

A reduced-basis element method

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Abstract

Reduced basis methods are particularly attractive to use in order to diminish the number of degrees-of-freedom associated with the approximation to a set of partial differential equations. The main idea is to construct ad hoc basis functions with a large information content. In this Note, we propose to develop and analyze reduced basis methods for simulating hierarchical flow systems, which is of relevance for studying flows in a network of pipes, an example being a set of arteries or veins. We propose to decompose the geometry into generic parts (e.g., pipes and bifurcations), and to construct a reduced basis for these generic parts by considering representative geometric snapshots. The global system is constructed by gluing the individual basis solutions together via Lagrange multipliers. *To cite this article: Y. Maday, E.M. Rønquist, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 195–200.* © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

Une méthode d'éléments en base réduite

Résumé

Les méthodes de base réduite sont particulièrement attractives par la diminution du nombre de degrés de liberté qu'elles entraînent pour l'approximation d'un système d'équations aux dérivées partielles. L'idée principale sur laquelle repose cette approche est la définition de fonctions de base ad hoc contenant une grande part d'information sur le système considéré. Dans cette Note nous proposons et analysons une méthode de base réduite pour la simulation d'écoulements dans un système hiérarchique comme ce peut être le cas dans un réseau de distribution de fluides ou le système sanguin. Nous proposons de décomposer la géométrie du domaine en un assemblage de formes génériques (des conduites et des bifurcations par exemple) et d'associer à ces sous parties des fonctions de bases réduites obtenues comme des instantanés géométriques représentatifs. Le système global est alors construit en recollant ces fonctions locales par des multiplicateurs de Lagrange. *Pour citer cet article : Y. Maday, E.M. Rønquist, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 195–200.* © 2002 Académie des sciences/Éditions scientifiques et médicales Elsevier SAS

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Les méthodes de base réduite [4] sont particulièrement attractives par la diminution du nombre de degrés de liberté qu'elles entraînent pour l'approximation d'un système d'équations aux dérivées partielles. L'idée principale sur laquelle repose cette approche est la définition de fonctions de base ad hoc contenant une grande part d'information sur le système considéré. Si l'on cherche $u(\mu)$ solution de (1) dans un espace fonctionnel approprié, où μ est un paramètre de \mathbb{R}^p , l'idée de base pour la définition de ces fonctions de base

est de calculer précisément des approximations de u pour un certain nombre de valeurs μ_i , $i = 1, \dots, n$, prédéfinies. Pour une valeur générique de μ , une approximation de $u(\mu)$ est alors recherchée dans l'espace engendré par ces solutions particulières. La conjonction de cette idée de base réduite avec la définition de bornes a posteriori proposée dans [2] permet de fiabiliser les résultats et l'utilisation de cette méthode avec confiance.

Dans cette Note nous proposons et analysons une méthode de base réduite pour la simulation d'écoulements dans un système hiérarchique comme ce peut être le cas dans un réseau de distribution de fluides ou le système sanguin. Nous proposons de décomposer la géométrie du domaine en un assemblage de formes génériques (des conduites et des bifurcations par exemple) et d'associer à ces sous-parties des fonctions de bases réduites obtenues comme des instantanés géométriques représentatifs. Le système global est alors construit en recollant ces fonctions locales par des multiplicateurs de Lagrange.

Nous considérons que le domaine Ω peut être décomposé en une union non recouvrante de sous domaines Ω_k , $k = 1, \dots, K$, de sorte que Ω_k est obtenu comme la déformation d'une forme de référence \mathcal{B}^m , $m = 1, \dots, M$ (disons un carré ou des bifurcations de référence) par une transformation régulière Φ_k . Nous supposons ensuite que chaque \mathcal{B}^m est muni de fonctions w_i^m , $i = 1, \dots, I$, solutions locales particulières pour des formes préchoisies. La méthode consiste alors à définir les espaces discrets (2), recollés globalement le long des interfaces suivant (3) pour un choix approprié des multiplicateurs de Lagrange $W_{k,\ell}$, sur chaque interface $\Gamma_{k,\ell}$ entre Ω_k et Ω_ℓ , puis de proposer une approximation de Galerkin du problème de départ. La méthode peut se révéler intéressante dans le cas où le domaine Ω présente une certaine complexité et où K est grand mais M petit. La complexité des calculs est alors faible si l'on peut choisir I assez petit (par exemple $I \leq 10$). Ce contexte entre dans le formalisme « en base réduite » de (1) comme on peut le voir en considérant que $\Omega = \Omega(\Phi)$ où le paramètre Φ désigne la collection des Φ_k . À notre connaissance, cette approche où la géométrie du domaine est le paramètre de la base réduite est nouvelle.

