Contents

Keynote Presentations ................................................. 2
Invited Presentations .................................................. 8
Contributed Presentations ............................................. 17
Poster Presentations ..................................................... 36
Keynote Presentations
# List of Keynote Presentations

<table>
<thead>
<tr>
<th>Title</th>
<th>Presenter</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model Order Reduction in Data Assimilation</td>
<td>C. A. Beattie</td>
<td>4</td>
</tr>
<tr>
<td>Nonlinear Model Reduction: Discrete Optimality, h-Adaptivity, and Error Surrogates</td>
<td>K. T. Carlberg</td>
<td>5</td>
</tr>
<tr>
<td>Some Issues on Stability, Accuracy and Behavior with Noisy Data Assimilation for EIM/GEIM/PBDW Approaches</td>
<td>Y. Maday</td>
<td>6</td>
</tr>
<tr>
<td>Conditional Mean Embeddings for Reinforcement Learning</td>
<td>J. Shawe-Taylor</td>
<td>7</td>
</tr>
</tbody>
</table>
Model Order Reduction in Data Assimilation

Christopher Beattie

1Virginia Tech, Blacksburg, USA

The prediction and estimation of spatially varying dynamic processes is an important component of weather prediction and ocean modeling. The processes of interest are represented typically by highly complex multiphysics models that are adjusted in response to observations that sample the true process evolution. This adaptation of computational models to accommodate observations of true process evolution is critical in bringing model fidelity up to a level that is required for them to be useful in predictive roles and this constitutes the ’data assimilation’ enterprise. Limited computational resources deployed on large scale computational models coupled to a mass of noisy observations within a context requiring rapid turn-around times creates an acute demand for effective strategies that can reduce the cost of evaluation of the related dynamic models without losing the level of accuracy necessary for mission requirements. The creation of reduced order process models is one response to this demand, yet in the data assimilation context, these process models are used typically to move information both forward and backward in time, complicating the usual notions of model reduction efficiency and optimality.

Variational data assimilation methods depend also on knowledge of the statistical covariance structure of quantities of interest (and its evolution). Typically, this covariance structure is unknown, yet in principle, it may be estimated from the same data that is used to predict or estimate the main quantities of interest. In many cases and especially for nonstationary random processes that commonly occur in atmospheric sciences and oceanography, the available data are too sparse in either space or time to provide reliable estimates, so additional structural features must be assumed and included to bridge the gap. A recent approach to this problem begins with the remarkable observation that two classes of covariance kernels commonly used in spatial statistics, the Gauss and the Matérn classes, may be identified with Green’s functions of differential operators. This interpretation allows for straightforward modeling of anisotropy and nonhomogeneity, through low-order models.

I will discuss these ways and some others in which systematic model order reduction methods can contribute to variational and ensemble-based data assimilation methods together with limitations seen in the current state-of-the-art. Some ideas described in this talk derive from collaboration with Volker Mehrmann at TU-Berlin, Peter Benner at MPI-Magdeburg, and Max Yaremchuk at NRL-Stennis.
Nonlinear model reduction:
discrete optimality, $h$-adaptivity, and error surrogates

K. Carlberg$^1$, M. Barone$^1$, H. Antil$^2$, and M. Drohmann$^1$

$^1$Sandia National Laboratories
$^2$George Mason University

Large-scale models of nonlinear dynamical systems arise in applications ranging from compressible fluid dynamics to structural dynamics. Due to the large computational cost incurred by these models, it is impractical to use them in time-critical scenarios such as control, design, uncertainty quantification. Model reduction aims to mitigate this computational burden. To date, reduced-order models (ROMs) for relatively simple models (e.g., linear-time-invariant systems; elliptic, parabolic, and linear hyperbolic PDEs) have been widely adopted, as researchers have developed methods that are accurate, reliable, and certified. In contrast, model reduction for nonlinear dynamical systems lacks these assurances and thus remains in its infancy; the most common method—POD–Galerkin—is often unstable.

This talk will describe several advances that have made nonlinear model reduction viable for a new frontier of problems. However, doing so has required fundamentally new data-driven approaches, as the critical tools leveraged for simpler models (e.g., Gramians, coercivity constants) are no longer available. First, I will introduce the notion of least-squares Petrov–Galerkin (LSPG) projection—and the associated GNAT method [3]—which enables accuracy via discrete optimality: it performs optimal projection after the dynamical system has been discretized in time. Comparative theoretical and numerical studies will highlight the benefits of LSPG projection over Galerkin projection [2].

Second, I will introduce a new approach for enabling reliability. This approach—which is a model-reduction analogue of mesh-adaptive $h$-refinement—combines ideas from goal-oriented adaptivity and machine learning [1]. The method enriches the low-dimensional basis by ‘splitting’ a given basis vector into multiple vectors, where the splitting scheme is defined by a tree structure constructed via recursive $k$-means clustering of snapshot data. The method selects vectors to split using a dual-weighted-residual approach. Numerical experiments on advection-dominated problems show that the method enables the ROM to satisfy any prescribed error tolerance without requiring any large-scale operations.

Finally, I will present a new approach for certification. Certification is typically pursued by deriving rigorous error bounds; however, such bounds have limited utility for nonlinear dynamical systems, as they often grow exponentially in time. To address this, we adopted a new perspective: rather than relying on error bounds, one can construct statistical reduced-order-model error surrogates (ROMES) via machine learning [4]. The hope is for a viable path toward certification: while no longer a bound on the error, the error surrogate can provide richer insight by generating a data-driven model that reflects our knowledge of the ROM error. This strategy is viable because ROMs produce inexpensive ‘error indicators’ (e.g., residual norms) that correlate with the ROM error.

References


Some issues on stability, accuracy and behavior with noisy data assimilation for EIM/GEIM/PBDW approaches

Yvon Maday

Sorbonne Universités, UPMC Univ Paris 06, CNRS, UMR 7598, Laboratoire Jacques-Louis Lions, 4, place Jussieu 75005, Paris, France and Institut Universitaire de France and, Division of Applied Mathematics, Brown University, Providence, RI, USA.


EIM (empirical interpolation methods) [1, 8, 3, 2], GEIM (generalized interpolation methods) [5] and PBDW (Parametrized-Background Data-Weak) [9, 4] allow to incorporate data measurements and assimilation in a frame where reduction of complexity approaches hold due to the fact that the functions we want to reconstruct are, for some reason, in a set with small Kolmogorov n-width.

These approaches — that are hierarchical thanks to a possible greedy construction of the basic ingredients — are viable approximation alternatives to best fit obtained by projection on optimal Kolmogorov spaces.

The understanding of the plain stability of these approaches is improving [6, 7] and I will present some of these aspects in this talk. In addition, there are many situations where the data are polluted with noise and some corrections have to be proposed so that these noises do not destroy the quality of the approximations. We shall also present some recent elements in the analysis of noisy data together with various applications of the method in industrial context.

References

Conditional Mean Embeddings for Reinforcement Learning

J. Shawe-Taylor

1University College London

Conditional Mean Embeddings (CME) provide a way of learning to estimate expectations under unknown distributions. We consider their application to learning the system dynamics for Markov Decision Processes (MDPs). This results in a model-based approach to their solution that reduces the planning problem to a finite (pseudo-) MDP exactly solvable by dynamic programming. Unfortunately the size of the finite MDP scales badly with the amount of experience. By approximating the loss function of the CME the size of the induced (pseudo-) MDP can be compressed while maintaining performance guarantees. At the same time the CME model can itself be approximated using a fast sparse-greedy kernel regression. The performance of the composite method compares favourably with the state-of-the-art methods both in accuracy and efficiency.
Invited Presentations
List of Invited Presentations

Improving the Data-Driven Identification of Nonlinearities in a Car Crash Simulation
J. Fehr ................................................................. 10

Operator Based Multi-Scale Analysis of Simulation Bundles
J. Garcke ............................................................... 11

Radial Basis Function Interpolation for Parametric Model Order Reduction
S. Grundel ............................................................. 12

Data-Driven H2-Approximation, Numerical Quadrature and Discretized H2-Minimization
S. Gugercin ............................................................ 13

Dynamic Mode Decomposition, Manifold Learning and Sparsity for Reduced Order Models
J. N. Kutz .............................................................. 14

Reliability and Computational Efficiency in RB Methods for Complex Nonaffine and Nonlinear PDEs
A. Manzoni ............................................................ 15

Gaussian Functional Regression for Model-Data Assimilation
N.-C. Nguyen .......................................................... 16
Improving the Data-driven Identification of Nonlinearities in a Car Crash Simulation

J. Fehr\(^1\) and D. Grunert\(^1\)

\(^1\)Institute of Engineering and Computational Mechanics, University of Stuttgart, [joerg.fehr,dennis.grunert]@itm.uni-stuttgart.de

Unlike several decades ago, hardware crash tests are now commonly substituted by simulations in the development phase of a new car. Usually, thousands of simulations are run for only one car to ensure its crash safety after changes in the model. Combined with detailed finite element (FE) models, this leads to a high demand of computing power and long response time for the design engineer. These problems can be solved by applying model order reduction (MOR) to the underlying system, i.e., substituting it by a smaller system with preferably low approximation error.

