An efficient reduced-order modeling approach for nonlinear parametrized partial differential equations

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An efficient reduced-order modeling approach for nonlinear parametrized partial differential equations

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SUMMARY

For general nonlinear parametrized partial differential equations, the standard Galerkin projection is no longer efficient to generate reduced-order models. This is because the evaluation of the integrals involving the nonlinear terms has a high computational complexity and cannot be pre-computed. This situation also occurs for linear equations when the parametric dependence is nonaffine. In this paper, we propose an efficient approach to generate reduced-order models for large scale systems derived from partial differential equations which may involve nonlinear terms and nonaffine parametric dependence. The main idea is to replace the nonlinear and nonaffine terms with a coefficient-function approximation consisting of a linear combination of pre-computed basis functions with parameter-dependent coefficients. The coefficients are determined efficiently by an inexpensive and stable interpolation at some pre-computed points. The efficiency and accuracy of this method are demonstrated on several test cases, which show significant computational savings relative to the standard Galerkin projection reduced-order approach.

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KEY WORDS: parametrized PDEs; reduced-order approximation; standard Galerkin reduced order model; coefficient-function approximation; elliptic equations; convection-diffusion equations

1. Introduction

Many systems/processes in engineering and science are described by parametrized partial differential equations (PDEs). Typically, the quantities of engineering interests are not the full field variables, but rather certain outputs, best articulated as functionals of the field variables. Typical outputs include flowrate, pressure drops, concentration and flux, critical stresses or maximum displacements, and lift and drag forces. These outputs are functions of system parameters, or inputs, that serve to identify a particular configuration of the system — geometry, material properties, initial and boundary conditions, and loads. The

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relevant system behavior is thus described by an implicit input-output relationship, evaluation of which demands solution of the underlying PDE. The design, optimization, control, and characterization of engineering systems requires repeated and real-time output prediction.

Our goal is to develop an efficient reduced-order modeling approach for the rapid prediction of functional outputs associated with parametrized PDEs. Our approach is based on past and recent development of the reduced-basis approaches [1, 2, 3, 4, 5, 6, 7] and reduced-order modeling techniques [8, 9, 10, 11, 12, 13, 14]. The fundamental observation is that the field variable is not an arbitrary member of the infinite-dimensional solution space associated with the underlying PDE; rather, it resides on a much lower-dimensional manifold induced by the parametric dependence. Low order methods explicitly recognize and exploit this observation to develop reduced-order modeling of parametrized PDEs, often at a reduction of several orders of magnitude in the degrees of freedom compared to the classical models generated by finite element (FE), finite volume (FV), or finite difference (FD) methods.

In particular, the reduced-basis method has been successfully developed for (a) parametrized linear elliptic and parabolic PDEs that are affine† in the parameter [7, 15, 16, 17, 18, 19] and (b) nonlinear PDEs that are at most quadratically nonlinear in the field variable [20, 21, 22]. In these cases, a very efficient reduced-basis approximation can be developed by exploiting the affine decomposition of the parametrized differential operator and resolving nonlinear terms into the sum of products of the basis functions and coefficients; in such cases, the reduced-basis method offers significant — several orders of magnitude — computational savings relative to classical solution methods. However, while the assumptions of affine parameter dependence and quadratic nonlinearity are crucial to computational efficiency, they restrict the application of the reduced-basis method to some specific domains. For example, problems involving nonaffine parameter dependence and highly nonlinear terms do not fall into the categories (a) and (b). Hence, when applied to such problems, the traditional reduced-basis method no longer provides efficiency to compete with classical solution methods.

The Proper Orthogonal Decomposition (POD)-Galerkin approach has been widely used to produce reduced-order modeling of time-dependent PDEs. Nevertheless, its success and thus applications remain very much limited to linear and quadratically nonlinear problems such as linearized Euler and parabolic equations [12, 13, 23], Burgers equation [10, 24], and incompressible Navier-Stokes equations [11, 25, 26]. Other model reduction techniques have also been developed for nonlinear time-dependent problems. In particular, linearization methods [27, 28, 29] and polynomial approximation methods [30, 31] have been proposed to treat certain (weakly) nonlinear problems quite satisfactorily. However, inefficient representation of the nonlinear terms and fast growth of the computational complexity in the presence of strong nonlinearity, render these methods impractical for more general applications.

The classes of parametrized PDEs we consider here include (i) linear elliptic equations with nonaffine parameter dependence, (ii) nonlinear elliptic equations, and (iii) nonlinear time-dependent convection-diffusion equations. For such classes of PDEs, the reduced-order modeling provided by the standard Galerkin projection is no longer efficient. This is because the evaluation of the integrals involving the nonaffine and nonlinear terms has a high computational complexity and can not be pre-computed. To recover efficiency, we replace the nonaffine and

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†“Affine parameter dependence” means that the parametrized differential operator can be expressed as a sum of products of parameter-dependent functions and parameter-independent operators [7, 15, 16, 17].

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nonlinear terms with a \textit{coefficient-function approximation} consisting of a linear combination of pre-computed basis functions with parameter-dependent coefficients. The coefficients are determined very efficiently by an inexpensive and stable interpolation at some pre-computed points. This allows us to apply an offline/online computational decomposition \cite{7,17,21} for the generation and simulation of the reduced-order model. Unlike the standard Galerkin reduced-order approach, our method has a low computational complexity for the (online) evaluation of the integrals associated with the nonaffine and nonlinear terms. The method can thus effect considerable computational economies relative to both the standard Galerkin reduced-order approach and classical solution methods.

Our work is in some aspects related to a new reduced-basis approach, first introduced in \cite{32} for linear elliptic problems with nonaffine parameter dependence and recently extended more broadly to nonlinear elliptic and parabolic problems \cite{33}. However, our method differs from these earlier efforts in two important aspects. Rather than a greedy basis construction approach, we employ the POD approach to construct our low-dimensional approximation spaces. The POD basis provides the most accurate representation of the given snapshot set in the mean square error sense. More importantly, rather than the empirical interpolation method (EIM) \cite{32,33}, we use the so-called \textit{best points interpolation method} (BPIM) first introduced in \cite{34} to develop coefficient-function expansions for the nonaffine and nonlinear terms. Compared to the EIM, the BPIM is more expensive in the construction of interpolation points and basis functions, but provides approximations with higher accuracy than the EIM. As a result, with the BPIM we can use a smaller number of basis functions to achieve the same accuracy, which in turn leads to a more economical reduced-order model than with the EIM.

The paper is organized as follows. In Section 2, we present a short review of the BPIM. In subsequent sections, we introduce the abstract formulation and develop the reduced-order approximation for linear elliptic problems in Section 3, nonlinear elliptic problems in Section 4, and nonlinear time-dependent convection-diffusion problems in Section 5. Numerical examples are presented in each section in order to assess the efficiency and accuracy of our approach. Finally, in Section 6, we present concluding remarks.

2. Best Points Interpolation Method

In this section, we briefly describe the BPIM to construct a "coefficient-function" approximation of parametrized functions. The approximation of such class of functions is important for the effective reduced-order treatment of nonaffine and nonlinear PDEs.

2.1. Coefficient–Function Procedure

We consider the problem of approximating a given \( \mu \)-dependent function \( g(x; \mu) \in L^\infty(\Omega) \cap C^0(\Omega), \forall \mu \in D \), by a coefficient-function expansion \( g_M(x; \mu) \); here \( x = (x^1, \ldots, x^d) \) is a point of the physical domain \( \Omega \subset \mathbb{R}^d \), and \( D \subset \mathbb{R}^P \) is the parameter space in which our \( P \)-tuple parameter vector \( \mu = (\mu^1, \ldots, \mu^P) \) resides. Toward this end, we assume that we are given an approximation space spanned by \( M \) orthonormal basis functions, \( \Phi_M = \text{span}\{\phi_1, \ldots, \phi_M\} \), with \( (\phi_i, \phi_j) = \delta_{ij}, 1 \leq i, j \leq M \); here \( \delta \) is the Kronecker symbol and \( (\cdot, \cdot) \) denotes the \( L^2(\Omega) \) inner product with an induced norm \( \| \cdot \| = \sqrt{(\cdot, \cdot)} \). We further assume that we are given an associated set of \( M \) interpolation points \( \{z_m \in \Omega\}_{m=1}^M \).
Next, we define our coefficient-function approximation as

\[ g_M(x; \mu) = \sum_{m=1}^{M} \beta_M m(\mu) \phi_m(x) \]  

(1)

where the coefficient vector \( \beta_M(\mu) \) is the solution of

\[ \sum_{m=1}^{M} \phi_m(z_i) \beta_M m(\mu) = g(z_i; \mu), \quad i = 1, \ldots, M. \]  

(2)

We observe from (1)-(2) that \( g_M(x; \mu) \) and \( g(x; \mu) \) are equal at the interpolation points \( \{z_m\}_{m=1}^{M} \).

