Abstracts of the Presentations

An adaptive POD approximation method for the control of evolutive equations

<u>A. Alla</u> and M. Falcone

Università degli studi di Roma "La Sapienza", Piazzale Aldo Moro, 2 0010 Roma Italy alla@mat.uniroma1.it

Keywords : Optimal Control, Proper Orthogonal Decomposition, Hamilton-Jacobi equations, advection-diffusion equations.

We consider the approximation of a finite horizon optimal control problem for an evolutive partial differential equation, choosing in particular there advection– diffusion equation. The basic ingredient of the method is the coupling between an adaptive reduced basis representation of the solution and a Dynamic Programming scheme for the evolutive Hamilton-Jacobi equation which gives the characterization of the value function.

Although the approximation schemes available for the HJB are shown to be convergent for any dimension, in practice we need to restrict the dimension to rather low number (typically 4) and this limitation affects the accuracy of the POD approximation. In fact with only few basis functions the POD method does not have enough informations to follow the solution of the advectiondiffusion problem. A way to circumvent this problem is to update our POD basis splitting the problem into subproblems. Every sub-problem is set in an interval $[t_j, t_{j+1}]$ and in that interval we recompute the POD basis. Several strategies can be applied to determine an optimal way to generate the partition of the time interval so to adapt the POD basis choice.

Since the solution based on the HJB equation allows to compute the value function and the optimal feedback for general nonlinear problems, this technique can be applied also to nonlinear cost functions.

We will show some numerical tests to explain our problem and to show the effectiveness of the method.

References

- A. Alla, M. Falcone An adaptive POD approximation method for the control of advection-diffusions equation, Preprint, 2012
- [2] M. Bardi e I. Capuzzo Dolcetta, Optimal control and viscosity solutions of Hamilton-Jacobi-Bellman equations. (Birkhauser, Basel, 1997)

- [3] E. Carlini, M. Falcone, R. Ferretti. An efficient algorithm for Hamilton-Jacobi equations in high dimension. Computing and Visualization in Science, Vol.7, No.1 (2004) pp. 15-29.
- [4] K. Kunisch, S. Volkwein, L. Xie. HJB-POD Based Feedback Design for the Optimal Control of Evolution Problems. SIAM J. on Applied Dynamical Systems, 4 (2004), 701-722.
- [5] K. Kunisch, L. Xie, POD-Based Feedback Control of Burgers Equation by Solving the Evolutionary HJB Equation, Computers and Mathematics with Applications. 49 (2005), 1113-1126.

On the greedy approach to the reduced basis method

<u>Peter Binev</u>

University of South Carolina, binev@math.sc.edu

Keywords : greedy algorithms, reduced basis method, parametric PDEs, optimal control problems

Many design problems in engineering can be formulated as optimal control problems with parametric PDE constraints. Typically, solving these control problems requires the frequent numerical solution of a PDE depending on dynamically updated parameters. The reduced basis method was introduced for the accurate online evaluation of solutions to a parameter dependent family of elliptic PDEs. Abstractly, it can be viewed as determining a "good" n dimensional space \mathcal{H}_n to be used in approximating the elements of a compact set \mathcal{F} in a Hilbert space \mathcal{H} .

One, by now popular, computational approach is to find \mathcal{H}_n through a greedy strategy. It is natural to compare the approximation performance of the \mathcal{H}_n generated by this strategy with that of the Kolmogorov widths $d_n(\mathcal{F})$ since the latter gives the smallest error that can be achieved by subspaces of fixed dimension n. The first such comparisons, given in [1], show that the approximation error, $\sigma_n(\mathcal{F}) := \text{dist}(\mathcal{F}, \mathcal{H}_n)$, obtained by the greedy strategy satisfies $\sigma_n(\mathcal{F}) \leq Cn2^n d_n(\mathcal{F})$.

The talk will present various improvements of this result. Among these, it is shown that whenever $d_n(\mathcal{F}) \leq Mn^{-\alpha}$, for all n > 0, and some $M, \alpha > 0$, we also have $\sigma_n(\mathcal{F}) \leq C_\alpha Mn^{-\alpha}$ for all n > 0, where C_α depends only on α . Similar results are derived for generalized exponential rates of the form $Me^{-an^{\alpha}}$. The exact greedy algorithm is not always computationally feasible and a commonly used computationally friendly variant can be formulated as a "weak greedy algorithm". The results are established for this version as well.

This is a joint research together with A. Cohen, W. Dahmen, R. DeVore, G. Petrova, and P. Wojtaszczyk published in [2].

References

- A. Buffa, Y. Maday, A.T. Patera, C. Prud'homme, and G. Turinici, A priori convergence of the greedy algorithm for the parameterized reduced basis, ESAIM Math. Model. Numer. Anal. 46 (2012), 595-603.
- [2] P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, and P. Wojtaszczyk, *Convergence Rates for Greedy Algorithms in Reduced Basis Meth*ods, SIAM J. Math. Anal. 43 (2011), 1457-1472.

Flow problems on varying spatial meshes

M. Braack, Jens Lang and N. Taschenberger

Mathematische Seminar, Christian-Albrechts-Universtät zu Kiel, braack@math.uni-kiel.de

Keywords : Adaptivity, Navier-Stokes, Stokes, stabilized finite elements

Changing the spatial mesh in transient flow computations may negatively affect the pressure on the new mesh due to the fact that the interpolated or L^2 -projected velocities usually violate the divergence constraint on the new mesh. It is proven that this pressure perturbation scales as k^{-1} when k denotes the time step. Hence, this phenomena becomes more and more relevant for small time steps. This is even more important due to the fact that this phenomena occurs independently whether the discrete scheme is inf-sup stable or not. In order to cure this problem, a divergence free projection should be applied instead of a simple interpolation or L^2 -projection of the velocities. For inf-sup stable finite elements, a recent published analysis (Besier & Wollner, 2011) shows how such a projection should be performed. For not inf-sup stable finite element pairs with stabilization techniques, as for instance equal-order elements, such an analysis is still missing. In this work, we tackle this problem, present a possible algorithm and prove bounds of the pressure in the linear Stokes case. The type of pressure stabilization is very general and includes the interior penalty method, local projection techniques and others.

