Efficient Reduced Basis Solution of Quadratically Nonlinear Diffusion Equations

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Abstract: We present reduced basis approximations and associated a posteriori error estimation procedures for a steady quadratically nonlinear diffusion equation. We develop an efficient computational procedure for the evaluation of the approximation and bound. The method is thus ideally suited for many-query or real-time applications. Numerical results are presented to confirm the rigor, sharpness and fast convergence of our approach.

Keywords: Parametrized partial differential equations, reduced basis approximation, a posteriori error estimation, nonlinear diffusion equations.

1. INTRODUCTION

Nonlinear diffusion problems appear in a large number of real world applications ranging from biology to ecology, heat radiation and fluid flows, see Vazquez (2006). These equations often involve a large number of parameters such as viscosity constants or diffusion coefficients which, in general, have a strong influence on the behavior of the system. Hence, to analyze and understand a specific model many different combinations of parameters have to be investigated.

However, classical discretization techniques such as finite element methods and finite volume methods often prove prohibitively expensive if the system has to be evaluated at a large number of different parameters. Efficient techniques to solve these parametric problems are therefore important. Our goal here is development of a numerical technique that permits rapid yet accurate and reliable prediction of quadratically nonlinear parametrized diffusion equations. To achieve this goal we pursue the reduced basis (RB) method. The reduced basis method is a model order reduction technique that has proven to admit efficient and reliable reduced-order approximations for a large class of parametrized partial differential equations; see Rozza et al. (2008) for a recent review.

The study of nonlinear diffusion problems started in 1831 with the evolution of a two-phase system (water and ice) and was led to a free boundary problem which came to be known as Stefan problem. It took more than 120 years until a complete solution of this problem with existence and uniqueness results in the context of weak solutions was given in Oleinik et al. (1958). In this paper we consider diffusion equations of the type

$$ \text{div}(D(u)\nabla u) = f, $$  \hspace{1cm} (1)

where $D(u)$ is a linear function of $u$. This problem is particularly important in heat transfer applications where the heat conductivity depends linearly on the temperature.

The rest of this paper is organized as follows: In Section 2 we introduce the problem statement as well as the notation required later; we also introduce a model problem to which we shall apply the new method. The reduced basis approximation and associated a posteriori error estimation are discussed in Section 3. Finally, in Section 4 we present numerical results for our model problem.

2. PROBLEM STATEMENT

2.1 Abstract Framework

We first define the Hilbert space $X^e \equiv H^1_0(\Omega)$, or more generally, $H^1_0(\Omega) \subset X^e \subset H^1(\Omega)$, where $H^1_0(\Omega) = \{v|v \in L^2(\Omega), \nabla v \in (L^2(\Omega))^d\}$, $H^1(\Omega) = \{v|v \in H^1(\Omega), v|_{\partial \Omega} = 0\}$, and $L^2(\Omega)$ is the space of square integrable functions over $\Omega$. Here $\Omega$ is a bounded domain in $\mathbb{R}^d, d = 1, 2, 3$, with Lipschitz continuous boundary $\partial \Omega$. The inner product and norm associated with $X^e$ are given by $(\cdot, \cdot)_{X^e}$ and $\| \cdot \|_{X^e} = (\cdot, \cdot)_{X^e}^{1/2}$; respectively. For example we may take

$$ (w,v)_{X^e} \equiv \int_{\Omega} \nabla w \nabla v, \quad \forall w, v \in X^e. \hspace{1cm} (2)$$

The abstract formulation can then be stated as follows: given any parameter $\mu \in (\mu_0, \mu_1) \in \mathcal{D} \subset \mathbb{R}^2$, we evaluate $u^e(\mu) \in X^e$, where $u^e(\mu)$ is the solution of

$$ a(u^e(\mu), v, G(u^e(\mu); \mu)) = f(v), \quad \forall v \in X^e. \hspace{1cm} (3)$$

Here $\mathcal{D}$ is the admissible parameter domain, $a$ is given by

$$ a(w,v, G(w; \mu)) = \int_{\Omega} G(w; \mu) \nabla w \nabla v, \quad \forall w, v \in X^e, \hspace{1cm} (4)$$

with $G(w; \mu) = \mu_0 + \mu_1 w$, and $f(v)$ is a $X^e$-continuous linear form. We can thus write
In order to formulate conditions for existence and unique-
approximation shall be built upon this truth finite element
subspace $X$. In actual practice, of course, we do not have access to the
well-posedness of (3) can be found in Caloz et al. (1997).

