Reduced Basis Modeling of Hierarchical Flow Systems

Proposal for BeMatA

Project Manager:

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June 8, 2001

Abstract

Reduced basis methods are particularly attractive to use in order to reduce the number of degrees-of-freedom associated with a given numerical approximation to a set of partial differential equations; the computational complexity can be reduced to a level where potentially very complex systems can be simulated. The main idea is to construct basis functions with a large information content in order to reduce the number of basis coefficients needed to reach a certain level of accuracy in the outputs of interest. In this project, we propose to develop and analyze reduced basis methods for simulating hierarchical flow systems, which is of relevance for studying flow in a set of arteries or veins, flow in a respiratory system, or flow in a network of pipes. We propose to decompose the geometry into generic parts (e.g., pipes and bifurcations), and to contruct a reduced basis for these generic parts by considering representative geometric snapshots. The global system will be constructed by gluing the individual basis solutions together via Lagrange multipliers. As far as we know, the use of reduced basis methods have previously been limited to finite-dimensional parameter spaces; defining the geometry as a generic "parameter" appears to be new.

1 Background

For complex systems, which can be modeled by a set of partial differential equations, numerical simulation has become an invaluable tool in order to gain insight into the behavior of such systems, and for design and control. This is true in many areas of science and engineering, in finance, and for medical applications. Computational tools typically gain acceptance as long as the reliability of the computations is acceptable, and as long as the computational cost is reasonable.

Despite the major advances that we see today both in terms of hardware development and advances in numerical algorithms, there are still many relevant systems that cannot yet be solved in a satisfactory manner. The reason may be that the resulting algebraic systems become too large to handle following a "conventional" approach; another reason may be that the resulting system takes too long to solve (e.g., in the context of real time control of distributed systems, or for design and optimization).

In the following, we shall limit ourselves to flow systems which can be modeled by the incompressible Navier-Stokes equations. The available computational methods for such problems comprise a plethora of techniques [14]. The methods may be classified according to the type of spatial discretization, e.g., finite element methods, finite difference methods, boundary element methods, etc. Another classification may emphasize the temporal treatment, e.g., operator splitting methods, explicit methods, implicit methods etc. In any case, a typical method will frequently involve the solution of large systems of algebraic equations, either as part of an outer Newton iteration or in the context of time advancement. Together with the specific solution algorithm, the size of these systems creates a practical limit to how large the computational model can be, or equivalently, how detailed we can simulate the underlying physical system. Further complications and challenges are created when we try to model *coupled problems* where several physical phenomena are present and interacting together at the same time; an example of this is fluid-structure interaction in time-dependent domains.

1.1 Hierarchical flow systems

As a particular example of a complex physical system, we consider the modeling of fluid flow in a network of deformable pipes with bifurcations. Obvious examples of such hierarchical flow systems are the flow in a set of arteries or veins, or the air flow in a respiratory tree. Despite the fact that such flows may be considered as being laminar, a detailed, realistic, time-dependent behavior is difficult to predict for a complete system due to the very large number of degrees-of-freedom required following a "conventional" modeling approach, i.e., via a direct simulation. The limit of what is feasible to compute is, of course, being pushed forward all the time; however, a detailed full-scale model is still far away.

On the other hand, a more feasible task is the detailed simulation of the flow in a single pipe or a single bifurcation. With a detailed simulation, we mean an accurate numerical solution of the incompressible Navier-Stokes equations with prescribed boundary conditions and initial conditions. However, even such limited systems can be computationally challenging. An additional problem (or challenge) is the definition of the proper boundary conditions that have to be applied on a truncated domain.