Adaptive finite elements for optimal experimental design

T. Carraro

Heidelberg University, thomas.carraro@iwr.uni-heidelberg.de

Keywords : Optimal Experimental Design, Goal-Oriented Adaptivity, FEM

The aim of OED is to increase the confidence level of an estimation process. In the last decades the application of optimal experimental design (OED) has been extended to various fields, which comprehend also the use of complex models based on partial differential equations (PDE).

Although important developments have been made on numerical methods for OED with differential equations, expecially for ordinary differential equations, further progresses must be done applying the state-of-the-art approaches for optimization problems constrained with PDE systems.

We present an adaptive finite element approach based on the dual weighted residual (DWR) method to discretize OED problems, showing numerical examples.

Towards a Fully Space-Time Adaptive Multilevel Optimization Environment

Debora Clever and Jens Lang

 $Technische \ Universit\"{a}t \ Darmstadt, \quad \texttt{clever@mathematik.tu-darmstadt.de}$

Keywords : space-time adaptivity, error estimation, embedding techniques, hierarchical bases, multilevel strategy

We present a multilevel optimization environment for PDAE constraint optimal control problems with pointwise constraints on control and state. The environment couples a Newton-iterative optimization algorithm with the fully space-time adaptive PDAE solver KARDOS and a multilevel strategy which balances accuracy and optimization progress. Reduced gradient and reduced Hessian are computed by continuous adjoint calculus. Inexactness between reduced derivatives and optimization problem itself are controlled by the multilevel strategy. Local errors in time are estimated by embedding techniques, local errors in space by hierarchical bases. We adjust local errors in state and adjoint system to a desired accuracy by fully adaptive mesh refinement in space and time. To bridge the gap between local error estimates used for grid adaption and global estimates considered within the multilevel strategy, we relay on tolerance proportionality. Considering a semi-discretization of Rothe's type the fully adaptive environment allows for independent spatial meshes in each time step, such that the number of unknowns can be reduced significantly. Furthermore, accuracy is increased and numerical effort reduced, by allowing for independent time integration schemes for the different PDAEs, exploiting the knowledge about the type of the underlying PDAE.

The presented algorithm is applied to the optimal boundary problem of glass cooling in two and three space-dimensions, where the cooling process is modeled by radiative heat transfer.

Indirect multiple shooting with spatial mesh adaptation for PDE constrained optimal control problems

Michael E. Geiger and Thomas Carraro

Ruprecht-Karls-Universität Heidelberg, michael.geiger@iwr.uni-heidelberg.de

Keywords : multiple shooting, DWR method, spatial adaptivity, parabolic optimal control problems

Multiple shooting methods are widely used in optimal control of ordinary differential as well as differential algebraic equations. We present an indirect shooting approach which is still novel for the solution of PDE constrained optimal control problems, thereby discussing the theoretical framework as well as the numerical realization. Indirect multiple shooting in this context is applied to the optimality system of the control problem, leading to a system of intervalwise boundary value problems.

Employing Rothe's method (and thereby leaving the ODE control framework), we discretize first the time variable and then the spatial variables, this procedure enabling us to choose dynamically changing spatial meshes. The dual weighted residual (DWR) method is applied which allows for goaloriented error estimation and spatial mesh adaptation. Due to discontinuities of the solution between the shooting intervals, we have to cope with an error protruding from possibly non-matching spatial meshes around the shooting points.

Our approach is based on preliminary work done by Hesse and Kanschat. The described methods are substantiated by numerical examples.

Hesse, H. & Kanschat, G.: Mesh adaptive multiple shooting for partial differential equations. Part I: linear quadratic optimal control problems, J. Numer. Math. 17, pp. 195-217 (2009)

A Certified Reduced Basis Approach for Parametrized Linear-Quadratic Optimal Control Problems

M.A. Grepl and M. Kärcher

Numerical Mathematics, RWTH Aachen University, Templergraben 55, 52056 Aachen grepl@igpm.rwth-aachen.de

Keywords : reduced basis methods, optimal control, *a posteriori* error estimation, parameter-dependent systems

The solution of optimal control problems governed by PDEs using classical discretization techniques such as finite elements or finite volumes is computationally very expensive and time-consuming since the PDE must be solved many times. One way of decreasing the computational burden is the surrogate model based approach, where the original high-dimensional model is replaced by its reduced order approximation. However, the solution of the reduced order optimal control problem is suboptimal and reliable error estimation is therefore crucial.

A posteriori error estimates have been proposed previously in [3] and [1], respectively. However, the bounds in [3], although rigorous, require solution of the high-dimensional problem and are thus online-inefficient; whereas the estimates in [1], although efficient, are not rigorous upper bounds for the error.

In this talk, we build upon and extend the preliminary results in [2] to linear-quadratic optimal control problems governed by parametrized parabolic PDEs. To this end, employ the reduced basis method as a surrogate model for the solution of the optimal control problem and develop rigorous and efficiently evaluable a posteriori error bounds for the optimal control and the associated cost functional. Besides serving as a certificate of fidelity for the suboptimal solution, our a posteriori error bounds are also a crucial ingredient in generating the reduced basis with greedy algorithms.

References

- L. Dedé, Reduced basis method and a posteriori error estimation for parametrized linear-quadratic optimal control problems. SIAM J. Sci. Comp., 32:2 (2010), pp. 997-1019.
- [2] M.A. Grepl, M. Kärcher, Reduced basis a posteriori error bounds for parametrized linear-quadratic elliptic optimal control problems. C. R. Acad. Sci. Paris, Ser. I, 349(2011), pp. 873-877.

[3] F. Tröltzsch and S. Volkwein, POD a-posteriori error estimates for linearquadratic optimal control problems. *Comp. Opt. Appl.*, 44(1)(2009), pp. 83-115.

