tikzcd}$$

Control methods

- Semidiscretization in space using FVM, FEM, FDM $\Longrightarrow$ large scale ODE/DAE-control problem.
- Model reduction to reduce state dimension.
- Computation of control for reduced model using standard software such as SLICOT
- Application of computed control in large semidiscretized model or infinite dimensional model.
- Inequality or equality constraints are included in outer loop (SQP, Newton).

Semidiscretized control problem

$$
\begin{aligned}
F(t, x, \dot{x}, u) &= 0, \quad x(t_0) = x_0 \\
y(t) &= g(x)
\end{aligned}
$$

- state $x \in \mathbb{R}^n$,
- control $u \in \mathbb{R}^m$,
- output $y \in \mathbb{R}^p$,
- n, the number of discretization points (elements) in space is large.
- $m, p << n$

Replace system

$$\begin{array}{rcl} F(t,x,\dot{x},u) & = & 0, \quad x(t_0) = x_0 \\ y(t) & = & g(x) \end{array}$$

with $x \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, and $y \in \mathbb{R}^p$, by a reduced model

$$\begin{array}{rcl} \tilde{F}(t,\tilde{x},\dot{\tilde{x}},u) & = & 0, \quad \tilde{x}(t_0) = \tilde{x}_0 \\ y(t) & = & \tilde{g}(\tilde{x}) \end{array}$$

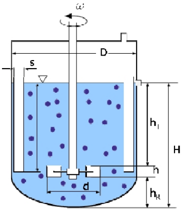
with $\tilde{x} \in \mathbb{R}^{\tilde{n}}$, $\tilde{n} << n$.

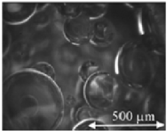
Goals

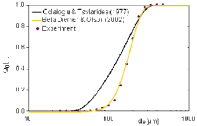
- Approximation error small, global error bounds
- Preservation of physics: stability, passivity, conservation laws
- Stable and efficient method for model reduction.

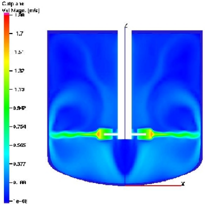
Outline

with M. Kraume from Chemical Engineering (S. Schlauch/Schmelter)









Chemical industry: pearl polymerization and extraction processes

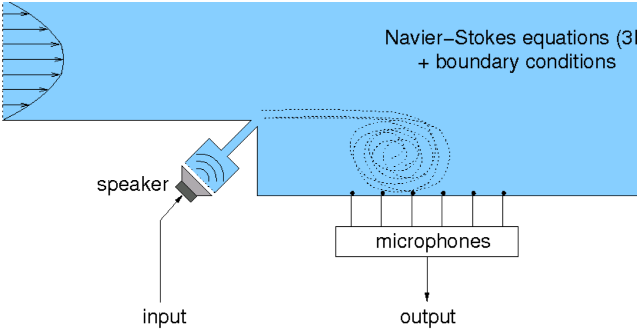
- Modelling of coalescence and breakage in turbulent flow.
- Numerical methods for simulation of coupled system of population balance equations/fluid flow equations.
- Development of optimal control methods for large scale coupled systems
- Model reduction and observer design.
- Feedback control of real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

Ultimate 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.


Navier–Stokes equations (3
+ boundary conditions
speaker
microphones
input
output

Control of detached turbulent flow on airline wing

- Test case (backward step to compare experiment/numerics.)
- Modelling 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.

Outline

Model reduction techniqes

SVD (singular value decomposition) based methods

- Balanced truncation (linear) Antoulas, Benner, Li, Moore, Penzl, Stykel, Sorensen, Varga, Wang, White, ...
- Hankel approximation: (linear) Adamjan, Anderson, Arov, Glover, Liu, Krein, ...
- Principal orthogonal decomposition (POD), (nonlinear) Banks, Hinze, King, Kunisch, Volkwein, ...

Krylov methods

- Pade' via Lanczos (moment matching) (linear) Boley, Freund, Gallivan, Gragg, Grimme, Jaimoukha, Kasenally, Van Dooren, ...