Note further that we can express \( g_M(x; \mu) \) in terms of the cardinal functions (Lagrange interpolation functions) as

\[ g_M(x; \mu) = \sum_{m=1}^{M} g(z_m; \mu) \psi_m(x). \]  

(3)

Here, the cardinal functions \( \{\psi_m\}_{m=1}^{M} \) are defined by \( \psi_j(z_i) = \delta_{ij} \), and hence given by

\[ \phi_i(x) = \sum_{j=1}^{M} \phi_i(z_j) \psi_j(x), \quad 1 \leq i \leq M. \]  

(4)

We point out that \( \{\psi_m\}_{m=1}^{M} \) depends on both \( \{\phi_m\}_{m=1}^{M} \) and \( \{z_m\}_{m=1}^{M} \).

The approximation quality depends critically both on the basis set \( \{\phi_m\}_{m=1}^{M} \) and the point set \( \{z_m\}_{m=1}^{M} \). In this paper, we use the POD method [35, 36, 37] to compute \( \{\phi_m\}_{m=1}^{M} \) from a suitably fine set of snapshots

\[ S^g_K = \{\xi^g_k(x) = g(x; \mu^g_k), \quad \mu^g_k \in S^g_K, 1 \leq k \leq K \}, \]  

(5)

where \( S^g_K = \{\mu^g_1, \ldots, \mu^g_K\} \) is a selected parameter sample set. Details of the POD procedure are given in the Appendix for reference. Once we have the basis set \( \{\phi_m\}_{m=1}^{M} \), we can determine the point set \( \{z_m\}_{m=1}^{M} \) as follows.

2.2. Interpolation Points

We first introduce the best approximations of the elements in the snapshot set as

\[ g^*_M(\cdot; \mu^g_k) = \arg \min_{w_M \in \Phi_M} \|g(\cdot; \mu^g_k) - w_M\|, \quad 1 \leq k \leq K. \]  

(6)

It is easily derived from the orthonormality of the \( \phi_m \) that

\[ g^*_M(x; \mu^g_k) = \sum_{m=1}^{M} \alpha_M m(\mu^g_k) \phi_m(x), \quad 1 \leq k \leq K, \]  

(7)

where the coefficients are given by

\[ \alpha_M m(\mu^g_k) = (\phi_m, g(\cdot; \mu^g_k)), \quad m = 1, \ldots, M, 1 \leq k \leq K. \]  

(8)
We now define our interpolation points \( \{ z_m \}_{m=1}^M \) as a minimizer of the following minimization problem

\[
\min_{x_1 \in \Omega, \ldots, x_M \in \Omega} \sum_{k=1}^K \left\| g_M^*(\cdot; \mu_k^q) - \sum_{m=1}^M \beta_{M_m}(x_1, \ldots, x_M; \mu_k^q) \phi_m \right\|^2 \tag{9}
\]

\[
\sum_{n=1}^M \phi_n(x_m) \beta_{M_n}(x_1, \ldots, x_M; \mu_k^q) = g(x_m; \mu_k^q), \quad 1 \leq m \leq M, 1 \leq k \leq K. \tag{10}
\]

By inserting (8) into (9) and invoking orthonormality of \( \{ \phi_m \}_{m=1}^M \), we obtain

\[
\min_{x_1 \in \Omega, \ldots, x_M \in \Omega} \sum_{k=1}^K \sum_{m=1}^M \left( \alpha_{M_m}(\mu_k^q) - \beta_{M_m}(x_1, \ldots, x_M; \mu_k^q) \right)^2 \tag{11}
\]

\[
\sum_{n=1}^M \phi_n(x_m) \beta_{M_n}(x_1, \ldots, x_M; \mu_k^q) = g(x_m; \mu_k^q), \quad 1 \leq m \leq M, 1 \leq k \leq K. \tag{12}
\]

In words, \( \{ z_m \}_{m=1}^M \) is determined so as to minimize the average error between the interpolants \( g_M(\cdot; \mu_k^q) \) and the best approximations \( g_M^*(\cdot; \mu_k^q) \). For this reason, the points \( \{ z_m \}_{m=1}^M \) shall be referred as “best points”.

2.3. Solution Procedure

We now find a solution of the least-squares minimization problem (10) using the Levenberg-Marquardt (LM) algorithm [38]. Let \( s = (x_1, \ldots, x_M) \), we write the objective in (10) as

\[
F(s) = \frac{1}{2} \sum_{q=1}^Q r_q^2(s), \tag{13}
\]

where \( r_q(s), 1 \leq q \leq Q = KM \), are given by

\[
r_q(s) = \alpha_{N_m}(\mu_k^q) - \beta_{N_m}(s; \mu_k^q), \quad 1 \leq k \leq K, 1 \leq m \leq M. \tag{14}
\]

The gradient and Hessian of the objective function \( F(s) \) can thus be computed as

\[
\nabla F(s) = \sum_{q=1}^Q r_q(s) \nabla r_q(s) = (J(s))^T r(s), \tag{15}
\]

\[
\nabla^2 F(s) = (J(s))^T J(s) + \sum_{q=1}^Q r_q(s) \nabla^2 r_q(s), \tag{16}
\]

where for \( 1 \leq q \leq Q, 1 \leq m \leq M \),

\[
J_{qm}(s) = \frac{\partial r_q(s)}{\partial x_m} = \frac{\partial \beta_{N_m}(s; \mu_k^q)}{\partial x_m}. \tag{17}
\]

Hence, when the residuals \( r_q(s) \) are small, we may approximately compute the Hessian in terms of only the Jacobian matrix \( J(s) \) as

\[
\nabla^2 F(s) \approx (J(s))^T J(s). \tag{18}
\]
The Jacobian matrix $J(s)$ is computed by differentiating both sides of the constraint (10) with respect to $s$. Finally, the interpolation points $z_m, 1 \leq m \leq M$ are determined by solving the problem (10). For the examples presented in this paper, the optimal solution is typically reached in less than 15 iterations of the LM algorithm. Further details and results about the BPIM method can be found in [34].

3. Nonaffine Linear Elliptic Equations

In this section, we develop the reduced-order approximation of linear elliptic equations with nonaffine parameter dependence. The basic idea is to replace the nonaffine terms with the coefficient-function expansions constructed using the BPIM. A model problem involving geometric variation is provided to demonstrate the application of our reduced-order approach to shape optimization problems.

3.1. Abstract Problem Formulation

We consider a suitably regular domain $\Omega \subset \mathbb{R}^{d-2}$ with spatial coordinate $x$ and define the Hilbert spaces $X \equiv H_0^1(\Omega)$ — or, more generally, $H_0^1(\Omega) \subset X \subset H^1(\Omega)$ — where $H^1(\Omega) = \{v \mid v \in L^2(\Omega), \nabla v \in (L^2(\Omega))^d\}$, $H_0^1(\Omega) = \{v \mid v \in H^1(\Omega), v|_{\partial \Omega} = 0\}$. We also recall the parameter domain $D \subset \mathbb{R}^{P}$ and parameter vector $\mu = (\mu^1, \ldots, \mu^P)$ introduced in the previous section.

The abstract formulation for a $\mu$-parametrized linear elliptic PDE can be stated as follows: given any $\mu \in D \subset \mathbb{R}^{P}$, we find

$$s(\mu) = \ell^O(u(\mu); \mu), \quad (17)$$

where $u(\mu) \in X(\Omega)$ is the solution of

$$a(u(\mu), v; \mu) = \ell(v; \mu), \quad \forall v \in X(\Omega). \quad (18)$$

Here, $\ell^O(\cdot; \mu), \ell(\cdot; \mu)$ are continuous functionals; and $a(\cdot; \mu)$ is a continuous bounded bilinear form. In addition, we make certain assumptions on the parametric dependence of $a, \ell,$ and $\ell^O$. In particular, we suppose that, for some finite $Q$, $a$ may be expressed as

$$a(w, v; \mu) = \sum_{q=1}^{Q} a^q(w, v, g^q(\cdot; \mu)), \quad (19)$$

and $\ell$ and $\ell^O$ are given by

$$\ell(v; \mu) = b(v, h(\cdot; \mu)), \quad (20)$$

$$\ell^O(v; \mu) = c(v, h^O(\cdot; \mu)). \quad (21)$$

Here $a^q: X \times X \times L^\infty(\Omega) \to \mathbb{R}, 1 \leq q \leq Q$, are continuous $\mu$-dependent trilinear forms; $b: X \times L^\infty(\Omega) \to \mathbb{R}$ and $c: X \times L^\infty(\Omega) \to \mathbb{R}$ are continuous $\mu$-dependent bilinear forms; and $h(x; \mu), h^O(x; \mu), g^q(x; \mu) \in L^\infty(\Omega) \cap C^0(\Omega): \Omega \times D \to \mathbb{R}, 1 \leq q \leq Q$, are known functions. We note that $a$ defined above is nonaffine in the parameter because the operators $a^q$ depend on $g^q(x; \mu)$ — general functions of spatial coordinate $x$ and parameter vector $\mu$.