1.2 Reduced order models

The idea of trying to contruct a low-dimensional model which provide good accuracy in outputs of interest has a lot of appeal, either in order to deal with a very complex system, or in the context of repetitive use of a model as in design, optimization, and real time control. In other cases, one would like to study a given physical problem with respect to variation in certain model parameters. One scenario is that the governing equations, the computational domain and the boundary conditions are all fixed, but the material properties (e.g., the Reynolds number) vary from case to case. For such problems, an alternative way to construct a low-dimensional model is to first use a high-resolution numerical model, and then "sample" the parameter space of interest by solving *selected* forward problems. From these sample solutions (or snapshots), one can construct a low-dimensional model which will capture the most important dynamical aspects of a fluid flow problem. We will refer to such a model as a *reduced-order model*.

The reduced basis approach is founded on the fact that many problems can be cast in the following framework: for a given value of μ, find $u(\mu) \in X$ such that

$$F(u(\mu); \mu) = 0,$$

where X is some functional space, the parameter μ belongs to some subset of $\mathbb{R}^p$ and F is a given mapping defined over $X \times \mathbb{R}^p$. The basic idea of the reduced basis method is that, as a function of the parameter μ, the solution $u(\mu)$ is often a smooth function so that, provided that some realizations $u(\mu_i)$ are known for a few values $\mu = \mu_i$, with $i = 1, .., n$, then by interpolation or extrapolation, we can predict a good approximation of $u(\mu)$ for a generic value of μ. In order to choose, among the many possible possibilities for inter- or extra-polation, a *Galerkin method* is most often used since, for many types of problems, it allows us to infer the best linear combination of the precomputed $u(\mu_i)$. The reduced basis methods are very attractive in the sense that, with very few basis functions, such methods may describe the solution for many values of μ with acceptable accuracy, even when n is small (perhaps $\mathcal{O}(100)$).

The methodology just described is often referred to as Karhunen-Loeve expansion or *Proper Orthogonal Decomposition (POD)*. The quality of the reduced order model strongly depends upon the selection of basis functions, i.e., how much of the "physics" in a new, unknown situation is captured by the previously preselected sample solutions (or basis functions). The term "orthogonal" is used because some of the preselected sample solutions (or snapshots) may be close to being linearly dependent; orthogonalization of the reduced basis with respect to some inner product is therefore preferred for numerical stability.

For evolution problems, the parameter μ is typically taken to be time, and the numerical solution is described as a linear combination of snapshots of the process. This way of applying the POD methodology has shown promise in the area of fluid mechanics; see [3, 5].

The potential benefits of using low-dimensional models may also be seen in the area of design and optimization because of the typically large parameter space that needs to be explored, and because of the associated huge reduction in the computational cost; see [8].

Another important application is real time control of physical systems. A full-scale model based upon a detailed numerical solution of the governing partial differential equations may simply not be feasible to use even when looking many years into the future. However, a carefully constructed low-dimensional model is a very interesting alternative that looks promising for real time control of distributed systems; see [1].

We also mention that, a completely different approach toward constructing a low order model is to use an *eigenfunction expansion* of the underlying spatial differential operators. For example, a finite number of eigenfunctions (or eigenvectors) of the discrete Stokes or singular Stokes operator may be used in order to construct a reduced (spatial) basis for the time-dependent Navier-Stokes equations; see [2]. The dimension of each eigenvector may still be very large (e.g., $\mathcal{O}(10^4) - \mathcal{O}(10^6)$), and each eigenvector may be computationally expensive to obtain. However, once the eigenvectors have been computed, a general and fairly complex solution may be spanned by a relatively small number of eigenvectors. In essense, the expensive part of the computation (the computation of the eigenvectors) is done in a pre-processing step, while a low-dimensional model (perhaps of dimension $\mathcal{O}(100)$) is subsequently used to follow the evolution of time-dependent solutions.

The idea of constructing a reduced basis is not only limited to POD methods or eigenfunction expansions. Another way is simply to use a large mesh size, although a naive approach will often produce unreliable answers in the outputs of interest (e.g., forces, displacements, various averages, etc). We should note, however, that significant progress has recently been made in developing alternative strategies to improve the accuracy in the output of interest (even on coarse meshes), while at the same time bound the error; the latter is very important for reliable use of reduced order methods.