In structural mechanics, linear model order reduction is applied for a long time and well understood. Small reduction errors and large acceleration of the simulation can be achieved with, e.g., modal reduction, Krylov methods or techniques based on SVD or Gramian matrices. While this is true for mechanical systems with small deformations, it is certainly not the case in a crash test simulation with large deformations, nonlinear material behavior and complex contact scenarios leading to nonlinear differential equations. Unfortunately, nonlinear reduction techniques are not yet as mature and can be found rarely in industrial applications. Therefore, one aim is the improvement of nonlinear reduction techniques in the field of crash test simulations.

Before using nonlinear MOR for the complete car model, it is beneficial to separate it in parts which can be considered to behave linear and on the other hand parts considered to behave nonlinear. Linear respectively nonlinear methods can then be applied accordingly, cf. [2]. Since our workflow should be easily applicable in the industry, we use the widely-used FE program LS-DYNA to simulate the crash. Unfortunately, it is not only feature-rich but closed-source, therefore, the underlying, nonlinear differential equations are not visible to the user. Thus, only heuristic identification remains. In [1], clustering algorithms were used to identify similar behaving parts of the car within a set of simulation runs. This approach was adopted to our use case and improved after some problems were identified.

First we define measures for scattering, defined as difference between several simulation runs with small parameter variations, and deformation, which both are indicators for nonlinear behavior. The measures allow to quantify these properties and judge the quality of the separation not only by engineering experience. They are also used as new input for the clustering algorithms ensuring that the clusters correspond to the desired separation. Furthermore, the rigid body movement is eliminated with the help of a reference node located in an undeformed part. It can be shown that most of the time clustering algorithms can be accelerated by simpler approaches. All these improvements contribute to a better separation in parts which corresponds to the experience of engineers. The 2001 Ford Taurus model of the National Crash Analysis Center serves as an example.

References


Operator Based Multi-Scale Analysis of Simulation Bundles

Garcke, Jochen¹ and Iza-Teran, Rodrigo²

¹University of Bonn / Fraunhofer SCAI
²Fraunhofer SCAI

We propose a new mathematical data analysis approach, which is based on the mathematical principle of symmetry, for the post-processing of bundles of finite element data from computer-aided engineering. Since all those numerical simulation data stem from the numerical solution of the same partial differential equation, there exists a set of transformations, albeit unknown, which map simulation to simulation. The transformations can be obtained indirectly by constructing a transformation invariant positive definitive operator valid for all simulations.

The eigenbasis of such an operator turns out to be a convenient basis for the handled simulation set due to two reasons. First, the spectral coefficients decay very fast, depending on the smoothness of the function being represented, and therefore a reduced multi-scale representation of all simulations can be obtained, which depends on the employed operator. Second, at each level of the eigendecomposition the eigenvectors can be seen to recover different independent variation modes like rotation, translation or local deformation. Furthermore, this representation enables the definition of a new distance measure between simulations using the spectral coefficients. From a theoretical point of view the space of simulations modulo a transformation group can be expressed conveniently using the operator eigenbasis as orbits in the quotient space with respect to a specific transformation group.

Based on this mathematical framework we study several examples. We show that for time dependent datasets from engineering simulations only a few spectral coefficients are necessary to describe the data variability, while the coarse variations get separated from the finer ones. Low dimensional structures are computed in this way, which are able to capture information about the underlying simulation space. Overall, due to the achieved dimensionality reduction, a mechanism to efficiently deal with the analysis of many numerical simulations is obtained.
Radial Basis Function Interpolation for Parametric Model Order Reduction

Sara Grundel\textsuperscript{1}, Nils Hornung\textsuperscript{1}, and Peter Benner\textsuperscript{2}

\textsuperscript{1}Max Planck Institute for Dynamics of Complex Technical Systems
\textsuperscript{2}Fraunhofer SCAI Bonn

Parametric Model Order Reduction is now an established field of research. We present an approach to create linear parametric reduced order models using $\mathcal{H}_2$-optimality interpolation together with information generated by measurements \cite{BennerGrundel2015}. In a parametric system these optimal interpolation points are nontrivial functions, depending on the parameter. If $r$ is the size of the reduced order model, we will have $r$ such functions. They behave similarly to eigenvalues of parametric matrices. Creating metamodels for these optimal interpolation points will be discussed in detail, and further, the efficient creation of reduced order models \cite{BennerGrundelHornung2015}. This will be illustrated by several numerical examples.

References


Data-driven H2-Approximation, Numerical Quadrature and Discretized H2-Minimization

S. Gugercin

1Department of Mathematics, Virginia Polytechnic Institute and State University, 460 McBryde, Virginia Tech, Blacksburg

Iterative Rational Krylov Algorithm (IRKA) of Gugercin et al. [2008] is an effective tool for optimal rational approximation in the H2 norm. The original formulation of IRKA uses the projection-framework; thus requires access to internal system dynamics. Using the data-driven Loewner-framework of Mayo and Antoulas [2007], Beattie and Gugercin [2012] has recently developed a data-driven formulation of IRKA that only uses transfer function evaluations, without requiring access to internal dynamics. This extended IRKA to H2 approximation of irrational, infinite-dimensional dynamical systems. The need to update the interpolation points during the iteration requires repeated transfer function evaluations at every iteration step. In this talk, we will present a quadrature-based formulation of IRKA where a number of transfer function evaluation are computed only at the beginning (the offline phase) and the IRKA steps (the online phase) never revisit the original transfer function, performing all the computations in the reduced order dimension. We will also investigate how a data-driven discretized-H2 approximation can lead to effective rational approximations and provide good initialization strategies for optimal H2 approximation.
Dynamic Mode Decomposition, Manifold Learning and Sparsity for Reduced Order Models

J. Nathan Kutz\textsuperscript{1}, Alessandro Alla\textsuperscript{2}, S. Sargsyan\textsuperscript{1}, and Steven L. Brunton\textsuperscript{3}

\textsuperscript{1}Department of Applied Mathematics, University of Washington, Seattle, WA 98195
\textsuperscript{2}Department of Mathematics, University of Hamburg, Hamburg, Germany
\textsuperscript{3}Department of Mechanical Engineering, University of Washington, Seattle, WA 98195

Machine learning strategies, which are often rooted in dimensionality reduction techniques, are beginning to play a transformative role in the sciences. They have also been recently advocated in model reduction methods as they provide a natural mathematical framework for building off-line libraries of dynamically relevant POD modes for use in online computation. We develop two innovations aimed at producing more efficient ROM reductions. First, we demonstrate a sparse sampling technique capable of optimally classifying a dynamic regime from learned POD libraries. The selected sampling points are shown to be effective sensing/measurement locations for characterizing the underlying dynamics, stability, and bifurcations of nonlinear dynamical systems. This work builds upon the greedy algorithm associated with the discrete empirical interpolation method (DEIM) and the sparse representation that facilitates a family of local reduced-order models for each physical regime. Indeed, the method advocated allows one to optimize for both the error in reconstructing the nonlinear terms of a ROM while still correctly performing a classification task for library mode selection. Additionally, as an alternative to the standard EIM/DEIM architecture, we propose using the recently developed Dynamic Mode Decomposition (DMD) for producing low-rank approximations of the PDE nonlinearities. We demonstrate that the POD-DMD method is even more numerically efficient than the standard POD-DEIM method for producing viable ROMs. DMD provides a decomposition of data into spatio-temporal modes that correlates the data across spatial features (like POD), but also pins the correlated data to unique temporal Fourier modes. More precisely, DMD computes a regression of the sampled data to a best fit (least-squares) linear, constant-coefficient, system of differential equations. This spatio-temporal regression allows us to directly project the nonlinear terms in the PDE to its best-fit time dynamics. Like EIM/DEIM, it requires a singular value decomposition to generate the approximation. At its core, the DMD method can be thought of as an ideal combination of spatial dimensionality-reduction techniques, such as POD, with Fourier Transforms in time. It also allows for further innovations that integrate the DMD with key concepts from wavelet theory, multi-resolution analysis and sparsity/compression. Moreover, the DMD is shown to have a strong connection to Koopman theory, which is one of the earliest examples of manifold learning. Thus the DMD/Koopman theory applied in a model reduction context is like a nonlinear manifold learning task of machine learning for discovering the nonlinear embeddings of dynamical systems.
Reliability and computational efficiency in RB methods for complex nonaffine and nonlinear PDEs

A. Manzoni

CMCS MATHICSE - Ecole Polytechnique Fédérale de Lausanne

Reduced basis (RB) methods represent a very efficient approach for the numerical approximation of problems involving the repeated solution of differential equations arising from engineering and applied sciences [3]. Noteworthy examples include partial differential equations (PDEs) depending on several parameters, PDE-constrained optimization, and optimal control and inverse problems. When dealing with these cases – and more in general with complex nonaffine and/or nonlinear problems – several challenges have to be faced to ensure reliability and computational efficiency of the RB method.