Books by Antoulas, 2005, Benner/M./Sorensen, 2005

Proper Orthogonal Decomposition (POD)

$$\begin{aligned} \dot{x} = f(t, x, u) &= 0, \quad x(t_0) = x_0 \\ y(t) &= g(x) \end{aligned}$$

- Consider snapshots for some control u.
- Determine (by solving the system)

$$\mathcal{X} = \left[\begin{array}{cccc} x(t_1) & x(t_2) & \ldots & x(t_N) \end{array}\right]$$

- SVD $\mathcal{X} = U_N \Sigma_N V_N^T \approx U_{\tilde{n}} \Sigma_{\tilde{n}} V_{\tilde{n}}^T$
- Truncate small singular values $\tilde{n} << n$
- Reduced system

$$\dot{\tilde{x}} = U_{\tilde{n}}^T f(t, U_{\tilde{n}} \tilde{x}, u) = 0$$

Analysis of POD

- Cheap and easy to use.
- 'Works' for nonlinear systems.
- Successful in practice.
- How to choose $u(t)$ for snapshots?
- Quite heuristic. Pure data compression.
- Little theory, Beattie, Kunisch/Volkwein, Tröltzsch.
- No preservation of physical properties.

Replace

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t), \quad x(t_0) = x_0 \\ y(t) &= Cx(t) \end{aligned}$$

by

$$\begin{aligned} \dot{\tilde{x}}(t) &= \tilde{A}\tilde{x}(t) + \tilde{B}u(t), \quad \tilde{x}(t_0) = \tilde{x}_0 \\ y(t) &= \tilde{C}x(t), \end{aligned}$$

with $\tilde{x} \in \mathbb{R}^{\tilde{n}}$, $\tilde{n} << n$.

Laplace transformation and approximation in frequency domain.

$$\begin{aligned} \hat{y} &= C(sI - A)^{-1} B\hat{u} \\ &= G(s)\hat{u}, \end{aligned}$$

with rational matrix valued transfer function $G(s)$ in Hardy space of functions that are analytic and bounded in the right half of complex plane.

$$\|G - \tilde{G}\|_{H_\infty} = \sup_{\omega \in \mathbb{R}} \|G(i\omega) - \tilde{G}(i\omega)\|$$

with $i = \sqrt{-1}$ and approximate transfer function $\tilde{G}(s) = \tilde{C}(sI - \tilde{A})^{-1}\tilde{B}$. ($G(i\omega)$: "frequency response matrix")

Moment matching, Pade' via Lanczos

Expand the transfer function $G(s)$ at point s_0

$$G(s) = M_0 + M_1(s - s_0) + M_2(s - s_0)^2 + \dots$$

and find approximate $\tilde{C}, \tilde{B}, \tilde{A}$ so that in the expansion of

$$\tilde{C}(sI - \tilde{A})^{-1}\tilde{B} = \tilde{M}_0 + \tilde{M}_1(s - s_0) + \tilde{M}_2(s - s_0)^2 + \dots$$

as many terms as possible are matched.

- $s_0 = \infty$: partial realization, Pade' approximation. Solution via Lanczos or Arnoldi method.
- $s_0 \in \mathbb{C}$ rational interpolation. Solution via rational Lanczos.

Analysis of Krylov Approach

- Fast and easy to use.
- Works for very large scale problems.
- Very successful in practice, VLSI simulation.
- Preservation of passivity, Sorensen 2002.
- Choice of s_0?
- Computation of moments problematic.
- No global error bound.
- Breakdown of Lanczos.

Outline

$$\dot{x} = Ax + Bu, \quad y = Cx$$

Consider Lyapunov equations:

$$\begin{aligned} AX_B + X_BA^T &= -BB^T \quad (X_B \text{ controllab. Gramian}) \\ A^TX_C + X_CA &= -C^TC \quad (X_C \text{ observab. Gramian}). \end{aligned}$$

- If A is stable and the system is controllable and observable, then X_B, X_C are positive definite.
- Idea: Make the system balanced, $X_B = X_C$ diagonal, and truncate small components.
- Every controllable and observable system can be balanced by a change of basis $\tilde{x} = Tx$.

1. Compute Gramians and Cholesky fact. $X_B = L_B L_B^T$, $X_C = L_C L_C^T$.
2. Compute the SVD of $U\Sigma V^T = L_B^T L_C$ with

$$\Sigma = \operatorname{diag}(\sigma_1, \ldots \sigma_n) = \begin{bmatrix} \Sigma_1 & \\ & \Sigma_2 \end{bmatrix},$$

   $\Sigma_2 = \operatorname{diag}(\sigma_{\tilde{n}+1}, \ldots, \sigma_n)$, $\sigma_{\tilde{n}+1}, \ldots, \sigma_n \leq tol$.
3. Set $T = \Sigma^{1/2} U^* L_B^{-1} = \Sigma^{-1/2} V^T L_C^T$.
4. Set $\tilde{x} = Tx$ and partition matrices as Σ.