In practice, the exact solution $u(\mu)$ is often not available, we thus replace $u(\mu)$ with a “truth” approximation, $u_h(\mu)$, which resides in (say) a suitably fine piecewise-linear FE approximation
space $X_h \subset X$ of very large dimension $\mathcal{N}$. The FE discretization of (17)-(18) is thus: given any $\mu \in \mathcal{D}$, we evaluate
\[
s_h(\mu) = \ell^O(u_h(\mu); \mu),
\]
where $u_h(\mu) \in X_h$ satisfies
\[
a(u_h(\mu), v; \mu) = \ell(v; \mu), \quad \forall v \in X_h.
\]

We shall assume that the discretization is sufficiently rich such that $u_h(\mu)$ and $u(\mu)$ and hence $s_h(\mu)$ and $s(\mu)$ are indistinguishable at the accuracy level of interest. Unfortunately, the computational cost associated with this FE approximation will depend on some power of $\mathcal{N}$. As a result, the evaluation $\mu \rightarrow s_h(\mu)$ is simply too costly in the many-query and real-time contexts often of interest in engineering.

In what follows, we develop a reduced-order approximation of th problem (17)-(18) for the rapid prediction of the output of interest. The reduced-order approximation shall be built upon the FE approximation, and the reduced-order error will thus be evaluated with respect to $s_h(\mu)$.

3.2. Reduced-Order Approximation

To begin, we introduce a parameter sample $S^u_K = \{\mu^u_1 \in \mathcal{D}, \ldots, \mu^u_K \in \mathcal{D}\}$ and an associated set of snapshots $S^u_K \equiv \{s^u_k = u_h(\mu^u_k), 1 \leq k \leq K\}$, where $u_h(\mu^u_k)$ is a solution of (23) for $\mu = \mu^u_k$. Upon the snapshot set $S^u_K$, we apply the POD procedure (see in the Appendix) to construct $N$ basis functions $\{\zeta_i\}_{i=1}^N$ and define an associated approximation space $W_N = \text{span}\{\zeta_1, \ldots, \zeta_N\}$.

Were we to follow the standard Galerkin reduced-order approach, we would obtain an approximation $u^SG_N(\mu) \in W_N$ that satisfies
\[
\sum_{q=1}^Q a^q(u^SG_N(\mu), v, g^q(\cdot; \mu)) = b(v, h(\cdot; \mu)), \quad \forall v \in W_N.
\]
Expressing $u^SG_N(\mu) = \sum_{j=1}^N u^SG_{N,j}(\mu) \zeta_j$ and choosing $v = \zeta_i$, $1 \leq i \leq N$, we arrive at
\[
A^SG_N(\mu)u^SG_N(\mu) = L^SG_N(\mu),
\]
where $A^SG_N(\mu) \in \mathbb{R}^{N \times N}$ and $L^SG_N(\mu) \in \mathbb{R}^N$ are given by
\[
A^SG_{ij}(\mu) = \sum_{q=1}^Q a^q(\zeta_j, \zeta_i, g^q(\cdot; \mu)), \quad 1 \leq i, j \leq N,
\]
\[
L^SG_{Ni}(\mu) = b(\zeta_i, h(\cdot; \mu)), \quad 1 \leq i \leq N.
\]
The output of interest would then be evaluated as
\[
s^SG_N(\mu) = \sum_{j=1}^N u^SG_{N,j}(\mu) c(\zeta_j, h^O(\cdot; \mu)).
\]
We note that since $N \ll \mathcal{N}$ the (full) linear system (25) of size $N \times N$ is very small compared to the (sparse) $\mathcal{N} \times \mathcal{N}$ linear system associated with the FE discretization (23). The standard Galerkin reduced-order approach can thus effect a significant reduction in the degrees of
freedom. Unfortunately, for any given parameter \( \mu \), the cost of assembling the stiffness matrix \( A^N_{\mu}^{SG}(\mu) \) depends on \( N \) because of the presence of the nonaffine functions \( g^q(\mathbf{x}; \mu), 1 \leq q \leq Q \), in the trilinear forms \( a^q, 1 \leq q \leq Q \). Similarly, the cost of assembling \( I^N_{\mu}^{SG}(\mu) \) and evaluating the output \( s^N_{\mu}^{SG}(\mu) \) also scales with \( N \). Consequently, although having much less degrees of freedom, the standard Galerkin reduced-order model may not offer significant computational savings relative to the FE approximation using advanced iterative methods.

To obtain an efficient reduced-order approximation, we first employ the BPIM to construct the point sets \( \{z^g_m\}^{M_g=1}, \{z^h_m\}^{M_h=1}, \{z^{h^{SG}}_m\}^{M_{h^{SG}}=1} \) and basis sets \( \{\psi^g_m\}^{M_g=1}, \{\psi^h_m\}^{M_h=1}, \{\psi^{h^{SG}}_m\}^{M_{h^{SG}}=1} \) for \( g^q(\mathbf{x}; \mu), 1 \leq q \leq Q; h(\mathbf{x}; \mu); h^O(\mathbf{x}; \mu) \), respectively, as described in Section 2. For notational simplification we presume that \( M^g = \ldots = M^h = M^{h^{SG}} = M \). We next replace \( g^q(\mathbf{x}; \mu), 1 \leq q \leq Q; h(\mathbf{x}; \mu); h^O(\mathbf{x}; \mu) \) with our coefficient-function expansions \( g^q_M(\mathbf{x}; \mu), 1 \leq q \leq Q; h_M(\mathbf{x}; \mu); h^O_M(\mathbf{x}; \mu) \), respectively. Our reduced-order approximation is thus: for any given \( \mu \in D \), we evaluate

\[
s_{N,M}(\mu) = c(u_{N,M}(\mu), h^O_M(\cdot; \mu)) ,
\]

where \( u_{N,M}(\mu) \in W_N \) satisfies

\[
\sum_{q=1}^{Q} a^q(u_{N,M}(\mu), v, g^q_M(\cdot; \mu)) = b(v, h_M(\cdot; \mu)), \quad \forall v \in W_N .
\]

In order derive the discrete equations for this reduced-order approximation, we write

\[
\begin{align*}
  u_{N,M}(\mu) &= \sum_{n=1}^{N} u_{N,M,n}(\mu) \zeta_i , \\
  g^q_M(\cdot; \mu) &= \sum_{m=1}^{M} g(z^g_m; \mu) \psi^g_m, \quad 1 \leq q \leq Q , \\
  h_M(\cdot; \mu) &= \sum_{m=1}^{M} h(z^h_m; \mu) \psi^h_m , \\
  h^O_M(\cdot; \mu) &= \sum_{m=1}^{M} h^O(z^{h^{SG}}_m; \mu) \psi^{h^{SG}}_m .
\end{align*}
\]

Inserting these representations into (29) and (28) and choosing \( v = \zeta_i, 1 \leq i \leq N \), we obtain

\[
\sum_{j=1}^{N} \left( \sum_{q=1}^{Q} \sum_{m=1}^{M} g^q(z^g_m; \mu) a^q(\zeta_i, \zeta_i, \psi^g_m) \right) u_{N,M,j}(\mu) = \\
\sum_{m=1}^{M} h(z^h_m; \mu) b(\zeta_i, \psi^h_m), \quad 1 \leq i \leq N ,
\]

and

\[
s_{N,M}(\mu) = \sum_{m=1}^{M} \sum_{j=1}^{N} h^O(z^{h^{SG}}_m; \mu) u_{N,M,j}(\mu) c(\zeta_j, \psi^{h^{SG}}_m) .
\]
Equivalently, we arrive at the linear system of \( N \) equations for the coefficient vector \( u_{N,M}(\mu) \)
\[ A_N(\mu)u_{N,M}(\mu) = L_N(\mu), \]
and then calculate
\[ s_{N,M}(\mu) = (L^O_N(\mu))^T u_{N,M}(\mu), \]
where
\[ A_N(\mu) = \sum_{q=1}^{Q} \sum_{m=1}^{M} g^q(z^q_m; \mu) A^q_m, \]
\[ L_N(\mu) = \sum_{m=1}^{M} h(z^m_m, \mu) L^m, \]
\[ L^O_N(\mu) = \sum_{m=1}^{M} h^O(z^O_m, \mu) L^O_m. \]

Here \( A^q_m \in \mathbb{R}^{N \times N}, 1 \leq q \leq Q, 1 \leq m \leq M \), and \( L^m, L^O_m \in \mathbb{R}^{N}, 1 \leq m \leq M \), are given by
\[ A^q_m_{ij} = a^q(\zeta_i, \zeta_j, \psi_g^q), \quad 1 \leq i,j \leq N, \]
\[ L^m_i = b(\zeta_i, \psi^h_m), \quad 1 \leq i \leq N, \]
\[ L^O_m_i = c(\zeta_i, \psi^O_{h^O}), \quad 1 \leq i \leq N. \]

The matrices and vectors in the above equation do not depend on the parameter vector \( \mu \) and can therefore be pre-computed offline. The remaining operations required to form (33)-(35) can be performed online.

We summarize the computational process in Figure 1 for the offline stage and in Figure 2 for the online stage. The offline construction of our reduced-order model is of course computationally intensive, but it is done only one time. However, in the online stage, we can compute \( s_{N,M}(\mu) \) with a total cost of \( O(N^3 + QMN^2) \) operations for any given new parameter vector \( \mu \).