As regards reliability, we propose some heuristic approaches to approximate the stability factor of parameterized (linear and) nonlinear PDEs, a key ingredient of any a posteriori error estimate [1]. The evaluation of stability factors is a computational bottleneck whenever a posteriori error estimates have to be rapidly evaluated – this occurs e.g. when a greedy algorithm is used to build a RB space.

Concerning computational efficiency, we show how to exploit a Matrix Discrete Empirical Interpolation Method (MDEIM) to recover in a non-intrusive, efficient and purely algebraic way an affine decomposition of the PDE operators [2]. This latter is mandatory to assemble the RB problem in an inexpensive way, without relying on arrays whose dimension is related to the high-fidelity problem. Moreover, we also show how to take advantage of MDEIM in order to efficiently build those structure of the RB problem which are related to (possibly, nonpolynomial) nonlinearities. Once MDEIM has been performed, a state approximation resulting either from a proper orthogonal decomposition or a greedy approach can be performed in a less expensive way.

The efficacy of the proposed methods is demonstrated on a variety of computationally-intensive problems occurring in engineering contexts, namely parameter-dependent fluid and structural dynamics problems, PDE-constrained shape optimization, parametrized coupled problems.

References


Gaussian Functional Regression for Model-Data Assimilation

C. Nguyen \(^1\) and J. Peraire\(^1\)

\(^1\)Massachusetts Institute of Technology

We introduce a Gaussian functional regression (GFR) technique [1, 2] that integrates multi-fidelity models with model reduction to efficiently predict the input–output relationship of a high-fidelity model. The GFR method combines the high-fidelity model with a low-fidelity model to provide an estimate of the output of the high-fidelity model in the form of a posterior distribution that can characterize uncertainty in the prediction. A reduced basis approximation is constructed upon the low-fidelity model and incorporated into the GFR method to yield an inexpensive posterior distribution of the output estimate. As this posterior distribution depends crucially on a set of training inputs at which the high-fidelity model are simulated, we develop a greedy sampling algorithm to select the training inputs. Our approach results in an output prediction model that inherits the fidelity of the high-fidelity model and has the computational complexity of the reduced basis approximation. Numerical results are presented to demonstrate the proposed approach.

References


List of Contributed Presentations

<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>On Probabilistic Transformations and Optimal Sampling Rules for Emulator Based inverse Uncertainty Quantification Problems</td>
<td>19</td>
</tr>
<tr>
<td>Causality Verification for Data-Driven Macromodeling</td>
<td>20</td>
</tr>
<tr>
<td>Kernel Methods for the Model Reduction of Nonlinear Control Systems</td>
<td>21</td>
</tr>
<tr>
<td>Model Reduction from Partial Observations</td>
<td>22</td>
</tr>
<tr>
<td>The Distributed Empirical Cross Gramian</td>
<td>23</td>
</tr>
<tr>
<td>Energy Stable Model Order Reduction for Gradient Systems</td>
<td>24</td>
</tr>
<tr>
<td>System Identification and Model Reduction for MIMO Systems via the Eigensystem Realization Algorithm</td>
<td>25</td>
</tr>
<tr>
<td>Neural Network Training Using Reduced Basis Approximation</td>
<td>26</td>
</tr>
<tr>
<td>Model Reduction for Convection-Diffusion Problems</td>
<td>27</td>
</tr>
<tr>
<td>Analysis of the Stability and Accuracy of Discrete Least Squares on Multivariate Polynomial Spaces with Evaluations at Random or Low-Discrepancy Point Sets</td>
<td>28</td>
</tr>
<tr>
<td>Model Order Reduction of Dynamic Skeletal Muscle Models</td>
<td>29</td>
</tr>
<tr>
<td>A Reduced-Order Strategy for Efficient State/Parameter Identification in Cardiac Electrophysiology</td>
<td>30</td>
</tr>
<tr>
<td>Minimum Residual Based Model Order Reduction Approach for Unsteady Nonlinear Aerodynamic Problems</td>
<td>31</td>
</tr>
<tr>
<td>Structure-Preserving Data-Driven Interpolation of Dynamical Systems</td>
<td>32</td>
</tr>
<tr>
<td>A Model Reduction Approach to Structural Health Monitoring</td>
<td>33</td>
</tr>
<tr>
<td>A Hybrid Ensemble Approach to the Adjoint-Free Data Assimilation into Geophysical Flows</td>
<td>34</td>
</tr>
<tr>
<td>On the Notion of Distance in Data-Driven Manifold Learning and Surrogate Modeling</td>
<td>35</td>
</tr>
</tbody>
</table>
On probabilistic transformations and optimal sampling rules for emulator based inverse uncertainty quantification problems

F. Franzelin¹, J. Jakeman², and D. Pflüger¹

¹University of Stuttgart, Germany
²Sandia National Laboratories, USA

December 15, 2015

The generalized polynomial chaos expansion (gPCE) [7] is a very attractive technique for uncertainty quantification. However, it assumes model inputs that are independent random variables. For non-independent random variables the basis polynomials of the gPCE are no longer orthogonal to the probability density, which decreases the efficiency of all PCE based methods. Moreover, they are not even applicable for data-driven problems, which arise in the context of data assimilation. A common way to overcome these issues are isoprobabilistic transformations, at least theoretically.

This talk will discuss isoprobabilistic transformations such as the Nataf [3] and the Rosenblatt transformation [5] that decorrelate random variables for improving the efficiency of emulator based Bayesian inverse problems. We will present numerical studies that demonstrate the effectiveness of these transformations and present some alternatives such as Leja sequences [1, 2, 4] in combination with arbitrary polynomial chaos expansion [6].

References


Causality Verification for Data-Driven Macromodeling

S. Grivet-Talocia\textsuperscript{1} and M. Bandinu\textsuperscript{2}

\textsuperscript{1}Dept. Electronics and Telecommunications, Politecnico di Torino, Italy
\textsuperscript{2}IdemWorks s.r.l., Torino, Italy

The automated design and verification of electronic systems relies on accurate and robust models of components, interconnects, and subsystems. In particular, Signal and Power Integrity verification requires low-complexity models for the numerical prediction of performance degradation effects due to parasitic couplings, near-field electromagnetic interaction, and non-ideal behavior of components and materials. These models, which are often derived from tabulated frequency responses obtained by direct measurements or commercial electromagnetic solvers, should be cast in state-space form or as equivalent circuit netlists, for enabling system-level verification based on standard circuit or ODE solvers.

This contribution considers the standard problem of identifying a reduced-order model with transfer function $H(s) = C(sE - A)^{-1}B + D$, where $\{E, A, B, C, D\}$ is a suitable (generalized) state-space realization, starting from a finite number of samples of the frequency response $\hat{H}_k$ available at frequencies $s_k = j\omega_k$, with $k = 1, \ldots, K$. Several reliable methods exist for this task, including Vector Fitting\textsuperscript{2} or Loewner approaches\textsuperscript{3}. When dealing with passive structures, such algorithms should be complemented by passivity verification and enforcement to ensure unconditional stability in subsequent transient simulation. An overview of passive macromodeling techniques is available in\textsuperscript{1}.

There are some situations where all these methods will fail. We discuss the possible reasons for such failures, and we review the various algorithms that can be used to predict them. A frequent scenario is encountered when the available frequency samples are affected by some hidden non-causal components, which may result from measurement errors or noise, as well as from inappropriate setup or usage of electromagnetic solvers. Causality, intended as compliance with a suitable set of dispersion relations\textsuperscript{5, 4}, is a fundamental prerequisite for successful extraction of a stable and passive model. Causality verification is in fact very challenging when a finite number of frequency samples is available, due to truncation and discretization errors that inevitably affect the numerical verification of dispersion relations. In addition, more subtle checks are required to verify that the sampling density of the raw data is sufficient for the extraction of a physically meaningful model. This contribution will show how robust and reliable data consistency checks can be performed, by comparing alternative approaches based on direct dispersion relation verification and stable/unstable rational approximation.