$$\begin{aligned} TAT^{-1} &= \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \; Tx = \begin{bmatrix} \tilde{x} \\ \tilde{x}_r \end{bmatrix}, \\ TB &= \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}, \; CT^{-1} = \begin{bmatrix} C_1 & C_2 \end{bmatrix}. \end{aligned}$$

5. Reduced system $\frac{d}{dt}\tilde{x} = A_{11}\tilde{x} + B_1 u$, $y = C_1 \tilde{x}$.

Analysis of balanced truncation

- Very good approximation properties.
- Exact error estimates.

$$\|G - \tilde{G}\|_{H_\infty} = 2(\sigma_{\tilde{n}+1} + \ldots + \sigma_n).$$

- Stability is preserved. Passivity with modification
- Energy interpretation.
- In this form not feasible for large sparse problems from semidiscretized PDEs.
- Expensive to solve large scale Lyapunov equations.
- However, the Lyapunov solution has fast decaying eigenvalues.

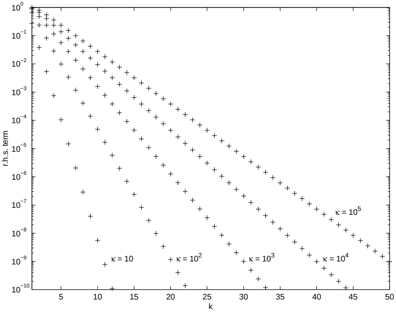
Theorem (Penzl '00)

A stable, symmetric, condition number $\kappa = \kappa(A)$, $m \ll n$. Then eigenvalues $\lambda_i(X)$ of Lyapunov solution satisfy

$$\frac{\lambda_{mk+1}(X)}{\lambda_1(X)} \leq \left(\prod_{j=0}^{k-1} \frac{\kappa^{(2j+1)/(2k)} - 1}{\kappa^{(2j+1)/(2k)} + 1} \right)^2 .$$

Extension to nonsymmetric case Antoulas et al, '01

Example: Heat equation



Low rank approx. of Lyapunov solutions

- We don't need the solution of Lyapunov equations.
- We need the product of Cholesky factors $L_B^T L_C$.
- Since we truncate anyway, it suffices to have low rank approximation of Cholesky factors

$$X = LL^T \sim \tilde{L}\tilde{L}^T,$$

where $\tilde{L}$ is rectangular with few columns.

Iterative methods for the computation of low rank factors: Penzl '99, Hackbusch/Khoromskij '00, Antoulas et al '05, Grasedyck '01-'04, Li '00, Gugercin '06, Sorensen et al '01., A Benner '02, Baur '08

Wachspress '88, Reichel '92, Starke '91, Penzl '98

Consider

$$A^T X + XA = W.$$

Split as forward

$$A^T X_{i+1/2} + X_i A = W$$

and backward solve

$$A^T X_{i+1/2} + X_{i+1} A = W$$

and iterate.

- We need sparse solver for A and A^T and shifts of these.
- Convergence acceleration by shifts.

Low rank version of classical ADI (LR-ADI) Penzl '00, Li '02, Stykel '04

Consider

$$A^T X + XA = BB^T$$

Iteration:

$$\begin{aligned} Z_1 &= \sqrt{-2p_1}(A + p_1 I)^{-1} B \\ Z_j &= [(A - p_j I)(A + p_j I)^{-1} Z_{j-1}, \\ &\quad \sqrt{-2p_i}(A + p_j I)^{-1} B] \end{aligned}$$

p_j's are scalar shift parameters.

LR-ADI computes sequence of rectangular Cholesky factors

$Z_1 =$  $,\qquad Z_2 =$  $,\qquad Z_3 =$  $,\qquad \ldots,$

s.t. $Z_j Z_j^T \to X$.

- Size grows by m in each step.
- Fixed storage version, Antoulas et al '01.
- Convergence analysis based on decay rates.

LR-Smith(l) Penzl '99 Efficient implementation of LR-ADI with cyclic shifts.

- LR-ADI/LR-Smith(l). More reliable and accurate than Krylov subspace techniques for Lyapunov equations
- Costs for LR-ADI/LR-Smith(l) comparable to Krylov methods.
- Compute low rank Cholesky factors Z_B and Z_C by LR-ADI or LR-Smith(l), such that $Z_B Z_B^T \approx X_B$ and $Z_C Z_C^T \approx X_C$.
- Balancing cheap since $Z_B^T Z_C$ small.
- Recent extensions using $\mathcal{H}$ matrix methods, Dissertation Baur 08, Grasedyck '07,...

