

# MoRePaS 09

## Workshop on Model Reduction of Parametrized Systems

# Book of Abstracts

University of Münster, Germany  
Sept. 16-18, 2009



<http://MoRePaS09.uni-muenster.de>



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Center for  
Nonlinear Science



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# Preface

The aim of this 3-day workshop is to bring together mathematicians and engineers working on model reduction of parametrized problems. In particular we aim at Reduced Basis (RB) methods for parametrized partial differential equations and Parametrized Model Order Reduction (PMOR) techniques for dynamical systems. It is also a specific intention to bring together experts from both pde and ode-based frameworks. The acronym *MoRePaS* stands for *Model Reduction of Parametrized Systems* and includes both areas.

We especially have in mind the following aspects of parametrized model reduction that also represents the wide scope of the program:

- Parametrized Partial Differential Equations
- Parametrized Dynamical Systems
- Reduced Basis Methods
- Proper Orthogonal Decomposition
- Krylov-Subspace Methods (Padé, Moment matching, etc.)
- Error Estimation (a priori, a posteriori, effectivities, etc.)
- Basis Construction
- Preservation of System-Properties (Conservation, Stability, etc.)
- Approximation of Nonlinearities
- Interpolation Methods
- Robust Optimization
- Applications of Reduced Models (Control, Parameter Identification, Inverse Problems, Hierarchical Models)
- Engineering Applications (CFD, MEMS, etc.)

The quality of the submissions for this workshop is impressive. Not only the invited sessions but also the contributed talks as well as the topics of the poster session represent the leading edge of research on MoRePaS. Furthermore, we are very happy to have such a broad internationality of participants coming from Austria, Belgium, Finland, France, Germany, Norway, Switzerland and the United States.

In order to maintain the character of a workshop, we have scheduled no parallel sessions. We do hope that this workshop will also serve as a platform for a scientific exchange with respect to the before-mentioned different aspects of MoRePaS.

## Acknowledgment

We acknowledge funding of this event by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG), the Landesstiftung Baden-Württemberg and the Universities of Münster, Stuttgart and Ulm. The funding of the DFG enabled us to support ten PhD-Students with accepted contributions. We also wish to thank the local organizers at the University of Münster for their support. In particular, we wish to thank Astrid Heitmann for her indispensable support in coordinating tasks including registration, accommodation and on-site organization. We also thank Oliver Kamps and Markus Wilczek for installing and maintaining the webpage of the workshop. Finally, we thank all participants for their contributions and joining the workshop and hope that everybody will benefit from this meeting.

Stuttgart, Münster and Ulm, September 2009

*Bernard Haasdonk*

*Mario Ohlberger*

*Timo Tonn*

*Karsten Urban*

## Schedule

Wednesday (Sept. 16, 2009):

8:00 - 8:45	<i>Registration</i>	
8:45 - 9:00	<i>Opening</i>	
9:00 - 9:45	INV	Patera, Anthony T.
9:45 - 10:35	CON	Veroy - Grepl, Karen Pomplun, Jan
10:35 - 11:15	<i>Coffee Break</i>	
11:15 - 12:30	CON	Zaslavsky, Mikhail Constantine, Paul G. Lebiedz, Dirk
12:30 - 14:00	<i>Lunch Break</i>	
14:00 - 14:45	INV	Benner, Peter
14:45 - 15:35	CON	Baur, Ulrike Farle, Ortwin
15:35 - 16:15	<i>Coffee Break</i>	
16:15 - 17:00	INV	Sorensen, Danny C.
17:00 - 17:25	CON	Chaturantabut, Saifon
17:25 - 19:00	<i>Break</i>	
19:00 - 22:00	<i>Conference Dinner</i>	

Thursday (Sept. 17, 2009):

9:00 - 9:45	INV	Maday, Yvon
9:45 - 10:35	CON	Løvgren, Alf E. Boyaval, Sébastian
10:35 - 11:15	<i>Coffee Break</i>	
11:15 - 12:30	CON	Liebermann, Chad Lohmann, Boris Eppler, André
12:30 - 14:00	<i>Lunch Break</i>	
14:00 - 14:45	INV	Volkwein, Stefan
14:45 - 15:35	CON	Schu, Matthias Kunkel, Martin
15:35 - 16:15	<i>Coffee Break</i>	
16:15 - 17:00	INV	Rønquist, Einar
17:00 - 17:25	CON	Grepl, Martin
17:25 - 20:00	POS	Poster Introduction Poster Presentation

Friday (Sept. 18, 2009):

9:00 - 9:45	INV	Stykel, Tatjana
9:45 - 10:35	CON	Vossen, Georg Antil, Harbir
10:35 - 11:15	<i>Coffee Break</i>	
11:15 - 12:05	CON	Knezevic, David J. Drohmann, Martin
12:05 - 12:50	INV	Rozza, Gianluigi
12:50 - 13:15	<i>Closing</i>	
13:15 - 15:00	<i>Break</i>	
15:00 - 16:00	<i>City Tour</i>	

## Venue

Alexander von Humboldt Haus, Room 50  
Hüfferstraße 61  
48149 Münster

# Invited Talks

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## Interpolatory and system-theoretic methods for parametric model reduction

Peter Benner

*Faculty of Mathematics  
Chemnitz University of Technology*

Model reduction has become an ubiquitous tool in simulation and control for dynamical systems arising in various engineering disciplines. Often, models of physical processes contain parameters describing material properties and geometry variations, or arising from changing boundary conditions. For purposes of design and optimization, it is often desirable to preserve these parameters as symbolic quantities in the reduced-order model (ROM). This allows the re-use of the ROM after changing the parameter so that the repeated computation of reduced-order models can be avoided. Significant savings in simulation times for full parameter sweeps or within optimization algorithms can be achieved this way.

In this talk, we study several approaches for computing ROMs for linear parametric systems. Parameter dependencies can be linear, polynomial, or nonlinear in general. We study methods based on multi-moment matching. We provide an interpretation of these methods as rational interpolation methods and combine them with optimal  $H_2$  model reduction. A further approach based on a combination of balanced truncation and sparse grid interpolation will also be discussed. Numerical results illustrate the performance of all the methods under consideration.



## A two-grid finite-element/reduced basis scheme for the approximation of the solution of parameter dependent P.D.E

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<sup>b</sup> *Division of Applied Mathematics, Brown University  
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In the frame of optimization process in industrial framework, where numerical simulation is used at some stage, the same problem, modeled with partial differential equations depending on a parameter has to be solved many times for different sets of parameters. The reduced basis method may be successful in this frame and recent progress have permitted to make the computations reliable thanks to *a posteriori* estimators and to extend the method to non linear problems thanks to the “magic points” interpolation. However, it may not always be possible to use the code (for example of finite element type that allows for evaluating the elements of the reduced basis) to perform all the “off-line” computations required for an efficient performance of the reduced basis method. We propose here an alternating approach based on a coarse grid finite element the convergence of which is accelerated through the reduced basis and an improved post processing.

This is a joint work with Rachida Chakir

## Reduced Basis Approximation and A Posteriori Error Estimation for Parametrized Partial Differential Equations

Anthony T. Patera

*Massachusetts Institute of Technology  
Department of Mechanical Engineering  
and  
Center for Computational Engineering*

We discuss reduced basis approximation and associated *a posteriori* error estimation for reliable and rapid solution of parametrized partial differential equations.

The crucial ingredients are rapidly convergent Galerkin approximations over a space spanned by “snapshots” on the parametrically induced solution manifold; effective constructions for stability-constant lower bounds; rigorous and sharp *a posteriori* error estimators for the outputs/quantities of interest; efficient POD (in time)/Greedy (in parameter) selection of quasi-optimal samples; and Offline-Online computational procedures for very rapid response in the real-time and many-query contexts.

Our approach is applicable to elliptic equations, parabolic equations, and hyperbolic equations. In this talk we focus on time-dependent phenomena including the (frequency domain) Helmholtz equation, linear and nonlinear convection–diffusion equations, and the second-order wave equation of acoustics and elastodynamics.

## An “*hp*” Reduced Basis Method for Parametrized Partial Differential Equations

Jens L. Eftang<sup>a</sup>, Anthony T. Patera<sup>b</sup> and Einar M. Rønquist<sup>a</sup>

<sup>a</sup> *Norwegian University of Science and Technology*

<sup>b</sup> *Massachusetts Institute of Technology*

We consider the numerical solution of parametrized partial differential equations where there is a premium on rapid output computation given any particular choice of the parameters over a predefined parameter domain. The reduced basis method provides a theoretical and computational framework specifically developed to address this class of problems; see [1]. The efficiency of the reduced basis method rests on an assumption about parametric smoothness, i.e., the solution is assumed to vary smoothly with the underlying parameters.

In this talk we propose an “*hp*” reduced basis method, where different reduced basis models (approximation spaces) are used in different parts of the parameter domain. We first adaptively partition the parameter domain into smaller and smaller subdomains (“*h*”-refinement) and then construct reduced basis models valid within each subdomain (“*p*”-refinement). Of particular interest are problems where the qualitative behavior of the solution is different in different parts of the parameter domain. The idea is that the “local” reduced basis models can be quite small compared to the standard “global” models, and hence reduce the online computational cost. Given any new set of parameters in the online stage, a key challenge is to find the associated reduced basis model in a computationally efficient way. Rigorous *a posteriori* error estimation plays an important role both in the offline/online parameter domain partitioning and model construction and in subsequent certification.

We present simple test problems to illustrate both the opportunities and the challenges with the proposed “*hp*” reduced basis method.

## References

- [1] G. Rozza, D.B.P. Huynh and A.T. 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(3)**, 229–275, (2008).

