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 knows 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

$$\mathbf{div}\Big(D(u)\nabla u\Big) = f, \tag{1}$$

⋆ Excellence Initiative of the German federal and state governments.

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 $X^e \equiv H_0^1(\Omega)$, or more generally, $H_0^1(\Omega) \subset X^e \subset H^1(\Omega)$, where $H^1(\Omega) = \Big\{v\Big|v \in L^2(\Omega), \nabla v \in \big(L^2(\Omega)\big)^d\Big\}$, $H_0^1(\Omega) = \big\{v\big|v \in H^1(\Omega), v\big|_{\partial\Omega} = 0\big\}$, and $L^2(\Omega)$ is the space of square integrable functions over Ω. Here Ω 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

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

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

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

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

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

with $G(w; \mu) = \mu_0 + \mu_1 w$, and $f(v)$ is a X^e-continuous linear form. We can thus write

$$a\big(w,v,G(w;\mu)\big) = \mu_0 \int_\Omega \nabla w \nabla v + \mu_1 \int_\Omega w \ \nabla w \nabla v \quad (5)$$

$$= \mu_0 \int_\Omega \frac{\partial w}{\partial x_j}\frac{\partial v}{\partial x_j} + \mu_1 \int_\Omega w \frac{\partial w}{\partial x_j}\frac{\partial v}{\partial x_j} \quad (6)$$

$$= \mu_0 a_0(w,v) + \mu_1 a_1(w,w,v), \quad (7)$$

where, for simplicity, we have used Einstein notation

$$\int_\Omega \frac{\partial w}{\partial x_j}\frac{\partial v}{\partial x_j} = \int_\Omega \sum_{j=1}^{d} \frac{\partial w}{\partial x_j}\frac{\partial v}{\partial x_j}. \quad (8)$$

We can also define an output $s^e : \mathcal{D} \mapsto \mathbb{R}$ as

$$s^e(\mu) = \ell\big(u^e(\mu)\big), \quad (9)$$

where $\ell(v)$ is a X^e-continuous linear form. Results about 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 $X \subset X^e$ and replace $u^e(\mu) \in X^e$ with a "truth" approximation $u(\mu) \in X$. Here, X is a suitably fine piecewise linear finite element approximation space with *very* large dimension $\mathcal{N}$. X shall inherit the inner product and norm from X^e. Our truth approximation is thus: for any $\mu \in \mathcal{D}$, evaluate the output $s : \mathcal{D} \mapsto \mathbb{R}$ from

$$s(\mu) = \ell\big(u(\mu)\big). \quad (10)$$

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

$$a\big(u(\mu), v, G(u(\mu);\mu)\big) = f(v), \quad \forall v \in X. \quad (11)$$

We shall assume that the discretization is sufficiently rich such that $u(\mu)$ and $u^e(\mu)$ 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 $w, v \in X$, we define the Frechet derivative form $dg : X^3 \times \mathcal{D} \mapsto \mathbb{R}$ as

$$dg(w,v;z;\mu) = a_0(w,v;\mu) + a_1(z,w,v;\mu) + a_1(w,z,v;\mu). \quad (12)$$

We also define the inf-sup constant

$$\beta_z(\mu) = \inf_{w\in X} \sup_{v \in X} \frac{dg(w,v;z;\mu)}{\|w\|_X \|v\|_X}, \quad z \in X, \quad (13)$$

and the continuity constant

$$\gamma_z(\mu) = \sup_{w\in X} \sup_{v \in X} \frac{dg(w,v;z;\mu)}{\|w\|_X \|v\|_X}, \quad z \in X. \quad (14)$$

We further assume that a_0 and a_1 satisfy

$$|a_0(w,v)| \le \|w\|_X \|v\|_X, \quad (15)$$

$$|a_1(z,w,v)| \le \rho \|z\|_X \|w\|_X \|v\|_X. \quad (16)$$

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

$$\beta_z(\mu) \ge \beta_0, \quad \forall \mu \in \mathcal{D}. \quad (17)$$

2.3 Algebraic Equations

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

$$u(\mu) = \sum_{j=1}^{\mathcal{N}} u_j(\mu)\phi_j, \quad (18)$$

where the $\phi_j, 1 \le j \le \mathcal{N}$, are the basis functions for our truth approximation space X. Choosing basis functions $\phi_i, 1 \le i \le \mathcal{N}$, as test functions v in (11) we can show that $\underline{u}(\mu) = [u_1(\mu), u_2(\mu), \cdots, u_{\mathcal{N}}(\mu)] \in \mathbb{R}^{\mathcal{N}}$ satisfies

