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

DFG Research Center MATHEON
Mathematics for key technologies

17.07.08

Outline

Physical system

↙ ↘

Modelling | **Modelling**

↓ | ↓

ODEs ⟵ *semidiscr.* **PDEs**

↓

Mod. reduction

↓

Reduced ODE ⟶ *Sim., Control*

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

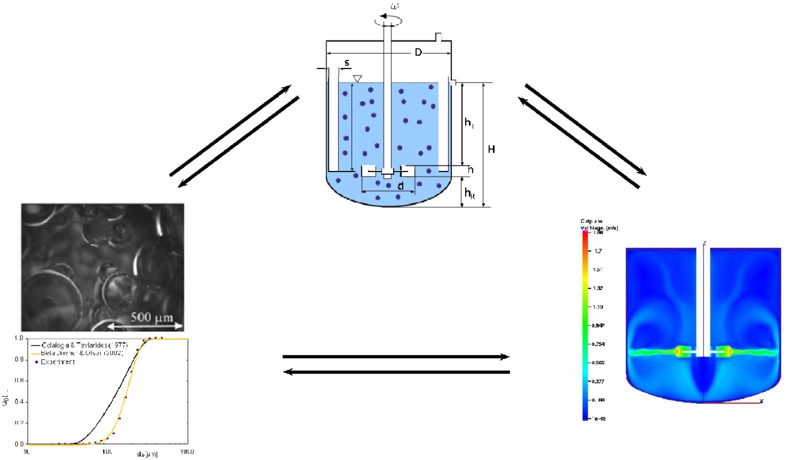
Goals

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

Outline

Drop size distributions in stirred systems

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



Technological Application, Tasks

Chemical industry: pearl polymerization and extraction processes

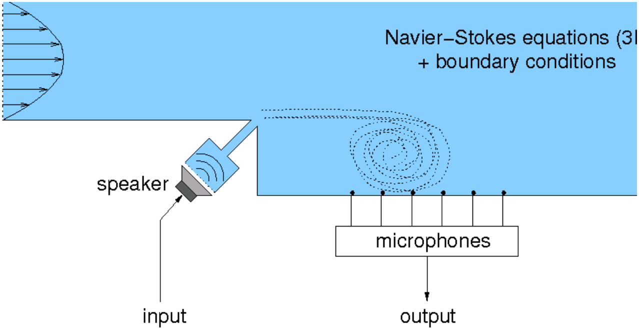
- ▷ Modelling of coalescence and breakage in turbulent flow.
- ▷ Numerical methods for simulation of coupled system of population balance equations/fluid flow equations.
- ▷ Development of optimal control methods for large scale coupled systems
- ▷ Model reduction and observer design.
- ▷ Feedback control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

Technological Application, Tasks

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.

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)

$$\mathcal{X} = \begin{bmatrix} x(t_1) & x(t_2) & \dots & x(t_N) \end{bmatrix}$$

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

Distance of control systems

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:

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

- 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

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

   $\Sigma_2 = \mathrm{diag}(\sigma_{\tilde{n}+1}, \ldots, \sigma_n)$, $\sigma_{\tilde{n}+1}, \ldots, \sigma_n \leq tol$.
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.

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

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.

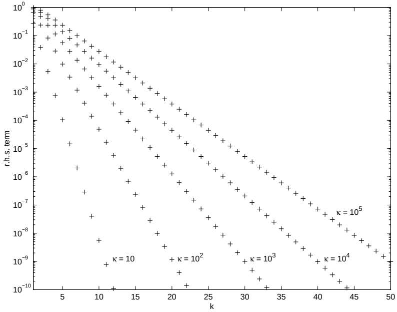
Theorem (Penzl '00)

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

ADI Method for Lyapunov equations

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 ADI for Lyapunov

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

Consider

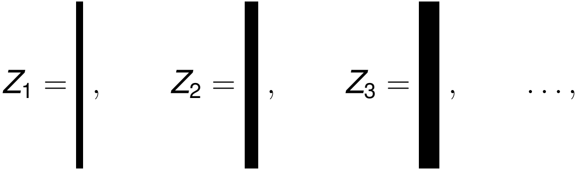
$$A^T X + XA = BB^T$$

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,...

Steel cooling example

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)

$$\begin{array}{lll} Z_B: & \text{rel. residual} = 9 \cdot 10^{-11}, & \text{rank } Z_B = 300 \\ Z_C: & \text{rel. residual} = 4 \cdot 10^{-12}, & \text{rank } Z_C = 360 \end{array}$$

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

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

Outline

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

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 $W_\ell = [L_p^T U_1 \Sigma_1^{-1/2}, L_i^T U_2 \Theta_1^{-1/2}]$, $T_\ell = [R_p^T V_1 \Sigma_1^{-1/2}, R_i^T V_2 \Theta_1^{-1/2}]$.

Analysis of method

- 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.

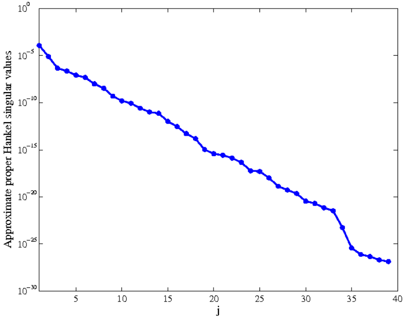
Discretization with FEM.