# Reduced Basis Method for Shape Design, Parametrization and Optimization

Gianluigi Rozza

*École Polytechnique Fédérale de Lausanne, Switzerland*

In the last decades optimal shape design problems have gained an increasing importance in many engineering fields and especially in structural mechanics and in thermo-fluid dynamics. The problems we consider, being related with optimal design and flow control, necessarily involve the study of an evolving system modelled by PDEs and the evaluation of functionals depending on the field variables, such as velocity, pressure, drag forces, temperature, energy, wall shear stress or vorticity.

Especially in the field of shape optimization, where the recursive evaluation of the field solution is required for many possible configurations, the computational costs can easily become unacceptably high. Nevertheless, the evaluation of an “input/output” relationship of the system plays a central role: a set of input parameters identifies a particular configuration of the system and they may represent design or geometrical variables, while the outputs may be expressed as functionals of the field variables associated with a set of parametrized PDEs. The rapid and reliable evaluation of many input/output relationships typically requires great computational expense, and therefore strategies to reduce the computational time and effort are being developed.

Among model order reduction strategies, reduced basis method represents a promising tool for the simulation of flow in parametrized geometries, for shape optimization or sensitivity analysis. An implementation of the reduced basis method is presented by considering different shape or domain parametrizations: from simple affine maps [3] to non-affine ones [2], transforming an original parametrized domain to a reference one. Our analysis will focus on the general properties and performance of the reduced basis method by highlighting with several examples its special suitability and considering parametrized wavy or curvy geometries. The proposed approach includes also a geometric model reduction resulting from a suitable low-dimensional parametrization of the geometry based on free-form deformations technique [4]. We focus on the possibility of handling very generic geometric parametrizations without requiring to create “ad hoc” affine representations necessary to solve the problem efficiently, but recovering this property by an empirical interpolation method [1] in order to take advantage of an offline-online decomposition [3]. We present in particular some examples of reduced basis method applied to external inviscid potential flow, internal viscous thermal flows and steady incompressible Stokes flows for shape optimization problems in cardiovascular geometries.

In collaboration with A. Manzoni, T. Lassila and L. Iapichino.

## References

- [1] M. Barrault, Y. Maday, N.C. Nguyen and A.T. Patera. An ‘empirical interpolation’ method: application to efficient reduced-basis discretization of partial differential equations. *C. R. Math. Acad. Sci. Paris*, 339(9):667-672, 2004.
- [2] G. Rozza. Reduced basis methods for Stokes equations in domains with non-affine parameter dependence. *Comput. Vis. Sci.*, 12(1):23-35, 2009.
- [3] G. Rozza, D.B.P. Huynh and A.T. Patera. Reduced basis approximation and a posteriori error estimation for affinely parametrized elliptic coercive partial differential equations. *Arch. Comput. Methods Engrg.*, 15:229-275, 2008.
- [4] T.W. Sederberg and S.R. Parry. Free-form deformation of solid geometric models. *Comput. Graph.*, 20(4), 1986.

## Discrete Empirical Interpolation for Nonlinear Model Reduction

S. Chaturantabut<sup>a</sup> and D.C. Sorensen<sup>a</sup>

<sup>a</sup> *Rice University*

A dimension reduction method called Discrete Empirical Interpolation is proposed and shown to dramatically reduce the computational complexity of the popular Proper Orthogonal Decomposition (POD) method for constructing reduced-order models for unsteady and/or parametrized nonlinear partial differential equations (PDEs).

In the presence of a general nonlinearity, the standard POD-Galerkin technique reduces dimension in the sense that far fewer variables are present, but the complexity of evaluating the nonlinear term remains that of the original problem. Empirical Interpolation (Barrault, Maday, Nguyen and Patera, 2004) posed in finite dimensional function space is a modification of POD that reduces complexity of the nonlinear term of the reduced model to a cost proportional to the number of reduced variables obtained by POD.

We propose a Discrete Empirical Interpolation Method (DEIM), which is a variant of EIM that is suitable for reducing the dimension of systems of ordinary differential equations (ODEs). In particular, it is applicable to ODEs arising from finite difference discretization of unsteady time dependent PDE and/or parametrically dependent steady state problems. However, the method applies to arbitrary systems of nonlinear ODEs, not just those arising from discretization of PDEs. Our contribution is a simplified description of EIM in a finite dimensional setting that possesses an error bound on the quality of approximation. An application of DEIM to a finite difference discretization of the 1-D FitzHugh-Nagumo equations is shown to reduce the dimension from 1024 to order 5 variables with negligible error over a long-time integration that fully captured non-linear limit cycle behavior. DEIM applied to the simulation of nonlinear miscible viscous fingering in a 2-D porous medium was able to reduce the dimension from 15,000 to 40 variables with negligible error in the solution. Computing time was reduced from 2,100 to 1.3 seconds.

## **Model reduction of differential-algebraic equations: algorithms and applications**

Tatjana Stykel

*Technische Universität Berlin*

We consider model order reduction of differential-algebraic equations (DAEs) that arise in many applications including computational fluid dynamics, circuit simulation and mechanical systems with constraints. We present an extension of balancing-related model reduction techniques to DAEs. Important properties of these methods are that physical properties such as stability and passivity are preserved in the reduced-order model and there exist computable error bounds. The balanced truncation methods and its relatives are based on balancing the solutions of projected Lyapunov, Lur'e or Riccati equations. We discuss the numerical solution of these matrix equations for large-scale problems. We also consider structure-preserving model reduction of coupled DAEs.

## POD a-posteriori error estimates for optimal control problems

Stefan Volkwein

*University of Konstanz*

*Department of Mathematics and Statistics*

The main focus of this talk is on an a-posteriori analysis for the method of proper orthogonal decomposition (POD) applied to optimal control problems governed by parabolic and elliptic PDEs. Based on a perturbation method it is deduced how far the suboptimal control, computed on the basis of the POD model, is from the (unknown) exact one. Numerical examples illustrate the realization of the proposed approach.





# Contributed Talks

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## Domain Decomposition, Model Reduction and Optimization of Time Dependent PDE-Constrained Optimization Problems

H. Antil<sup>a</sup>, M. Heinkenschloss<sup>b</sup>, R.H.W. Hoppe<sup>a</sup>, D.C. Sorensen<sup>b</sup>

<sup>a</sup> *University of Houston, Houston*

<sup>b</sup> *Rice University, Houston*

We introduce a technique for the dimension reduction of a class of PDE constrained optimization problems governed by linear time dependent advection diffusion equations [1] for which the optimization variables are related to spatially localized quantities. Our approach uses domain decomposition applied to the optimality system to isolate the subsystem that explicitly depends on the optimization variables for the remaining linear optimality subsystem. We apply balanced truncation model reduction to the linear optimality subsystem. The resulting coupled reduced optimality system can be interpreted as the optimality system of a reduced optimization problem. We derive estimates for the error between the solution of the original optimization problem and the solution of the reduced problem. The approach is demonstrated numerically on an optimal control problem and on a shape optimization problem.

Also we extend our approach to the problems governed by the time dependent Stokes [2, 5] or the linearized Navier-Stokes equations, linearized around a steady state. Although conceptually the approach in this case is same as above, the extension requires several important changes. These are due to the presence of the incompressibility constraints that affect the model reduction, the domain decomposition, the coupling of both, and the analysis. As an application we will be concerned with the optimal design of capillary barriers as a part of a network of microchannels and reservoirs on microfluidic biochips [3]. The problem amounts to solving a shape optimization problem governed by Stokes equations.

Our approach (in both cases) leads to a reduced optimization problem with the same structure as the original one, but a potentially much smaller dimension. The numerical results confirms the error estimates derived. Our approach can be extended to admit localized nonlinearities in the PDE, such as those considered in [4] or to model reduction techniques for nonlinear systems such as POD [6]. However, currently no a-priori error estimates exists for these model reduction techniques.

## References

- [1] H. Antil *et al.* Domain decomposition and model reduction for the numerical solution of PDE constrained optimization problems with localized optimization variables. *Comput. Vis. Sci.* submitted.
- [2] H. Antil *et al.* Domain decomposition and balanced truncation model reduction for shape optimization of the Stokes system. *Optimization Methods and Software* submitted.
- [3] H. Antil *et al.* Modeling and simulation of piezoelectrically agitated acoustic streaming on microfluidic biochips. *Lect. Notes in Comput. Sci. & Engg.* 60 (2008), pp. 305–312.
- [4] M. Heinkenschloss *et al.* Domain decomposition and model reduction of systems with local nonlinearities. *Num. Math. & Adv. App.* (2008) pp. 389-396
- [5] M. Heinkenschloss *et al.* Balanced truncation model reduction for a class of descriptor systems with application to the Oseen equations. *SIAM Jour. on Sci. Comput.*, 30(2) (2008) pp. 1038–1063.
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# Model Reduction for Parametric Systems Using Balanced Truncation and Interpolation

Ulrike Baur<sup>a</sup>

<sup>a</sup> Chemnitz University of Technology, Germany

Model reduction is common in simulation, control and optimization of complex dynamical systems. Quite often, these systems contain additional parameters, e.g., to allow for geometrical variation or modifications of boundary conditions. The preservation of the parameters in the reduced-order system is a highly desired task. Since usual approaches for model reduction of linear, time-invariant systems are not suitable, we derive a method which preserves the parameters  $p = \{p_1, \dots, p_d\}$  in a linear system

$$\dot{x}(t) = A(p)x(t) + B(p)u(t)$$

with parameter-dependent matrices  $A(p) \in \mathbf{R}^{n \times n}$ ,  $B(p) \in \mathbf{R}^{n \times m}$  and a matrix  $C(p) \in \mathbf{R}^{n \times q}$  in the output equation

$$y(t) = C(p)^T x(t).$$

The matrix  $A(p)$  is assumed to be stable for all parameter values in the considered parameter interval. The transfer function of the system is  $G(s, p) = C(p)^T (sI_n - A(p))^{-1} B(p)$ .