2D Semi-discretization of heat equation (with boundary control term) from a steel cooling example Penzl 99, without constraints, using FEM

$$\begin{aligned} M\dot{\hat{x}}(t) &= -N\hat{x}(t) + \hat{B}u(t) \\ y(t) &= \hat{C}\hat{x}(t) \end{aligned}$$

- "stiffness matrix" N: large, sparse, symmetric, positive definite
- "mass matrix" M: large, sparse (same pattern as N), symmetric, positive definite, well-conditioned
- dimensions of example: $m = q = 6$, $n = 12113$

Model reduction with LR-Smith(l)

Z_B: rel. residual $= 9 \cdot 10^{-11}$, rank $Z_B = 300$
Z_C: rel. residual $= 4 \cdot 10^{-12}$, rank $Z_C = 360$

$$\text{“Error”} = \text{Error}(\omega) = \|G(i\omega) - \tilde{G}(i\omega)\|/c, c = \|G\|_{L_\infty}$$

Reduction $n = 12113 \searrow \tilde{n} = 600$, but difference in “frequency response” is tiny. For larger error much smaller $\tilde{n}$.

$$\begin{aligned} \frac{\partial v}{\partial t} &= \nabla(K(\nabla v)) + \nabla p + u(t), \\ 0 &= \mathrm{div}\ v, \end{aligned}$$

plus initial and boundary conditions Semidiscretization in space gives descriptor system

$$\begin{aligned} \frac{dv_h}{dt} &= \Delta_h(K_h \Delta_h v_h(t)) + \nabla_h p_h(t) + Bu(t), \\ 0 &= \mathrm{div}_h v_h(t), \end{aligned}$$

where v_h is the semidiscretized vector of velocities and p_h is the semidiscretized vector of pressures.
Linearization and robust H_∞ control to take care of nonlinearity.

$$
\begin{aligned}
E\dot{x}(t) &= Ax(t) + Bu(t), \quad x(t_0) = x_0 \\
y(t) &= Cx(t)
\end{aligned}
$$

Replace by

$$
\begin{aligned}
\tilde{E}\dot{\tilde{x}}(t) &= \tilde{A}\tilde{x}(t) + \tilde{B}u(t), \quad \tilde{x}(t_0) = \tilde{x}_0 \\
y(t) &= \tilde{C}\tilde{x}(t),
\end{aligned}
$$

If E is singular, then

$$
G(s) = C(sE - A)^{-1}B = G_p(s) + P(s),
$$

where $G_p(s)$ is the proper rational part and $P(s)$ is the polynomial part, associated with the singular part of E.

Gramians for descriptor systems.

Stykel, Diss. '02 Let P_l, P_r be left, right spectral projectors onto deflating subspace of $\lambda E - A$ to finite eigenvalues.

- $EX_{pc}A^T + AX_{pc}E^T = -P_lBB^TP_l^T, \quad X_{pc} = P_rX_{pc}$ proper controllability Gramian.
- $E^TX_{po}A + A^TX_{po}E = -P_r^TC^TCP_r \quad X_{pc} = X_{pc}P_l$ proper observability Gramian.
- $AX_{ic}A^T - EX_{ic}E^T = (I - P_l)BB^T(I - P_l)^T, \quad P_rX_{ic} = 0$ improper controllability Gramian.
- $A^TX_{io}A - E^TX_{io}E = (I - P_r)^TC^TC(I - P_r) \quad X_{pc}P_l = 0$ improper observability Gramian.

Proper Hankel singular values: $\xi_j = \sqrt{\lambda_j(X_{pc}E^TX_{po}E)}$, $j = 1, \ldots, n_f$.
Improper Hankel singular values: $\theta_j = \sqrt{\lambda_j(X_{ic}A^TX_{io}A)}$, $j = 1, \ldots, n_\infty$.

Balanced truncation descriptor systems

- Compute (low rank) Cholesky factors

$$X_{pc} = R_p R_p^T, X_{po} = L_p^T L_p, X_{ic} = R_i R_i^T, X_{io} = L_i^T L_i$$

- Form singular value decompositions

$$L_p E R_p = \begin{bmatrix} U_0 & U_1 \end{bmatrix} \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_0 \end{bmatrix} \begin{bmatrix} V_0 & V_1 \end{bmatrix}^T$$

with $\Sigma_1 = \mathrm{diag}(\xi_1, \ldots, \xi_{\tilde{n}_f})$, $\tilde{n}_f << n_f$ and

$$L_i E R_i = \begin{bmatrix} U_2 & U_3 \end{bmatrix} \begin{bmatrix} \Theta_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V_2 & V_3 \end{bmatrix}^T$$

with $\Theta_1 = \mathrm{diag}(\theta_1, \ldots, \theta_{\tilde{n}_\infty})$ invertible.