References

Kernel Methods for the Model Reduction of Nonlinear Control Systems

Dr. Hamzi, Boumediene\textsuperscript{1} and Dr. Bouvrie, Jake\textsuperscript{2}

\textsuperscript{1}AlFaisal University
\textsuperscript{2}MIT

We introduce a data-driven order reduction method for nonlinear control systems, drawing on recent progress in machine learning and statistical dimensionality reduction. The method rests on the assumption that the nonlinear system behaves linearly when lifted into a high (or infinite) dimensional feature space where balanced truncation may be carried out implicitly. This leads to a nonlinear reduction map which can be combined with a representation of the system belonging to a reproducing kernel Hilbert space to give a closed, reduced order dynamical system which captures the essential input-output characteristics of the original model. Empirical simulations illustrating the approach are also provided.
Model Reduction from Partial Observations

C. Herzet\(^1\) and P. Heas\(^1\)

\(^1\)Institut National de Recherche en Informatique, 35000 Rennes, France

Our contribution takes place in the context of model reduction for parametric partial differential equation:

\[
PDE(u, \mu) = 0, \tag{1}
\]

where \(u\) belongs to an Hilbert space \(\mathcal{H}\) (with inner product \((\cdot, \cdot)\) and induced norm \(\| \cdot \|\)) and \(\mu \in \mathcal{P}\) is a parameter. When the solution \(u(\mu)\) of (1) has to be evaluated for many different values \(\mu \in \mathcal{P}\), the computational cost may become prohibitive. To circumvent this issue, model reduction intends to simplify the resolution of (1) by constraining \(u\) to belong to some low-dimensional subspace \(S\). The choice of \(S\) should be made so that all the elements of the solution manifold \(\mathcal{M} = \{u(\mu) \in \mathcal{H} : \mu \in \mathcal{P}\}\) are well-approximated by some element in \(S\). Many techniques have been proposed in the literature to identify such subspaces: reduced basis \(^3\), POD \(^1\), etc. However, all these methods presuppose the knowledge of the solution manifold \(\mathcal{M}\) (or the parameter set \(\mathcal{P}\)) although the latter may not always be available. On the other hand, since the advent of numerical acquisition, it has become quite common to have (incomplete) measurements of the elements of \(\mathcal{M}\) at our disposal. In this work, we thus address the following question: can we build a good approximation subspace for \(\mathcal{M}\) by exploiting these measurements?

More formally, the setup considered in our work is as follows. We assume that: \(i)\) for each \(u \in \mathcal{M}\), we collect a set of observations \(\{w_i, u\}_{i=1}^m\), where \(\{w_i\}_{i=1}^m\) is an orthogonal basis of some subspace \(W\); \(ii)\) we have a “rough” prior knowledge of \(\mathcal{M}\), that is we are given some \(\hat{\Sigma}\) such that \(\mathcal{M} \subseteq \hat{\Sigma}\). We assume that \(\hat{\Sigma} = \{u : \text{dist}(u, V) \leq \epsilon\}\) for some \(\epsilon \geq 0\) and \(n\)-dimensional subspace \(V\). We address the two following questions: \(i)\) how can we combine the observations \(\{w_i, u\}_{i=1}^m\) and the prior \(\hat{\Sigma}\) to derive a “good” approximation subspace for \(\mathcal{M}\)? \(ii)\) can we derive guarantees on the quality of this approximation subspace?

The first question has a simple (theoretical) answer. Letting \(\Sigma_{\text{post}} \triangleq \bigcup_{u \in \mathcal{M}} (\hat{\Sigma} \cap H_u)\), with \(H_u = \{u' : (w_i, u') = (w_i, u)\text{ for }i = 1, \ldots, m\}\), it can be seen that \(S^* = \arg\min_{S, \dim(S) = j} \max_{u \in \Sigma_{\text{post}}} \text{dist}(u, S)\) is the best \(j\)-dimensional approximation subspace for \(\mathcal{M}\) from a “worst-case” perspective. As for the second question, we provide an upper bound on the approximation quality achieved by \(S^*\) by elaborating on the recent results by Binev et al. \(^2\). More specifically, assuming that \(\mathcal{M} \subseteq \{u : \text{dist}(u, U) \leq \epsilon'\}\) where \(0 \leq \epsilon' \leq \epsilon\) and \(U \subseteq V\) is a \(k\)-dimensional subspace, we show that

\[
\max_{u \in \mathcal{M}} \text{dist}(u, S^*) \leq C_j \epsilon', \tag{2}
\]

for some constant \(C_j \geq 1\). The value of \(C_j\) is related to the singular values of the projection operator from \(V\) to \(W\). In particular, when \(V\) and \(W\) obey some simple non-degeneracy conditions, we have \(C_j < \infty\) for \(j \geq k\). This shows that, under a proper choice of \(V\) and \(W\), one can essentially achieve the same reduction performance (up to some constant factor) as in the fully informed setup.

References


The Distributed Empirical Cross Gramian

C. Himpe¹, M. Ohlberger¹, and S. Rave¹

¹University of Münster

A well known projection-based model reduction technique for input-output systems is balanced truncation, which utilizes the controllability and observability gramians to determine the states with the least input-output coherence of the underlying system. The related, approximately balancing direct truncation method is based on the cross gramian [1], a linear operator that combines controllability and observability information.

The system gramians can be computed as solutions to matrix equations or alternatively, empirically in a data-driven manner. These empirical gramians broaden the scope of gramian-based model reduction to nonlinear systems [3]. Additionally, the empirical cross gramian can also encode parameter identifiability information [2].

However, the empirical gramians are dense matrices, and may be numerically challenging to assemble for large-scale systems. To overcome this limitation, a partitioned variant of the empirical cross gramian method is presented, which allows a separate assembly of the partitions. Due to the self-contained construction, this distributed empirical cross gramian can be parallelized efficiently on a distributed memory system.

To obtain a truncated approximate balancing projection from this distributed empirical cross gramian, a distributed singular value decomposition maintains the isolated partitioning. This procedure is demonstrated to yield a reduced order model, assembled in parallel with minimal communication.

References


Energy stable model order reduction for gradient systems

Bülent Karasözen\textsuperscript{1} and Murat Uzunca\textsuperscript{2}

\textsuperscript{1,2}Department of Mathematics \& Institute of Applied Mathematics, Middle East Technical University, 06800, Ankara, Turkey

It is well known that Allen-Cahn and Schlögel(nagumo) equations are gradient systems, where the free-energy functional decreases monotonically in time. In this talk, we present energy stable reduced order modeling for gradient systems, which inherits the energy decreasing property of the full order model (FOM). The equations are discretized in space by discontinuous Galerkin (dG) method and in time by second order unconditionally stable average vector field (AVF) method. For an efficient computation of the nonlinear terms as variational derivatives of the quartic and logarithmic free energy, we apply the proper orthogonal decomposition (POD) with greedy discrete empirical interpolation (DEIM). For affine parameterized gradient systems, we construct reduced order models (ROMs) with the POD greedy adaptive sampling strategy of the snapshots in time, by selecting the parameters as the interfacial length for the Allen Cahn equation, and as the diffusion coefficient for the Schlögel equation. We show that the FOMs and ROMs preserve the energy decreasing property of both equations. The computational efficiency and accuracy of the reduced solutions are demonstrated numerically for Allen-Cahn and Schlögel equations.
Subspace based system identification provides a framework to determine state space representations of dynamical systems from experimental or synthetic data. The Eigensystem Realization Algorithm (ERA) [1] is a commonly used data-driven method for the joint task of system identification and reduced-order modeling, and has been used in the engineering community for almost four decades [2]. The algorithm produces system matrices $A, B, C, D$ in a numerically stable way and retains stability.

The main computational difficulty in ERA arises when the system under consideration has a large number of inputs and outputs, requiring to compute an SVD of a large-scale dense Hankel matrix. In this talk, we present an algorithm that aims to resolve this computational bottleneck via tangential interpolation. This involves projecting the original impulse response sequence onto suitably chosen directions. The resulting data-driven reduced-model preserves stability and is endowed with an a priori error bound. Numerical examples demonstrate that the modified ERA algorithm with tangentially interpolated data produces accurate reduced models while, at the same time, reducing the computational cost and memory requirements significantly compared to the standard ERA. We also give an example to demonstrate the limitations of the proposed method and the standard ERA in general.

References


Neural Network Training Using Reduced Basis Approximation

O. Kunc¹ and F. Fritzen¹

¹Institute of Applied Mechanics (CE), University of Stuttgart

Neural networks (NN) are gaining significance in modern computational sciences [2]. The key advantage of neural networks are their high numerical performance and the possibility to parallelize the operations on neuron/perceptron level in a rather straightforward way. Additionally, neural networks allow the processing of data with little a priori knowledge of the resulting model while they can still produce reliable yet rapid models. In the past neural networks have been applied massively in pattern recognition, characterization and in finance to mention only a few applications.

We propose the use of neural networks in order to provide an efficient computer assisted homogenization scheme for the prediction of the mechanical response of strongly nonlinear solid materials, cf., e.g., [4]. A three-dimensional nonlinear finite element problem of a microstructured solid is considered. We investigate the effective response of the reference volume element. The material law under consideration is assumed hyperelastic for now, but extensions towards dissipative (i.e. path-dependent) materials are also planned, cf. [1]. In the hyperelastic case the effective material is also hyperelastic. Hence, a parameterization of the effective strain energy and of its first and second gradient with respect to the six independent components of the macroscopic strain tensor is sought-after. More precisely six inputs (the macroscopic strains) and six outputs (the resulting effective stress tensor) have to be related to each other. While this task appears to be rather straightforward, the complication is found in the training of the neural network: for each pair of input/output vectors, a nonlinear finite element simulation involving thousands of degrees of freedom is required. While a couple of these simulations can be realized at a reasonable computational expense, the amount of feasible training simulations is still limited, e.g., to a few dozen computations in total. In order to provide more reliable training data, we suggest to feed the neural network by a reduced order model (ROM), cf., e.g., [3]. The ROM itself is trained by means of few finite element simulations with systematically chosen boundary conditions. Thereby a two-stage OFFLINE/ONLINE decomposition is achieved: first, the finite element model is used to provide the input data for the ROM. The reduced order model is then used ONLINE in order to generate thousands of data points. These are then used in order to train the neural network, i.e., the ONLINE ROM calculations represent the OFFLINE stage of the neural network. First results for highly nonlinear solids are anticipated.