Here, we should stress the fact that the reduced order methods need to be used with a lot of care. Without any estimate for the error in the outputs of interest, we may not know whether the model has enough basis functions to approximate the solution well. This is why the recent development of *a posteriori* tools to certify the computed solutions has been a very important step for the development of this approach; see [9, 13, 12].

2 Objectives

Main objective:

To develop reduced basis methods for solving complex hierarchical flow problems.

Partial objectives:

- To develop reduced basis methods for computational domains comprising a network of deformed pipes and bifurcations, and in the context of solving the unsteady heat equation as well as the unsteady Stokes and Navier-Stokes equations.
- To develop reduced basis methods for time-dependent domains.
- To propose and implement *a posteriori* estimators in order to certify the reduced basis results.

- To investigate the potential, as well as the limitations, of using reduced order models to solve complex problems in science and engineering.
- To contribute to the education of doctoral students.

3 Method

In this project, we will consider the possibility of constructing a more complete model for hierarchical flow systems by extending the concepts from reduced-order modeling and combining these with domain decomposition. Of particular interest is to understand to what extent one can use the *geometry* of the computational domain as a generic parameter.

The basic idea can be described as follows: we first construct a series of flow solutions for individual (and representative) pipes and bifurcations. In the case of a simple pipe, this can be considered as being in the range of a reference pipe through a regular mapping. With each pipe or bifurcation, we will associate a set of Navier-Stokes solutions. These flow solutions will be precomputed *individually* by considering a set of preselected deformed geometries obtained by mapping the reference domains through some regular mappings. The challenge is then to construct a reduced discrete space on the composed domain by "gluing" these precomputed basis functions together with some Lagrange multipliers (in a mortar-like approach; see [4]). The objective is to generate a discrete approximation space for a new and *unknown* configuration with a tractable number of degrees-of-freedom, yet providing a good accuracy.

Note that the key steps (and challenges) in this approach are: (i) to decompose the network into nonoverlapping generic parts (pipes or bifurcations, say); (ii) to precompute a family of generic solutions which is associated with a single generic part of the network; (iii) to contruct a reduced order model on each part where the geometry is the generic parameter; (iv) to glue the individual parts together, both geometrically and functionally; (v) to certify the computational results for the global problem.

We now make several comments on the proposed approach.

1. *Boundary conditions*: We will consider problems where the boundary conditions on all the external surfaces are fixed in *type and value*. This fact will be exploited when constructing the basis functions. Note that the *shape* of the surfaces on which the given boundary conditions are imposed can vary.
2. *Geometric variation*: The idea of constructing a reduced basis in order to incorporate variation in the solution due to variation in geometric shape is new. As far as we know, the use of reduced basis methods have previously been limited to finite-dimensional parameter spaces; defining the geometry as a generic "parameter" appears to be new.
3. *Basis functions*: The basis functions will be constructed as discrete solutions (or snapshots) on various preselected deformed pipes and bifurcations, but the solutions will be represented on the associated reference domains (one for a pipe, and one for a bifurcation). The computation of the discrete solutions will be based upon the finite (or spectral) element methodology.