Nous avons testé cette approche sur le problème (5) avec la géométrie présentée à la Fig. 1. Les résultats sont particulièrement encourageants et une convergence exponentielle par rapport nombre de degré de liberté peut être exhibée.

1. Introduction

Reduced basis methods [4] are particularly attractive to use in order to diminish the number of degrees-of-freedom associated with the 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, or where the highly repetitive use of the underlying model becomes feasible, e.g., for design, optimization and real time control. 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.

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

$$F(u(\mu); \mu) = 0, \tag{1}$$

where X is some functional space, the parameter μ (e.g., representing material properties, geometric parameters, time, or some control) 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 very nice function so that, provided that some realizations $u(\mu_i)$ are known for some values $\mu = \mu_i$, with $i = 1, \dots, n$, 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 possibilities for inter- or extra-polation,

a Galerkin method is most often involved since for many types of problems, it allows us to infer the best linear combination of the various $u(\mu_i)$. The reduced basis methods are very attractive since, with very few basis functions, they describe the solution very well for many values of μ . However, these methods can also be deceptive, because the computation may involve too few basis functions to approximate the solution sufficiently well over the entire parameter space of interest. The reduced basis approach and the associated recent definition of bounds for outputs of interest are two coherent tools that allow us to extend the domain of applicability of numerical simulation by both increasing the speed of the computations and by providing conservative error bars on the outputs; see [2].

So far, the use of such reduced basis methods has been limited to finite dimensional parameter spaces. For evolution problems, time has been used as a parameter, and the solutions are found as linear combinations of snapshots of the process. Our approach here is to understand to what extent one can use the geometry of the computational domain as a generic parameter. We think of using “geometric snapshots” to approximate generically new situations.

In order to define our approach in more detail, we focus on geometries which can be decomposed into relatively simple parts, but where the overall system may be complex. An example of such a system is the flow in a network of pipes that can easily be decomposed, through a nonoverlapping domain decomposition, into a few generic shapes like deformed pipes and deformed bifurcations. The overall network is then comprised of the assembly of these simple generic parts, hereafter called elements, and each of these elements are provided with a family of generic solutions. Our objective is to glue both the shapes with identification of interfaces and the functions with Lagrange multipliers (in a mortar-like approach; see [1]). This allows us to define global functions by which we shall approximately solve the global problem.

This Note is a very first presentation of the results we have obtained so far, together with some heuristic analysis. We think that these results indicate that the proposed “reduced-basis element” method appears to have a potential interest. The particular PDE will be the Laplace equation, but this may already provide some hints to the behaviour of fluids through potential flow analysis.

2. Definition of the approach

We consider first the Poisson problem in a two-dimensional domain Ω with f given in $L^2(\Omega)$: find $u \in H^1(\Omega)$ such that $-\Delta u = f$ in Ω , complemented with appropriate boundary conditions.

We assume that the domain Ω can be decomposed into a nonoverlapping union of subdomains Ω_k , $k = 1, \dots, K$, such that each Ω_k is obtained as the deformation of a reference shape by a regular one to one transformation Φ_k . The reference shape will either be a square $]-1, 1[^2$ or a reference bifurcation. In general, we denote these reference shapes as \mathcal{B}^m , $m = 1, \dots, M$, and we assume that M is very small; here, we consider $M = 1$ or $M = 2$ for the sake of simplicity. Each Ω_k is thus a deformation of some $\mathcal{B}^{m(k)}$. We also make the assumption of “geometrical conformity” in the sense that each interface $\Gamma_{k,\ell}$ between two adjacent subdomains Ω_k and Ω_ℓ is assumed to be a whole common side of both Ω_k and Ω_ℓ .