$$\big[\mu_0 A_0 + \mu_1 A_1(\underline{u})\big]\underline{u} = F, \quad (19)$$

where $A_0 \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$ and $F \in \mathbb{R}^{\mathcal{N}}$ are parameter-independent matrix and vector with entries $A_0^{i,j} = a_0(\phi_j, \phi_i),\ 1 \le i,j \le \mathcal{N}$, and $F^i = f(\phi_i),\ 1 \le j \le \mathcal{N}$, respectively. Furthermore $A_1(u) \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$ has entries $A_1^{i,j}(\underline{u}) = \sum_{n=1}^{\mathcal{N}} u_n A_{1,n}^{i,j},\ 1 \le i,j \le \mathcal{N}$, where

$$A_{1,n}^{i,j} = a_1\big(\phi_n, \phi_j, \phi_i\big), \qquad 1 \le i,j,n \le \mathcal{N}. \quad (20)$$

We now solve (19), for $\underline{u}(\mu)$, using a Newton iterative scheme as follows: starting with an initial value $\underline{u}_0$, we find an increment $\delta\underline{u}_0$ such that

$$\Big[\mu_0 A_0 + \mu_1\big(A_1(\underline{u}_0) + \widetilde{A}_1(\underline{u}_0)\big)\Big]\delta\underline{u}_0 = F - \Big[\mu_0 A_0 + \mu_1 A_1(\underline{u}_0)\Big]\underline{u}_0. \quad (21)$$

We update $\underline{u}_1 = \underline{u}_0 + \delta\underline{u}_0$ and continue this process until $\|\delta\underline{u}_k\|_1 < \varepsilon_{\text{tol}}^{\text{newton}}$ is satisfied for some $k \ge 0$. The matrices $A_1(\underline{u}_0) \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$ and $\widetilde{A}_1(\underline{u}_0) \in \mathbb{R}^{\mathcal{N}\times\mathcal{N}}$ have entries

$$A_1^{i,j}(\underline{u}_0) = \sum_{n=1}^{\mathcal{N}} u_{0n} A_{1,n}^{i,j}, \quad (22)$$

$$\widetilde{A}_1^{i,j}(\underline{u}_0) = \sum_{n=1}^{\mathcal{N}} u_{0n} \widetilde{A}_{1,n}^{i,j}, \quad (23)$$

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

$$\widetilde{A}_{1,n}^{i,j} = a_1\big(\phi_j, \phi_n, \phi_i\big), \qquad 1 \le i,j,n \le \mathcal{N}. \quad (24)$$

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

$$s(\mu) = L^T \underline{u}(\mu), \quad (25)$$

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

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 Ω. We assume zero Dirichlet boundary condition on $\partial\Omega$ and consider a linear finite element truth approximation subspace X of dimension $\mathcal{N} = 2601$. We also define $(\cdot,\cdot)_X \equiv a_0\big(\cdot,\cdot\big)$ and $\ell(v) = \displaystyle\int_\Omega d\Omega$.

Our parameter domain $\mathcal{D}$ is defined as $\mathcal{D} \equiv (\mu_0, \mu_1) = [0.01, 1]^2$. We note that μ_1 represents the strength of the nonlinearity in the temperature-dependent conductivity

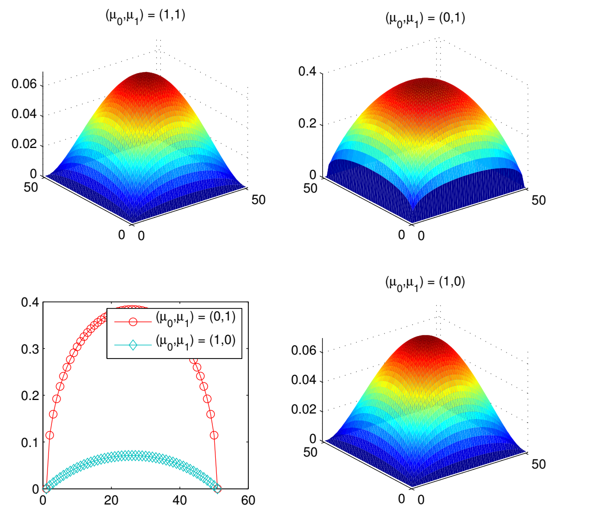

Fig. 1. Behavior of the solution for different parameter values.