The parameter space is discretized, e.g. by sparse grids; the resulting linear, time-invariant systems are reduced by the usual balanced truncation technique. The overall reduced-order system containing all parameters is obtained by interpolation [1]. Thereby, we will show the influence of different interpolation methods on the numerical results.

The error between the original and the reduced-order system in frequency domain is shown in Figure 1 for a one-parameter example from a semi-discretized diffusion-convection equation. In this example, the parameter influences the intensity of the convection and polynomial interpolation is used for computing the reduced transfer function  $G_r$  in the whole parameter space from six reduced-order systems at fixed parameter points.

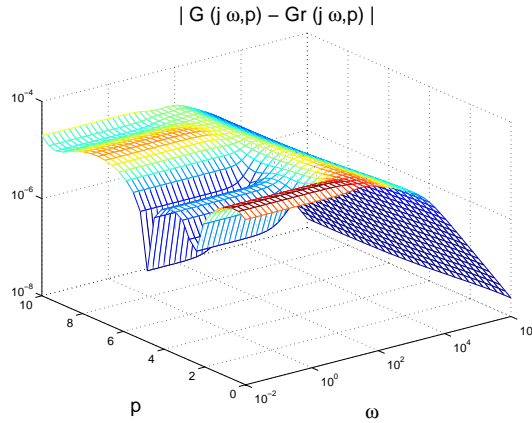


Figure 1: Error between  $G(j\omega, p)$  and  $G_r(j\omega, p)$ .

## References

- [1] Baur, U.; Benner, P.: Modellreduktion für parametrisierte Systeme durch balanciertes Abschneiden und Interpolation, to appear in at-Automatisierungstechnik, 2009.

## Reduced-Basis Approaches for Multiscale Problems

Sébastien Boyaval<sup>a</sup>, Claude Le Bris<sup>a</sup>, Tony Lelièvre<sup>a</sup>,  
Yvon Maday<sup>b</sup>, Cuong Ngoc Nguyen<sup>c</sup> and Anthony T. Patera<sup>c</sup>

<sup>a</sup>*Université Paris-Est, CERMICS (Ecole des Ponts ParisTech) & INRIA, MICMAC project*

<sup>b</sup>*University Paris VI & Brown University* <sup>c</sup>*MIT*

Mathematical models of multiscale problems, *e.g.* in material science, often rely on a separation of scales. Assuming the separation of the macroscopic and the microscopic scales indeed usually allows one to derive coarse-graining procedures for the explicit computation of quantities of interest at the macroscopic scale, like in homogenization theory. But then, *a large number* of (decoupled) microscopic problems, parameterized by the macroscopic scale, still have to be solved, for many values of the macroscopic parameter ; this is the case of the cell problems in homogenization theory.

We will show how Reduced-Basis methods can efficiently handle, at a low computational cost, the reiterated computation of many microscopic problems parameterized by the macroscopic scale, first in the case of the two-scale homogenization of elliptic operators [1], second in the case of stochastic differential equations coupled to an evolution problem through a mean-field assumption [3].

On the other hand, assuming a separation of scales is sometimes idealistic. It often corresponds to thought experiences in physics. On the contrary, multiscale models in engineering are often calibrated on data, and there is no reason then why the noisy field introduced at the macroscopic scale (by “oscillations” of the microscopic scale) should have zero correlation length. For instance, this is the case of uncertainty quantification for PDEs parametrized by colored noise through stochastic coefficients. We will show then how Reduced-Basis methods can still efficiently compute the first moments of the stochastic PDE solution, based on a Karhunen-Löve decomposition of the random parameter field [2].

## References

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- [2] S. Boyaval, C. Le Bris, Y. Maday, N.C. Nguyen, and A.T. Patera. A reduced basis approach for variational problems with stochastic parameters: Application to heat conduction with variable robin coefficient. Research Report 6617, INRIA, 08 2008. Accepted for publication in CMAME.
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## Application of POD and DEIM to Dimension Reduction of Nonlinear Miscible Viscous Fingering in Porous Media

Saifon Chaturantabut<sup>a</sup> and Danny C. Sorensen<sup>a</sup>

<sup>a</sup> *Rice University*

Proper Orthogonal Decomposition (POD) in conjunction with a Discrete Empirical Interpolation Method (DEIM) is applied to construct a reduced-order model of a finite difference discretized system used to simulate nonlinear miscible viscous fingering in a 2-D porous medium. POD is first used to extract a low-dimensional basis that optimally captures the dominant characteristics of the sampled trajectory of the system. This POD basis is truncated according to decay of the singular values and the resulting low dimensional reduced basis is then used in a Galerkin projection to construct a reduced-order system. However, this POD based reduced system still has complexity of the full system present in evaluation of the projected nonlinear term and hence provides no computational savings. DEIM is applied to reduce the complexity of the projected nonlinear term to be proportional to the number of reduced variables. Numerical results demonstrate that the dynamics of the viscous fingering in the full-order system of dimension 15000 can be captured accurately by the POD-DEIM reduced system of dimension 40 with the computational time reduced by factor of  $\mathcal{O}(1000)$  as shown in Figure 1 and Table 1.

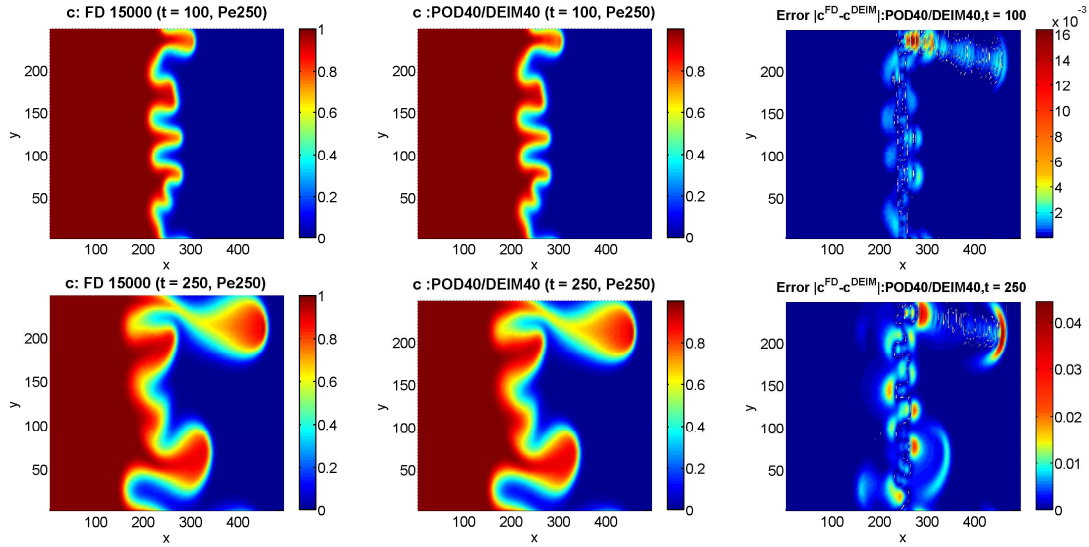


Figure 1: Concentration plots of the injected fluid at time  $t = 100$  and  $t = 250$  from the full-order system of dimension 15000 and from the POD-DEIM reduced system with both POD and DEIM having dimension 40 with the corresponding absolute error at the grid points (Péclet number  $Pe = 250$ ).

Dimension	Avg Rel Error of $c$	CPU time (sec)
Full 15000 (FD)	-	$2.138 \times 10^3$
POD40	$4.066 \times 10^{-4}$	$2.442 \times 10^2$
POD40/DEIM40	$2.045 \times 10^{-3}$	1.275

Table 1: Average relative error of the concentration  $c$  and CPU time of full-order system, POD reduced system, and POD-DEIM reduced system.

# An ANOVA-based Multivariate Spectral Galerkin Scheme for Parameterized Matrix Equations

Paul G. Constantine<sup>a</sup> and David F. Gleich<sup>a</sup>

<sup>a</sup> *Stanford University*

We examine the model problem of a linear system of equations where the matrix of coefficients and right hand side depend on a set of independent parameters, where we assume the system is non-singular for any parameter value chosen from a given parameter space – typically a hyper-rectangle. We extend the spectral Galerkin method for single parameter systems presented in [1] to the case of multiple parameters by employing product-type orthogonal polynomials as the multivariate basis functions.

The extension to multiple parameters induces a choice in the multivariate basis functions not present in the single parameter systems, and we use classical results from Fourier analysis to motivate effective basis reduction strategies. We develop an iterative scheme for choosing an efficient basis set using the so-called Sobol indices from an approximate functional ANOVA decomposition [2] of the solution. This scheme is naturally anisotropic, i.e. if some parameters contribute to the total variance of the solution more than others, then the ANOVA-based scheme discovers this property and exploits it. The scheme also reveals potential decouplings in the Galerkin projection that can dramatically reduce the required computational effort.

We derive the method in detail and present computational results for large-scale problems with up to eleven independent parameters.

## References

- [1] P. G. Constantine, D. F. Gleich, and G. Iaccarino. *Spectral Methods for Parameterized Matrix Equations*. arXiv:0904.2040v1.
- [2] R. Liu and A. B. Owen. *Estimating Mean Dimensionality of Analysis of Variance Decompositions*. JASA, vol. 101 (2006).

## A reduced basis method for evolution equations on parametrized geometries

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Reduced basis (RB) methods are a model reduction technique for parametrized applications requiring time-consuming parameter studies or rapid simulations. In this presentation, we discuss RB methods for parametrized evolution equations. In particular, we focus on nonlinear equations with geometry parametrizations leading to non-affine parameter dependence in the underlying partial differential equation (PDE) transformed on a reference domain.