Hence, as required in the many-query or real-time contexts, the online complexity is independent of \( N \) — the dimension of the FE approximation space. Since \( N,M,Q \ll N \), we expect significant computational savings in the online stage relative to the FE approximation (23) and relative to the standard Galerkin reduced-order model built upon (24).

### 3.3. Example 1: A Problem of Geometric Variation

We consider Poisson’s equation with homogenous Dirichlet condition solved on a parametrized domain \( \Omega(\mu) \),
\[ -\nabla^2 \Psi = 1, \quad \text{in} \ \Omega(\mu), \]
\[ \Psi = 0, \quad \text{on} \ \partial \Omega. \]

The parameter vector is given by \( \mu = (\mu^1, \mu^2) \equiv (R, \kappa) \in D \equiv [1, 10] \times [1, 10] \) where \( R \) and \( \kappa \) control the size and shape of the domain as shown in Figure 3; the inner and outer boundaries of the cross-section are described by the closed curves \( |z^1|^{\kappa} + |z^2|^{\kappa} = 1 \) and \( |z^1|^{\kappa} + |z^2|^{\kappa} = (R + 1)^{\kappa} \), respectively. Finally, the output of interest is the integral of \( \Psi \).
Over a "fixed" reference domain $\Omega \equiv \Omega^o$, we establish a one-to-one mapping between $\Omega$ and $\Omega^\ast$, over $\hat{\Omega}$. Although simple enough, this example serves to demonstrate the usefulness of our reduced-order approach for shape optimization problems.

Due to geometric symmetry, the problem can be reformulated as $-\nabla^2 u^o = 1$ in $\Omega^o(\mu)$ with homogeneous Neumann condition on $\Gamma_N^o \equiv \Gamma_1^o \cup \Gamma_3^o$ and homogeneous Dirichlet condition on $\Gamma_D^o \equiv \Gamma_2^o \cup \Gamma_4^o$; here $\Omega^o(\mu)$ is a "cut" domain as shown in Figure 4(b). Hence, $u^o(\mu) \in X^o$, $X^o \equiv \{ v \in H^1(\Omega^o(\mu)) | v|_{\Gamma_D^o} = 0 \}$, is the solution of
\[
\int_{\Omega^o(\mu)} \nabla u^o(\mu) \cdot \nabla v d\Omega^o = \int_{\Gamma_N^o(\mu)} v d\Gamma^o, \quad \forall v \in H^1(\Omega^o(\mu)).
\]
(37)

The output of interest is then $s^o(\mu) = 8 \int_{\Omega^o(\mu)} u^o(\mu) d\Omega^o$.

We treat geometric variation in an indirect way by transforming the equation (37) on $\Omega^o(\mu)$ to a new equation on a "fixed" reference domain $\Omega \equiv [0, 1] \times [0, 1]$ shown in Figure 4(a). To do this, we establish a one-to-one mapping between $\Omega$ and $\Omega^o(\mu)$. The geometric mapping $\mathcal{F}$ from $x = (x^1, x^2) \in \Omega$ to $x_o = (x_o^1, x_o^2) \in \Omega^o(\mu)$ is given by
\[
x^1_o = \frac{(x^1)((x^2)R + 1)}{(1 + (x^1)^{\kappa})^{1/\kappa}}, \quad x^2_o = \frac{(x^2)R + 1}{(1 + (x^1)^{\kappa})^{1/\kappa}}.
\]
(38)

Our exact solution on the original domain, $u^o(\mu)$, can then be expressed in terms of the solution on the mapped domain, $u(\mu)$, as $u^o(x_o; \mu) = u(\mathcal{F}^{-1}(x_o); \mu)$. The solution on the mapped domain satisfies a weak formulation of the form (18) in which the trilinear forms,
Figure 3. The cross-section $\hat{\Omega}$ varies with geometric parameters $R$ and $\kappa$. The “cut” domain $\Omega^o$ is formed by the dash lines and the boundary of the cross-section.

Figure 4. The computational domains: (a) reference domain $\Omega$ and (b) original cut domain $\Omega^o$.

Figure 5. The FE solutions on the physical domain $\hat{\Omega}$ for: (a) $\mu = (1,1)$, (b) $\mu = (1,2)$, and (c) $\mu = (1,10)$. Note how the geometry and solution change as $\mu^2$ increases.
bilinear forms, and nonaffine functions are given by

\[
a^1(w, v, g^1(x; \mu)) = \int_{\Omega} g^1(x; \mu) \frac{\partial w}{\partial x^1} \frac{\partial v}{\partial x^1} d\Omega,
\]

\[
a^2(w, v, g^2(x; \mu)) = \int_{\Omega} g^2(x; \mu) \frac{\partial w}{\partial x^1} \frac{\partial v}{\partial x^2} d\Omega,
\]

\[
a^3(w, v, g^3(x; \mu)) = \int_{\Omega} g^3(x; \mu) \left( \frac{\partial w}{\partial x^1} \frac{\partial v}{\partial x^2} + \frac{\partial w}{\partial x^2} \frac{\partial v}{\partial x^1} \right) d\Omega,
\]

\[
b(v, h(x; \mu)) = \int_{\Omega} h(x; \mu) v d\Omega,
\]

\[
c(v, h^O(x; \mu)) = \int_{\Omega} h^O(x; \mu) v d\Omega,
\]

\[
g^1(x; \mu) = \frac{R(1 + (x^1)^2)}{R(x^2) + 1},
\]

\[
g^2(x; \mu) = \frac{R(1 + (x^1)^{2\kappa} - (x^1) + (x^1)^{2\kappa} + 1)}{R((x^1)^\kappa + 1)^2},
\]

\[
g^3(x; \mu) = \frac{(x^1)^{\kappa - 1} - (x^1)^{\kappa + 1}}{(x^1)^{\kappa} + 1},
\]

\[
h(x; \mu) = R(1 + (x^1)^{\kappa} - 2/\kappa (R(x^2) + 1),
\]

\[
h^O(x; \mu) = R(1 + (x^1)^{\kappa} - 2/\kappa (R(x^2) + 1).
\]

Here \(X \equiv \{v \in H^1(\Omega) \mid v|_{\Gamma_{\partial_3}} = 0\}\). The output is evaluated as \(s(\mu) = \ell^O(u(\mu); \mu)\); note for this example \(\ell^O = \ell\) and \(h^O(x; \mu) = h(x; \mu)\).

The computational domain is discretized uniformly into piecewise-linear resulting in a FE approximation space \(X_h \in X\) of dimension \(N = 10,000\). We present in Figure 5 the computed solutions for different parameter values. As regards the offline construction, we choose for \(S^O_K\) a regular grid of 15 \times 15 points over \(\mathcal{D}\) and construct \(\{\psi_h^m\}_{m=1}^{M_{\max}}, \{z_h^m\}_{m=1}^{M_{\max}}, \{u_h^m\}_{m=1}^{M_{\max}}, \{z_{\max}^m\}_{m=1}^{M_{\max}}, 1 \leq q \leq Q, M_{\max} = 12\); we then take \(S^K_u = S^K_v\) and compute the associated snapshot set \(S^K_x\) upon which the basis set \(\{\zeta^n\}_{n=1}^{N_{\max}}\) is constructed for \(N_{\max} = 30\). We plot in Figure 6 the point sets corresponding to \(g^O(x; \mu)\) and \(h(x; \mu)\) for \(M = M_{\max}\). We see that most interpolation points are distributed along the \(x^2 = 0.6\) and \(x^2 = 0\) lines. Since these functions are linear in \(x^2\), only two points suffice to capture their behavior in the \(x^2\) direction.

We now present results obtained with our reduced-order approach. For this purpose, we choose a test sample \(\Xi_{\text{Test}}\) as a regular \(20 \times 20\) grid over \(\mathcal{D}\) and define the average relative error norm as

\[
\epsilon_{\text{ave,rel}}^u = \text{mean}_{\mu \in \Xi_{\text{Test}}} \frac{\|u_h(\mu) - u_{N,M}(\mu)\|}{\|u_h(\mu)\|}.
\]

Figure 7 shows \(\epsilon_{\text{ave,rel}}^u\) as a function of \(N\) and \(M\). We observe very rapid convergence of \(u_{N,M}(\mu)\) to \(u_h(\mu)\). The quality of the reduced-order approximation depends on \(N\) and \(M\) in a strongly coupled manner: for a fixed value of \(M\) the error initially decreases with increasing \(N\) and then levels off for \(N\) large enough; when the error does not improve with increasing \(N\), increasing \(M\) tends to reduce the error. This behavior of the error is expected because the accuracy of our reduced-order approximation is limited by the coefficient-function approximation error which is decreased with increasing \(M\). It basically suggests that optimal combinations of \(N\) and \(M\) are
at the “knees” of the error curves: for example, the combination $M = 6$ and $N = 12$ appears to be nearly optimal. Furthermore, we note that our coefficient-function approximation can lead to a very accurate representation of the nonaffine terms and indeed, for this example, $M$ can be chosen smaller than $N$ without sacrificing the accuracy.