We assume further that each reference domain \mathcal{B}^m comes with a set of functions w_i^m , $i = 1, \dots, I$, so that, over Ω , a finite dimensional space can be introduced:

$$Y_\delta = \left\{ v \in L^2(\Omega), v|_{\Omega_k} \circ \Phi_k \in \text{Vect}\{w_i^{m(k)}\} \right\}. \quad (2)$$

In order to propose an admissible discrete space for $H^1(\Omega)$, we have to glue together the values of elements of Y_δ through each interface $\Gamma_{k,\ell}$. The exact coincidence of the traces of the discrete functions is generally too stringent, and the gluing process is done in a dual way through Lagrange multipliers. We denote by $W_{k,\ell}$ a set of functions over each interface $\Gamma_{k,\ell}$, and we define

$$X_\delta = \left\{ v \in Y_\delta, \forall k, \ell, \forall \psi \in W_{k,\ell}, \int_{\Gamma_{k,\ell}} (v^+ - v^-)\psi = 0 \right\}, \quad (3)$$

where, for a given v in Y_δ and any interface $\Gamma_{k,\ell}$, $v_{\Gamma_{k,\ell}}^+ (= v^+)$ and $v_{\Gamma_{k,\ell}}^- (= v^-)$ stand for the two values that v takes on each side of $\Gamma_{k,\ell}$. The definition of the Lagrange multiplier space $W_{k,\ell}$ has to be done in a proper way and can also be defined through a mapping from a reference space of test functions over $]-1, 1[$. If we assume that $\chi_{k,\ell}$ is a parametrization from $]-1, 1[$ onto $\Gamma_{k,\ell}$, then a possible choice is $W_{k,\ell} = \{\psi \circ \chi_{k,\ell}, \psi \in \mathcal{W}_\delta\}$ where \mathcal{W}_δ is some given finite dimensional space.

The discrete problem can now be defined as: find $u_\delta \in X_\delta$ such that $\int_\Omega \nabla u_\delta \nabla v_\delta = \int_\Omega f v_\delta$ for all $v_\delta \in X_\delta$. It is an easy matter to check that this problem is well posed as soon as there exists a part of the boundary of Ω on which a Dirichlet boundary condition is imposed on u , and as soon as the constant functions belong to $W_{k,\ell}$, i.e., to \mathcal{W}_δ . In addition the following error estimate holds

$$\|u - u_\delta\|_* \leq c \inf_{v_\delta \in X_\delta} \|u - v_\delta\|_* + c \max_{v_\delta \in X_\delta} \max_{k,\ell} \frac{\int_{\Gamma_{k,\ell}} \frac{\partial u}{\partial n_{k,\ell}} (v^+ - v^-)}{\|v_\delta\|_*}, \tag{4}$$

where in the last expression — known as the consistency error — $n_{k,\ell}$ stands for the normal to the interface $\Gamma_{k,\ell}$. The first term in this error estimate is known as the best fit error and its smallness relies on the approximation properties of the basis functions $w_i^{m(k)}$.

The smallness of the consistency terms relies on the orthogonality property indicated in (3) that allows us to write $\int_{\Gamma_{k,\ell}} \frac{\partial u}{\partial n_{k,\ell}} (v^+ - v^-) = \int_{\Gamma_{k,\ell}} \left[\frac{\partial u}{\partial n_{k,\ell}} - \psi \right] (v^+ - v^-)$. It remains to choose a ψ in $W_{k,\ell}$ close enough to $\partial u / \partial n_{k,\ell}$. This remark helps us in choosing the space \mathcal{W}_δ . In contrast to general purpose methods such as finite element or spectral element methods, the evaluation of the best fit is not based on a density result formally written as $\bigcup_{\delta \rightarrow 0} X_\delta = H^1(\Omega)$, but on the fact that $u(\mu)$ is regular in μ . This is the main difference between a general purpose method and the reduced-basis element method: the dimension of the approximation space for the latter is much smaller, and the corresponding computational complexity is also smaller.

The previous definition of the space X_δ is general enough so that many methods fit into this framework. Our approach differs in the definition of the discrete functions $w_i^m, i = 1, \dots, I$. These are obtained by solving the problem we are interested in (here the Laplace problem) in some snapshots of deformed geometries and then mapped back over \mathcal{B}^m . This is the basic idea that was introduced in the Introduction, and which will be detailed further in the next section.