References

Model reduction for convection-diffusion problems

Guanglian Li\(^\dagger\) and Daniel Peterseim\(^\dagger\)

\(^\dagger\)Institute for Numerical Simulation, University of Bonn

We consider convection-diffusion equations of the form,

\[
-\epsilon \Delta u + b \cdot \nabla u = f \text{ in } \Omega,
\]
\[
u = g, \text{ on } \partial \Omega,
\]

where \(\Omega\) is a regular domain in \(\mathbb{R}^d\), \(\epsilon(0 < \epsilon \leq 1)\) is the molecular diffusivity characterizing the Brownian motion, \(b(x)\) is the given velocity field, \(f \in L^2(\Omega)\) is the forcing and \(g \in H^\frac{1}{2}(\partial \Omega)\) is the boundary condition. We assume that the velocity field \(b(x)\) is incompressible, i.e., \(\nabla \cdot b(x) = 0\). We are interested in the convection-dominant case with large Peclet number \(\text{Pe} = \frac{\|b(x)\|_{L^{\infty}(\Omega)}}{\epsilon}\). Our method is based on Localized Orthogonal Decomposition Method (LOD) [1].

References

Analysis of the stability and accuracy of discrete least squares on multivariate polynomial spaces with evaluations at random or low-discrepancy point sets

G. Migliorati

1Laboratoire Jacques-Louis Lions, UPMC Univ Paris 6, France

We review the main results achieved in the analysis of the stability and accuracy of the discrete least-squares approximation on multivariate polynomial spaces, with noiseless evaluations at random points [1], with noisy evaluations at random points [3], or with evaluations at low-discrepancy point sets [2].

References


Model order reduction of dynamic skeletal muscle models

M. Mordhorst\textsuperscript{1,2}, D. Wirtz\textsuperscript{1,2}, and O. Röhrle\textsuperscript{1,2}

\textsuperscript{1}University of Stuttgart, Institute of Applied Mechanics (CE), Germany
\textsuperscript{2}Stuttgart Research Centre for Simulation Technology, Germany

December 15, 2015

Forward-dynamics simulations of three-dimensional continuum-mechanical skeletal muscle models are a complex and computationally expensive problem. The governing equations yield a nonlinear second-order differential algebraic equation (DAE), which represents a challenge to model order reduction techniques.

In detail, the governing equations describe the motion and deformation of a continuous muscle, whose shape corresponds to the reference domain $\Omega_0 \subset \mathbb{R}^3$, over time by means of the balance of momentum, which is subject to the incompressibility constraint

$$
\rho_0(\mathbf{X}) \frac{\partial \mathbf{v}}{\partial t}(\mathbf{X}, t) = \nabla \cdot \mathbf{P}(\mathbf{X}, t) + \mathbf{B}(\mathbf{X}, t), \quad \text{s.t.} \quad J(\mathbf{X}, t) - 1 = 0, \quad \forall \mathbf{X} \in \Omega_0, \quad (1)
$$

and a nonlinear constitutive equation of the form

$$
\mathbf{P}(\mathbf{X}, t) = \mathbf{P}^{\text{iso}}(\mathbf{X}, t) + \mathbf{P}^{\text{oniso}}(\mathbf{X}, t) + \mathbf{P}^{\text{active}}(\mathbf{X}, t) + \mathbf{P}^{\text{viscous}}(\mathbf{X}, t) + p(\mathbf{X}, t) \mathbf{F}^{-T}(\mathbf{X}, t). \quad (2)
$$

Therein, $\rho_0$ is the muscle density, $\mathbf{v}$ is the velocity field, $\mathbf{P}$ is the first Piola-Kirchhoff stress tensor, $\mathbf{B}$ denotes the body forces, $J := \det \mathbf{F}$ is the Jacobian or volume ratio, $\mathbf{F}$ is the deformation gradient and $p$ is the hydrostatic pressure.

Introducing a parameter $\mu \in \mathcal{P} \subset \mathbb{R}^p$, which comprises any property of the muscle model that shall be varied, and using the finite element method to discretise Equation (1), leads to the following parametric nonlinear dynamical system

$$
M \dddot{\mathbf{u}}(t, \mu) + D(\mu)\dot{\mathbf{u}}(t, \mu) + K(\mathbf{u}(t, \mu), \mathbf{w}(t, \mu), \mu) = 0, \quad \text{s.t.} \quad g(\mathbf{u}(t, \mu)) = 0. \quad (3)
$$

Herein, $\mathbf{u}$ is the vector of position coefficients, $\mathbf{w}$ contains the pressure coefficients, $M$, $D$ and $K$ are the mass, viscous damping and generalised stiffness matrix, respectively, and $g$ is the operator associated with the incompressibility constraint.

To decrease the computational effort of solving this system, projection based model order reduction techniques are applied, where the reduced basis is obtained by means of a proper orthogonal decomposition (POD) on precomputed training data. The approach of first projecting the second-order system and subsequently transforming the reduced second-order system into a first-order system for the solution process has shown to produce a stable and accurate reduced model. Furthermore, the online evaluation of the projected nonlinear operator needs to be accelerated. Approaches that have been investigated so far include the discrete empirical interpolation method (DEIM) and the energy conserving sampling and weighting hyper reduction method (ECSW). Here, we will show current results and discuss open questions.
A reduced-order strategy for efficient state/parameter identification in cardiac electrophysiology

S. Pagani¹, A. Manzoni², and A. Quarteroni²

¹MOX Dipartimento di Matematica - Politecnico di Milano
²MATHICSE CMCS - Ecole Polytechnique Fédérale de Lausanne

A reduced basis (RB) ensemble Kalman Filter is proposed for the efficient solution of Bayesian inverse problems, namely state/parameter identification and uncertainty quantification, arising from cardiac electrophysiology. Starting from noisy boundary measurements, our goal is to identify the presence and the form of ischemic regions described through suitable parametrized quantities or fields.

The ensemble Kalman Filter (like other Bayesian filtering techniques [1]) requires a huge amount of queries to the forward problem; for the case at hand, the latter is given by a system of nonlinear unsteady PDEs, entailing an often prohibitive computational cost. Reduced order modeling (ROM) techniques, such as the reduced basis method [5], enable to approximate the forward problem efficiently and, as a matter of fact, to speed up the entire inversion procedure. In particular, we adopt a RB method relying on (i) proper orthogonal decomposition for the construction of RB spaces, (ii) clustering techniques for the sake of selection of local RB spaces and (iii) suitable hyper-reduction techniques, such as the discrete empirical interpolation method, for the evaluation of nonlinear terms [3].

A relevant question, arising when ROM techniques are exploited to solve inverse problems, is related to the propagation of reduction errors – i.e. the error between the high fidelity and the reduced-order model – along the filtering process [2]. In order to quantify reduction errors, we propose a reduction error model based on kriging interpolation, which is then integrated within the Bayesian filtering procedure to achieve a more accurate state/parameter identification [4].

As a proof of concept, we present some numerical results exploiting the proposed procedure where both a monodomain and a bidomain model are used to describe the evolution of the electrical potential in presence of ischemic areas, modeled through unknown or uncertain parameters/fields.

References

Minimum residual based model order reduction approach for unsteady nonlinear aerodynamic problems

M. Ripepi¹, R. Zimmermann², and S. Görtz¹

¹German Aerospace Center (DLR), Institute of Aerodynamics and Flow Technology, Braunschweig, Germany
²Institute Computational Mathematics, TU Braunschweig, Braunschweig, Germany

The advent and development of large-scale high-fidelity computational fluid dynamics (CFD) in aircraft design is requiring, more and more, procedures and techniques aimed at reducing its computational cost in order to afford accurate but fast simulations of, e.g., the aerodynamic loads. The adoption of reduced order modeling techniques in CFD represents a promising approach to achieve this goal. Several methods have been developed to obtain reduced order models (ROMs) for the prediction of steady aerodynamic flows using low-dimensional linear subspaces (cf. [1]) as well as nonlinear manifolds (cf. [4]), whose performances may be further improved by applying hyper-reduction procedures (cf. [3]).

In this talk, a model order reduction approach (cf. [2]) for unsteady aerodynamic applications is presented. Following the idea of Ref. [4], the problem of finding the CFD ROM is formulated as a non-linear least-squares optimization problem, by searching in a subspace for an approximate flow solution having a minimum norm least-squares solution for the corresponding unsteady (flow solver) residual. The reduced basis for representing the reduced-order solutions of the governing equations is obtained through a Proper Orthogonal Decomposition (POD) applied to a given set of solutions of the full-order model at different time steps.