- $(\tilde{E}, \tilde{A}, \tilde{B}, \tilde{C}) = (W_\ell^T E T_\ell, W_\ell^T A T_\ell, W_\ell^T B, C T_\ell)$, where $W_\ell = [L_p^T U_1 \Sigma_1^{-1/2}, L_i^T U_2 \Theta_1^{-1/2}]$, $T_\ell = [R_p^T V_1 \Sigma_1^{-1/2}, R_i^T V_2 \Theta_1^{-1/2}]$.

- Balancing for dynamic and algebraic part.
- Reduction for dynamic and algebraic part.
- Good approximation properties.
- Exact error estimates.

$$\|G - \tilde{G}\|_{H_\infty} = 2(\xi_{\tilde{n}_f+1} + \ldots + \xi_{n_f}).$$

- Stability is preserved. Passivity with modification.
- Low Rank methods for gen. Lyapunov/Riccati equations Stykel '04.

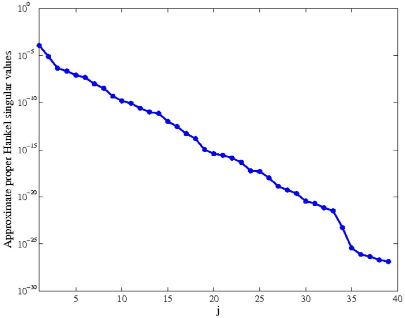
Discretization with FEM.

$$
\begin{aligned}
E &= \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}, \; A = \begin{bmatrix} \Delta_h & \nabla_h \\ \mathrm{div}_h & 0 \end{bmatrix}, \\
B &= \begin{bmatrix} B_1 \\ 0 \end{bmatrix}, \; C = \begin{bmatrix} 0 & C_2 \end{bmatrix}, \\
P_r &= P_l^T = \begin{bmatrix} \Pi & 0 \\ -(\nabla_h^T \mathrm{div}_h)^{-1} \nabla_h^T \Delta_h \Pi & 0 \end{bmatrix}, \\
\Pi &= I - \mathrm{div}_h (\nabla_h^T \mathrm{div}\ _h)^{-1} \nabla_h^T
\end{aligned}
$$

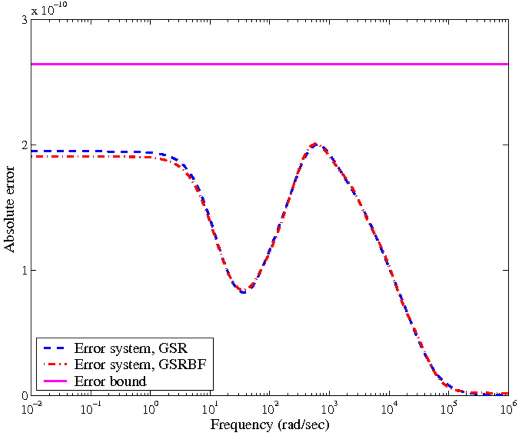
- We need only solutions with discrete Laplace Δ_h.
- Projectors P_l, P_r are easy to get.
- Reduced models are 'discretizations' of Stokes equation.
- Discretized conservation law.

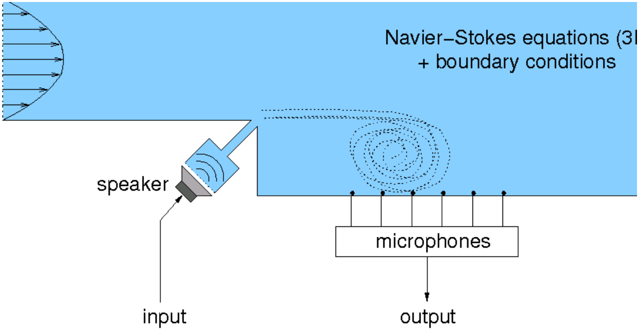
Semidiscretized model with $n = 19520$, $n_f = 6400$ and $n_\infty = 13120$. Approximation with $\tilde{n} = 11$, $\tilde{n}_f = 10$, $\tilde{n}_\infty = 1$.