The main ingredient is a discrete version of the empirical interpolation [3] of the spatial discretization operator which brings the operator into a form, where it can be computed affinely in the parameter. This is necessary for efficient online computations. For the discrete empirical interpolation, we assume that the discretization operator has a local stencil, which is typical for finite volume/finite element operators. In addition to collateral basis vectors and corresponding interpolation points, we need further precomputed quantities. These are a numerical subgrid and partial reconstruction of the RB vectors. Based on these quantities, an approximation of the discretization operator can be obtained in an effective offline/online fashion. The approach was successfully applied in our previous work [1], [2] where the numerical scheme was restricted to explicit discretization operators. Explicit discretizations of higher order terms in the PDE, however, lead to very small time steps and are therefore computationally expensive.

As an extension, we now demonstrate how empirical interpolation of implicit discretization operators can be integrated into a solver for nonlinear equation systems like the Newton method. Experimental results are presented for a diffusion equation equation which gets transformed to a convection-diffusion-reaction equation including an anisotropic diffusion tensor by a diffeomorphic geometry mapping. This demonstrates the applicability of the presented RB method and allows us to discuss the observed computational time gain. The experiments are implemented with our RB software package *RBmatlab*.

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## Structure preserving Krylov-Subspace methods for solving large Lyapunov equations

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We consider descriptor system arising from circuit equations. When applying model order reduction techniques such as balanced truncation to these systems, one of the main tasks consists of solving large scale Lyapunov equations efficiently. This is because balanced truncation desires to solve these equations frequently. Specifically one is interested in finding the solution of generalized, projected Lyapunov equations

$$EXA^T + AXE^T = -P_l BB^T P_l^T, \quad X = P_r^T X P_r \quad (1)$$

$$E^T Y A + A^T Y E = -P_r^T C^T C P_r, \quad Y = P_l Y P_l^T \quad (2)$$

with  $E, A \in R^{n \times n}$ ,  $B, C^T \in R^{n \times ns}$ .

When dealing with circuit equations the matrix  $E$  is usually a sparse, singular matrix. (cf.[1]) The right hand side is a symmetric low rank matrix. It can be shown that for passive systems the solution  $X$  is of low rank as well. So the aim is to find an iterative solver, which preserves the symmetry structure and low rank property in every iteration step. For this purpose Krylov-subspace methods fit perfectly. In particular we choose the **F**lexible-**G**eneral-**M**inimal-**R**esidual (cf.[2]) but other methods are possible as well. The drawback of these methods is often the slow convergence so it is essential to use a preconditioner which also fulfills these structure preserving properties. Here we apply the **C**holesky-**F**actor-**A**lternating-**D**irect-**I**mplicit-**I**teration (cf.[3]) as preconditioner rather than as a stand-alone method since by construction this method also preserves the structure properties. The success of the CF-ADI method strongly depends on the choice of the so called shift parameters  $\tau_i$ . The goal of combining these two methods is to use the robustness of the FGMRES together with the good convergence speed of the CF-ADI method. As a first result we will demonstrate that the combined method is less sensitive to disturbances in the shift parameters  $\tau_i$ .

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## A Numerically Robust Moment-Matching Algorithm for Multivariate Polynomially Parameterized Systems

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In recent years, model order reduction has been extended from the single-parameter to the multi-parameter case. The class of multivariate polynomially parameterized systems arises naturally in many applications, e.g. in structural mechanics or microwave engineering, and is considered in this contribution. Projection-based order reduction methods can mainly be divided into single-point and multi-point approaches. Multi-point methods utilize the solution vectors at different points in parameter space as projection basis, which results in high flexibility but also the need for a separate system matrix factorization at every expansion point. In contrast, single-point methods require just one matrix factorization, but the development of numerically stable algorithms is more challenging.

In principle, polynomially parameterized systems can be reduced to the multi-linear case by introducing auxiliary unknowns, and then treated by algorithms from the literature, e.g. [1]. For complicated real-world applications, however, the memory requirements of this approach are prohibitive. For this reason, we propose a new method that can deal with polynomial dependence on multiple parameters directly, without linearization. The main idea is to decompose the multivariate problem into a series of single-parameter problems that are easier to handle. The key features of the proposed method are as follows:

- Improved numerical stability compared to existing methods [2]: The reduction to single-parameter Krylov spaces allows the application of robust univariate order reduction methods [3].
- Straightforward parallelization: As in a recent method for the multi-linear case [1], the resulting single-parameter models are decoupled, so that the respective projection bases can be computed independently.
- Reduced memory requirement: The number of vectors to be kept in main memory is significantly reduced. No auxiliary matrices are needed.

In our presentation, we will introduce multivariate Krylov spaces of higher order, which form the theoretical foundation of our solver, explain the details of the proposed algorithm, and give numerical examples that support our findings.

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## A reduced-basis approach to real-time parameter estimation for parametrized parabolic partial differential equations

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We present a reduced-basis (RB) approach to real-time parameter estimation for parametrized parabolic partial differential equations with (non)affine parameter dependence. The fast and reliable evaluation of the input-output relationship – afforded by the RB method and associated *a posteriori* error estimators – is the basis for the efficient and robust solution of the estimation problem.

We first review the RB approximation method for linear parabolic problems with nonaffine dependence on the parameter (cf. [3]). The method replaces the nonaffine terms with a coefficient function approximation which then permits an efficient offline-online computational decomposition (cf. [2]). We also introduce – under certain restrictions on the function approximation – rigorous *a posteriori* error estimators for the RB approximations.

We next illustrate how the RB approach lends itself naturally to existing solution methods for parameter estimation and inverse problems (cf. [5]), and furthermore allows the development of new techniques to solve these problems. While the efficient evaluation of the input-output relationship is essential to achieve real-time solutions, the *a posteriori* error bounds let us pursue a robust parameter estimation procedure which takes into account explicitly and rigorously the uncertainty due to errors in the measurement and in the RB approximation. To this end, we introduce the “uncertainty region” as a measure of the degree of uncertainty in the parameter estimate. From a theoretical point of view, the “uncertainty region” may serve as an indication of (i) the parameter identifiability of the specific problem (cf. [1, 4]), and (ii) the sensitivity with respect to, e.g., measurement errors or sensor placement. To illustrate the applicability of our method, we present numerical examples for the dispersion of a pollutant in a flow field, i.e., the characterization of the unknown source location given sensor measurement data.

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# Certified reduced basis methods for the Fokker–Planck equation of dilute polymeric fluids

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The flow of dilute polymeric fluids can be described by a coupled Stokes Fokker–Planck system, where Stokes provides Fokker–Planck with a strain rate from the Newtonian solvent, and Fokker–Planck provides Stokes with an “extra polymeric stress” due to the microscopic polymer molecules in the fluid. The Fokker–Planck equation is posed over a high-dimensional physical–configuration space, but through standard Lagrangian manipulations it can be reformulated as a *large* number of instantiations of the Fokker–Planck equation — parametrized by the macroscopic strain rate — over configuration space only; the components of the polymeric extra stress tensor are the output functionals of interest for this parametrized problem. We apply the certified reduced basis method to this parametrized Fokker–Planck equation in order to obtain a reliable and highly efficient scheme in this many-query context.

We consider both the time-dependent and steady state cases. The new ingredients in our computational framework for the time-dependent case are a finite-time *a posteriori* bound for the error in the reduced basis prediction of the output quantities of interest, and a projection-based POD-greedy sampling procedure for the identification of effective reduced basis spaces. In the steady case, we utilize a Successive Constraint Method (SCM) for construction of a lower bound for the inf-sup constant of the Fokker–Planck convection-diffusion problem (which is non-standard due to the presence of an unbounded convection term), and (motivated by parameter estimation applications) we introduce parameters that characterize polymer molecule structure into the formulation.

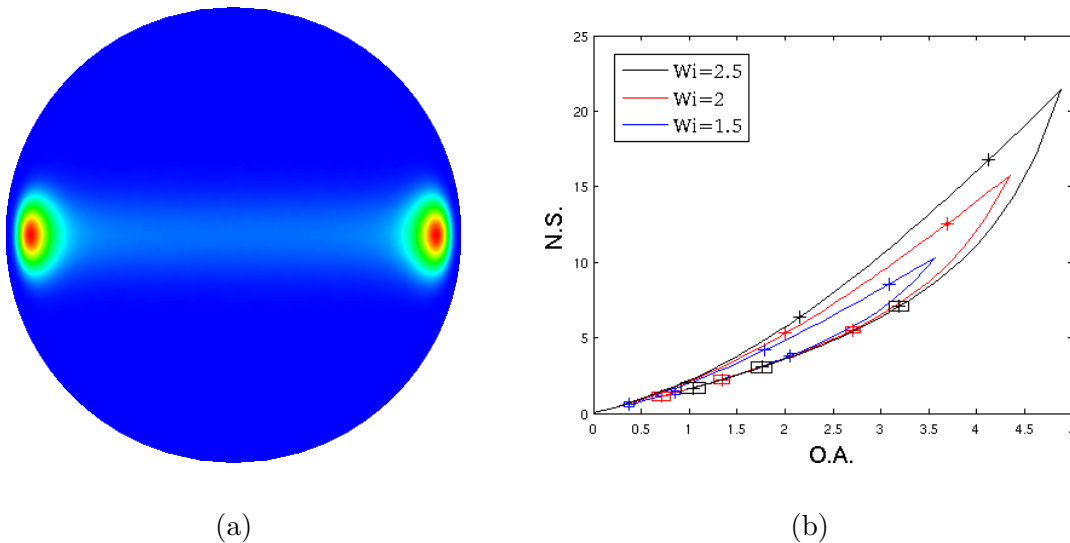


Figure 1: (a) Probability density of “model” polymer molecules in extensional flow, and (b) reduced basis stress hysteresis plot with error boxes.