Finally, we compare the results obtained with the proposed reduced-order approach (ROA) to those obtained with the standard Galerkin reduced-order approach (SGA). In Table I, we present the maximum relative error in the output over the test sample $\Xi_{\text{Test}}$ and computational times as a function of $N$ for both the ROA (with $M = 12$) and SGA. Here, the computational
times are normalized with respect to the time required to compute the finite element approximation (FEA) output \( s_h(\mu) \) shown in the last column of Table I. Since the standard Galerkin reduced-order model suffers from a \( N \)-dependent cost of assembling the reduced stiffness matrix and load vector, its computational advantage relative to the FE approximation is very modest as observed in Table I. In contrast, our reduced-order approximation achieves significant computational savings relative to the FE approximation and yields a convergence rate which is very similar to that of the standard Galerkin reduced-order model. Of course, this comparison is only meaningful if we are in the real-time or many-query contexts — in which the offline cost can be amortized over many output predictions.

4. Nonlinear Elliptic Equations

In this section, we illustrate how the proposed approach can be applied to nonlinear elliptic equations. The numerical difficulty is the presence of strong nonlinearities in the differential operator; we shall simply treat nonlinear terms as “functions” and construct associated coefficient-function approximations. In what follows, we introduce the abstract formulation of nonlinear elliptic equations and develop the associated reduced-order approximation; we then discuss numerical results obtained for a model problem.

4.1. Abstract Problem Formulation

We consider the following problem: for any \( \mu \in D \), find

\[
    s(\mu) = \ell^O(u(\mu)) ,
\]

where \( u(\mu) \) satisfies the weak form of the \( \mu \)-parametrized nonlinear elliptic PDE

\[
    \Theta(\mu)a_L(u(\mu), v) + \int_\Omega g(u(\mu); \mu)vd\Omega = \ell(v), \quad \forall v \in X .
\]

Here \( g(w; \mu) : X \times D \to \mathbb{R} \) is a general nonlinear function of \( w \in X \) and the parameter vector \( \mu; \Theta : D \to \mathbb{R} \) is a \( \mu \)-dependent function; \( a_L : X \times X \to \mathbb{R} \) is a continuous bounded bilinear and \( \ell^O, \ell : X \to \mathbb{R} \) are continuous bounded functionals. Here for simplicity, we shall assumed that
REDUCED ORDER MODELING FOR PARAMETRIZED NONLINEAR PDES

Our abstract problem is well-posed in the sense of Hadamard, meaning that its solution exists, is unique and depends continuously on the data functional $\ell$.

Next, we recall our FE approximation space $X_h(\subset X)$ of dimension $N$. Our FE approximation is then: given $\mu \in \mathcal{D}$, we find

$$s_h(\mu) = \ell^O(u_h(\mu)),$$

where $u_h(\mu) \in X_h$ is the solution of the discretized weak statement

$$\Theta(\mu)a_L(u_h(\mu), v) + \int_{\Omega} g(u_h(\mu); \mu)v d\Omega = \ell(v), \quad \forall v \in X_h. \tag{42}$$

We assume that $|s(\mu) - s_h(\mu)|$ is suitably small and hence that $\mathcal{N}$ will typically be very large.

4.2. Reduced-Order Approximation

We first introduce a sample set $S^u_K = \{\mu^u_1 \in \mathcal{D}, \ldots, \mu^u_K \in \mathcal{D}\}$, associated snapshot set $S^g_k = \{\xi_k = u_h(\mu^u_k), 1 \leq k \leq K\}$, and reduced basis space $W_N = \text{span}\{\zeta_n, 1 \leq n \leq N\}$; here $u_h(\mu^u_k)$ is the solution of (42) at $\mu = \mu^u_k$ and $\zeta_n, 1 \leq n \leq N$, are the POD basis functions. The standard Galerkin reduced-order model $\{7, 15, 16, 17, 18\}$ is then obtained by a standard Galerkin projection: given $\mu \in \mathcal{D}$, we evaluate

$$s^{SG}_N(\mu) = \ell^O(u^{SG}_N(\mu)),$$

where $u^{SG}_N(\mu) \in W_N$ satisfies

$$\Theta(\mu)a_L(u^{SG}_N(\mu), v) + \int_{\Omega} g(u^{SG}_N(\mu); \mu)v d\Omega = \ell(v), \quad \forall v \in W_N. \tag{44}$$

Unfortunately, the presence of strong nonlinearity in $g$ does not allow for the efficient offline-online procedure outlined in Section 3.2. As a result, although the dimension of the system (44) is small, solving it is actually expensive: the evaluation of the integral $\int_{\Omega} g(u^{SG}_N(\mu); \mu)v d\Omega$ will scale as some power of $\mathcal{N}$. Therefore, it is somewhat disingenuous to interpret (44) as a reduced-order model.

We seek to develop a reduced-order approximation with an online evaluation cost independent of $\mathcal{N}$. Towards this goal, we compute a set of snapshots

$$S^g_K = \{\xi^g_k = g(u_h(\mu^u_k); \mu), 1 \leq k \leq K = IJ\}.$$

(Recall that the $u_h(\mu_k)$ were already computed for all $\mu^u_k \in S^u_K$.) We then construct $\{z^g_m\}_{m=1}^M$ and $\{\psi^g_m\}_{m=1}^M$ by following the procedures described in Section 2. Then, for any given $w \in X_h$, we approximate $g(w; \mu)$ by $g_M^w = \sum_{m=1}^M g(w(z^g_m); \mu)\psi^g_m$.

We may now replace $g(u^{SG}_N(\mu); \mu)$ — as required in our reduced basis projection for $u^{SG}_N(\mu)$ — with $g_M^{u_{N,M}}(\mu; \mu)$. Our reduced basis approximation is thus: given $\mu \in \mathcal{D}$, we evaluate

$$s_{N,M}(\mu) = \ell^O(u_{N,M}(\mu)),$$

where $u_{N,M}(\mu) \in W_N$ satisfies

$$\Theta(\mu)a_L(u_{N,M}(\mu), v) + \int_{\Omega} g_{N,M}(\mu; \mu)v d\Omega = \ell(v), \quad \forall v \in W_N. \tag{46}$$
We expand our reduced-order approximation and coefficient-function approximation as
\[ u_{N,M}(\mu) = \sum_{j=1}^{N} u_{N,M,j}(\mu) \zeta_j , \]
\[ g_N^{u_{N,M}}(x; \mu) = \sum_{m=1}^{M} g(u_{N,M}(z_m^\mu); \mu) \psi_m^\mu = \sum_{m=1}^{M} g \left( \sum_{j=1}^{N} u_{N,M,j}(\mu) \zeta_j(z_m^\mu); \mu \right) \psi_m^\mu . \]

Inserting these representations into (46) yields
\[ \Theta(\mu) A_N u_{N,M}(\mu) + C_{N,M} g(D_{M,N} u_{N,M}(\mu); \mu) = L_N , \]
where \( A_N \in \mathbb{R}^{N \times N}, C_{N,M} \in \mathbb{R}^{N \times M}, D_{M,N} \in \mathbb{R}^{M \times N}, L_N \in \mathbb{R}^{N}, L_N^O \in \mathbb{R}^N \) are given by
\[ A_{N,ij} = a_L(\zeta_j, \zeta_i), \quad 1 \leq i, j \leq N \]
\[ C_{N,M,im} = \int_{\Omega} \psi_m^\mu d\zeta, \quad 1 \leq i \leq N, 1 \leq m \leq M \]
\[ D_{M,N,mj} = \tilde{\zeta}_j(z_m^\mu), \quad 1 \leq m \leq M, 1 \leq j \leq N \]
\[ L_{N,i} = \ell(\zeta_i), \quad 1 \leq i \leq N \]
\[ L_{N,i}^O = \ell^O(\zeta_i), \quad 1 \leq i \leq N ; \]
these reduced-order matrices and vectors are parameter-independent.

To solve (47) for \( u_{N,M}(\mu) \), we may apply a Newton iterative scheme: given a current iterate \( \bar{u}_{N,M}(\mu) \) we must find an increment \( \delta u_{N,M}(\mu) \) such that
\[ (\Theta(\mu) A_N + \bar{E}_N(\mu)) \delta u_{N,M}(\mu) = L_N - \Theta(\mu) A_N \bar{u}_{N,M}(\mu) - C_{N,M} g(D_{M,N} \bar{u}_{N,M}(\mu); \mu) . \]

Here, \( \bar{E}_N(\mu) \in \mathbb{R}^{N \times N} \) must be calculated at every Newton iteration as
\[ \bar{E}_{N,i,j}(\mu) = \sum_{m=1}^{M} C_{N,M,im} g_1 \left( \sum_{n=1}^{N} D_{M,N,mn} \bar{u}_{N,M,n}(\mu); \mu \right) D_{M,N,mj}, \quad 1 \leq i, j \leq N , \]
where \( g_1(w; \mu) \) is the first derivative of \( g \) with respect to \( w \). Note that calculating \( \bar{E}_N(\mu) \) has a cost of \( O(MN^2) \).