4. *Domain decomposition*: For two or more parts (pipes and bifucations), the constructed basis solutions associated with the individual parts will be glued together using a FETI-type approach; see [6]. The global domain will be decomposed into non-overlapping subdomains (i.e., individual pipes and bifurcations), and Lagrange multipliers will be used to enforce matching conditions along the subdomain interfaces (e.g., minimize the jump in the solution with respect to some polynomial trace space; see [4]).
5. *Self-adaptation*: If the shape of a part (pipe or bifurcation) is very different from previously preselected shapes (as measured in some norm), we may use this shape to enrich our previously constructed basis.
6. *Exploitation of symmetry*: For a two-dimensional deformed pipe, the associated reference domain is a square. The precomputed solution for a given shape may easily be reflected and rotated in order to enrich the basis and make the basis insensitive to directional effects.
7. *Time-dependent problems*: The Galerkin approach used to construct a reduced order model for steady probems can also be used to construct a low-dimensional model for time-dependent problems. It will be particularly interesting to investigate the quality of such a model in the case where not only the governing equations are time-dependent, but also the computational domain varies with time.
8. *Computational complexity*: Each precomputed solution (associated with a preselected pipe or bifurcation) preassumes the availability of an appropriate simulation tool; in principle, this tool may be non-scalable or otherwise non-optimal. However, the important thing is that the reduced order basis can be precomputed and stored for future use. In this sense, one may consider building up a data base of pertinent basis solutions which may be expanded as needed. On the other hand, the memory requirement to store the basis functions associated with the individual parts will grow linearly with the number of geometric snapshots. Note, however, that the idea is to *reuse* the basis functions associated with the individual parts to similar parts in the global, hierarchical system. In this sense, the memory requirement has the potential to be quite modest. Finally, note that the dimension of the reduced space is essentially the number of basis functions for a particular part (a pipe or a bifurcation) times the number of parts, plus the number of interface constraints associated with the subdomain interfaces.
9. *Simulation tool*: As a point of departure, we plan to use a spectral-element-based code for constructing the individual basis functions; see for example [10, 7, 15, 16].

We have done some preliminary investigation in terms of trying to understand some of the basic concepts of this approach. In particular, we have considered the solution of the Laplace equation and the Poisson equation in preselected deformed domains. All the computational domains considered in these tests have been various deformed two-dimensional pipes. The solution in a new and unknown domain (also a pipe) has then been spanned by the precomputed solutions as defined on the reference domain (a square) and mapped to the new domain. The results we have obtained in these preliminary tests have been very encouraging. We have followed the proposed approach on, admittedly, simpler model problems than the incompressible Navier-Stokes equations. However, the reduced order results, as applied to variation in geometric shapes, are encouraging. We have tried the approach in the single-domain case, and in the multi-domain case where the proposed FETI-type (or mortar-like) "gluing" process is required.

The methodology proposed in this project, as well as the preliminary results that we have obtained, will be presented at the Fifth International Conference on Spectral and High Order Methods (ICOSAHOM) which will be held in Uppsala, Sweden, June 11-15, 2001.

4 Time Schedule and Budget

4.1 Project period

The proposed project period is 01.01.2002 - 31.08.2006. Please note that the last year of the PhD scholarship will be paid for by the Department of Mathematical Sciences at NTNU.

4.2 Budget

The budget througout the period is as follows (all numbers are in 1000 NOK):

	2002	**2003**	**2004**	**2005**	**2006**	**Total**
PhD scholarship	170	423	438	264		**1295**
Stay abroad for PhD student				114		**114**
Travel expenses	50	50	50	50	50	**250**
Inviting guests	30	30	30	30	30	**150**
Total	**250**	**503**	**518**	**458**	**80**	**1809**

Comments to the budget:

1. Due to the proposed collaboration between NTNU and Paris VI, we have included a modest travel budget for mutual visits; we consider this as important. The travel expenses will also be used in order to disseminate the research results at conferences, meetings, and seminars, both at an international and national level.
2. We have added a small budget for inviting guests to NTNU who are working in areas related to the proposed work (e.g., researchers from MIT).
3. Again, please note that we expect the PhD candidate to finish in the middle of 2006, where the last year of the PhD scholarship will be paid for by the Department of Mathematical Sciences at NTNU.
4. The annual budget for the PhD scholarship is based on the rate for 2002 (408.000 kr.), plus a yearly increase of 15.000 kr.
5. We propose that the doctoral candidate visit a foreign univeristy for half a year. One alternative could be Paris VI given the proposed collaboration between NTNU and Paris VI. We propose that such a visit will occur during the first half of 2005.