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## Residual based POD Model Order Reduction of Drift Diffusion Equations in parametrized Electrical Networks

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In order to obtain a highly accurate model for integrated circuits (e.g. electrical networks containing semiconductors) it has been proposed by various authors to simulate the semiconductor components by drift-diffusion (DD) equations:

$$\begin{aligned}\operatorname{div}(\varepsilon \operatorname{grad} \psi) &= q(n - p - C), \\ -q \partial_t n + \operatorname{div} J_n &= q R(n, p, J_n, J_p), \\ q \partial_t p + \operatorname{div} J_p &= -q R(n, p, J_n, J_p), \\ J_n &= \mu_n q (U_T \operatorname{grad} n - n \operatorname{grad} \psi), \\ J_p &= \mu_p q (-U_T \operatorname{grad} p - p \operatorname{grad} \psi).\end{aligned}$$

The coupling with the network DAE then yields a nonlinear partial-differential algebraic equation (PDAE), see [2, 3].

We discretize the DD-equations in space by Raviart-Thomas elements and simulate the resulting high dimensional DAE. Snapshots of the semiconductor state variables are selected from one or multiple simulations with different sets of parameters (e.g. frequency of input source, length of semiconductor, doping). From these snapshots a reduced state space approximation is obtained by applying proper orthogonal decomposition (POD). The projection of the DD-equations onto the reduced state space yields a nonlinear low-dimensional model for the DD-equations. This low-dimensional model then serves as surrogate for the DD-equations in the integrated circuit.

In this talk we present an adaptive approach to construct POD models which are valid over certain parameter ranges. We use the residual as an estimate for the quality of the reduced model. The residual is constructed (as in [1] for the linear case) by introducing the solution of the reduced model into the unreduced model. Then we refine the reduced model by adding snapshots from additional simulations of the unreduced model at local maxima of the residual. Numerical results for this approach are presented which indicate that the method is applicable despite the nonlinearities.

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## Model reduction in chemical kinetics: Approximating slow attracting manifolds by computing minimal curvature trajectories

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The need for model reduction in chemical kinetics is mainly motivated by the fact that the computational effort for a simulation of reactive flows involving multiple time scale chemical reaction processes is computationally extremely expensive for detailed chemical reaction mechanisms with a large number of chemical species.

In dissipative ordinary differential equation systems modeling chemical reaction kinetics, different time scales cause anisotropic phase volume contraction along solution trajectories. Model reduction methods exploit this for simplifying chemical kinetics via a time scale separation into fast and slow modes. The aim is to approximate the system dynamics with a dimension-reduced model after eliminating the fast modes by enslaving them to the slow ones via computation of a slow attracting manifold. We present a novel and efficient numerical method for computing accurate approximations of such manifolds using trajectory-based optimization. We discuss Riemannian geometry concepts as a basis for suitable optimization criteria characterizing trajectories near slow attracting manifolds. Our approach is based on the solution of the trajectory optimization problem

$$\min_c \int_0^{t_f} \Phi(c(t)) \, dt$$

subject to the constraints

$$\begin{aligned} \frac{dc(t)}{dt} &= f(c(t)) \\ 0 &= g(c(0)) \\ c_k(0) &= c_k^0, \quad k \in I_{\text{fixed}}. \end{aligned}$$

$f$  describes the chemical reaction kinetics for the chemical species vector  $c(t)$ , chemical element mass conservation relations are collected in  $g$ .  $I_{\text{fixed}}$  is the index set of reaction progress variables chosen for parameterization of the reduced model. The key for the identification of trajectories approximating slow attracting manifold is the optimization criterion  $\Phi(c(t))$  which is supposed to characterize the relaxation of “chemical forces”. From a physical point of view, curvature (in the sense of rate of change of reaction velocity) is closely related to the geometric interpretation of force. Based on earlier ideas [1] we recently demonstrated [2, 3] that the curvature-based criterion  $\Phi(c) = \|J_f(c) f\|_W$  ( $J_f$ : Jacobian) with a particular thermodynamically motivated norm  $W$  is a suitable optimization criterion and allows the computation of accurate approximations of slow attracting manifolds in chemical kinetics.

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# Model Reduction for Partial Differential Equations with Distributed Parameters

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**Motivation.** Partial differential equations (PDEs) parameterized by distributed quantities arise frequently in several disciplines of engineering. In some cases, we control the parameter through structural and material design choices; other times, we must estimate an uncontrolled parameter in order to make subsequent decisions. Due to the complexity of simulating the governing equations, it is computationally expensive to explore the parameter space, e.g., in design optimization and statistical inverse problems. It is necessary to develop a systematic method by which we compute outputs of interest at much lower expense without sacrificing the integrity of the physics important to the input-output map. Projection-based model reduction techniques express state variables as a linear combination of basis vectors spanning a low-dimensional subspace. As a result, the forward map from parameter to state can be computed more cheaply; the cost is determined by the solution of a small dense linear system. The exploration of the parameter space, however, can still be prohibitively expensive for discretized distributed parameters.

**Approach.** In order to address this challenge, we extend projection-based reduction to the parameter space. We introduce an  $L_2$  map from the infinite-dimensional parameter space to one defined by a reduced parameter basis. Design exploration and statistical sampling take place in the reduced space at lower cost. To identify the reduced parameter and state subspaces, we utilize the greedy algorithm [1]. Iteratively, we identify the parameter which maximizes the output error between a refined computational model and the current reduced-order model. Through Gram-Schmidt orthogonalization, the parameter which maximizes output error and the corresponding state are appended to the current parameter and state bases, respectively. Reduced bases for both parameter and state are constructed by repeating this process iteratively until the desired reduction in the output error is achieved. Each greedy iteration requires the solution of a large-scale nonlinear program with PDE-constraints in an offline phase. Then, the reduced model may be used repeatedly online.

**Results.** Our approach is demonstrated for model groundwater statistical inverse problems in one- and two-dimensions. From synthetic pressure head well data, we attempt to infer the hydraulic conductivity in the subsurface. We demonstrate that a parameter- and state-reduced model is a sufficient surrogate for a refined computational model for the Markov chain Monte Carlo (MCMC) sampling required in the Bayesian solution to the inverse problem. In the two-dimensional model problem, we obtain a speedup of almost two orders of magnitude in the CPU time required for the statistical sampling. The reduction in state accelerates forward model evaluations, while reduction in parameter permits usage of a hand-tuned Metropolis-Hastings sampler. Without this reduction, the statistical inverse problem is beyond the current means: efficient samplers do not exist for high-dimensional nonlinear posteriors and the forward model computations are too costly for repeated evaluation to be feasible. Our approach makes tractable statistical inverse problems which depend on PDEs with distributed parameters.

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## A New Framework for Order Reduction of Parametric Models by Superposition of Locally Reduced Ones

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Starting from a given parametric state-space model, the goal of *parametric model order reduction* is finding a reduced model that preserves the parameter-dependency, thus allowing a variation of any of the parameters without the need to repeat the reduction step.

One of the first works in this direction is [1]: Assuming a linear model with affine parameter dependency, a projection  $\mathbf{V}$  can be calculated, such that the reduced model not only matches some of the first moments of the transfer function  $\mathbf{G}(s, \mathbf{p})$  with respect to  $s$ , but also with respect to the parameters. The method suffers from the curse of dimensionality where the order of the reduced system grows very rapidly even for small numbers of parameters. Another well-known technique (also used in TPWL) is to calculate local projection matrices from several local models in the parametric space, merge them together, and then apply a common order reducing projection to the original parametric (or nonlinear) model. Also this method leads to a relatively high reduced order. In [2], a TBR-based method using an interpolation and a soft switching between the reduced order transfer functions of different non-parametric models (obtained by varying the parameters using sparse grids) is suggested.

In this contribution, a novel framework, inspired from the work in [3], for the reduction of linear parametric systems is introduced. It consists of an interpolating representation of the linear parametric model as:

$$\dot{\mathbf{x}} = \sum_{i=1}^s \omega_i(\mathbf{p}) [\mathbf{A}(\mathbf{p}_i)\mathbf{x} + \mathbf{B}\mathbf{u}], \quad \mathbf{y} = \mathbf{C}\mathbf{x}, \quad (1)$$

and then *separately* reducing all the local models by using separate  $q$ -dimensional subspaces as follows:

$$\dot{\mathbf{x}}_r = \sum_{i=1}^s \omega_i(\mathbf{p}) \left[ \tilde{\mathbf{V}}_i^T \mathbf{A}(\mathbf{p}_i) \tilde{\mathbf{V}}_i \mathbf{x}_r + \tilde{\mathbf{V}}_i^T \mathbf{B}\mathbf{u} \right], \quad \mathbf{y} = \mathbf{C}\tilde{\mathbf{V}}\mathbf{x}_r. \quad (2)$$

The main features of the new approach are: 1) The parametric matrix  $\mathbf{A}(\mathbf{p})$  needs only to be known and evaluated at  $s$  discrete values of the vector  $\mathbf{p}$  (no analytical or affine dependency needed; also  $\mathbf{B}$  and  $\mathbf{C}$  may depend on  $\mathbf{p}$ ), 2) the order of the reduced model will equal  $q$ , independent of the number  $s$  of local models considered, 3) by suitable state transformations, the state vector of the reduced interpolating model is given a clear physical interpretation, 4) the reduction method to be applied can be freely chosen, e.g. TBR or Krylov-subspace method, 5) when using a Krylov-subspace reduction method, it is possible to show that the moments are matched for any parameter value, 6) the framework can be applied to nonlinear reduction as well.

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# Stabilized reduced basis approximation of the incompressible three-dimensional Navier–Stokes equations in parametrized deformed domains

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In this work we are interested in the numerical solution of the steady incompressible Navier-Stokes equations for fluid flow in pipes with varying orientations and cross-sections. We intend to compute a reduced basis element approximation of the solution, employing the geometry as a parameter in the reduced basis method. This has previously been done in a spectral element  $P_N - P_{N-2}$  setting in  $2D$  for the steady Stokes equations[1, 2]. To compute the necessary basis functions in the reduced basis method, we propose to use a stabilized  $P_1 - P_1$  finite element method for solving the Navier-Stokes equations on different geometries. By employing the same stabilization method in the reduced basis approximation, we avoid having to enrich the velocity basis in order to satisfy the inf-sup condition. This reduces the complexity of the reduced basis method for the Navier-Stokes problem, while keeping the good approximation properties. We present numerical results for selected parameter dependent  $3D$  pipes. The reduced basis approximation error relative to the finite element solution shows exponential convergence with respect to the number of basis functions.