2.2 Truth Approximation

In actual practice, of course, we do not have access to the
exact solution. We thus introduce a “truth” approximation
subspace $X \subset X^*$ and replace $w^*(\mu) \in X^*$ with a “truth”
approximation $u(\mu) \in X$. Here, $X$ is a suitably fine
piecewise linear finite element approximation space with
very large dimension $N$. $X$ shall inherit the inner product
and norm from $X^*$. Our truth approximation is thus: for
any $\mu \in \mathcal{D}$, evaluate the output $s : \mathcal{D} \mapsto \mathbb{R}$ from

$$ s(\mu) = \ell(u(\mu)), $$

where $u(\mu) \in X$ satisfies

$$ a(u(\mu), v, G(u(\mu); \mu)) = f(v), \quad \forall v \in V. $$

We shall assume that the discretization is sufficiently rich
such that $u(\mu)$ and $w^*(\mu)$ are indistinguishable. The RB
approximation shall be built upon this truth finite element
approximation and the RB error will thus be evaluated with
respect to $u(\mu) \in X$.

In order to formulate conditions for existence and uniqueness
of the solution, for given $z \in X$ and every $v, w \in X$, we define the Frechet derivative
form $dg : X^3 \times \mathcal{D} \mapsto \mathbb{R}$ as

$$ dg(w, v, z; \mu) = a_0(w, v; \mu) + a_1(z, w, v; \mu) + a_1(w, v, z; \mu). $$

We have also defined the inf-sup constant

$$ \beta_{\infty}(\mu) = \inf_{w \in X} \sup_{v \in X} \frac{dg(w, v; z; \mu)}{\|w\| X \|v\| X}, \quad z \in X, $$

and the continuity constant

$$ \gamma_{\infty}(\mu) = \sup_{w \in X} \sup_{v \in X} \frac{dg(w, v; z; \mu)}{\|w\| X \|v\| X}, \quad z \in X. $$

We further assume that $a_0$ and $a_1$ satisfy

$$ |a_0(w, v)| \leq \|w\| X \|v\| X, $$

$$ |a_1(z, w, v)| \leq \rho \|z\| X \|w\| X \|v\| X. $$

Assumptions (15), (16) immediately imply boundedness of
dg. We also assume that there exists a constant $\beta_0 > 0$, such that

$$ \beta_{\infty}(\mu) \geq \beta_0, \quad \forall \mu \in \mathcal{D}. $$

2.3 Algebraic Equations

We now express the solution $u(\mu)$ as

$$ u(\mu) = \sum_{j=1}^{N} u_j(\mu) \phi_j, $$

where the $\phi_j, 1 \leq j \leq N$, are the basis functions for our
approximation space $X$. Choosing basis functions
$\phi_j$, $1 \leq i \leq N$, as test functions $v$ in (11) we can show that

$$ u(\mu) = [u_1(\mu), u_2(\mu), \ldots, u_N(\mu)] \in \mathbb{R}^N $$

satisfies

$$ [\mu_0 A_0 + \mu_1 A_1(u)] \mu = F, $$

where $A_0 \in \mathbb{R}^{N \times N}$ and $F \in \mathbb{R}^N$ are parameter-
indepedent matrix and vector with entries $A_{ij}^{1,0} = a_0(\phi_j, \phi_i),
1 \leq i, j \leq N$, and $F_i = f(\phi_i), 1 \leq j \leq N$, respectively.
Furthermore $A_1(u) \in \mathbb{R}^{N \times N}$ has entries

$$ A_{ij}^{1,1} = a_1(\phi_j, \phi_i), $$

where

$$ A_{ij}^{1,1} = a_1(\phi_j, \phi_i), \quad 1 \leq i, j, n \leq N. $$

We now solve (19), for $u(\mu)$, using a Newton iterative
scheme as follows: starting with an initial value $\tilde{u}_0$, we find an increment $\Delta u_0 \in \mathbb{R}^N$ such that

$$ \left [ \mu_0 A_0 + \mu_1 (A_1(u_0) + \tilde{A}_1(u_0)) \right ] \Delta u_0 = F - \left [ \mu_0 A_0 + \mu_1 A_1(u_0) \right ] u_0. $$