Approximate proper Hankel singular values for the semidiscretized Stokes equation

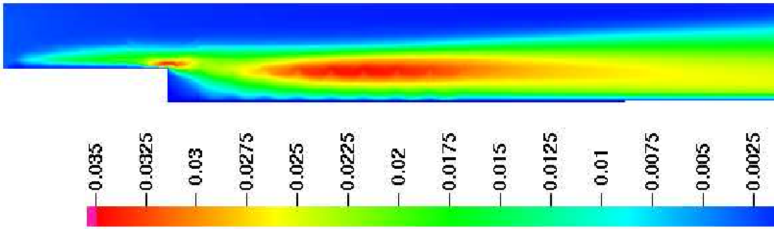


Absolute error plots and bound for semidiscretized Stokes eq.

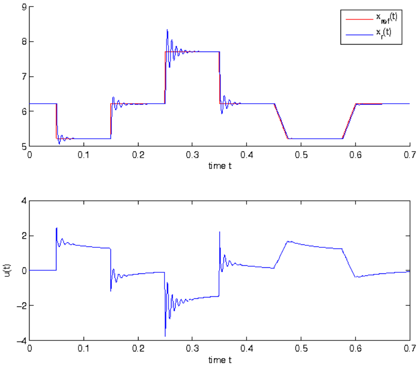



Navier–Stokes equations (3
+ boundary conditions
speaker
microphones
input
output

Simulated flow with FEATFLOW

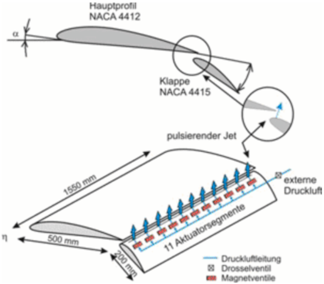


Henning/ Kuzmin/M./Schmidt/Sokolov/Turek '07. Movement of recirculation bubble following reference curve.



Results obtained with the DFG Collaborative research center SFB 557 TU Berlin.

- Closed loop separation control Becker/King/Petz/Nitsche 07.
- Computational investigation of separation for high lift airfoil flows Schatz/Günther/Thiele ’07
- Systematic Discretization of Input/Output Maps Dissertation Schmidt ’07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NACA 4412
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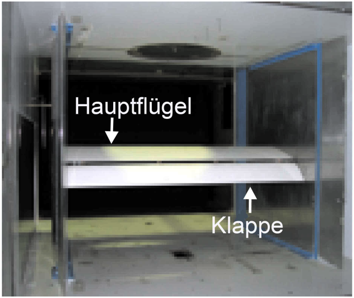
Hauptflügel
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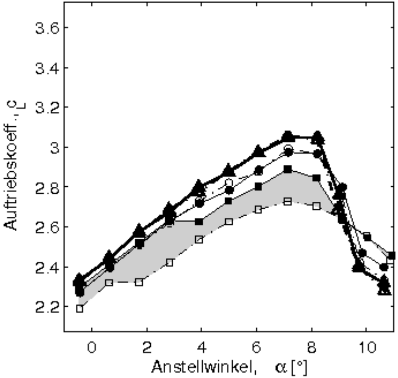
Auftriebskoeff., c_L
3.6
3.4
3.2
3
2.8
2.6
2.4
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0
2
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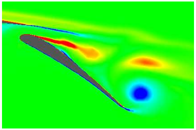
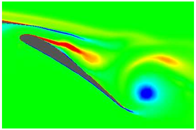
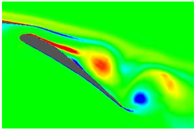
6
8
10
Anstellwinkel, α [°]

Flow field for different excitations







Current work

- Solution representations and model reduction for Oseen equations (see also Heinkenschloss, Sorensen, et al. ’07)
- Extension of theory and efficient reduction methods to linear time varying systems.
- Adaptive grid refinement for input/output maps, as in Becker, Heuveline, Rannacher, . . .

Conclusions

- Control problems for PDEs.
- Semidiscretization leads to large sparse control problems with few inputs and outputs.
- Model reduction is used to reduce the order.
- Control is determined from small model.
- Large scale and generalized balanced truncation. Penzl '00, Benner '03, Stykel 04', Baur '08
- Descriptor case: Dissertation Stykel, '02
- Error and perturbation bounds.
- Discretization of input output maps M. Schmidt 2007.
- MATLAB package **LYAPACK**, Penzl '00 available. New Version from TU Chemnitz soon.

Thank you very much
for listening to me for 3 hours.