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## Accelerated a posteriori error estimation for the reduced basis method with application to 3D electromagnetic scattering problems

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We present a new technique for fast estimation of error bounds in the reduced basis context, efficiently applicable to real world 3D problems. Geometric parametrizations of complicated 2D or even simple 3D structures easily leads to affine expansions consisting of a high number of terms (100-1000) [1]. Application of state-of-the-art reduced basis techniques for computation of error bounds becomes practically impossible. As way out we propose a new error estimator which leads to substantial savings regarding online and offline computational times and memory consumption.

We apply the reduced basis method and the developed estimator to inverse scattering applications in electromagnetics and examples from computational lithography in 2D and 3D as shown in Figure 1.

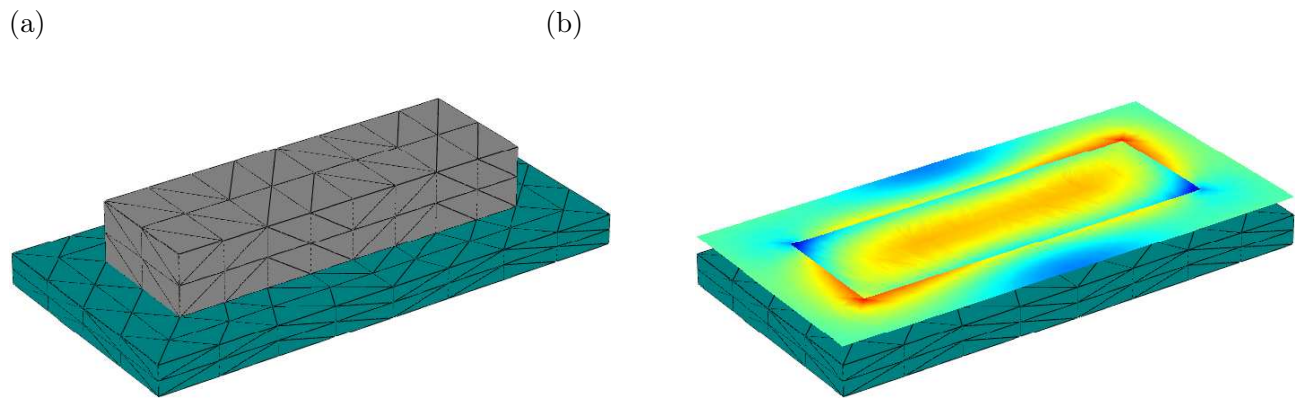


Figure 1: (a) 3D periodic grating for reduced basis computations. (b) Intensity of electric field obtained from FEM computation.

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## Multi-level trust region POD algorithms

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Optimization problems with parabolic differential equation constraints are by themselves often difficult to solve. If, in addition an integral term is added to the PDE, its numerical solution becomes more complex and also more expensive. One example for such a problem is the calibration of improved option pricing models, namely jump-diffusion models, which are gaining importance in practice (cf. [1], e.g.). Discretizing the space variable by a finite element approach requires first a proper variational formulation. A general optimal control problem would then be given by

$$\begin{aligned} & \min_u J(y, u) \\ \text{s.t. } & \frac{d}{dt} \langle y(t), v \rangle_H + a(u; t; y(t), v) = \langle f(u; t), v \rangle_H, \quad v \in \mathcal{V}, \quad t \in (0, T] \\ & \text{i.c. } \langle y(0), v \rangle_H = \langle y_0, v \rangle_H \end{aligned} \quad (1)$$

with hopefully an elliptic time- and control-dependent bilinear form  $a$ . The time variable can be discretized by a finite difference approach, which in case of integro differential equations generally leads to dense stiffness matrices. Implicit methods are hard to implement and using these for a solution is quite expensive.

We propose to use proper orthogonal decomposition (**POD**) in order to avoid the solution of these large, dense, linear systems of equations. Given one solution of the full discretized problem for a specific control  $u_k$  we accumulate significant information of this solution in only a few new basis functions  $\Psi_1, \dots, \Psi_p$  via POD. We can use these basis functions in the variational formulation (1) instead of the finite element functions, that are normally used to discretize  $\mathcal{V}$ . The result is a much smaller system, but well-known error estimates for PDEs, see e.g. Kunisch, Volkwein [4], can be extended also to PIDEs and numerical results show that the finite element and the POD solution are very close.

However these error estimates only hold true for unchanged controls, and if we veer away from the starting control  $u_k$ , where the POD model is based on, the results get worse. The solution is to use the model in a trust region framework. The usually used quadratic model function here is replaced by a model function based on the POD model and one only has to find an appropriate minimizer of the reduced function in the trust region in each step. To verify the POD model, the full finite element solution has to be calculated once per step, what is the most expensive part of the algorithm.

To further reduce the costs of the algorithm a multi-level approach is introduced. A hierarchy of grids from coarse to fine is set up (cf. [3]) and controlled via a nested iteration. Gratton, Sartenaer and Toint [2] could even show convergence for quadratic model functions. We show some promising numerical results using a multi-level strategy in the trust region POD algorithm in the context of calibrating option pricing models.

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## Reduced-basis *a posteriori* error estimation for the parametrized steady incompressible Navier-Stokes equations

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We review the recent work on *a posteriori* error estimation techniques for reduced-basis (RB) approximations for quadratically nonlinear elliptic partial differential equations, particularly for the steady incompressible Navier-Stokes equations. The key ingredient is the Brezzi-Rappaz-Raviart (BRR) theory (cf. [1, 2, 6, 8]) for analysis of variational approximations of nonlinear PDEs. Typically, the BRR framework provides a non-quantitative *a priori* or *a posteriori* justification of asymptotic convergence. However, we show that the RB context is a unique opportunity to render the BRR theory completely predictive. We elucidate the application of the BRR theory in our context, i.e., in the construction of rigorous, quantitative, sharp, and inexpensive (real-time) *a posteriori* error estimators for RB approximations to quadratically nonlinear PDEs (cf. [3, 5, 9, 12]). The main components are appropriate approximations and associated computational procedures for (a) the dual norm of the requisite residuals, (b) an upper bound for the  $L^4(\Omega) - H^1(\Omega)$  Sobolev embedding continuity constant (cf. [10, 11]), (c) a lower bound for the Babuška inf-sup stability factor (cf. [4, 7]), and (d) the adjoint contributions associated with the output. In all these components – as in the reduced-basis approximations – we exploit affine parametric structure and offline-online computational decompositions to provide real-time response.

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## $\mathcal{H}_{2,\alpha}$ -norm optimal model reduction for computation of a parametrized volume source in laser welding

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The physical phenomena in laser welding processes can yet not completely be described by mathematical models. It is therefore common to describe the effects of the heat energy by means of a parametrized volume source. The parameters of the volume source are obtained in several steps by a calibration of computed and experimental values of the temperature. In each step, a time-dependent partial differential equation on a domain of up to three spatial dimensions has to be solved.

This procedure can be mathematically modelled by the optimization problem

$$\text{Minimize}_{p \in P} \quad \|T - T_e\|_{\Omega_e \times (0, t_f)}^2 + \gamma \|p\|_P^2 \quad (1)$$

where  $T$  is the solution of the parametrized partial differential equation

$$T_t + v \nabla T = \kappa \Delta T + f(p), \quad T \in \Omega \times (0, t_f) \quad (2)$$

with appropriate initial and boundary conditions. Here,  $T$  denotes the temperature on a spatial domain  $\Omega \subset \mathbb{R}^3$  and the time interval  $[0, t_f]$ ,  $v$  the convection velocity and  $\kappa$  the thermal diffusivity. The parameters  $p \in P$  of the volume source are to be determined such that the temperature is close to experimental data  $T_e$  for the temperature on a domain  $\Omega_e \times (0, t_f)$  with  $\Omega_e \subset \Omega$  while  $\gamma$  is a small regularization parameter. The overall computation time for solving Problem (1) numerically is very high since the partial differential equation (2) has to be solved in each iteration step of the optimization routine. This precludes the direct application of this method for real-world problems.

In this talk, we present a method for finding a reduced model to compute the temperature  $T$  on  $\Omega_e \times (0, t_f)$  from the parametrized partial differential equation (2) subject to the parameters  $p$ . After linearization of  $f$  and spatial discretization of (2),  $p$  can be interpreted as the input of a large-scale linear dynamical system with the temperature  $T$  on  $\Omega_e \times (0, t_f)$  as the output of the system. We use a model reduction method where the transfer function is approximated optimally with respect to the  $\mathcal{H}_{2,\alpha}$ -norm. The reduced system satisfies certain tangential interpolation conditions and can be computed with the algorithm MIRIAM [1], [2]. Instead of Problem 1, one can then solve

$$\text{Minimize}_{p \in P} \quad \|T_r - T_e\|_{\Omega_e \times (0, t_f)}^2 + \gamma \|p\|_P^2 \quad (3)$$

where  $T_r$  is the output of the reduced system. We present a numerical solution for Problem (3) and results for the error  $\|\bar{p} - \bar{p}_r\|$  where  $\bar{p}$  and  $\bar{p}_r$  are the optimal solutions for Problem (1) and (3), respectively.

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## On combining model reduction and Gauss-Newton algorithms for inverse PDE problems

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We suggest an approach to speed up the Gauss-Newton solution of inverse PDE problems by minimizing the number of forward problem calls. The acceleration is based on effective incorporation of the information from the previous iterations via a reduced order model (ROM).