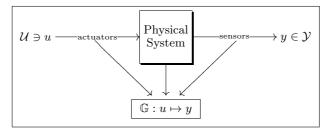
Direct Discretization of Input/Output Maps and Application to Flow Control

J. Heiland and V. Mehrmann

TU Berlin, heiland@math.tu-berlin.de

Keywords : Reduced order modeling, input/output maps, flow control

We propose a model reduction method that focuses on the input/output behavior rather than on the state dynamics. We consider the so called *input/output* (I/O) map that describes a physical system equipped with actuators and sensors in terms of the relation between an actuation (input) u and the related output y:



The basic idea is to approximate the spaces of inputs \mathcal{U} and outputs \mathcal{Y} by finite dimensional subspaces \mathcal{U}_h and \mathcal{Y}_h . With this, one can approximate the I/O map $\mathbb{G} : \mathcal{U} \to \mathcal{Y}$ by a finite dimensional map \mathbb{G}_h that maps \mathcal{U}_h onto \mathcal{Y}_h . Thus, \mathbb{G}_h is a reduced order model of the system.

If \mathbb{G} is linear, then \mathbb{G}_h can be represented as a matrix and the computation of the reduced system's response for a given input u can be realized via a matrix vector multiplication.

This approach of directly discretizing the input/output map was introduced for abstract linear time-invariant systems in [1]. Here, we are going to present the abstract framework of the approach, it's extension to linear time-invariant descriptor systems and it's application to optimal control of flows, see [2] for details. The given references are available for download on our homepage http://www.tu-berlin.de/?id=99416.

[1] —, M. SCHMIDT, A new discretization framework for input/output maps and its application to flow control, 2010.

[2] —, Distributed control of linearized Navier-Stokes equations via discretized input/output maps, 2011.

Snapshot Location by Error Equilibration in Proper Orthogonal Decomposition for Linear and Semilinear Parabolic Partial Differential Equations

R.H.W. Hoppe and Z. Liu

University of Augsburg and University of Houston, hoppe@math.uni-augsburg.de

Keywords : proper orthogonal decomposition, parabolic PDEs

It is well-known that the performance of snapshot based POD and POD-DEIM for spatially semidiscretized parabolic PDEs depends on the proper selection of the snapshot locations. In this contribution, we present an approach that for a fixed number of snapshots selects the location based on error equilibration in the sense that the global discretization error is approximately the same in each associated subinterval. The global discretization error is assessed by a hierarchical-type a posteriori error estimator known from automatic timestepping for systems of ODEs. We study the impact of this snapshot selection on error equilibration for the ROM and provide numerical examples that illustrate the performance of the suggested approach.

Adaptive Discontinuous Symmetric Interior Penalty Galerkin (SIPG) method for Convection Dominated Distributed Optimal Control Problems

<u>B. Karasözen</u> and H. Yücel

Middle East Technical University, bulent@metu.edu.tr

Keywords : Optimal control problems, convection dominated equations, discontinuous Galerkin methods, a posteriori error estimates, adaptive finite elements

Adaptive mesh refinement is particularly attractive for convection dominated optimal control problems, since the solution of the governing state partial differential equation (PDE) or the solution of the associated adjoint PDE may exhibit interior or boundary layers, localized regions where the derivative of the PDE solution is large, and adaptivity allows to refine the mesh locally around the layers as needed. The numerical solution of optimization problems governed by convection dominated PDEs provides additional challenges. The state and the adjoint PDEs are convection dominated, but the convection term of one PDE is the negative of the convection term of the other PDE. As a result, errors in the solution can potentially propagate in both directions and meshes may be refined unnecessarily because of this error propagation.

We prove residual based a-posteriori error estimates for the solution of distributed linear-quadratic optimal control problems governed by an elliptic convection diffusion PDE using the SIPG method with upwinding for the convection term, and we demonstrate the application of our a-posteriori error estimators for the adaptive solution of these optimal control problems with and without control constraints. Our numerical results show that meshes are only refined in regions where states or adjoints exhibit layers.

Based on joint work with M. Heinkenschloss, Rice University.

A posteriori error estimation in shape optimization

Bernhard Kiniger and Boris Vexler

Technical University of Munich, kiniger@ma.tum.de

 ${\bf Keywords}: {\rm shape \ optimization, \ optimal \ control, \ a \ posteriori \ error \ estimation}$

We consider a model shape optimization problem with a tracking-type functional. The state variable solves an elliptic equation on a domain with one part of the boundary described as the graph of a control function. First, we show higher regularity of the optimal control and the corresponding state as well as a convergence result of optimal order for the finite element discretization of the problem under consideration. Second, we derive an a posteriori error estimator which separates the error in the control and the state and then use an equilibrium strategy to balance these two error types. A numerical example is also presented.

Reduced models and adaptive simulation of chemical degradation mechanisms in porous media with evolving microstructure

C.-J. Heine¹ and C. A. Möller² and <u>M. A. Peter³</u> and K. G. Siebert⁴

¹Universität Stuttgart, claus-justus.heine@ians.uni-stuttgart.de, ²Universität Augsburg, christian.moeller@math.uni-augsburg.de, ³Universität Augsburg, malte.peter@math.uni-augsburg.de, ⁴Universität Stuttgart, kg.siebert@ians.uni-stuttgart.de.

 ${\bf Keywords}$: Reaction–diffusion, adaptive finite elements, homogenization, concrete carbonation

Concrete carbonation is a chemical degradation mechanism compromising the service life of reinforced concrete structures. Using a homogenization approach to upscale the associated reaction-diffusion system given in a porous medium, whose microstructure undergoes an evolution with respect to time, an effective reduced macroscopic limit model is obtained. In order to lower the complexity of numerical simulations of the process even further, an efficient adaptive finite element scheme for the resulting limit problem is presented. While the approach is motivated by concrete carbonation, it is generally applicable to reaction-diffusion problems in porous media.

Simulation and Optimization of large bore combustion engines using model order reduction

<u>A. Rieß</u> and R. H.W. Hoppe

MAN Diesel & Turbo SE, alexander.riess@man.eu University of Houston, rohop@math.uh.edu

$\mathbf{Keywords}: \mathrm{MOR}$

Very large 4-stroke combustion engines are commonly used for power production and marine applications. These engines may weight more than 100 t. An adequate model is typically a multi body system. This so-called virtual engine consists of several modules. In general the crankshaft, main bearings and conrod have to be described as flexible bodies. These flexible bodies are based on finite element models and take global and local stiffness effects into account. The underlying mathematical model is described by a second order system of ordinary differential equations. It must be solved in time domain which contains at least one combustion cycle. In order to reduce calculation time, model order reduction technique is necessary. Proper orthogonal decomposition method is successfully applied to the main bearing simulation. In an optimization of friction loss, the surfaces of the main bearings are parameterized by splines. Different optimization algorithms are applied to this problem. In overall a friction loss of 28 % is indicated.