$G(u) = \mu_0 + \mu_1 u$. As $\mu_1 \longrightarrow 0$, we have $G(u) \longrightarrow \mu_0$ and the solution thus tends to the solution of a linear heat equation. Fig(1) shows three snapshots of the solution for three different parameters.

3. REDUCED BASIS METHOD

3.1 Approximation

We first introduce a nested set of parameter samples $S_1 \equiv \{\mu_1 \in \mathcal{D}\} \subset \cdots \subset S_{N^{\max}} \equiv \{\mu_1, \mu_2, \cdots, \mu_{N^{\max}} \in \mathcal{D}\}$ and associated reduced basis spaces $X^N \subset X$ as

$$X^N \equiv \text{span}\{\xi_j,\ 1 \le j \le N\} = \text{span}\{u(\mu_j),\ 1 \le j \le N\}, \qquad (26)$$

where the ξ_j, $1 \le j \le N$, are mutually $(\cdot,\cdot)_X$-orthogonal basis functions. We construct the samples using a weak greedy algorithm based on the inexpensive *a posteriori* error estimators introduced later.

The RB approximation is then clear. For every $\mu \in \mathcal{D}$, we find $u_N(\mu) \in X^N$ such that

$$a\big(u_N(\mu), v, G(u_N(\mu);\mu)\big) = f(v), \qquad \forall v \in X^N. \qquad (27)$$

We also calculate the RB output $s_N(\mu)$ from

$$s_N(\mu) = \ell\big(u_N(\mu)\big). \qquad (28)$$

3.2 Computational Procedure

In this section we develop an efficient computational procedure to recover online $\mathcal{N}$-independence for our nonlinear problem. First we express $u_N(\mu)$ as

$$u_N(\mu) = \sum_{j=1}^{N} u_{Nj}(\mu)\xi_j, \qquad (29)$$

and choose $v = \xi_i$, $1 \le i \le N$ in (27). It then follows that the vector $\underline{u}_N = [u_{N1}(\mu), u_{N2}(\mu), \cdots, u_{NN}(\mu)]^{\mathrm{T}} \in \mathbb{R}^N$, satisfies

$$[\mu_0 A_{0N} + \mu_1 A_{1N}(\underline{u}_N)]\underline{u}_N = F_N, \qquad (30)$$

where $A_{0N} \in \mathbb{R}^{N\times N}$ and $F_N \in \mathbb{R}^N$ are parameter-independent matrix and vector with entries $A_{0N}^{i,j} = a_0(\xi_j, \xi_i)$, $1 \le i,j \le N$, and $F_N^i = f(\xi_i)$, $1 \le i \le N$, respectively. $A_{1N}(\underline{u}_N) \in \mathbb{R}^{N\times N}$ has entries $A_{1N}^{i,j}(\underline{u}_N) = \sum_{n=1}^{N} u_{Nn} A_{1N,n}^{i,j}$, $1 \le i,j \le N$, where

$$A_{1N,n}^{i,j} = a_1(\xi_n, \xi_j, \xi_i), \qquad 1 \le i,j,n \le N. \qquad (31)$$

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

$$\Big[\mu_0 A_{0N} + \mu_1 \left(A_{1N}(\underline{u}_{0N}) + \widetilde{A}_{1N}(\underline{u}_{0N})\right)\Big]\delta\underline{u}_{0N} = F_N - \Big[\mu_0 A_{0N} + \mu_1 A_{1N}(\underline{u}_{0N})\Big]\underline{u}_{0N}, \qquad (32)$$

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

$$A_{1N}^{i,j}(\underline{u}_{0N}) = a\sum_{n=1}^{N} u_{0Nn} A_{1N,n}^{i,j}, \qquad (33)$$

$$\widetilde{A}_{1N}^{i,j}(\underline{u}_{0N}) = \sum_{n=1}^{N} u_{0Nn} \widetilde{A}_{1N,n}^{i,j}, \qquad (34)$$

where the matrix $A_{1N,n}^{i,j}$ is defined in (31) and

$$\widetilde{A}_{1N,n}^{i,j} = a_1(\xi_j, \xi_n, \xi_i), \qquad 1 \le i,j,n \le N. \qquad (35)$$

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

$$s_N(\mu) = L_N^T \underline{u}_N(\mu), \qquad (36)$$

where $L_N \in \mathbb{R}^N$ is defined as $L_{Ni} = \ell(\xi_i)$, $1 \le i \le N$.