Let

$$A(\rho)u_k = s_k, \quad k = 1, \dots, m_s \quad (1)$$

be a FE or FD approximation of a linear second order PDE with symmetric (or complex symmetric) operator with variable coefficient. Here  $\rho$  is a finite-dimensional vector of the discrete PDE coefficient,  $m_s$  is the number of sources. Let

$$F(\rho) \in C^{m_s \times m_r}$$

be the matrix with elements  $u_i^T r_j$ , where  $r_1, \dots, r_{m_r}$  is a linearly independent set of weight functions  $r_j \in C^N$  (corresponding to receivers). In the inverse problem we reconstruct the distribution of  $\rho$  under known measurement at receivers.

Due to the nonlinear dependence of  $F$  on  $\rho$  the conventional Gauss Newton algorithm may require many iterations. Instead we propose a so-called Model Reduction Gauss-Newton (MRGN) algorithm, that converges much faster with approximately the same cost as the GN per iteration. Basic idea of that algorithm is that on the  $n$ -th iteration we construct a multivariate rational (with respect to the components of  $\rho$ ) approximation  $F^n(\rho)$  of function  $F(\rho)$  such that  $F^n(\rho)$  is easily computable and  $\max_{\rho} \|F^n - F\| \rightarrow 0$ . The approximation is designed with the help of Galerkin and pseudo-Galerkin methods for self-adjoint and complex symmetric problems respectively. In order to construct  $F^n$  we use all the information from previous steps. Therefore the constructed ROM generates effective multivariate rational interpolation matching the forward solutions and the Jacobians from the previous iterations. Numerical examples for the inverse conductivity problem for the 3D Maxwell system show significant accelerations.



# Poster Presentations

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## Combining moment matching and balanced truncation for order reduction of bilinear systems

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As a first step from the linear to the nonlinear world, bilinear systems are of special interest. For example the method of Carleman linearization allows to approximate nonlinear systems with affine control input by high-dimensional bilinear control systems.

There have been several attempts to transfer methods of model order reduction like balanced truncation and moment matching from linear to bilinear systems (see the references). In this talk we review these results, and point out some extensions. In particular, we suggest a mixed approach which combines the two methods. The results are illustrated by a number of examples of large-scale bilinear systems.

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## Snapshot-based Approximation of Frequency-weighted Gramian Matrices for Model Reduction in Multibody Dynamics

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One important issue for the simulation of flexible multibody systems is the reduction of the flexible body's degrees of freedom. By the use of second order frequency weighted Gramian matrix based reduction techniques the distribution of the loads is taken into account a priori and very accurate models can be obtained within a predefined frequency range. Furthermore, an energy interpretation of the reduction procedure and a priori error bounds are available [1]. Hence, using this method only the load distribution, the frequency range of interest and a measure for the desired accuracy have to be provided by the user. That is why the method is especially attractive as far as engineering applications are concerned. However, the calculation of the frequency weighted Gramian matrices requires high computational effort. Hence, appropriate approximation schemes have to be used to find the dominant eigen space of the matrices.

The matrix integral needed for calculating the Gramian matrices can be approximated by quadratures using integral kernel snapshots. This method can be viewed as an extension of the Poor Man's TBR [2] scheme for second order systems. The number and location of these snapshots have a big influence on the reduction results. In Reduced Basis methods, sophisticated snapshot-selection methods are used for basis construction [3]. In the current study we transfer some of these methods to Gramian matrix based model reduction. The method can be viewed as an automatic determination of optimal frequency weighting and as an adaptive learning of quadrature rules.

In a first step, a greedy search algorithm is used for the calculation of the next snapshot at the maximum of an error measure calculated for the finite training set  $\omega_t \in \mathcal{F}_{training}$  of training frequencies  $\omega_t$ . Possible error measures are the absolute error  $e = \|\mathbf{H}(\omega_t) - \bar{\mathbf{H}}(\omega_t)\|_F$  or the relative error  $\epsilon = (\|\mathbf{H}(\omega_t) - \bar{\mathbf{H}}(\omega_t)\|_F) / \|\mathbf{H}(\omega_t)\|_F$  between the transfer matrix of the original model  $\mathbf{H}(\omega_t)$  and the reduced model  $\bar{\mathbf{H}}(\omega_t)$ . By a sensitivity analysis the appropriate size of the training set and the correct error measure are determined. The results of the greedy search algorithm are compared with uniformly and randomly chosen basis construction strategies. Then, an adaptive basis construction scheme, derived from [3], is used for further improvement of the snapshot selection. Due to the fact that only the dominant eigen space of the POD Kernel is used as projection matrix the influence of some snapshots on the reduced system is marginal. These snapshots are removed from the training set as well as from the POD kernel. Afterwards, based on a newly developed strategy, the training set is extended by using frequencies originating in more influential regions. The applicability of the approaches is demonstrated on a small academic benchmark model but is additionally tested for a demanding technical system with more than 30 000 degrees of freedom.

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## Efficient reduced models and a posteriori error estimation for parametrized dynamical systems by offline/online decomposition

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Reduced basis (RB) methods are effective methods for model reduction of parametrized partial differential equations (P<sup>2</sup>DEs). During the last years various types of stationary and time-dependent, linear and nonlinear P<sup>2</sup>DEs have been treated [2, 3]. In the field of model order reduction for dynamical systems [1], these methods are largely unknown, but the interest in reduction of parametrized systems is increasing. In the current presentation, we show that some characteristic components of RB-methods can be transferred to model reduction of parametrized dynamical systems [4]. We exemplify this for linear systems with output estimation. We assume an affine decomposition of the system components in parametric coefficient functions and parameter-independent components. In particular, this covers more than linear or polynomial parametrizations. An offline/online decomposition is the key for efficient simulation: In the offline phase, one prepares the reduced basis and auxiliary parameter-independent quantities. These preparations allow rapid online simulations for varying parameters. The possibly extensive offline phase pays off in case of a multi-query context, where sufficiently many reduced simulations with different parameter constellations are expected. In addition to the effective reduced simulation schemes, rigorous error control is possible by a posteriori error estimators for the state and output. These are based on residual analysis and can also be effectively decomposed in an offline/online fashion and hence allow fast and rigorous error guarantees. The output estimates can be improved by primal-dual techniques similar to [3] and corresponding a posteriori error estimators can be derived. Experiments with simple dynamical systems demonstrate the applicability of the reduced parametrized systems and the reliability of the error estimators.

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## Error Estimators for Projection-Based Order Reduction Methods

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In order reduction of systems in engineering applications it is a priori unclear how small a reduced system could be and it is necessary to control the error made by reduction. Thus we present error estimators ensuring that the error which is made by the reduction does not exceed a given tolerance and allowing a suitable choice of the reduced dimension. The error estimators are applicable to linear PDEs. We consider time discrete state space systems of the form  $Ex^k - Ex^{k-1} = \Delta t Ax^k + \Delta t Bu^k$  where  $k = 1, \dots, K$  indicates the discrete time step.

We present two different residuum-based strategies to estimate the error between the full order and the reduced order approximation without computing the full order one. The first error estimator, see Figure 1 b), is applicable to coercive problems and measures the error in the energy norm. The energy norm,  $\|x^k\|_E^2 = (x^k)^T Ex^k - \Delta t \sum_{k=1}^K (x^k)^T Ax^k$ , is physically motivated and the derivation is according to [1]. After an offline/online decomposition the computational complexity is independent of the full order dimension. The disadvantage is that this error estimator is restricted to coercive problems and the error might be overestimated. The second error estimator demands weaker assumptions on the system than coercivity. The exact error is computed in a problem specific norm that is an upper bound for the  $L^2$  space-time norm. The exactness is shown in Figure 1 c). In general, the error estimators are applicable to projection-based reduction methods, e.g. Krylov Reduction Method or the Proper Orthogonal Decomposition.

As an example we apply the theory to the academic Benchmark problems, CD player and the beam model. We compare the different reduction methods and the error estimators to each other. Concerning the CPU times, the speed-up factor achieved by calculating the error estimator instead of the real error is up to 100. Additionally, we consider a solenoid actuator, see Figure 1 a). Similar actuators are used in the common rail injectors. The underlying PDEs are the heat equation and the Maxwell equations.

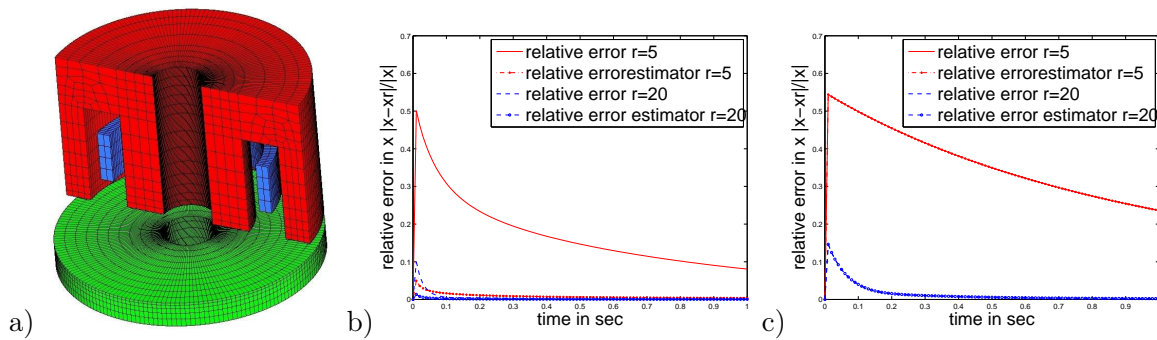


Figure 1: a) Solenoid actuator structure; comparison of the real error and the b) first error estimator and c) second error estimator applied where the reduced model is achieved by Krylov reduction method. The order of the reduced system is  $r$ .