Shape parametrization and computational reduction for viscous flows simulations in varying geometries

Gianluigi Rozza, Toni Lassila, Andrea Manzoni

EPFL, MATHICSE, CMCS Station 8-MA, CH-1015 Lausanne, Switzerland gianluigi.rozza@epfl.ch

Keywords : Reduced basis method, shape optimization, free form deformations, radial basis functions

Many problems in scientific computing, such as shape optimization [4], shape registration [5], and more general inverse problems [1], are formulated on parametrized domains.

We review some flexible and general methods used to represent shapes, either implicitly or explicitly, with a special emphasis on choosing methods that can be combined with existing model reduction approaches for PDEs. We present techniques developed recently for treating the complexities related to model reduction of PDEs on varying domains. Two different approaches may be considered: free-form deformations [3] and radial basis functions [5]. In both cases the problem is reduced to a fixed mesh with parameter-dependent coefficients, allowing us to apply the reduced basis method. Some remarks regarding the optimal choice of the shape parametrization will also presented in view of reducing the parametric dimension of the problem to a more tractable one.

Numerical examples of the proposed techniques are presented for the rapid solution of shape-related inverse-like problems [2].

[1] T. Lassila, A. Manzoni, A. Quarteroni, G. Rozza. A reduced computational and geometrical framework for inverse problems in haemodynamics, submitted, 2012.

[2] T. Lassila, A. Quarteroni, G. Rozza. *Reduced Formulation of Steady Fluid-structure Interaction with Parametric Coupling*, SIAM J. Sci. Comput., in press, 2012.

[3] T. Lassila, G. Rozza. Parametric free-form shape design with PDE models and reduced basis method, Comput. Methods Appl. Mech. Engrg., 199: 1583-1592, 2010.

[4] A. Manzoni, A. Quarteroni, G. Rozza. Shape optimization of cardiovascular geometries by reduced basis methods and free-form deformation techniques, Int. J. Numer. Meth. Fluids, in press, 2012.

[5] A. Manzoni, A. Quarteroni, G. Rozza. *Model reduction techniques for fast blood flow simulation in parametrized geometries*, Int. J. Numer. Meth. Biomed. Engrg., in press, 2012.

Preconditioning for PDE-constrained optimization using proper orthogonal decomposition

$\underline{\mathrm{E.\ Sachs}}$ and X. Ye

Uni Trier, sachs@uni-trier.de

Keywords : preconditoner, POD, PDE constrained optimization

The main effort of solving a PDE constrained optimization problem is devoted to solving the corresponding large scale linear system, which is usually sparse and ill conditioned. As a result, a suitable Krylov subspace solver is favourable, if a proper preconditioner is embedded. Other than the commonly used block preconditioners, we exploit knowledge of proper orthogonal decomposition (POD) for preconditioning and achieve some interesting features. Numerical results on nonlinear test problems are presented.

A Reduced Basis Approach for Multiscale Optimization Problems

Mario Ohlberger and <u>Michael Schaefer</u>

University of Münster, {ohlberger,michael.schaefer}@uni-muenster.de

Keywords : Reduced basis method, multiscale modelling, homogenization, parameter optimization

As a model reduction technique for parameterized problems, reduced basis methods (RBM) have become very popular over the last years. The method was originally studied for elliptic PDEs ([4]). In recent years many extensions were made, including nonlinear evolution equations ([1]) and variational inequalities ([2]).

The general idea in RBM is to generate a low-dimensional *reduced basis space* which approximates well the set of all admissible solutions; a Galerkin projection then yields an efficient reduced scheme. The key feature is the *offline-online splitting*: An *offline phase* includes expensive computations like the generation of the reduced basis space, while the cheap reduced simulations take place in the *online phase*. This fast online phase allows the efficient handling of *multi-query* applications like extensive parameter studies or optimal control.

Parameter optimization with elliptic constraints has already been studies in [3]. The aim of this talk is to present an RB approach for the following *multiscale* optimization setting:

Find
$$\mu^* = \arg \min J(u^{\varepsilon}(\mu), \mu)$$

subject to $C_j(u^{\varepsilon}(\mu), \mu) \le 0 \quad \forall j = 1, \dots, N, \quad \\ \mu \in \mathcal{P}$ (0.1)

with a compact parameter set $\mathcal{P} \subset \mathbb{R}^{P}$. In (0.1), the state variable $u^{\varepsilon}(\mu)$ is solution of the following (parameterized) multiscale problem:

$$-\nabla \cdot (A^{\varepsilon}(x;\mu)\nabla u^{\varepsilon}(x;\mu)) = f(x;\mu) \quad (x \in \Omega)$$

+ suitable BC
$$(0.2)$$

with a bounded domain $\Omega \subset \mathbb{R}^d$. The diffusion tensor is assumed to be rapidly oscillating: $A^{\varepsilon}(\cdot;\mu) = A(\cdot|\varepsilon;\mu)$, and $A : \mathbb{R}^d \times \mathcal{P} \to \mathbb{R}^{d \times d}$ is periodic w.r.t. $(0,1)^d$.

References

- M. Drohmann, B. Haasdonk and M. Ohlberger, "Reduced basis approximation for nonlinear parametrized evolution equations based on empirical operator interpolation". Technical report, FB10, University of Münster, 2010.
- [2] B. Haasdonk, J. Salomon and B. Wohlmuth, "A Reduced Basis Method for Parametrized Variational Inequalities". SimTech Preprint 2011-17, University of Stuttgart. Submitted to SINUM, 2011.
- [3] I. Oliveira and A. Patera, "Reduced-basis techniques for rapid reliable optimization of systems described by affinely parametrized coercive elliptic partial differential equations". Optim. Eng., 8 (2007), pp. 43–65.
- [4] G. Rozza, D. Huynh and A. Patera, "Reduced Basis Approximation and a Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations. Application to Transport and Continuum Mechanics". Archives of Computational Methods in Engineering, 15 (2008), pp. 229–275.