We update $u_1 = u_0 + \Delta u_0$ and continue this process until

$$ ||\Delta u_0|| < \epsilon_{tol} $$

is satisfied for some $k \geq 0$. The matrices
$A_1(u_0) \in \mathbb{R}^{N \times N}$ and $\tilde{A}_1(u_0) \in \mathbb{R}^{N \times N}$ have entries

$$ A_{ij}^{1,1} = \sum_{n=1}^{N} u_{0n} A_{ij}^{1,1,n}, $$

where

$$ \tilde{A}_{ij}^{1,1} = \sum_{n=1}^{N} u_{0n} \tilde{A}_{ij}^{1,1,n}, $$

and matrix $A_{ij}^{1,1,n}$ is defined in (20) and

$$ \tilde{A}_{ij}^{1,1,n} = a_1(\phi_j, \phi_n, \phi_i), \quad 1 \leq i, j, n \leq N. $$

Finally, we evaluate the output function $s(\mu)$ from

$$ s(\mu) = L^T \tilde{u}(\mu), $$

where $L \in \mathbb{R}^N$ is the output vector defined as $L_i = \ell(\phi_i)$, $1 \leq i \leq N$.

2.4 Model Problem

We introduce a “thermal block” elliptic nonlinear diffusion
problem. We specify the spatial domain (the thermal
block) as a unit square $\Omega = [0,1]^2$, and shall consider
the non-dimensional temperature $u(\mu)$ over $\Omega$. We assume
zero Dirichlet boundary condition on $\partial \Omega$ and consider
a linear finite element truth approximation subspace $X$ of
dimension $N = 2601$. We also define $(\cdot, \cdot)_X \equiv a_0(\cdot, \cdot)$ and

$$ \ell(v) = \int_{\Omega} \delta v. $$

Our parameter domain $\mathcal{D}$ is defined as
$\mathcal{D} = (0,1)^2$. We note that $\mu_1$ represents the strength of the nonlinearity in the temperature-dependent conductivity
where $A_{0N} \in \mathbb{R}^{N \times N}$ and $F_N \in \mathbb{R}^N$ are parameter-independent matrix and vector with entry $A_{i,j}^{0,N} = a_0(\xi_j, \xi_j)$, $1 \leq i, j \leq N$, and $F_i = f(\xi_i)$, $1 \leq i \leq N$, respectively. $A_{1N}(u_N) \in \mathbb{R}^{N \times N}$ has entries $A_{i,j}^{1,N}(u_N) = \sum_{n=1}^N u_{nN} A_{i,j,N,n}$, $1 \leq i, j \leq N$, where

$$A_{i,j,N,n} = a_1(\xi_n, \xi_n, \xi_i), \quad 1 \leq i, j, n \leq N.$$  

(31)

We again use Newton’s method to solve the nonlinear system (30). Starting with $u_{0N}$ as initial value for the Newton iterations, we calculate $\delta u_{0N}$ from the system

$$[\mu_0 A_{0N} + \mu_1 (A_{1N}(u_{0N}) + A_{1N}(\tilde{u}_{0N}))] \delta u_{0N} = F_N - [\mu_0 A_{0N} + \mu_1 A_{1N}(u_{0N})] u_{0N},$$  

(32)

update $u_{N}(\mu)$ and continue this process until a certain level of accuracy satisfied. The matrices $A_{1N}(u_{0N})$ and $\tilde{A}_{1N}(u_{0N})$ are defined as

$$A_{1,j,N,n}^{1,N} = \sum_{n=1}^N u_{nN} A_{i,j,N,n}, \quad \tilde{A}_{1,j,N,n}^{1,N} = \sum_{n=1}^N u_{nN} \tilde{A}_{i,j,N,n},$$  

(33)

(34)

where the matrix $A_{i,j,N,n}$ is defined in (31) and $\tilde{A}_{i,j,N,n}$ is as initial value for the a posteriori error bound $\Delta_N(\mu)$ for the error $||u(\mu) - u_N(\mu)||_X$. To this end, we follow the idea in Caloz et al. (1997) and employ the Brezzi-Rappaz-Raviart (BRR) theory. The BRR framework was successfully used for the Navier-Stokes equations in Veroy et al. (2005). To begin, we first define the residual operator $g(w_N, v; \mu)$ as follows:

$$g(w_N, v; \mu) = a(w_N, v, G(w_N; \mu)) - f(v).$$  

(37)

Based on the residual function, we define the dual norm of the residual as

$$\varepsilon_N(\mu) = \sup_{v \in X} \frac{g(w_N, v; \mu)}{\|v\|_X}, \quad \forall \mu \in \mathcal{D}. \tag{38}$$

We also require the inf-sup constant $\beta_N(\mu)$ which is defined as

$$\beta_N(\mu) = \inf_{w \in X} \sup_{v \in X} \frac{dg(w, v; u_N; \mu)}{\|v\|_X \|w\|_X}. \tag{39}$$