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## Model Reduction Method in Multi-Parameter Domain

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The reduction process is a construction of a low-order model that minimizes the defined error between the solution of the detailed reference model and the reduced low-order one. In this work, projection methods are used. Depending on the projection error definition, different methods can be constructed. For example, the efficient reduced-basis method is proposed in [1] using  $L$ -infinity norm for the error. Another option is to use  $L^2$ -norm that will lead to “Proper Orthogonal Decomposition”-type methods with spatially-distributed basis functions and time-dependent coefficients [2] or, vice versa, time-distributed basis functions and coefficients of a reduced model that are spatially distributed [3]. In applications it is also quite important to estimate the approximation quality of the reduced model with some quantitative measure.

In this contribution, we propose an extension of the model reduction based on the POD-like approach that differs from the original one in a way that the reduction is performed for snapshot solutions distributed not only in time and space but also in a multi-parameter space. The reduction procedure can be used for the construction of a low-order model with an approximation quality chosen in advance. The reduction method consists of three steps:

- Finding of the optimal basis set of spatially orthonormal functions that is a *best approximation* to the model reference data.
- Computing of coefficient matrices of the reduced model with a Galerkin approximation.
- Optimization or *calibration* of the model coefficients to minimize the approximation error.

The necessity of the calibration is shown in recent studies [4]. In this work, the last step is crucial in the model reduction and can not be avoided. >From this point of view, the first two steps can be treated as a computation of an initial point for the calibration process. Results of the reduction procedure are shown by an example of the confined square cylinder wake flow in laminar regimes.

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## Shape optimization in cardiovascular geometries using reduced basis and free-form deformations

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Optimal shape design problems play an important part in structural mechanics and fluid dynamics; however, they require large computational effort and one option to counter this is to use model order reduction. Reduced Basis methods (RB) coupled with a suitable tool for shape parametrization are a very promising tool in flow control and shape optimization problems. An implementation of the reduced basis method for the resolution of viscous interior flows in parameterized geometries is presented. We discuss some applications based on Free-Form Deformation (FFD) techniques [1] for the reduction of the number of parameters, combined with reduced basis methods for the reduction of the dimension of the parameterized PDE system compared with the one obtained with finite element methods (FEM).

The proposed approach includes two different types of model reduction: a geometric reduction resulting from a suitable low-dimensional parameterization of the geometry and a linear system reduction by using RB methods [2, 3, 4] to solve the partial differential equations. In particular, we focus on the possibility of handling very generic geometric parameterizations and solving the problem efficiently, taking advantage of an offline-online decomposition [3]. For this reason, all problems are treated with the empirical interpolation method [5]. We present in particular some examples of reduced basis methods applied to steady incompressible Stokes equations for shape optimization problems in cardiovascular modelling.

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# A Matlab-Toolbox for Parametric Reduction of Multi-Field FE-Models

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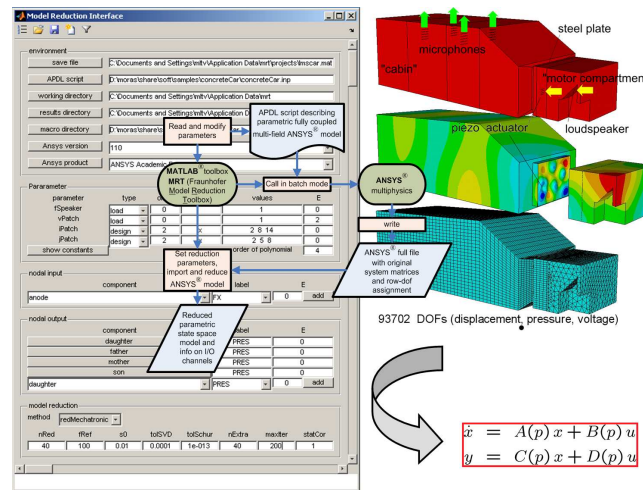


Figure 1: Illustration of the Fraunhofer parametric model reduction toolbox.

Up to now there seems to be no software package covering all aspects of designing mechatronic systems for active noise and vibration control: on the one hand coupled FE models of structure, aero acoustics, or piezo actuators, and on the other hand DAE's describing electronic components or methods for controller design and parametric optimization. Therefore, we have developed a toolbox which enables engineers to transfer and reduce automatically linear multi-field ANSYS models into parametric Matlab state space models. Note that the considered FE models are, in general, characterized by large non-symmetric and singular matrices due to fluid-structure coupling or neglecting piezo inductance. Hence, neither the built in model reduction of ANSYS can be applied, which is restricted to symmetric systems with proportional damping, nor the one of Matlab, which requires small full storage systems. Therefore, we implemented a modal reduction for singular non-symmetric systems.

The other focus of the article will be on parametric model reduction. Fitting models to measurements or optimizing designs requires parameterized models allowing fast evaluation. Common approaches rely on expansions of the full system matrices with respect to the parameters. However, this requires FE-meshes to be smoothly deformable into each other, which is a hard restriction for more realistic geometries. Alternatively, transfer functions can be interpolated rather than system matrices. This gives good results away from poles, but fails close to them. Therefore, we follow another approach: models are reduced independently to systems with standardized structure and size and interpolated only on this level. The main result is related to finding system realizations suitable for interpolation. It is motivated why realizations for new parameter sets should be chosen as close as possible to some reference realization. The corresponding similarity transform is found by solving a generalized Lyapunov equation. Results are illustrated by applying the toolbox to some benchmark problems, e.g. finding optimal positions of piezo patches for active noise reduction.

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## An Error Bound for Linear Spline Interpolation Based Parametric Model Reduction

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Large dynamical systems whose behavior depend on a small number of parameters occur in various fields of application. They may be design parameters in the design of micro-electronic-mechanical systems for instance and very many simulations have to be performed varying these parameters. If reduced models are needed for the simulations it is crucial to preserve the parameters in the reduced model. One possible approach consists in reducing the original system for certain (few) parameters points and receive a global reduced system by interpolation. Here we consider linear time invariant systems depending on one parameter in an interval and suggest a linear spline interpolation based reduction. The reduced system is asymptotically stable for all parameters, if this holds for the reduced systems at the given points. An error bound for the global system is presented, which only requires a Lipschitz condition for the parameter.

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## Adaptivity and aspects of implementation for the reduced basis method applied to parametrized evolution equations

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In this presentation we are going to discuss two issues concerning efficient reduced basis methods for parametrized evolution equations [1]. The first issue is a methodological aspect and aims at adaptivity in both the offline phase and the online phase in order to obtain accelerations over corresponding non-adaptive approaches. In the offline phase, a compact reduced basis can be constructed by a greedy search using adaptive grids in parameter space and incremental training set extension with overfitting control [2]. In the online phase, the model dimension can be adjusted over time according to the solution complexity [3]. Both adaptive approaches considerably rely on the availability of a posteriori error estimators that can be computed efficiently.

The second issue concerns implementational questions that are related to coupling the reduced basis library RBmatlab [6] with available Finite Element, or Finite Volume libraries. In particular, we present an abstract interface for such coupling with the numerical software environment DUNE and the module DUNE-FEM [4, 5].

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# On Dominant Poles and Model Reduction of Time-Delay Systems

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Time-delay systems (TDS's) appear in a wide variety of problems (e.g. the electronic signal of the control of a robot [3]). There is a tendency to analyze and design systems of ever increasing size. Large scale models are more difficult to analyze. As a result it is also harder to develop control algorithms. Model order reduction (MOR) is of great importance since it reduces the size of the model while keeping most of its characteristics. The dominant pole algorithm (DPA) has proven to be an efficient tool for reducing the computational complexity of the solution of ODE's arising from large interconnected electrical networks [2]. We introduce the dominant pole algorithm as a new MOR method for TDS's.

Consider the TDS,

$$\Sigma = \begin{cases} \dot{\mathbf{x}}(t) &= \mathbf{A}_0 \mathbf{x}(t) + \mathbf{A}_1 \mathbf{x}(t - \tau) + \mathbf{b}u(t) \\ y(t) &= \mathbf{c}^* \mathbf{x}(t) + du(t), \end{cases} \quad (1)$$

where  $\mathbf{A}_0, \mathbf{A}_1 \in \mathbb{R}^{n \times n}$ ,  $\mathbf{b}, \mathbf{c}, \mathbf{x}(t) \in \mathbb{R}^{n \times 1}$ ,  $d, y(t) \in \mathbb{R}$  and where  $\tau \geq 0$  is the delay and  $n$  is the dimension of the system. The idea of MOR is to approximate  $\Sigma$  by  $\tilde{\Sigma}$  with dimension  $k \ll n$ . The transfer function of the system (1) is

$$H(s) = \mathbf{c}^*(s\mathbf{I} - \mathbf{A}_0 - \mathbf{A}_1 e^{-s\tau})^{-1} \mathbf{b} + d.$$

If all eigenvalues are simple then  $H$  can be expressed as,

$$H(s) = \sum_{i=1}^{\infty} \frac{R_i}{s - \lambda_i}. \quad (2)$$

It turns out that the residues  $R_i$  in (2) can be computed from the right and left eigenvectors,  $\mathbf{x}_i, \mathbf{y}_i$  respectively, as

$$R_i = \frac{(\mathbf{c}^* \mathbf{x}_i)(\mathbf{y}_i^* \mathbf{b})}{\mathbf{y}_i^* (\mathbf{I} + \lambda_i \tau \mathbf{I} - \tau \mathbf{A}_0) \mathbf{x}_i}, \quad (3)$$

where  $\lambda_i$  is the corresponding eigenvalue. Unlike the ODE case,  $\Sigma$  has no finite dimension linearization and the proof of (3) relies on a more general theory [1]. Using this result, we can adapt the dominant pole algorithm (DPA) to TDSs. We will present the theory for DPA for delay systems, develop an algorithm and show numerical results for an academic example.

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