The arising nonlinear least-squares problem for the POD coefficients is solved by using a Levenberg-Marquardt (LM) algorithm. A Broyden update procedure is employed to approximate the Jacobian of the reduced-order system of equations, and it is further exploited to reduce the computational costs to generate the approximate Hessian matrix for the LM procedure. In addition, the potential of masked projection approaches, such as the missing point estimation (MPE) (cf. [5]), is going to be investigated.

The proposed approach is demonstrated for the Navier-Stokes equations by modeling the transonic flow around the LANN wing oscillating in pitch at different reduced frequencies.

References


Structure-preserving data-driven interpolation of dynamical systems

B. Unger\textsuperscript{1}, P. Schulze\textsuperscript{1}, C. Beattie\textsuperscript{2}, and S. Gugercin\textsuperscript{2}

\textsuperscript{1}Technische Universität Berlin, Germany
\textsuperscript{2}Virginia Tech, Blacksburg, VA, USA

The task of finding a dynamical system that interpolates input/output data in the frequency domain is investigated. Hereby, we assume knowledge of the structure of the system from which the data originates. Examples for structure are internal state delays or second order formulation, which we would like to preserve in the realization. More precisely, we consider realizations with transfer function

\[ H_r(s) = C_r \left( \sum_{k=1}^{N} h_k(s) A_{k,r} \right)^{-1} B_r \]

with known analytic functions \( h_k \). In this talk we present sufficient conditions for interpolation, which are based on a result from [1]. For the special case \( N = 2 \), this condition yields a realization that generalizes the Loewner realization [2], which is based on \( h_1(s) = s \) and \( h_2(s) = -1 \). In this case the Loewner realization is the only realization that satisfies the sufficient conditions for interpolation.

In the case that \( N > 2 \), we generalize the proportional ansatz from [3] that allows us to use the results from the \( N = 2 \) case with some additional degrees of freedom. We present two strategies to take advantage of these: One leads to matching of additional interpolation points. The other allows for Hermite interpolation in the given set of interpolation points. Neither of the strategies increases the state-space dimension. The results are illustrated by numerical examples.

References

A Model Reduction Approach to Structural Health Monitoring

Tommaso Taddei\textsuperscript{1}, James D Penn\textsuperscript{1}, and Anthony T Patera\textsuperscript{1}

\textsuperscript{1}Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

February 15, 2016

We present a Data-Based Approach to the problem of Structural Health Monitoring with synthetic training. The approach exploits (i) synthetic results obtained by repeatedly solving a PDE model for different values of the parameters, and (ii) machine-learning algorithms to generate a classifier that monitors the state of damage of the system.

Our approach is based on an offline/online computational decomposition. In the offline stage, the field associated with many different system configurations, corresponding to different states of damage, are computed and then employed to teach a classifier. Model reduction techniques, ideal for this many-query context, are employed to reduce the computational burden associated with the parameter exploration. In the online stage, the classifier is used to associate measured data to the relevant diagnostic class.

We prove that, given upper bounds for the model error related to the assumed damage configurations, we can provide upper bounds for the misclassification error associated with the classifier.

We illustrate our method through a companion micro-truss experiment. We show that the use of simulations allows us to drastically reduce the number of physical experiments needed during the offline stage, and also to improve the design of the experiment. We also present a synthetic acoustic duct example\textsuperscript{1} to show the importance of model order reduction.

\textsuperscript{1}Work in collaboration with Dr. D. B. P. Huynh (Akselos SA).
A hybrid ensemble approach to the adjoint-free data assimilation into geophysical flows

M. Yaremchuk\textsuperscript{1}, P. Martin\textsuperscript{1} and C. Beattie\textsuperscript{2}

\textsuperscript{1}Naval Research Laboratory, Stennis Space Center, USA
\textsuperscript{2}Virginia Tech, USA

The ongoing parallelization trend in computer technologies facilitates the use of ensemble approach in geophysical data assimilation. Of particular interest are ensemble techniques which do not require the development of tangent linear numerical models and their adjoints for optimization. These “adjoint-free” methods minimize the cost function within the sequence of subspaces spanned by a chosen sets perturbations of the control fields.

In this presentation, an adjoint-free variational technique (a4dVar) is investigated in an application estimating initial conditions of the Navier-Stokes system constrained by a sparse data set. It is shown that enriching the ensemble of search directions by the leading eigenmodes of the background error covariance and (by the leading) EOFs of the model trajectory provides a significant improvement of the convergence rate while keeping optimal corrections to the control fields on the slow (geostrophic) manifold. Comparison of the a4dVar method with traditional (4dvar) technique [utilizing tangent linear and adjoint numerical models of the original system] shows similar performance both in terms of the CPU time requirements and the forecast skill.
On the notion of distance in data-driven manifold learning and surrogate modeling

R. Zimmermann\textsuperscript{1} and T. Franz\textsuperscript{1,2}

\textsuperscript{1}Institute ’Computational Mathematics’, TU Braunschweig
\textsuperscript{2}Institute of Aerodynamics and Flow Technology, German Aerospace Center (DLR), Braunschweig

A fundamental challenge in manifold learning and dimensionality reduction is to estimate the intrinsic interpoint distances of a given data set. For example, the method of Isomap\textsuperscript{3} is, in essence, a method for approximating the Riemannian distance inherent to a point cloud that is assumed to lie on a differentiable manifold. The notions of distance and locality are also key to an adaptive construction and refinement of reduced order and surrogate models, because a reliable distance measure can be used to detect gaps in the underlying design of experiment. In particular, this holds true for non-intrusive data-driven approaches. Related is the task of estimating the spatial correlation in a data set of multivariate sample points, which is critical to the design and analysis of computer experiments\textsuperscript{2}. Using the example of the non-intrusive dimensionality reduction method for nonlinear parametric Navier-Stokes flow problems introduced in [1], we expose how these ingredients are combined and we discuss their impact on the resulting reduced model.

References


Poster Presentations
# List of Poster Presentations

<table>
<thead>
<tr>
<th>Title</th>
<th>Authors</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability in MOR Using the Loewner Framework</td>
<td>A. C. Antoulas</td>
<td>38</td>
</tr>
<tr>
<td>Data-Driven Time-Parallelism for Reduced-Order Models via Forecasting</td>
<td>L. Brencher</td>
<td>39</td>
</tr>
<tr>
<td>POD-DEIM Based Model Reduction for Multi-Component Porous-Media Models</td>
<td>D. Fink</td>
<td>40</td>
</tr>
<tr>
<td>Efficient Snapshot Generation for the POD Basis Identification</td>
<td>F. Fritzen</td>
<td>41</td>
</tr>
<tr>
<td>Robust Fuzzy Regression by alpha-cutting the cost</td>
<td>M. Janev</td>
<td>42</td>
</tr>
<tr>
<td>Data-Driven Optimization Procedure for Black-Box Objective Functions</td>
<td>S. Kaul</td>
<td>43</td>
</tr>
<tr>
<td>Black-Box Model Order Reduction Technique for Nonlinear Dynamical Systems by Kernel Approximation</td>
<td>L. Kazaz</td>
<td>44</td>
</tr>
<tr>
<td>Model Order Reduction for Nonlinear Multiscale Materials with Imperfect Interfaces</td>
<td>M. Leuschner</td>
<td>45</td>
</tr>
<tr>
<td>High-Performance Data Mining for Large, Moderate-Dimensional Regression Problems Using Spatially-Adaptive Sparse Grids</td>
<td>D. Pfander</td>
<td>46</td>
</tr>
<tr>
<td>Hierarchical Approximate POD</td>
<td>S. Rave</td>
<td>47</td>
</tr>
<tr>
<td>Greedy Kernel Interpolation Surrogate Modeling</td>
<td>G. Santin</td>
<td>48</td>
</tr>
<tr>
<td>Reduced Basis Method for H2 Optimal Feedback Control Problems</td>
<td>A. Schmidt</td>
<td>49</td>
</tr>
<tr>
<td>Nonlinear Model Order Reduction on the Substructure Level Through POD-Based CMS and Bonded Contact for the Interface Coupling</td>
<td>L. Zhou</td>
<td>50</td>
</tr>
</tbody>
</table>
Stability in MOR using the Loewner Framework

I.V. Gosea\textsuperscript{1} and A.C. Antoulas\textsuperscript{2}

\textsuperscript{1}Jacobs University Bremen
\textsuperscript{2}Rice University, Houston

One of the issues with the Loewner Framework is that stability is in general not preserved. In this contribution we show how to address this issue by post-processing of the reduced model. The procedure will be performed both in the H-2 and the H-infinity norms. Several examples illustrate the approach.
Data-driven time-parallelism for reduced-order models via forecasting

Lukas Brencher¹, Kevin Carlberg², Bernard Haasdonk¹, and Andrea Barth¹

¹University of Stuttgart, Stuttgart, Germany
²Sandia National Laboratories, Livermore, CA, USA *

Model order reduction techniques have been successfully approved to decrease the computational costs of simulations, measured in cores × hours [1]. Unfortunately, they do not show significant speedup regarding the wall-time as spatial parallelism is quickly saturated. This becomes a major roadblock for solving problems where near-real-time solutions are needed. To improve the time to solution, parallel-in-time methods (e.g. parareal-in-time [3], PITA) have shown significant speedup, even though time stepping does not easily lend itself to parallelism due to its sequential nature.