Almost third order convergent time discretization for control constrained parabolic optimal control problems

Andreas Springer and Boris Vexler

Technische Universität München, springer@ma.tum.de

Keywords : optimal control, heat equation, control constraints, discontinuous Galerkin methods, error estimates

We consider a linear quadratic optimal control problem built around the heat equation with time-dependent control and box constraints on the control. For such problems it is straightforward to show that a time-discrete solution with second order convergence can be obtained either by the variational discretization approach or by a post-processing strategy. Here, we present an approach that achieves almost third order convergence with respect to the size of the time steps by combining those two ideas.

To this end we discretize the state variable in time with the piecewise linear discontinuous Galerkin (dG(1)) method. The control is not discretized but instead computed from the semidiscrete adjoint state through the first order optimality condition. Exploiting superconvergence properties of the dG(1)method at the nodes of the Radau quadrature, we reconstruct an improved adjoint state from the optimal adjoint of the semidiscrete equation by piecewise quadratic interpolation. It is shown that this reconstructed adjoint converges with almost third order as the fineness of the time discretization approaches zero. An improved control solution is obtained by pointwise projection of this reconstructed adjoint, again employing the first order optimality condition. This post-processed solution also converges with almost order three with respect to the size of the time step.

We present numerical results supporting our theoretical findings.

L^2 -projection and quasi-optimality in the spatial discretization of the heat equation

F. Tantardini and A. Veeser

Università degli Studi di Milano, francesca.tantardini1@unimi.it

Keywords : Galerkin methods, quasi-optimality, heat equation, L^2 -projection, finite element methods, semidiscrete a priori error bounds

We analyze Galerkin approximation in space of the heat equation with particular attention to quasi-optimality, in the sense of Cea's Lemma. The error norms we consider are associated to the standard weak formulation of parabolic problems. In this setting, quasi-optimality has been derived in [2] for a mesh-depending norm close to the one of $H^1(H^{-1}) \cap L^2(H^1)$. Other works in this direction are [1] and [3], which require the additional assumption of the H^1 -stability of the L^2 -projection onto the discrete space. Under this hypothesis, quasi-optimality in $H^1(H^{-1}) \cap L^2(H^1)$ and stability in $L^2(H^1)$ have been established in [1] and [3], respectively. By means of the inf-sup theory, we unify the existing results and reveal that this hypothesis is also necessary. More precisely, we show that the results in [1] and [3] are essentially equivalent, and that [2], together with the H^1 -stability of the L^2 -projection implies quasi-optimality in $H^1(H^{-1}) \cap L^2(H^1)$. As application, we consider the finite element approximation in space and derive a priori error bounds in terms of the local meshsize that are of optimal order under minimal additional regularity.

- K. Chrysafinos, L. S. Hou: Error estimates for semidiscrete finite element approximations of linear and semilinear parabolic equations under minimal regularity assumptions. SIAM J. Numer. Anal., 40 (2002), 282–306.
- [2] T. Dupont: Mesh modification for evolution equations. Math. Comp., 39 (1982), 85–107.
- [3] W. Hackbusch: Optimal H^{p,p/2} error estimates for a parabolic Galerkin method, SIAM J. Numer. Anal., 18 (1981), 681–692.

On adaptive numerical methods for elliptic optimal control problems of semi-infinite type

Pedro Merino, Ira Neitzel, and Fredi Tröltzsch

EPN Quito, pedro.merino@epn.edu.ec TU München, neitzel@ma.tum.de TUBerlin, troeltzsch@math.tu-berlin.de

Keywords : elliptic equation, semi-infinite optimization, adaptive method

We consider a class of semi-infinite optimal control problems for linear elliptic PDEs. In this class of problems, finitely many control parameters are to be optimized while pointwise state constraints are given in all points of the spatial domain. We apply a standard finite element method for the numerical approximation of the problem. It is known that the optimal control parameters can be fairly sensitive with respect to the location of active grid points, hence a very fine uniform mesh would be needed for a high precision solution.

We suggest two adaptive methods for reducing the size of the associated discretized optimization problems. The first relies on our error estimates in [1], [2]. Based on them, in all steps of the method we determine the set of those grid points of the uniform finite element mesh, where the unknown optimal state cannot be active. In the next step, after refining the mesh, we concentrate on the remaining grid points. The method permits to compute a very good approximation of the optimal control while the size of the discretized problems remains small.

In the second method, we use an adaptive method for solving the elliptic PDE. Here, the mesh is refined by standard mesh adaptation strategies applied to the currently optimal discretized state function. We combine this method with the first idea of reducing the number of state constraints. A method of a posteriori error estimation is suggested as optimality test.

[1] P. Merino, I. Neitzel, F. Tröltzsch: On linear-quadratic elliptic control problems of semi-infinite type. Applicable Analysis, 90(6), 1047-1074, 2011.

[2] P. Merino, I. Neitzel, F. Tröltzsch: Error Estimates for the Finite Element Discretization of Semi-infinite Elliptic Optimal Control Problems. Discussiones Mathematicae. Differential Inclusions, Control and Optimization 30(2), 221-236, 2010.

Discontinuous Symmetric Interior Penalty Galerkin (SIPG) method for Nonlinear Diffusion-Convection-Reaction Problems

M. Uzunca and B. Karasözen

Middle East Technical University, uzunca@metu.edu.tr

Keywords : Discontinuous Galerkin methods, nonlinear diffusion-convectionreaction equations, adaptive mesh, Newton's method, automatic differentiation

Coupled diffusion-convection-reaction equations are widely used modelling chemical reaction and combustion problems. For linear convection dominated problems, the stabilized finite element methods and the discontinuous Galerkin methods are capable of handling the boundary and interior layers. On the other hand, due to the strong nonlinear reaction terms, sharp layers and discontinuities occur. So far, the most common and known technique to solve the nonlinear diffusion-convection-reaction equations is SUPG with some additional stabilization schemes such as shock-capturing to handle the local oscillations.