Finally, we evaluate the reduced-order output as
\[ s_{N,M}(\mu) = (L_N^O)^T u_{N,M}(\mu) . \]

Similarly as in Section 3.2, we can develop an efficient offline-online procedure for the rapid evaluation of \( s_{N,M}(\mu) \) for each \( \mu \) in \( D \).

The operation count of the online stage is essentially the predominant Newton update component (49): at each Newton iteration, we first assemble the right-hand side and compute \( \bar{E}_N^N \) at cost \( O(MN^2) \); we then form and invert the left-hand side (Jacobian) of (49) at cost \( O(N^3) \). The online complexity depends only on \( N, M \), and the number of Newton iterations; we thus recover \( N \) independence in the online stage.
4.3. Example 2: Non-polynomial Nonlinearity

We consider a particular instantiation of our abstract statement in which

$$
\Theta(\mu) = \mu^1, \quad a_L(w, v) = \int_\Omega \nabla w \cdot \nabla v d\Omega, \quad g(w; \mu) = |w|^2 - 1 w,
$$

and $\ell^O(v) = \ell(v) = \int_\Omega v d\Omega$. Here, $\Omega = [0, 1] \times [0, 1]$, $D = [0.01, 1] \times [1, 10] \in \mathbb{R}^2$, and $X = H^1_0(\Omega)$. Our model problem is well-posed and becomes linear for $\mu^2 = 1$.

We present in Figure 8 two typical solutions obtained with a regular linear triangular FE approximation space $X_h$ of dimension $N = 10,000$. We see that as $\mu^1$ decreases and $\mu^2$ increases, the solution develops a boundary layer. For the offline construction, we choose $S_K$ as the nodes of a regular $12 \times 12$ grid over $D$ and generate $\{\zeta_n\}_{n=1}^{N_{\text{max}}}$, $\{\psi_m\}_{m=1}^{M_{\text{max}}}$, and $\{\zeta_m\}_{m=1}^{M_{\text{max}}}$ for $N_{\text{max}} = 9$ and $M_{\text{max}} = 10$. We plot the interpolation point set $\{\zeta_m\}_{m=1}^{M_{\text{max}}}$ in Figure 9. We see that all the points lie in one quarter of the domain due to the symmetry in the solution; and that many points lie close to the boundary due to the presence of the boundary layer.

We now present numerical results for the reduced-order approximation. We show in Figure 10 the convergence of $e_{\text{ave,rel}}^N$ with respect to $N$ and $M$. Here $e_{\text{ave,rel}}^N$ is the average relative error norm over the parameter sample $\Xi_{\text{Test}} \subset D$ of size $16 \times 16$. The reduced-order approximation converges very rapidly to the FE approximation. Furthermore, the error behavior is similar to that of the linear example of Section 3.3: the errors initially decrease, but then “plateau” in $N$ for a particular value of $M$; then increasing $M$ reduces the errors further. This implies that for a given $N$, we can always choose $M$ large enough that the error induced by the coefficient-function approximation does not affect the desired accuracy of our reduced-order approximation.

We compare numerical results obtained with our reduced-order approach and with the standard Galerkin reduced-order approach. We tabulate in Table II the maximum relative error in the output over $\Xi_{\text{Test}}$ and computational times as a function of $N$ (for $M = 10$) for both the ROA and SGA. Here, the computational times are normalized with respect to the time to compute $s_h(\mu)$ in the last column of Table II. We observe very high accuracy of the
Figure 9. Distribution of the interpolation points \( \{ z_m \}_{m=1}^{M_{\text{max}}} \) over the physical domain \( \Omega \) for \( M_{\text{max}} = 10 \).

Figure 10. Average relative error norm \( \epsilon_{\text{ave,rel}}^u \) as a function of \( N \) and \( M \) for the Example 2.

output approximation and significant computational savings: for a relative accuracy of less than 0.0002 \((N = 4, M = 10)\), the online time to compute \( s_{N,M}(\mu) \) is less than 1/30,000 the time to compute \( s_h(\mu) \). In addition, thanks to fast convergence of the coefficient-function and reduced-order approximations and thanks to the \( N \)-independent computational cost of the online stage, our reduced-order model is almost four orders of magnitude less expensive than the standard Galerkin reduced-order model, while yielding practically the same convergence and accuracy.
Table II. Numerical results for the Example 2: Maximum relative error in the output over $\Xi_{\text{test}}$ and normalized computational time as a function of $N$ for the ROA (with $M = 10$) and SGA. The computational times are normalized with respect to the computational time for $s_h(\mu)$.

<table>
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<th>$M$</th>
<th>ROA Max. rel. error</th>
<th>ROA Online time</th>
<th>SGA Max. rel. error</th>
<th>SGA Online time</th>
<th>FEA Comp. time</th>
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5. Nonlinear Convection-Diffusion Equations

In order to illustrate how our proposed approach can accommodate time-dependent problems, we consider a scalar nonlinear convection-diffusion problem with only one parameter $\mu \in \mathbb{R}$. We note that the approach can be easily extended to multi-parameter systems of PDEs. The essential new ingredient is the presence of time; we shall simply treat time as an additional, albeit special, parameter. We briefly describe the abstract formulation of nonlinear convection-diffusion equations and then develop the associated reduced-order approximation. Finally, we discuss the results obtained using our approach and the reduced-basis approach presented in [32, 33] for the two-dimensional Buckley-Leverret equation.

5.1. Abstract Problem Formulation

We consider the following problem: for any given $\mu \in \mathcal{D} \subset \mathbb{R}$, we find the output of interest as

$$s(\mu, t) = \ell^O(u(\mu, t)),$$

where $u(\mu, t)$ is the solution of

$$m \left( \frac{\partial u(\mu, t)}{\partial t}, v \right) - \int_{\Omega} \left( \frac{\partial f^1(u(\mu, t))}{\partial x^1} + \frac{\partial f^2(u(\mu, t))}{\partial x^2} \right) d\Omega + \mu a_L(u(\mu, t), v) = 0, \quad \forall v \in X, t \in (0, T] ,$$

with initial condition $u(\mu, 0) = u_0(x)$ and appropriate boundary condition. Here, $\mu$ is a viscosity parameter varying in the parameter space $\mathcal{D} \subset \mathbb{R}$; the fluxes, $(f^1(u(\mu, t)))$ and $(f^2(u(\mu, t)))$, are nonlinear functions of the field variable $u(\mu, t)$; $a_L$ and $m$ are parameter-independent bilinear forms; and $\ell^O$ is a linear functional. We note that the output and field variable are now functions of both the parameter $\mu$ and time $t$.

We consider a discretization of (52)-(53) using the FE approximation and the second-order backward difference formula. We denote the number of time steps by $J$ and let $\Delta t = T/J$. We further introduce a piecewise-linear FE approximation space $X_h$ of very large dimension $N$. Our FE discretization is thus: given any $\mu \in \mathcal{D}$, for $j = 2, \ldots, J$, evaluate

$$s_h(\mu, t^j) = \ell^O(u_h(\mu, t^j)) ,$$


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Then for any given \( w \) following the procedures described in Section 2. (For notational simplification, we assume \( u \) forward in time requires \( u_h(\mu, t^j) \) from \( u_h(\mu, 0) \).) In essence, (55) yields a nonlinear discrete system of equations which can be solved by Newton's method at each timestep.

5.2. Reduced-Order Approximation

We introduce an approximation subspace \( W_N = \text{span}\{\xi_1, \ldots, \xi_N\} \), where the basis functions \( \xi_n \) are constructed using the POD procedure on a set of snapshots

\[
S_n^w \equiv \{ \xi_k^w = u_h(\mu^w, t^j) \}, 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K = IJ \}
\]

Here, \( u_h(\mu^w, t^j) \), \( 1 \leq j \leq J \), are solutions of (55) at parameter points \( \mu_i, 1 \leq i \leq I \), belonging to the sample set \( S_n^w = \{ \mu^w_i \in D, \ldots, \mu^w_J \in D \} \).

We next consider the standard Galerkin projection: for \( \mu \in D \), we find

\[
s_N^G(\mu, t^j) = \ell^j(u_N^G(\mu, t^j)), \quad 2 \leq j \leq J,
\]

where \( u_N^G(\mu, t^j) \in W_N \) satisfies

\[
m(u_N^G(\mu, t^j), v) - \frac{2}{3} \Delta t \int_{\Omega} f^1(u_N^G(\mu, t^j)) \frac{\partial v}{\partial x_1} d\Omega
- \frac{2}{3} \Delta t \int_{\Omega} f^2(u_N^G(\mu, t^j)) \frac{\partial v}{\partial x_2} d\Omega
+ \frac{2}{3} \Delta t \partial x a_L(u_N^G(\mu, t^j), v)
= \frac{4}{3} m(u_N^G(\mu, t^j-1), v) - \frac{1}{3} m(u_N^G(\mu, t^j-2), v), \quad v \in W_N.
\]

As pointed out earlier, this standard Galerkin reduced-order model is not efficient.