5 Information

The research results obtained through the proposed project will be published in international journals and at conferences. We believe that the proposed work and methodology is fairly generic and interdisciplinary in nature, and that advances made during the course of the project could benefit a wider group of medical researchers, engineers, and scientists involved in simulating and analyzing complex physical systems described by partial differential equations.

Given the fact that we propose to investigate a new computational paradigm, it is difficult at this stage to predict all the implications and applications of the proposed approach besides those we believe could be “natural” candidates: (i) medical applications: simulation of fluid structure interaction phenomenon for blood and air circulation; (ii) oil and gas transport: simulation of the flow in a network of pipes. (iii) architectural engineering: simulation of ventilation systems.

6 Professional position

Within NTNU:
If funded, the proposed research project will complement other onging research activities at the Department of Mathematical Sciences at NTNU. In particular, it will complement an already ongoing Strategic University Program in Computational Science and Engineering. It will complement and strengthen the expertise and research in the numerical solution of partial differential equations in general and in finite element methodology in particular, while at the same time have a focus on applications related to the physical sciences and to engineering, as well as to the medical field.

We also believe that the proposed project could be connected to the future teaching activities within the numerical subjects in the Department of Mathematical Sciences at NTNU. Besides learning about the more “conventional” methods for solving partial differential equations, learning how to develop and use reduced order models could also be a good way for students to better appreciate different ways of modeling the same underlying physical phenomenon.

Co-operation with Paris VI:
The preliminary results we have obtained so far have been obtained in collaboration with Prof. Yvon Maday at Laboratoire d’Analyse Numerique at Universite Pierre et Marie Curie (Paris VI); Prof. Maday was recently named Director of this laboratory. The project manager and Prof. Maday have enjoyed fruitful collaboration in the past, and both are looking forward to a continued interaction and collaboration on the proposed ideas.

Prof. Yvon Maday is an internationally recognized numerical analyst who has made major contributions to the analysis of methods for solving partial differential equations, in particular, in areas concerned with spectral methods, variational methods, domain decomposition methods, wavelets, fluid mechanics and quantum chemistry. Enclosed is a letter from Prof. Maday regarding his interest in the proposed project as well as his intent to collaborate.

Co-operation with MIT:
The project manager has also enjoyed more than 15 years of collaboration and interaction with Prof. Anthony T. Patera and his research group at Massachusetts Institute of Technology, Cambridge, USA. We anticipate that this collaboration and interaction will continue in the future. Given the fact that the research topics proposed here are related to Prof. Patera's own current research activities in reduced order modeling and *a posteriori* error estimation, we consider it natural that we will discuss and exchange ideas with him and his group.

7 Additional comments

It should be noted that the project manager for the proposed work has only worked in Norway for $1\frac{1}{2}$ years after studying and working in the United States for a total of 14 years. During the relatively short working period at NTNU, it has not been enough time to establish sufficient working relations with researchers at other universities and research institutions in Norway.

We believe that the proposed approach is at a too early stage to justify a large interdisciplinary team at this point. We believe that the focus should first be on investigating the basic concepts of the proposed approach with a nimble and complementary group of people.

Although fundamental research in numerical algorithms is always associated with risk, we are optimistic about the proposed ideas. We believe that new and promising computational paradigms and approaches to simulating complex systems are needed, and that the proposed project will give constructive insight into the opportunities, as well as the limitations, of using reduced basis models to this end.

Finally, we note that this project represents a good opportunity for a doctoral student to get trained in a variety of numerical methods and methodologies. We have not yet identified a potential doctoral candidate for the proposed work. With the new 5 year study program at NTNU, we anticipate that the most likely starting point for a doctoral candidate is in the middle of 2002. We will be actively looking for a good and motivated candidate for the proposed project.

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