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

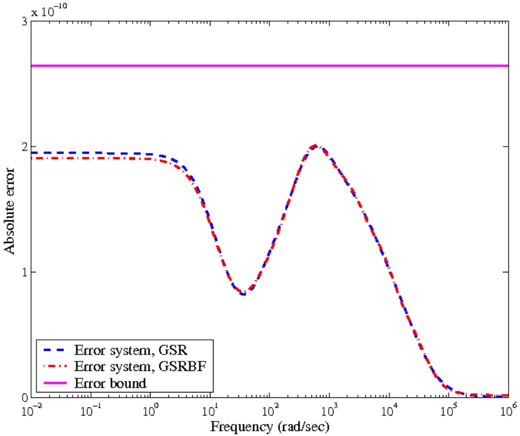
- We need only solutions with discrete Laplace Δ_h.
- Projectors P_l, P_r are easy to get.
- Reduced models are ‘discretizations’ of Stokes equation.
- Discretized conservation law.

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

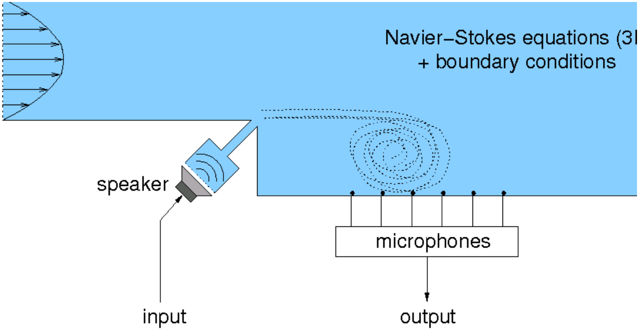


Absolute error plots and bound for semidiscretized Stokes eq.

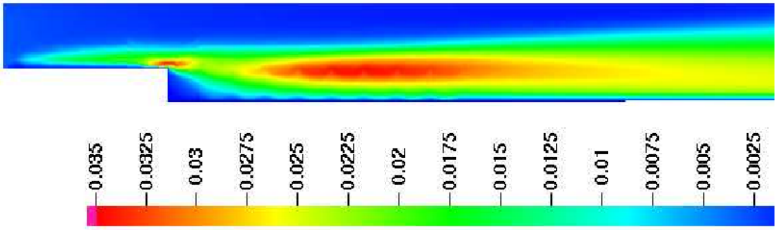


Outline

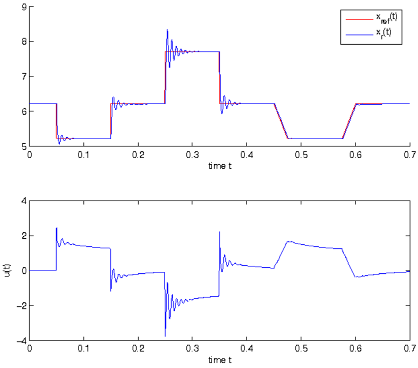
Active flow control, M. Schmidt ’07



Simulated flow with FEATFLOW



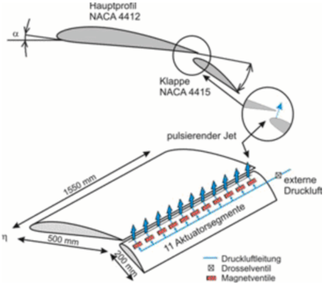
Henning/ Kuzmin/M./Schmidt/Sokolov/Turek '07. Movement of recirculation bubble following reference curve.

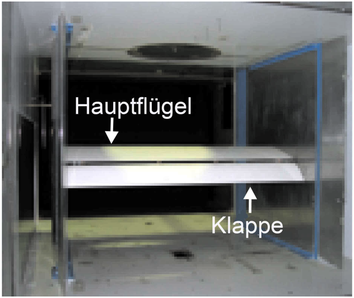


Results obtained with the DFG Collaborative research center SFB 557 TU Berlin.

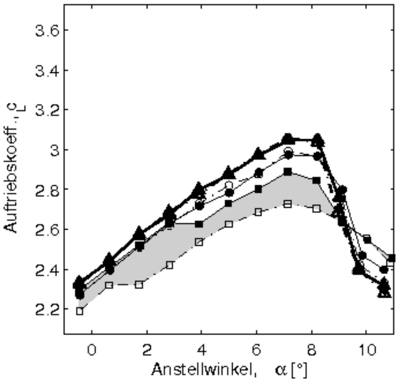
- Closed loop separation control Becker/King/Petz/Nitsche 07.
- Computational investigation of separation for high lift airfoil flows Schatz/Günther/Thiele '07
- Systematic Discretization of Input/Output Maps Dissertation Schmidt '07

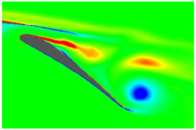
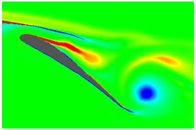
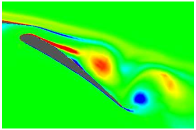
Experiment/Simulation





Lift optimization



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.