We apply the discontinuous Symmetric Interior Penalty Galerkin (SIPG) method to nonlinear diffusion-convection-reaction equations. We show that SIPG gives more reliable and accurate results for convection/reaction dominated problems with nonlinear reaction term. Moreover, using adaptive meshes, we show that the algorithm becomes efficient.

On the reliability of the dual weighted residual method

Andreas Veeser

Università degli Studi di Milano, andreas.veeser@unimi.it

Keywords : quantity of interest, adaptive finite element methods, dual weighted residual method, a posteriori error estimates, convergent algorithms

The dual weighted residual method, or in short DWR method, is an adaptive finite element method for the approximation of so-called quantities of interest. The latter are motivated by the underlying application and are given by evaluating a known functional at the exact solution of a partial differential equation. There is a lot computational evidence that the DWR method is an efficient tool for the afore-mentioned task.

This talk discusses the reliability of the DWR method and variants, focusing on theoretical results concerning a posteriori error estimates as well as the convergence of the algorithm.

Model Order Reduction for Aerodynamics

<u>A. Vendl</u> and H. Faßbender

TU Braunschweig, a.vendl@tu-braunschweig.de

Keywords : Model order reduction, CFD, aerodynamics

In this talk model order reduction techniques for aerodynamical applications are presented. In this context usually proper orthogonal decomposition (POD) [1] is used. Given a set of snapshots, which are solutions of the governing equations characteristic of the model to be constructed, POD yields a basis for the solution space of the model. This is achieved by storing the snapshots as columns vectors in a matrix and subsequently computing the SVD of this matrix.

Having established a suitable basis, a reduced order model can then be constructed with the help of projection techniques like Galerkin projection. While in literature the projection is frequently applied to the continuous governing equations (e.g. [2]), in this talk it is applied to the discrete equations. This has the advantage that the reduced order model is closely connected to the discrete full order model and in this way the capabilities of the full model, like highly advanced turbulence models etc., can be exploited.

The disadvantage of such an approach is however that the nonlinear terms of full order have to be computed. In order to alleviate this negative property another kind of projection is implemented which evaluates the spatial discretization not at every point, but a subset of all points of the computational mesh. This method is referred to as Missing Point Estimation (MPE) [3]. It is applied to obtain steady state flows for relevant flow parameters such as the angle of attack.

In the end ideas of how to use steady model reduction techniques in order to construct an unsteady reduced order model are presented. This is based on the so-called dual-time stepping approach (see e.g. [4]), which formulates an unsteady problem as a steady one.

The work of the author is supported by the German Federal Ministry of Economics and Technology (BMWi).

References

 P. Holmes, J.L. Lumley and G. Berkooz: Turbulence, Coherent Structures, Dynamical Systems and Symmetry, Cambridge, New York 1996.

- [2] D. M. Luchtenburg, B. Günther, B. R. Noack, R. King, and G. Tadmor. A generalized mean-field model of the natural and high-frequency actuated flow around a high-lift configuration. Journal of Fluid Mechanics, 623:283–316, 2009.
- [3] P. Astrid, S. Weiland, K. Willcox and T. Backx: Missing point estimation in models described by proper orthogonal decomposition, IEEE Transactions on Automatic Control, Vol. 53, No. 10, pp. 2237-2251, 2008.
- [4] J. Blazek. Computational Fluid Dynamics: Principles and Applications. Elsevier, first edition, 2001.

Accelerating PDE-Constrained Optimization by Model Order Reduction with Error Control

Y. Yue and K. Meerbergen

KU Leuven, yao.yue@cs.kuleuven.be

Keywords : PDE-constrained optimization, model order reduction, Krylov methods, design optimization, vibrations and structures

Design optimization problems are often formulated as PDE-constrained optimization problems where the objective is a function of the output of a largescale parametric dynamical system, obtained from the discretization of a PDE. To reduce its high computational cost, model order reduction techniques can be used. Two-sided Krylov-Padé type methods are very well suited since also the gradient to the design parameters can be computed accurately at a low cost. In our previous work, we embedded model order reduction and parametric model order reduction in the damped BFGS method. In this talk, we present a new provable convergent error-based trust region method that allows to better exploit interpolatory reduced models. Then, we propose two practical algorithms, ETR and EP, to fit in this framework. For our benchmark problems, we use a simple interpolatory model order reduction method based on two-sided Krylov methods for a single interpolatory point. Numerical experiments from civil engineering show that the new methods outperform damped BFGS accelerated by non-interpolatory reduced models.

Fast reduced-order steady-state solutions to the Navier-Stokes equations for full-scale aircraft configurations at cruise conditions

Ralf Zimmermann

ICM, TU Braunschweig, ralf.zimmermann@tu-braunschweig.de

Keywords : Computational Fluid Dynamics, Proper Orthogonal Decomposition (POD), Least-Squares Residual Optimization, Extrapolation

A reduced-order modeling (ROM) approach for predicting steady, turbulent aerodynamic flows based on Computational Fluid Dynamics (CFD) and Proper Orthogonal Decomposition (POD) will be presented.

Model-order reduction is achieved by restricting a given full-order CFD solver to the reduced POD basis. More precisely, solving the Navier-Stokes equations of viscous fluid dynamics is replaced by solving a non-linear least-squares optimization problem restricted to the low-dimensional POD subspace [1,2]. The method will be referred to as LSQ-ROM method. Similarities and differences to projection-based ROMs will be discussed.

Applications of the LSQ-ROM method to 2D airfoil (NACA 64A010) as well as to a complete industrial aircraft configuration (NASA Common Research Model) in the transonic flow regime will be presented with a special emphasis of the methods extrapolation capabilities. For the industrial aircraft configuration, the cost of computing the reduced-order solution is shown to be two orders of magnitude lower than that of computing the reference CFD solution. Moreover, by adding constraints to the least-squares optimization problem, it will be demonstrated how the approach can be applied for fusing experimental data, e.g. obtained via wind tunnel measurements, and CFD data.