The idea of time-parallel methods is to decompose the time interval into time sub-intervals and construct independent initial value problems by introducing initial conditions on each time-slice. These initial conditions are computed by a coarse propagator, which typically is a traditional time integrator with a large time step. Therefore, the initial values are not necessarily accurate and the solution computed in parallel is likely to have jumps (discontinuities) on the border of the sub-intervals. To correct these discontinuities, an iterative correction step is performed. For inaccurate coarse propagators, these iterations limit or even eliminate the speedup of the time-parallelism.

To open up this bottleneck, this work proposes a new method—data-driven time-parallelism— which reduces the number of iterations needed for convergence if time parallelism is used for computing model-order-reduction simulations. The proposed method applies the temporal complexity reduction method introduced in Ref. [2], which computes a data-driven forecast of the solution at future time steps, as an accurate coarse propagator to obtain the initial conditions on the sub-intervals. Exploiting time-evolution data from offline training simulations allows the method to converge faster than typical time integrators.

References


*Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.
POD-DEIM based model reduction
for multi-component porous-media models

D. Fink and W. Ehlers

1Institute of Applied Mechanics (CE), Chair of Continuum Mechanics, University of Stuttgart

A broad variety of materials in geomechanical and biomechanical engineering, such as porous soils, intervertebral discs or human-brain tissue, exhibit a porous microstructure. In order to evaluate the overall response of these materials, a macroscopic continuum-mechanical modelling approach is used. Therefore, the complex inner structure is regarded in a multi-phasic manner by means of the Theory of Porous Media (TPM), see [2]. Furthermore, the finite-element method (FEM) is used to approximate the solution of the descriptive set of coupled partial differential equations (PDE), see [3] among others.

In the context of FE simulations, computing time and numerical effort is an important issue because the number of degrees of freedom (DOF) of such coupled problems can become very large. Following this, model reduction plays an important role to reduce the computing time of the FE simulations. Therefore, the main target of this work is to apply the proper-orthogonal-decomposition (POD) method in combination with the discrete-empirical-interpolation method (DEIM), see [1], on the global FE equation for models of porous materials. Applying the POD method, a given data set is approximated with a low-dimensional subspace which ensures a high flexibility in application, see [4]. Therefore, representative state variables (and thus the vector of unknowns of the FE simulation, which contains the values of the primary variables at each node of the FE grid), the so-called “snapshots” of the system, are stored in a pre-computation using the initial full system. Additionally, snapshots of the nonlinear terms of the coupled differential equations (occurring from geometrical and material nonlinearities) are stored to further approximate the nonlinearities using the DEIM. Following the concept of offline/online decomposition, the time-consuming offline phase (including the pre-computations and the basis generation) is separated from the time-efficient online phase with reduced simulations.

Dealing with porous-media problems, the primary variables (e.g. the solid displacement, the pore pressure and, depending on the particular problem, other primary variables such as molar concentrations of therapeutic agents) have a different temporal behaviour. This may lead to problems when applying the POD method by default. To overcome this problem, the snapshots are divided in separated parts for each primary variable and, consequently, separated reduction matrices for all primary variables are computed.

References


Efficient snapshot generation for the POD basis identification

F. Fritzen

Efficient Methods for Mechanical Analysis Group, Institute of Applied Mechanics (CE), University of Stuttgart, fritzen@mechbau.uni-stuttgart.de

The author has recently proposed reduced basis (RB) methods for the numerically efficient computational homogenization of the mechanical properties of dissipative solid materials [2, 1]. Similar to many other RB methods, they require a reduced basis of the internal variables as input, i.e. the RB for the plastic strain and for the hardening variables are needed. In previous works a low number of manually chosen loading paths was assigned to the unreduced finite element problem in order to provide the input data for the snapshot proper orthogonal decomposition. As was already emphasized in [3], the choice of these loading paths in the OFFLINE stage has a significant impact on the accuracy and on the computational efficiency.

In this presentation we focus on the OFFLINE stage rather than on the reduced order model itself. The kinematic approach proposed in [4] for the identification of cohesive interface modes is used in order to determine optimal loading directions automatically. Then different ensembles of load cases are considered in the OFFLINE stage and a total of more than 1,000 finite element analyses (each having more than 400,000 DOF) with full-consideration of the path-dependency of the microscopic visco-plasticity model with nonlinear hardening are conducted. The resulting 16,000 output fields are then examined in detail. The results are compared to randomly chosen loadings in order to outline the advantages of systematically chosen OFFLINE calculations. By incorporating simple micro-mechanical aspects into the snapshot POD a new strategy for the mode identification is proposed. It can help to reduce the dimension of the RB while preserving the accuracy of the ROM.

References


Robust Fuzzy Regression by $\alpha$-cutting the cost

Dragan Kukolj$^1$, Lidija Krstanovic$^1$, Ratko Obradovic$^1$, Nebojsa Ralevic$^1$, Vladimir Zlokocica$^1$, and Marko Janev$^2$

$^1$Faculty of Engineering, University of Novi Sad, Novi Sad, Serbia
$^2$Institute of Mathematics, Serbian Academy of Sciences and Arts, Serbia

Classical regression models are used as a statistical tool in order to deliver the relationship between the independent and dependent variables, assuming that the difference between the observed and the dependent variables, who are crisp numbers, is due to the additive noise.

In the case of robust noise, as for example Laplace or heavy tailed additive noise, or the mixture of Gaussian and Heavy tailed additive noise, the robust $M$-estimators are introduced, where those that utilize Huber norm are the most common and one of the most effective.

Contrary to the situation when there is no uncertainty regarding the measurement process of the system variables, fuzzy regression models are developed to construct the relationship between explanatory variables and response in a fuzzy environment, i.e., explanatory variables and response are considered to be fuzzy numbers. Those are mostly used in the problems of prediction in various applications that deal with uncertainty, as in many real world problems, the actual observations are usually described by approximate values, which is due to the fact that the measurement process is inherently more or less uncertain. A number of fuzzy regression models which had been developed, could be roughly divided into following categories: 1) Linear programming methods, 2) least-squares, and similar cost methods 3) support vector machines methods. For all fuzzy regression models linguistic terms can be used to describe fuzzy observations which are quantitatively described by their corresponding fuzzy numbers.

In our work, we propose the novel Robust Fuzzy Regression model, by introducing fuzzy $M$-estimator that utilize Huber robust norm, in order to handle outliers present in the fuzzy data which are modelled by the usage of heavy tailed noise. The estimator is obtained by $\alpha$-cutting the cost function which contains the unknown regression coefficients. Actually, the unconstrained optimization problem is obtained whose solution is desired estimate of the regression parameters. We confirm the proposed method on the syntectic data, and also analyze possibilities to apply the obtained result on real datasets, in various fuzzy regression tasks.
Data-driven Optimization procedure for black-box objective functions

Shehjar Kaul¹ and Thomas Baumeister²

¹Ex-employee of TUM CREATE Centre of Electromobility, Singapore
²Masters Student of Technische Universität München, München

An Optimization procedure is proposed which uses machine learning techniques for speeding up the procedure and identifying patterns in the input variables affecting the objective function. The objective function is termed as black-box as there is no clear relation between the input variables to the objective function value. This situation complicates the optimization problem and most of the deterministic optimization procedures, where there is a need for derivatives calculation, are rendered ineffective.

The stochastic approach to optimization therefore becomes more relevant and despite their robustness, the algorithm requires numerous iteration runs which is computationally expensive. There have been previous work done [1] on reducing the computation time of the objective function using Machine Learning approaches and its applications are tremendous. However, the work presented through this paper would focus solely on the application of Machine Learning as a tool for reducing the design search space.

The proposed semi-automatic algorithm would try to first find the optimum or reduced search space within the originally defined Design search space as shown in fig 1. This is would be achieved by a series of point distribution generations within the search space, using clustering algorithms in Machine Learning to find the best working cluster and lastly, identifying the search direction by the use of principle components of the covariance matrix generated by the point distribution outcome. The optimum or reduced search space would be a small subset of the originally defined space, which would later be bounded to an approximate objective function leading to a global optimum.

![Schematic diagram of overall Optimization procedure](image)

**Figure 1: Schematic diagram of overall Optimization procedure**

References

Black-box model order reduction technique for nonlinear dynamical systems by kernel approximation

Lorin Kazaz\textsuperscript{1}, Daniel Wirtz\textsuperscript{1}, and Bernard Haasdonk\textsuperscript{1}

\textsuperscript{1}University of Stuttgart

The complexity of full state evaluation needed in projection-based reduced nonlinear systems has led to the Discrete Empirical Interpolation Method (DEIM, cf. [1]) which takes care of nonlinearity. Yet, the DEIM needs the assumption that each component of the right-hand side function can be evaluated cheaply and individually. This may be highly nontrivial or impossible, e.g. when given third party solver packages.