We obtain the following result, see Rasty et al. (2012).
Proposition 1. For 
\[ \tau_N = \frac{4\mu e_N(\mu)}{2\beta_N^{BL}(\mu)^2} < 1, \]  
(40) 
and for every \( \mu \in \mathcal{D} \), there exists a unique solution \( u(\mu) \in X^N \) in the neighborhood of \( u_N(\mu) \in X^N \). Furthermore, there exists a rigorous upper bound for the RB error, \( \| u(\mu) - u_N(\mu) \| \) given by 
\[ \Delta_N^u(\mu) = \frac{\beta_N^{BL}(\mu)}{2\rho} \left( 1 - \sqrt{1 - \tau_N(\mu)} \right). \]  
(41) 
Here, \( \beta_N^{BL}(\mu) \) is a lower bound for the inf-sup constant \( \beta_N(\mu) \) which we calculate by the SCM method, Huynh et al. (2007); and \( \rho \) is the Sobolev embedding constant. For more details we refer the interested reader to Rasty et al. (2012). We can also prove 

Proposition 2. If 
\[ \tau_N = \frac{4\mu e_N(\mu)}{2\beta_N^{BL}(\mu)^2} < 1, \]  
(42) 
the error in the output satisfies: \( | s(\mu) - s_N(\mu) | \leq \Delta_N^s(\mu), \) \( \forall \mu \in \mathcal{D} \), where 
\[ \Delta_N^s(\mu) = \| \ell(v) \|_X X^{\Delta(\mu)}. \]  
(43) 
and \( \| \ell \|_X^* = \sup_{v \in X} \| v \|_X \) is the dual norm the residual function \( \ell \).

4. NUMERICAL RESULTS

In this section, we present some numerical results to verify the efficiency and accuracy of the presented method. We consider the model problem introduced in Section 2.4. The output is defined as the average temperature over \( \Omega \).

Table 1. Maximum relative values for \( e_N^s, \Delta_N^s \) and average effectivity \( \eta_N^s(\mu) \). \( \ell_{u,v},s_N^u \) are the average normalized times needed to calculate \( u_N, \Delta_N(\mu) \).

<table>
<thead>
<tr>
<th>N</th>
<th>( e_{N_{\max\text{rel}}}^s )</th>
<th>( \Delta_{N_{\max\text{rel}}}^s )</th>
<th>( \eta_N^s )</th>
<th>( \ell_{u,v} )</th>
<th>( s_N^u )</th>
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<td>2.91e-1</td>
<td>1.45</td>
<td>2.08e4</td>
<td>4.51e2</td>
</tr>
<tr>
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<td>1.50e-2</td>
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<td>1.24e4</td>
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<td>4.09e-6</td>
<td>1.44</td>
<td>4.53e3</td>
<td>1.89e2</td>
</tr>
</tbody>
</table>

We generate the RB approximation by running a weak greedy algorithm on a test sample \( \Xi_{\text{test}} \) of size \( n_{\text{test}} = 2000 \).

We define the effectivities \( \eta_N^s(\mu) \) and \( \eta_N^s(\mu) \) as follows:
\[ \eta_N^s(\mu) = \frac{\Delta_N^s(\mu)}{e_N^s(\mu)}, \quad \eta_N^s(\mu) = \frac{\Delta_N^s(\mu)}{e_N^s(\mu)} \]  
(44) 
where \( e_N^s(\mu) = \| u(\mu) - u_N(\mu) \|_X \) and \( s_N^s(\mu) = s(\mu) - s_N(\mu) \).

In Table 1 we present, as a function of \( N \), the maximum relative error \( e_{N_{\max\text{rel}}}^s \), maximum realtive error bound \( \Delta_{N_{\max\text{rel}}}^s \), and the average effectivity \( \eta_N^s \). Here, the maximum and average are taken over a train sample of size 225. We observe that the error and bound converge very fast and that we obtain very sharp bounds.

In Table 1, we also present the ratio of the online computational time and the computational time to solve the truth approximation. We observe that the computational saving are considerable.

In Table 2 we present, as a function of \( N \), the maximum relative output error, maximum relative output bound, and also average effectivity for the output.

Table 2. Maximum relative values for \( e_N^s(\mu), \Delta_N^s(\mu) \) and average effectivity \( \eta_N^s(\mu) \).

<table>
<thead>
<tr>
<th>N</th>
<th>( e_{N_{\max\text{rel}}}^s )</th>
<th>( \Delta_{N_{\max\text{rel}}}^s )</th>
<th>( \eta_N^s )</th>
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REFERENCES