3.3 A posteriori Error Estimation

In this section we introduce an *a posteriori* error bound $\Delta_N^u(\mu)$ 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:

$$g(w_N, v;\mu) = a\big(w_N, v, G(w_N;\mu)\big) - f(v). \qquad (37)$$

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

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

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

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

We obtain the following result, see Rasty et al. (2012).

Proposition 1. For

$$\tau_N = \frac{4\rho\varepsilon_N(\mu)}{2\beta_N^{\rm LB}(\mu)^2} < 1, \tag{40}$$

and for every $\mu \in \mathcal{D}$, there exists a unique solution $u(\mu) \in X^{\mathcal{N}}$ 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

$$\Delta_N^u(\mu) = \frac{\beta_N^{\rm LB}(\mu)}{2\rho}\Big(1 - \sqrt{1-\tau_N(\mu)}\Big). \tag{41}$$

Here, $\beta_N^{LB}(\mu)$ is a lower bound for the inf-sup constant $\beta_N(\mu)$ which we calculate by the SCM method, Huynh et al. (2007); and ρ 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

$$\tau_N = \frac{4\rho\varepsilon_N(\mu)}{2\beta_N^{\rm LB}(\mu)^2} < 1, \tag{42}$$

the error in the output satisfies: $|s(\mu) - s_N(\mu)| \le \Delta_N^s(\mu)$, $\forall \mu \in \mathcal{D}$, where

$$\Delta_N^s(\mu) = \|\ell\|_{X'}\Delta_N^u(\mu). \tag{43}$$

and $\|\ell\|_{X'} = \sup\limits_{v\in X} \dfrac{\ell(v)}{\|v\|_X}$ is the dual norm the residual function ℓ.

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 Ω.

Table 1. Maximum relative values for e_N^u, Δ_N^u and average effectivity $\bar{\eta}_N^u(\mu)$. $t_{u,u_N}, t_{u,\Delta_N}$ are the average normalized times needed to calculate $u_N, \Delta_N(\mu)$.

N	$e^u_{N,\max,\rm rel}$	$\Delta^u_{N,\max,\rm rel}$	$\bar{\eta}^u_N$	t_{u,u_N}	t_{u,Δ_N}
2	9.97e-2	2.91e-1	1.45	2.08e4	4.51e2
4	8.72e-3	1.50e-2	1.39	1.24e4	3.39e2
8	4.61e-4	5.11e-4	1.30	7.77e3	2.36e2
12	3.42e-6	4.09e-6	1.44	4.53e3	1.89e2

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

We define the effectivities $\eta_N^u(\mu)$ and $\eta_N^s(\mu)$ as follows:

$$\eta_N^u(\mu) = \frac{\Delta_N^u(\mu)}{e_N^u(\mu)}, \qquad \eta_N^s(\mu) = \frac{\Delta_N^s(\mu)}{e_N^s(\mu)}, \tag{44}$$

where $e_N^u(\mu) = \|u(\mu) - u_N(\mu)\|_X$ and $e_N^s(\mu) = |s(\mu) - s_N(\mu)|$.

In Table 1 we present, as a function of N, the maximum relative error $e^u_{N,\max,\rm rel}$, maximum realtive error bound $\Delta^u_{N,\max,\rm rel}$, and the average effectivity $\bar{\eta}^u_N$. 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 $\bar{\eta}_N^s(\mu)$.

N	$e^s_{N,\max,\rm rel}$	$\Delta^s_{N,\max,\rm rel}$	$\bar{\eta}^s_N$
2	3.85e-3	3.01e-3	0.76
4	3.11e-5	2.42e-4	55.6
8	2.80e-7	7.76e-6	31.8
12	2.53e-8	5.90e-8	2.45

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