3. Definition of the basis functions in one domain

In what follows, we assume that the domain Ω is the range of $]-1, 1[^2 = \mathcal{B}^1$ by a regular mapping Φ . The domain of interest is thus a deformed square with 4 curved edges $\Gamma_1, \Gamma_2, \Gamma_3$ and Γ_4 . We then consider the Laplace problem ($f = 0$): find $u \in H^1(\Omega)$ such that

$$-\Delta u = 0 \quad \text{in } \Omega \quad \text{such that} \quad u = 1 \text{ over } \Gamma_1, \quad u = 0 \text{ over } \Gamma_3, \quad \frac{\partial u}{\partial n} = 0 \text{ over } \Gamma_2 \text{ and } \Gamma_4. \tag{5}$$

Let us now describe the approach for defining the discrete basis functions w_i^1 over \mathcal{B}^1 . We choose I geometric shapes, i.e., we choose I deformation mappings Φ_i from \mathcal{B}^1 into \mathbb{R}^2 , and solve as accurately as possible the corresponding problems of the type (5). The resulting solutions are denoted as u_i and are mapped onto \mathcal{B}^1 ; we then set $w_i^1 = u_i \circ \Phi_i$.

As a numerical example, we consider the solution of the Laplace equation in a deformed 90 degree bend; see Fig. 1a. We choose mappings $\Phi_i, i = 1, \dots, I$, corresponding to deformed squares as well as other deformed 90 degree bends; see [3] for more details. In all cases, only the edges Γ_2 and Γ_4 are curved; the edges Γ_1 and Γ_3 are straight sides which are either parallel to each other or perpendicular to each other. All the problems are discretized and solved using a single spectral element of order $p = 25$. Armed with a set of precomputed basis functions w_i^1 , we compute a reduced-basis element solution and compare this solution

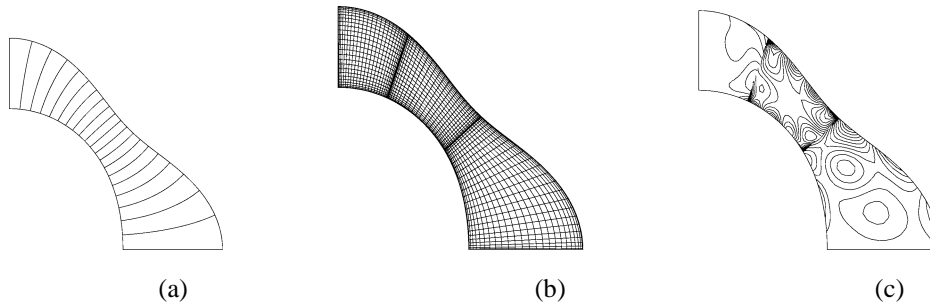


Figure 1. – (a) Contours of the solution; (b) three-domain case and spectral element grid; (c) error contours using $(11 + 20 + 10)$ basis functions and $n = 3$.

with the precomputed “exact” solution. We report the numerical results as the triplets (I, e_∞, e_N) where I is the number of basis functions, e_∞ is the corresponding maximum pointwise relative error, and e_N is the maximum of the error in the integrated fluxes along Γ_2 and Γ_4 . Our results are as follows: $(7, 0.098, 0.093)$, $(9, 0.019, 0.13)$, $(11, 0.0058, 0.011)$, $(15, 0.0030, 0.0069)$. In conclusion, for the computational problem considered here, and for the particular mappings chosen, rapid convergence is obtained in the maximum norm; the error in the fluxes is also decreasing significantly, although not monotonically.

It is of interest to understand to which extent this method enters within the framework of the reduced basis methods. Through a simple change of variable, the problem (5) can be set over \mathcal{B}^1 . Indeed, it takes the form $\int_{\mathcal{B}^1} \mathcal{J}(\Phi^{-1}) \widehat{\nabla} \hat{u} \mathcal{J}(\Phi^{-1}) \widehat{\nabla} \hat{v} J(\Phi) d\hat{x} d\hat{y} = \int_{\mathcal{B}^1} \hat{f} \hat{v} J(\Phi) d\hat{x} d\hat{y}$ where \hat{v} stands for $v \circ \Phi$, $\mathcal{J}(\Phi^{-1})$ is the jacobian matrix Φ^{-1} and $J(\Phi)$ is the jacobian of Φ . The dependency of this problem on the shape Φ is thus made explicit, and the problem can be written in the form (1). We may thus consider Φ as a parameter and write $\hat{u} \equiv \hat{u}(\Phi)$. In addition, it is an easy matter to verify that, at least in the neighborhood of the identity mapping $\Phi = \text{Id}$, the solution $\hat{u}(\Phi)$ together with $u(\Phi)$ are \mathcal{C}^∞ functions of Φ . This allows us to predict a good approximation property of $\hat{u}(\Phi)$ by a linear combination of the w_i^1 .