We present a black-box model order reduction technique for nonlinear dynamical systems based on the assumption that only global snapshots of the nonlinearity can be requested. Kernel methods can provide suitable kernel approximations for the relevant function components. Thus, we investigate the combination of the DEIM with the Kernel Orthogonal Greedy Algorithm yielding the Kernel-DEIM (cf. [3],[2]). We highlight the advantages of Kernel-DEIM for non-linear MOR. Furthermore, we provide background on evaluation complexity and efficient implementation. Numerical examples confirm the applicability of this approach.

**Keywords**: Nonlinear Model Order Reduction, Greedy, Kernel, DEIM

**References**


Model order reduction for nonlinear multiscale materials with imperfect interfaces

M. Leuschner¹ and F. Fritzen¹

¹Efficient Methods for Mechanical Analysis Group, Institute of Applied Mechanics (CE), University of Stuttgart

Composite materials are increasingly used in various engineering applications. In mechanical analyses, the heterogeneous microstructure of such materials is accounted for via homogenization schemes. Physical nonlinearities, e.g. due to viscoplasticity or imperfect interfaces at the phase boundaries, are treated numerically. To circumvent prohibitive numerical cost related to full-field homogenization methods, the Nonuniform Transformation Field Analysis (NTFA, first presented in [3]) has been proposed.

The key idea of the NTFA is to introduce a reduced basis for the plastic strain field, which is in contrast to many other reduced order methods for mechanical applications using a reduced basis for the displacement field. This approach has been generalized and applied to a more comprehensive class of problems in the potential-based Reduced Basis Model Order Reduction technique (pRBMOR, cf. [1]). The pRBMOR homogenization scheme relies on potential-based microscale constitutive models from the class of Generalized Standard Materials (GSM). GSM models have a variational structure which is transferred to the macroscale. In combination with the reduced basis ansatz, the macroscale variational problem can be solved in an efficient algorithm without costly iterations at the microscale.

The pRBMOR technique has recently been extended towards microstructures with imperfect interfaces (cf. [2]) by introducing a reduced basis for the displacement jump field (see Figure 1). First results for dissipative interfaces, also in combination with viscoplasticity in the matrix material, are available and will be presented.

Figure 1: Representative volume element of a particle reinforced material (left) and the first four elements of the reduced basis for the displacement jump field (right).

References


High-Performance Data Mining for Large, Moderate-Dimensional Regression Problems Using Spatially-Adaptive Sparse Grids

David Pfander$^1$ and Dirk Pflüger$^1$

$^1$Universität Stuttgart, Germany

Due to the availability of cheap sensors, higher-bandwidth communication devices and a generally intensified collection of data, datasets have become larger and larger. To extract useful information from these datasets, machine learning methods have to be employed that scale well with the size of the datasets. Specifically for large, moderate-dimensional regression problems, sparse grids are a good choice.

Sparse grids are a spatial discretization technique that is able to mitigate the curse of dimensionality to some extent [1, 2]. Due to the spatial discretization approach, sparse grids scale only linearly in the number of data points, which is a highly-beneficial attribute for large datasets [4]. Additionally, the efficiency of the sparse grid approach can be further increased by employing spatial adaptivity which permits a grid to have a higher resolution at localized regions in the domain [4]. However, to actually learn large datasets within reasonable timespans, it is not only necessary to choose appropriate algorithms, the implementation has to be highly-efficient as well.

In this work, we present new high-performance implementations for spatially-adaptive sparse grid regression with different basis functions. These implementations feature Auto-Tuning techniques that use code generators to generate architecture-specific optimized code. The code generation approach makes it possible to fit the algorithms to the low-level aspects of the hardware platform, e.g., by adjusting the algorithm to the length of the pipelines, to the sizes of the cache and the register file and by making use of the vector units. The optimizations that consider these low-level aspects are implemented in the code generator in a parameterized way. By searching the optimal values for these parameters, the fastest compute kernel for the platform at hand is obtained.

To validate our approach, we performed regression experiments with several datasets, grid configurations and grid adaptivity settings. From these experiments, we conclude that the performance of our compute kernels is competitive with the fastest known implementations [3]. The underlying sparse grid algorithm even scales up to whole clusters of hybrid compute nodes with Intel MIC accelerators. This enables the processing of vast datasets.

References


Hierarchical Approximate POD

C. Himpe\textsuperscript{1} and S. Rave\textsuperscript{1}

\textsuperscript{1}University of Münster

Proper orthogonal decomposition (POD) is a widely-used data compression method which is also a popular tool in the context of model order reduction for the computation of reduced state approximation spaces from given solution snapshot data. However, performing a POD is often a computationally demanding task as the effort for computing the POD depends quadratically on the number of snapshots. This is especially the case for time-dependent parametric problems where a single solution trajectory already can contain hundreds of state vectors.

To mitigate this issue, parallelizable algorithms for (approximate) POD computation have been proposed in [1, 2] where the ‘tall and skinny’ matrix of high-dimensional column snapshot vectors is horizontally sliced and the main computational work is performed locally on these slices. As a drawback of this approach, parts of every snapshot vector must be available on all compute nodes. This is typically not the case for distributed computing architectures. Moreover, all snapshots must have been computed before the POD computation can be started.

Another nearby solution to overcome the algorithmic limitations of POD is to compute, when and where available, PODs of subsets of the global snapshot set (i.e. slicing the snapshot matrix vertically), and then to use the resulting POD modes as input for an additional POD. We formalise this approach as ‘hierarchical approximate POD’ (HAPOD), allowing arbitrary trees of localized PODs, making HAPOD suitable for distributed, heterogeneous compute environments. As a special case of HAPOD we consider a ‘rolling approximate POD’ to compute approximate PODs of time trajectories on-the-fly, even when a whole trajectory would not fit into memory. Besides numerical examples underlining the capabilities of this very simple approach, we give rigorous bounds for the error introduced by the additional approximation steps.

References


Greedy kernel interpolation surrogate modeling

B. Haasdonk1 and G. Santin1

1University of Stuttgart, Institute of Applied Analysis and Numerical Simulation

In the construction of surrogate models, kernel methods are successfully applied to the reconstruction of functions from high dimensional and unstructured data.

Although these methods produce dense and generally ill-conditioned matrices, numerical evidence and theoretical results show the existence of suitable reduced spaces that provide stable and fast approximate solutions, while retaining the accuracy expected from the solution of the full problem. Greedy point-selection algorithms are an effective way to construct near-optimal and data dependent subspaces.

We present here a new approach to the kernel interpolation problem. Namely, we decouple the location of the data from the placement of the centers of the kernel. This strategy allows to control both the error and the stability of the reconstruction problem, and comprises as a special situation the usual kernel-based interpolation.

We will discuss a preliminary theoretical study of this approximation setting, and introduce different data-dependent greedy techniques that are motivated by these results. Numerical experiments will be presented to support our findings.
Reduced basis method for $\mathcal{H}_2$ optimal feedback control problems

A. Schmidt$^1$ and B. Haasdonk$^1$

$^1$University of Stuttgart

In this contribution we examine the application of known parametric model reduction techniques to the $\mathcal{H}_2$ optimal feedback control problem. The $\mathcal{H}_2$ control problem provides a realistic framework for control applications, since it considers disturbances in the system and in the measurement outputs. Furthermore it employs state-estimation techniques to reconstruct the unknown state from the noisy measurements. It turns out, that the controller is a dynamical system and two solutions of algebraic Riccati equations (AREs) are required to form it. We apply parametric model order reduction techniques to the AREs and to the state equation of the observer and show by numerical examples, that this approach can yield a significant speed-up in multi-query scenarios for large scale parametric problems for the control of partial differential equations (PDE).
Abstract

The shell is an optimal structural form in nature, but its design and analysis methods are very complex and thus the application is limited. In this research project, a more efficient method is developed, for the analysis of shell structures, which consist of many planar modular structural elements. The displacement fields of these structural elements can be approximated with less independent variables, leading to a reduction of the dimension of the global system and hence of computational effort. In this paper a new class of Component Mode Synthesis (CMS) method based on Proper Orthogonal Decomposition (POD) is presented (named in our approach as POD-based CMS). This application belongs to the framework of Model Order Reduction, which is carried out on the substructure level. Different from the classical CMS methods like Guyan or Craig-Bampton, this method can reduce the boundary nodes together with the internal nodes on each substructures, with no need to treat them separately, by using unified POD-based basis functions. Additionally the coupling of interfaces between two substructures is ensured through using bonded contact. The coupling term increases the computational effort, nevertheless is limited only on the boundaries. Both the reduced and unreduced parts are considered in the same way, which shows the flexibility for solving problem with locally higher nonlinearity. This method can be applied, not only for geometrical and material nonlinear cases through quasi-static analysis, but also for implicit dynamic analysis straightforwardly. Several numerical examples are presented, and the deformation responses are compared to results obtained by the standard finite element method, in order to show the efficiency of this method.