To recover efficiency, we develop the coefficient-function approximation for the nonlinear terms in (57). Henceforth, we compute two sets of snapshots

\[
F_K^1 \equiv \{ \xi_k^f = f^1(u_h(\mu^w, t^j)), 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K = IJ \},
\]

\[
F_K^2 \equiv \{ \xi_k^f = f^2(u_h(\mu^w, t^j)), 1 \leq i \leq I, 1 \leq j \leq J, 1 \leq k \leq K = IJ \},
\]

from which we construct \( \{ z_{m}^{f1} \}_{m=1}^{M} \), \( \{ \psi_{m}^{f1} \}_{m=1}^{M} \), \( \{ z_{m}^{f2} \}_{m=1}^{M} \), \( \{ \psi_{m}^{f2} \}_{m=1}^{M} \), respectively, following the procedures described in Section 2. (For notational simplification, we assume that the number of basis functions for both the coefficient-function expansions are the same.) Then for any given \( w \in X_h \), we approximate \( f^1(w) \) by \( f^1_M = \sum_{m=1}^{M} f^1(w(z_{m}^{f1}))/\psi_{m}^{f1} \) and \( f^2(w) \) by \( f^2_M = \sum_{m=1}^{M} f^2(w(z_{m}^{f2}))/\psi_{m}^{f2} \).
Our reduced-order approximation is obtained by replacing $f^1(u_N^S(\mu, t^j))$ and $f^2(u_N^S(\mu, t^j))$ with $f_M^{1,u,M}(\mu, t^j)$ and $f_M^{2,u,M}(\mu, t^j)$: given any $\mu \in D$, for $j = 2, \ldots, J$, we evaluate

$$s_{N,M}(\mu, t^j) = t^j(u_{N,M}(\mu, t^j)),$$

where $u_{N,M}(\mu, t^j) \in W_N$ satisfies

$$m(u_{N,M}(\mu, t^j), v) = -\frac{2}{3} \Delta t \int_\Omega f^{1,u,M}(\mu, t^j) \frac{\partial v}{\partial x_1} d\Omega$$

$$- \frac{2}{3} \Delta t \int_\Omega f^{2,u,M}(\mu, t^j) \frac{\partial v}{\partial x_2} d\Omega + \frac{2}{3} \Delta t a_L(u_{N,M}(\mu, t^j), v)$$

$$= \frac{4}{3} m(u_{N,M}(\mu, t^{j-1}), v) - \frac{1}{3} m(u_{N,M}(\mu, t^{j-2}), v), \quad v \in W_N. \quad (59)$$

Furthermore, we expand

$$u_{N,M}(\mu, t^j) = \sum_{n=1}^N u_{N,M,n}(\mu, t^j) \zeta_n,$$

$$f_M^{1,u,M}(\mu, t^j) = \sum_{m=1}^M f^1(u_{N,M}(z_m^j; \mu, t^j)) \psi_m = \sum_{m=1}^M f^1 \left( \sum_{n=1}^N u_{N,M,n}(\mu, t^j) \zeta_n(z_m^j) \right) \psi_m,$$

$$f_M^{2,u,M}(\mu, t^j) = \sum_{m=1}^M f^2(u_{N,M}(z_m^j; \mu, t^j)) \psi_m = \sum_{m=1}^M f^2 \left( \sum_{n=1}^N u_{N,M,n}(\mu, t^j) \zeta_n(z_m^j) \right) \psi_m.$$

Inserting these representations into (59), and choosing $v = \zeta_{n'}, 1 \leq n' \leq N$, we immediately obtain the nonlinear algebraic system: for $j = 2, \ldots, J$, $u_{N,M}(\mu, t^j) = [u_{N,M,1}(\mu, t^j), \ldots, u_{N,M,N}(\mu, t^j)]^T \in \mathbb{R}^N$ satisfies

$$M_{N} u_{N,M}(\mu, t^j) - \frac{2}{3} \Delta t (C_{N,M}^{1} F_{M}(u_{N,M}(\mu, t^j)) + C_{N,M}^{2} F_{M}(u_{N,M}(\mu, t^j)))$$

$$+ \frac{2}{3} \Delta t \mu A_{N} u_{N,M}(\mu, t^j) = \frac{1}{3} M_{N} (4 u_{N,M}(\mu, t^{j-1}) - u_{N,M}(\mu, t^{j-2})),$$

with the initial vector $u_{N,M,n}(0) = (u_h(0), \zeta_n), 1 \leq n \leq N$ and with the coefficient vector $u_{N,M}(\mu, t^1)$ being computed by the Crank-Nicolson scheme.

In the above, $M_N \in \mathbb{R}^{N \times N}$ and $A_N \in \mathbb{R}^{N \times N}$ are matrices with entries

$$M_{N,n,m} = m(\zeta_n, \zeta_n), \quad A_{N,n,m} = a_L(\zeta_n, \zeta_n), \quad (61)$$

for $1 \leq n, n' \leq N$; $C_{N,M}^{1} \in \mathbb{R}^{N \times M}$ and $C_{N,M}^{2} \in \mathbb{R}^{N \times M}$ are given by

$$C_{N,M}^{1,n,m} = \int_\Omega \psi_m \frac{\partial \zeta_n}{\partial x_1}, \quad C_{N,M}^{2,n,m} = \int_\Omega \psi_m \frac{\partial \zeta_n}{\partial x_2}, \quad (62)$$

for $1 \leq n \leq N, 1 \leq m \leq M$; and $F_{M}(u_{N,M}(\mu, t^j)) \in \mathbb{R}^M$ and $\tilde{F}_{M}(u_{N,M}(\mu, t^j)) \in \mathbb{R}^M$ are given by

$$F_{M}^{1}(u_{N,M}(\mu, t^j)) = f^1(D_{M,N}^{1} u_{N,M}(\mu, t^j)), \quad (63)$$

$$F_{M}^{2}(u_{N,M}(\mu, t^j)) = f^2(D_{M,N}^{2} u_{N,M}(\mu, t^j)), \quad (64)$$
where \( D_{M,N}^1 \in \mathbb{R}^{M \times N} \) and \( D_{M,N}^2 \in \mathbb{R}^{M \times N} \) are matrices with entries
\[
D_{M,N}^1_{mn} = \zeta_n(z_m^1), \quad D_{M,N}^2_{mn} = \zeta_n(z_m^2),
\]
for \( 1 \leq m \leq M, 1 \leq n \leq N \).

The nonlinear algebraic system (60) can be readily solved by using the Newton’s method at each timestep for the coefficient vectors \( u_{N,M}(\mu, t^j) \), \( 1 \leq j \leq J \). The reduced-order output is then calculated as
\[
s_{N,M}(\mu, t^j) = (L^O_N)^T u_{N,M}(\mu, t^j), \quad 1 \leq j \leq J.
\]
Here \( L^O_N \in \mathbb{R}^N \) is the output vector with entries \( L^O_n = \ell^O(\zeta_n), 1 \leq n \leq N \). The offline-online procedure can be developed as follows.

In the offline stage, we compute and store \( u_{N,M}(0), A_N, M_N, C^1_{N,M}, C^2_{N,M}, D_{M,N}, L^O_N \). In the online stage — for each new parameter value \( \mu \) — we solve the nonlinear system (60) at each timestep for the coefficient vector \( u_{N,M}(\mu, t^j) \) and evaluate the output \( s_{N,M}(\mu, t^j) \) with a computational cost (per Newton iteration per timestep) of only \( O(MN^2 + N^3) \).

5.3. Example 3: Buckley-Leverett equation

Our example is the two-dimensional Buckley-Leverett equation
\[
\frac{\partial u}{\partial t} + \frac{\partial f^1(u)}{\partial x} + \frac{\partial f^2(u)}{\partial y} - \mu \nabla^2 u = 0, \quad \text{in } \Omega \times (0, T],
\]
with initial condition \( u_0(x) = \exp(-16((x_1)^2 + (x_2)^2)) \) and homogeneous boundary condition on \( \partial \Omega \). Here \( \Omega = [-1.5, 1.5]^2 \), \( \mu \in \mathcal{D} \equiv [0.05, 0.1], t \in (0, T] \) with \( T = 0.5 \), and \( f^1(u) \) and \( f^2(u) \) are the fluxes which are nonlinear functions of the field variable \( u \),
\[
f^1(u) = \frac{u^2}{u^2 + (1 - u)^2}, \quad f^2(u) = f_1(u)(1 - 5(1 - u)^2).
\]
The output of interest is the average of the field variable over the physical domain.