4. Definition of the basis functions in the multi-domain case

For purposes of exposition, we revisit our sample problem from the previous section, but now in the multi-domain case. We now need to generate basis functions with good approximation properties also at the level of the elements interfaces. In addition, we would like to reuse our set of generic basis functions over similar parts (in our case, deformed pipes). In order to meet these objectives, our approach is as follows. As in the single-domain case, we compute reference solutions in preselected geometries Ω_i , but where the domains are obtained through the deformation of the rectangle $]-1, 3[\times]-1, 1[$; see [3] for more details. The basis functions w_i^1 are then chosen to be the restrictions of these computed solutions (mapped back over the rectangle) to $]-1, 1[$. This way, on the boundary $1 \times]-1, 1[$ — that corresponds to an interface, say — the shape of w_i^1 is not predefined. The set of basis functions must be general enough to also be applicable to the case with two interfaces on a single element Ω_k (i.e., when $K \geq 3$). This can readily be achieved by using the precomputed set of basis functions, and then add their symmetric variants over $]-1, 1[$; by using reflection with respect to both spatial directions, the constructed basis will also have reduced sensitivity to directional effects in the preselected mappings (or preselected deformed geometries).

In the spirit of the mortar spectral element method, see [1], we choose here the Lagrange multiplier space $W_{k,\ell}$ to be the space of polynomials of degree less than or equal to n , with $n < p$. Fig. 1b depicts the computational domain using 3 subdomains, and with each subdomain discretized using a single spectral element of order $p = 25$. Fig. 1c shows the contours of the error when $n = 3$ ($n \ll p$), and using $(11 + 20 + 10)$ basis functions in the 3 subdomains; in this particular case, $\dim(X_\delta) < 11 + 20 + 10 = 41$.

The maximum pointwise relative error is $e = 0.0017$. Since the error in this case appears to be located mainly at the level of the interfaces, this reveals that the choice of (low order) polynomials ($n = 3$) is not completely appropriate, and that we should better define a space of Lagrange multipliers based on snapshots of $\partial u / \partial n$.

5. Complexity analysis

The computational cost associated with the reduced-basis element method comprises the cost of performing the following operations: (i) precomputing the functions w_i^m for each generic part m ; (ii) constructing the reduced-basis element stiffness matrix and the associated right-hand side; (iii) solving for the basis coefficients.

Step (i) can be done off-line using potentially a non-scalable or non-optimal simulation tool; the important thing is that the reduced order basis can be precomputed and stored for future use.

The cost of step (ii) depends on the dimension of the reduced basis system. For the multi-domain case considered in Section 4, the dimension of the reduced-basis stiffness matrix is bounded by $K \times I + (K - 1)(n + 1)$; the dimension 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.

Assume further that each discrete basis function $w_i^m(k)$ can be represented as a vector of dimension N (here, $N = (p + 1)^2$). Overall, for the spectral element systems considered here, and with $p > I$, the total cost is dominated by the cost of constructing the reduced-basis element stiffness matrix for each element Ω_k , i.e., performing I global matrix-vector products.

If $\dim(X_\delta)$ is reasonably small, the simplest and best way to solve for the basis coefficients is to use a standard LU-decomposition, and the cost of step (iii) is subdominant to the cost of step (ii).

6. Future work

Future work will focus on three central aspects of the proposed methodology. The first one is the question of how to choose the geometric snapshots in order to ensure good approximation properties in the case of more general domains/parts and boundary conditions.

The second aspect is related to the reuse of the same set of basis functions for similar parts. When extending the proposed methodology to fluid flows, the complexity of the physics could have an impact on which set of basis functions would be the best choice for a particular part. We expect that this could be an issue for convection-dominated flows.

Finally, if the discrete approach maintains its appealing properties, the next step will be to derive *a posteriori* tools in order to provide confidence in the numerical results and in order to allow us to the use of the proper number of basis functions over each generic element.

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