References

- 1 P.A. LeGresley, J. J. Alonso: Investigation of Non-Linear Projection for POD Based Reduced Order Models for Aerodynamics, AIAA Paper 2001-0926 (2001)
- 2 R. Zimmermann, S. Görtz: Improved Extrapolation of Steady Turbulent Aerodynamics using a Non-Linear POD-Based Reduced Order Model. Preprint, to appear in 'The Aeronautical Journal' (2012)

Abstracts of the Postersession

Space-Time Adaptivity of Convection Dominated Optimal Control Problems by Discontinuous Symmetric Interior Penalty Galerkin (SIPG)

T. Akman and H. Yücel and B. Karasözen

Middle East Technical University, takman@metu.edu.tr

Keywords : Time-dependent PDE-constrained optimization, convection dominated equations, discontinuous Galerkin methods, space-time adaptivity

When convection dominates diffusion, the solutions of these PDEs typically exhibit interior or boundary layers. In the case of optimal control problems, the convection term of the adjoint equation is opposite of the state equation's; therefore, the error propagates in both directions. The state and the adjoint equation are discretized by discontinuous symmetric interior penalty Galerkin (SIPG) method in space and by the θ -family of methods in time. For steadystate problems, the adaptive finite element methods are an effective numerical resolution to resolve the boundary and/or interior layers by refining the mesh where necessary. For time-dependent problems the spatial adaptivity must also allow for a local mesh coarsening. We use residual-based estimators which bound the error of the computed approximate solution by a suitable norm of its residual with respect to the strong form of a differential equation. Numerical solutions for uniform and adaptive refined meshes are computed for several examples.

Spatio-temporal models of organogenesis

Ph. Germann, D. Menshykau, S. Tanaka and D. Iber

ETH Zürich, philipp.germann@bsse.ethz.ch

Keywords : Developmental biology, reaction diffusion equation, continuum physics, cellular Potts models, FEM

We build mathematical models for organogenesis – e.g. long bone growth, branching morphogenesis and limb development – based on reaction diffusion equations, potentially coupled to measured growth fields, cellular Potts models or continuum physics.

Developing these models involves a lot of trial and error, solving them numerically is challenging and they contain many parameters that have not been measured or cannot even be identified with measurable quantities. We developed a strategy to optimize the implementation in the commercial finite elements package COMSOL Multiphysics [1] allowing us to generate a sufficient number of solutions, but with our models evolving we are facing limitations.

References

 P. Germann, D. Menshykau, S. Tanaka, and D. Iber, Simulating Organogenesis in COMSOL, Proceedings of COMSOL Conference, 2011.

Reduced Basis Method for Time-Harmonic Maxwell's Equations

<u>M. Hess</u> and P. Benner

MPI Magdeburg, hessm@mpi-magdeburg.mpg.de

Keywords : Certified Reduced Basis Method, Time-Harmonic Maxwell's Equations

The Reduced Basis Method [1] generates low-order models to parametrized PDEs to allow for efficient evaluation of parametrized models in many-query and real-time contexts. The Reduced Basis approach is decomposed into a time-consuming offline phase, which generates a surrogate model and an online phase, which allows fast parameter evaluations. Rigorous and sharp a posteriori error estimators play a crucial role in this process, in that they define which snapshots are to be taken into the reduced space and give bounds to the output quantities during the online phase.

We apply the Reduced Basis Method to systems of Maxwell's equations arising from electrical circuits [2]. Using microstrip models as a microscopic view of interconnect structures, the input-output behaviour is approximated with low order reduced basis models for a parametrized geometry, like distance between microstrips and/or material coefficients, like permittivity and permeability of substrates.

We show the theoretical framework in which the Reduced Basis Method is applied to Maxwell's equations and present first numerical results.

- G. Rozza, D.B.P. Huynh, A.T. Patera, Reduced Basis Approximation and a Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations, Arch. Comput. Methods Eng. 15 (2008), 229 – 275.
- [2] R. Hiptmair, Finite Elements in computational electromagnetism, Acta Numerica (2002) 237 – 339.

High-order finite element methods for optimal control problems

K. Hofer, S. Beuchler and D. Wachsmuth

University of Bonn, Institute for Numerical Simulation, hofer@ins.uni-bonn.de

 ${\bf Keywords}: \ {\rm Optimal\ boundary\ control,\ Boundary\ concentrated\ finite\ element\ method}$

Considered is a linear-quadratic elliptic boundary control problem on twodimensional polygonal domains, where the observation domain for the state is either the whole domain Ω or a part of the boundary $\partial\Omega$. For solving these problems the boundary concentrated finite element method (BC-FEM), a highorder finite element method, can be used. After getting a general idea of the BC-FEM, a discretization error estimate for the case, where the observation domain is a part of the boundary, is given.

Approximation of Optimal Control Problems for the Boltzmann Transport Equation

Christian Jörres, Martin Grepl and Michael Herty

RWTH Aachen University, joerres@mathc.rwth-aachen.de

 ${\bf Keywords}$: Boltzmann Transport Equation, Model Order Reduction, Optimization

We discuss the discretization of optimal control problems for the stationary Boltzmann transport equation arising in radiotherapy treatment planning.

Currently, there exist several discretization approaches for the transport equation, e.g P_N -approximation. We present a new approach of choosing the discretization points Ω_k in order to minimize the current objective functional. Therefore we apply technics from the field of model order reduction and regard the velocity space as parameter space.

We present an algorithm which takes into account the specific structure of the solution for the Boltzmann transport equation and show numerical results in 1-D slab geometry.

Numerical Simulation of Elastic Wave Propagation in Composite Material

Markus Bause and Uwe Köcher

Helmut Schmidt University, University of the Federal Armed Forces Germany Hamburg, bause@hsu-hamburg.de uwe.koecher@hsu-hamburg.de

Keywords : Elastic wave propagation, discontinuous Galerkin methods.

Composites are one of the most promising materials to build light-weight structures for several fields of application, e.g. for wind energy plants and aerospace applications. Piezoelectric induced ultrasonic waves can be used for the development of structural health monitoring (SHM) systems. Numerical simulation can help to understand wave propagation in heterogeneous and composite media.