The weak formulation is stated as: given \( \mu \in \mathcal{D} \), find \( s(\mu, t) = \int_\Omega u(\mu, t), \) where \( u(\mu, t) \in X = H^1_0(\Omega) \equiv \{ v \in H^1(\Omega) \mid v|_{\partial \Omega} = 0 \} \) is the solution of
\[
\int_\Omega \frac{\partial u}{\partial t} v d\Omega - \int_\Omega \frac{\partial f^1(u)}{\partial x} v d\Omega - \int_\Omega \frac{\partial f^2(u)}{\partial y} v d\Omega + \mu \int_\Omega \nabla u \cdot \nabla v = 0, \quad \forall v \in X, t \in (0, T].
\]

Our abstract statement (53)-(52) thus obtains for
\[
m(w, v) = \int_\Omega w v d\Omega, \quad a(w, v) = \int_\Omega \nabla w \cdot \nabla v d\Omega, \quad \ell^O(v) = \int_\Omega v d\Omega.
\]
For the FE discretization, we use \( \Delta t = 0.02 \) (\( J = 25 \) time steps) and a uniform triangular piecewise-linear FE approximation space of dimension \( N = 10,000 \). Figure 11 shows two typical solutions at time \( t^j = 10 \Delta t \) for different values of \( \mu \). We see that when \( \mu = 0.05 \), the solution develops sharp gradient due to the strong effect of nonlinearity. However, as \( \mu \) increases, the effect of nonlinearity is dominated by the viscous effects, and the solution spreads out.
Figure 11. Numerical solutions for the Example 3 at $t^j = 10\Delta t$: (a) $\mu = 0.05$ and (b) $\mu = 0.1$.

We now present the results obtained. For this purpose we define the average relative error in the solution as

$$
\epsilon_{u,\text{ave,rel}} = \frac{\text{mean}_{\mu \in \Xi_{\text{Test}}, 1 \leq j \leq J} \left\| u_h(\mu, t^j) - u_{N,M}(\mu, t^j) \right\|}{\left\| u_h(\mu, t^j) \right\|}.
$$

Here $\Xi_{\text{Test}} \subset \mathcal{D}$ is the parameter test sample of size 21. Figure 12 shows $\epsilon_{u,\text{ave,rel}}$ as a function of $N$ and $M$. We observe very rapid convergence of our reduced-order approximation and a similar convergence behavior as already seen in the previous examples. Note our offline construction is based on $\mathcal{S}_K^u$ which consists of the initial solution $u_h(t^0)$ and $11 \times 25$ solutions corresponding to the parameter sample $\mathcal{S}_I^u = \{\mu_1^I, \ldots, \mu_I^I\}$ of size $I = 11$. We include $u_h(t^0)$ in $\mathcal{S}_K^u$ to render the error at time $t = 0$ as small as possible.

Figure 12. Average relative error $\epsilon_{u,\text{ave,rel}}$ as a function of $N$ and $M$ for the Example 3.
We next compare numerical results obtained with the proposed approach, the reduced-basis approach (RBA) of [32, 33], and the standard Galerkin reduced-order approach. In Table III, we present the maximum relative error in the output as a function of \( N \) and \( M \) for the ROA, RBA, and SGA. We first see that the three approaches yield uniform and rapid convergence of the reduced-order output approximation. However, the ROA results in smaller errors than the RBA for all values of \( N \) and \( M \): for example, for the case of \((N, M) = (30, 40)\), the error is \(9.51 \times 10^{-4}\) for the ROA and is \(3.10 \times 10^{-3}\) for the RBA. Furthermore, we observe that the differences in the results obtained with the ROA and SGA are very small.

Finally, in Table IV, we present the computational times to calculate the output as a function of \( N \) and \( M \). Here the computational times are normalized with respect to the time to compute the FE approximation output shown in the last column of Table IV. For a relative accuracy of less than 0.1 percent (corresponding to \((N, M) = (30, 40)\) with the ROA and \((N, M) = (40, 50)\) with the RBA), the reduction in online response time for both the ROA and RBA is more than four orders of magnitude compared to the SGA and FEA. This is due to the dramatic dimension reduction provided by the Galerkin projection on the reduced-basis space and the coefficient-function approximation of the nonlinear terms. We notice however that the offline computations are expensive since we must solve for the FE solutions over the parameter sample set. Hence, if a many-query context, or a clear demand for real-time response, can justify the offline cost, the proposed approach and the reduced-basis approach presented in [32, 33] can be gainfully employed.

6. Conclusions

We have presented an efficient numerical approach for developing reduced-order models of nonaffine and nonlinear parametrized PDEs. Although we discuss scalar problems and linear functionals, our approach can be easily extended to systems of equations and nonlinear functionals. It is demonstrated through numerical examples that the approach provides computational savings of many orders of magnitude relative to both the FE approximation and standard Galerkin reduced-order approach. Compared to the reduced basis approach of [32, 33], the proposed method is found to produce better, more accurate, models at a slightly higher computational cost in the offline stage. Therefore, the proposed approach can be gainfully used...
Table IV. Online computational times (normalized with respect to the computational time of the FE approximation) for different values of $N$ and $M$ for the Example 3.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$M$</th>
<th>ROA Online time</th>
<th>RBA Online time</th>
<th>SGA Online time</th>
<th>FEA Comp. time</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>20</td>
<td>2.58E-05</td>
<td>2.58E-05</td>
<td>4.35E-01</td>
<td>1</td>
</tr>
<tr>
<td>20</td>
<td>30</td>
<td>3.16E-05</td>
<td>3.16E-05</td>
<td>4.37E-01</td>
<td>1</td>
</tr>
<tr>
<td>30</td>
<td>40</td>
<td>5.34E-05</td>
<td>5.34E-05</td>
<td>4.38E-01</td>
<td>1</td>
</tr>
<tr>
<td>40</td>
<td>50</td>
<td>8.50E-05</td>
<td>8.50E-05</td>
<td>4.40E-01</td>
<td>1</td>
</tr>
<tr>
<td>50</td>
<td>60</td>
<td>1.38E-04</td>
<td>1.38E-04</td>
<td>4.42E-01</td>
<td>1</td>
</tr>
</tbody>
</table>

to generate efficient low order models of nonlinear large-scale systems, which are of considerable interest in the parameter estimation, design, optimization, and control contexts.

In this paper, we have not considered the selection of snapshots and a posteriori error estimation. The accuracy, efficiency, and reliability of a reduced-order model depend crucially on the quality of the snapshot set for guaranteeing stable and rapid convergence, and a posteriori estimator for quantifying the error in the approximation process. While these important issues need to be addressed in the reduced-order modeling of parametrized partial differential equations, they remain very open and challenging especially for nonlinear problems, the discussion of which is beyond the scope of this paper. Instead, we refer the reader to [39, 40] for a greedy algorithm for the judicious selection of snapshots and a posteriori error estimation procedures for linear and certain nonlinear problems.

APPENDIX

II. POD Procedure

We describe the POD procedure to generate an orthonormal basis set $\{\varphi_n\}_{n=1}^N$ from any given set of linearly independent snapshots $\{\xi_k\}_{k=1}^K$. First, a two-point spatial correlation function is defined as

$$\mathcal{K}(x, x') = \frac{1}{K} \sum_{k=1}^{K} \xi_k(x)\xi_k(x')$$

(69)

which accepts the following spectral decomposition

$$\mathcal{K}(x, x') = \sum_{k=1}^{K} \lambda_k \varphi_k(x)\varphi_k(x')$$

(70)

Here, the set of basis functions $\varphi_k, 1 \leq k \leq K$, are ordered such that the associated eigenvalues

$$\lambda_k = \frac{1}{K} \sum_{l=1}^{K} (\varphi_k, \xi_l)^2$$

(71)

satisfy $\lambda_k \geq \lambda_{k+1}$. 

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Next, for a given $N < K$, the POD procedure consists in finding $\varphi_n, 1 \leq n \leq N$, so as to maximize the captured energy

$$\max E_N = \sum_{n=1}^{N} \left( \frac{1}{K} \sum_{k=1}^{K} (\varphi_n, \xi_k)^2 \right) = \sum_{n=1}^{N} \lambda_n,$$

subject to the constraints $(\varphi_n, \varphi_n')_X = \delta_{nn'}, 1 \leq n, n' \leq N$. The first few basis functions represent the main energy-containing structures in the snapshots, with their relative importance quantified by $\lambda_n$. It can be shown that problem (72) amounts to solve the eigenfunction equation

$$(K(x, x'), \varphi(x'))_X = \lambda \varphi(x)$$

for the first $N$ eigenfunctions.

The method of snapshots [37] expresses a typical empirical eigenfunction $\varphi(x)$ as a linear combination of the $\xi_k$

$$\varphi(x) = \sum_{k=1}^{K} a_k \xi_k(x).$$

Inserting this representation and (69) into (73), we immediately obtain

$$C a = \lambda a,$$

where $C \in \mathbb{R}^{K \times K}$ is given by $C_{ij} = \frac{1}{K} (\xi_i, \xi_j)_X, 1 \leq i, j \leq K$. The eigenproblem (75) can then be solved for the first $N$ eigenvectors from which the POD basis functions $\varphi_n, 1 \leq n \leq N$, are constructed using (74).

The optimality of the POD basis can be shown by considering an arbitrary set of orthonormal basis functions, $\{v_n\}_{n=1}^{N}$, and demonstrating that the POD basis $\{\varphi_n\}_{n=1}^{N}$ minimizes

$$\min_{\alpha_1, \ldots, \alpha_N} \frac{1}{K} \left( \inf_{\alpha_k \in \mathbb{R}^N} \left\| \xi_k - \sum_{n=1}^{N} \alpha_k^N v_n \right\|_X^2 \right).$$

Indeed, this minimization problem is equivalent to the maximization problem (72), which in turn asserts the optimality of $\{\varphi_n\}_{n=1}^{N}$.

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