Recently, there has been an increased interest in applying the discontinuous Galerkin method (DGM) to wave propagation. Some of the advantages of the finite element method are the flexibility with which it can accomodate the underlying geometry, discontinuities in the model and boundary conditions, and the ability to approximate the wavefield with high-degree polynomials. The DGM has the further advantage that it can accomodate discontinuities, not only in the media parameters, but also in the wavefield, it can be energy conservative, and it is suitable for (massively) parallel computation.

We present a poster about the application of continuous and discontinuous Galerkin methods for analyzing elastic wave propagation in heterogeneous media. Moreover, wave propagation in various composite materials and the potential of using guided waves for detecting strutural damages is analyzed.

In particular, a positive impact of higher order approximations for heterogeneous materials will be illustrated; cf. also [2] for the application of higher order techniques to convection-dominated transport problems. Elastic wave propagation in various composite materials and the potential of using guided waves for detecting structural damages is considered further; cf. Figure 0.1.

References

 V. Giurgiutiu: Structural Health Monitoring, with piezoelectric wafer active sensors. Academic Press, Elsevier, 2008.

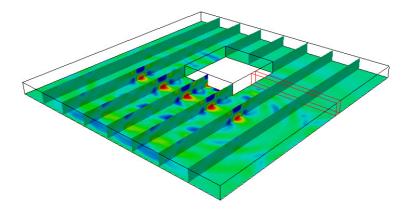


Figure 0.1: Elastic wave propagation.

- [2] M. Bause, K. Schwegler: Analysis of stabilized higher-order finite element approximation of nonstationary and nonlinear convection-diffusionreaction equations. *Comput. Methods Appl. Mech. Engrg.*, 209-212 (2012), 184–196.
- [3] W. Bangerth, G. Kanschat: deal.II differential equations analysis library, Technical reference, 2012, http://www.dealii.org.

A POD study for a coupled Burgers Equation

Boris Krämer and John Burns

Virginia Tech, bokr@vt.edu

Keywords : Group POD, Burgers Equation, Parameter Dependence

In this work, we present a numerical study of the coupled Burgers equation. The coupled Burgers equation is motivated by the Boussinesq equations that are often used to model the thermal-fluid dynamics of air in buildings. To deal with the nonlinear term, the convective nonlinearity is written in conservation form. The numerical results in the first part show that the Group Finite Element Method appears to be more stable than the standard Finite Element Method.

Using a "training" set generated by the Group Finite Element Method, we apply a POD model reduction scheme based on the Group Finite Element idea. The computational speed up, as well as the accuracy of the reduced order model, are compared to the high fidelity solution. The actual dynamics of the system can vary from the dynamics that are contained in the training set. Hence, we investigate the dependence of the reduced order model on the input parameters (especially the Reynolds number).

Optimal feedback control of the wave equation by solving the HJB equation

<u>A. Kröner</u> and K. Kunisch

Johann Radon Institute for Computational and Applied Mathematics axel.kroener@oeaw.ac.at

 $\label{eq:constraint} \begin{array}{l} \textbf{Keywords}: \ Dynamic \ programming, \ Hamilton-Jacobi-Bellman \ equation, \ closed \ loop \ control, \ wave \ equation, \ spectral \ elements \end{array}$

An approach for solving an optimal finite-time horizon feedback control problem for the wave equation is presented. The feedback law can be derived from the dynamic programming principle and requires to solve the evolutionary Hamilton-Jacobi-Bellman (HJB) equation. Since solving the discretized HJB equation in a high-dimensional finite dimensional space, as it is typically the case if the discretization bases on finite elements, is unfeasible, in this approach spectral elements are used to discretize the wave equation. The effect of noise is considered and numerical examples are presented.

Goal-oriented inference for PDE-constrained inverse problems

C. Lieberman and K. Willcox

Massachusetts Institute of Technology, celieber@mit.edu

Keywords : inverse problems, PDEs, model reduction

Inference of model parameters is one step in an engineering process often ending in predictions that support decision in the form of design or control. Incorporation of end goals into the inference process leads to more efficient goaloriented algorithms that automatically target the most relevant parameters for prediction. In the linear setting the control-theoretic concepts underlying balanced truncation model reduction can be exploited in inference through a dimensionally-optimal subspace regularizer. The inference-for-prediction method exactly replicates the prediction results of either truncated singular value decomposition, Tikhonov-regularized, or Gaussian statistical inverse problem formulations independent of data; it sacrifices accuracy in parameter estimate for online efficiency. The new method leads to low-dimensional parameterization of the inverse problem enabling solution on smartphones or laptops in the field.

Our method does not consist of traditional model reduction techniques, but instead exploits a traditional construction (namely, balanced truncation) in the recognition of analogy between the low-dimensional input-output maps exploited for state-space systems and the low-dimensional data-prediction maps observed in many invert-then-predict scenarios. In state-space systems, it is a high-dimensional state vector that is reduced. In the invert-then-predict scenario, the analogous role is played by a high-dimensional parameter. The dimensionality reduction takes place exclusively in the parameter space. We solve the inverse problem more efficiently in this reduced space without loss of accuracy in the required future predictions.

The poster will demonstrate the key idea behind our approach, present the primary theorem of prediction exactness for the linear setting, and provide results for several test cases in a contaminant identification and prediction problem, governed by advection-diffusion in two dimensions.

Solving the feedback optimal control problem using SDRE method

A. Owis

Astonomy, Space and Meteorology Department-Cairo University, aowis@cu.edu.eg

Keywords : Feedback, Hamilton Jacobi Bellman, SDRE, Orbit Transfer

In this work we solve the problem of feedback optimal control problem via solving the Hamilton-Jacobi-Bellman equation using the State Dependent Riccati Equation(SDRE) method. We formulate the dynamic of the system in the State space form and then we factorize the dynamics of the system into linear, state dependent, factors and then check the controllability of the factorized system and finally we apply the method of SDRE to the factorized system. We apply the method to the motion of a spacecraft under the influence of the gravitational attraction of a central body, the Sun in our case, and we would like to transfer the spacecraft from Earth to Mars. Both orbits of Earth and Mars around the Sun are assumed to be circular and coplanar. we use radial and tangential thrust control. The SDRE is solved to get the optimal control.