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Certified real-time solution of the parametrized steady incompressible Navier–Stokes equations: rigorous reduced-basis *a posteriori* error bounds

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SUMMARY

We present a technique for the evaluation of linear-functional outputs of parametrized elliptic partial differential equations in the context of *deployed* (in service) systems. Deployed systems require *real-time* and *certified* output prediction in support of *immediate* and *safe* (feasible) action. The two essential components of our approach are (i) rapidly, uniformly convergent reduced-basis approximations, and (ii) associated rigorous and sharp *a posteriori* error bounds; in both components we exploit affine parametric structure and offline–online computational decompositions to provide real-time deployed response. In this paper we extend our methodology to the parametrized steady incompressible Navier–Stokes equations.

We invoke the Brezzi–Rappaz–Raviart theory for analysis of variational approximations of non-linear partial differential equations to construct *rigorous*, *quantitative*, *sharp*, *inexpensive a posteriori* error estimators. The crucial new contribution is offline–online computational procedures for calculation of (a) the dual norm of the requisite residuals, (b) an upper bound for the '$L^4(\Omega) - H^1(\Omega)$' Sobolev embedding continuity constant, (c) a lower bound for the Babuška inf–sup stability 'constant,' and (d) the adjoint contributions associated with the output. Numerical results for natural convection in a cavity confirm the rapid convergence of the reduced-basis approximation, the good effectivity of the associated *a posteriori* error bounds in the energy and output norms, and the rapid deployed response. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: reduced-basis; *a posteriori* error estimation; output bounds; offline–online procedures; incompressible Navier–Stokes; natural convection; parametrized partial differential equations

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1. INTRODUCTION

We consider here the parametrized steady incompressible Navier–Stokes equations: Given $\mu \in \mathscr{D} \subset R^P$, we find a $u^{\mathrm{e}}(\mu)$ in X such that $g(u^{\mathrm{e}}(\mu), v; \mu) = 0$, $\forall v \in X$. Here, μ represents an *input* parameter; $\mathscr{D}$ is the associated parameter domain; $u^{\mathrm{e}}(\mu) = (u_1^{\mathrm{e}}(\mu), u_2^{\mathrm{e}}(\mu))$ is the velocity; $X(\Omega)$ is an appropriate divergence-free space (in Reference [1] we consider treatment of the pressure and hence non-divergence-free velocity spaces); $\Omega \subset \mathbb{R}^2$ is the spatial domain, a typical point of which shall be denoted $x = (x_1, x_2)$; and g is the weak form of the Navier–Stokes equations. Our interest is typically not in the velocity field *per se*, but rather in a (say, single) *output* $s^{\mathrm{e}}(\mu)$ expressed as $L(u^{\mathrm{e}}(\mu))$; in this paper L is a bounded linear functional, though more generally we may consider non-linear outputs. We thus arrive at an implicit *input–output* relationship $\mu \to s^{\mathrm{e}}(\mu)$, evaluation of which requires solution of the underlying partial differential equation.

Our (or an) interest is in 'deployed' systems: systems that are in service, in operation, in the field. Typical computational tasks include parameter estimation (inverse problems) and adaptive design (optimization) in support of an *action*. The computational requirements on the forward evaluations $\mu \to s^{\mathrm{e}}(\mu)$ are formidable: the evaluation must be *real-time*—as the action must be *immediate*; and the evaluation must be *certified* (endowed with a rigorous error bound)—as the action must be *safe* and *feasible*.

The two essential components of our approach are (i) rapidly, uniformly convergent reduced-basis (RB) approximations, and (ii) associated rigorous and sharp *a posteriori* error bounds; in both components we exploit affine parametric structure and offline–online computational decompositions to provide extremely rapid deployed/marginal response time. (Low marginal cost implies low asymptotic average cost; our methods are thus also relevant to non real-time many-query applications.) RB approximation [2–7] takes advantage of the dimension reduction afforded by the (smooth) parametrically-induced solution manifold: successful application to the incompressible Navier–Stokes equations [8–10] is well documented; our emphasis is thus on the development and application of rigorous *a posteriori* error estimation procedures.

To construct our *a posteriori* estimators, we invoke the Brezzi–Rappaz–Raviart (BRR) theory for analysis of variational approximations of nonlinear partial differential equations [11–14]. Typically, the BRR framework provides a non-quantitative *a priori* or *a posteriori* justification of asymptotic convergence. In our context, the challenge—and contribution—is the development of actual *a posteriori* error estimators that are *rigorous*, *quantitative*, *sharp*, and *inexpensive* (*real-time*); we shall see that the RB/offline–online context is a unique opportunity to render the BRR theory completely predictive.

Our key new ingredients are appropriate approximations and associated offline–online computational procedures for calculation of (a) the dual norm of the requisite residuals, (b) an upper bound for the '$L^4(\Omega) - H^1(\Omega)$' Sobolev embedding continuity constant [15, 16], (c) a lower bound for the Babuška inf–sup stability factor, and (d) the adjoint contributions associated with the output. Our constructions, applied to the Burgers problem in Reference [17], derive from our earlier work on RB *a posteriori* error estimators for somewhat simpler parametrized elliptic equations: coercive linear [18], non-coercive linear [1, 19], and monotonic non-linear problems [19].

In Section 2 we present our model problem, in Section 3 we summarize the RB approximation, in Section 4 we develop the *a posteriori* error estimators and in Section 5 we present numerical results.

2. NATURAL CONVECTION AT $Pr=0$

We consider the problem of natural convection at Prandtl number $Pr=0$ (see Reference [1] for treatment of $Pr \neq 0$) in a cavity $\Omega=[0,4]\times[0,1]$ [20, 21]: Given $\mu \equiv Gr$ (the Grashof number) in $\mathscr{D} \equiv [1,10^5]$, we find a velocity $u^{\mathrm{e}}(Gr)\in X$ such that $g(u^{\mathrm{e}}(Gr),v;Gr)=0$, $\forall v\in X$. Here, X is the divergence-free subspace of $(H_0^1(\Omega))^2$ imbued with inner product $(w,v)_X=\int_\Omega v_{i,j}w_{i,j}$ (here $v_{i,j}$ denotes $\partial v_i/\partial x_j$ and repeated physical indices imply summation) and norm $\|w\|_X=\sqrt{(w,w)_X}$; and $g(\cdot,\cdot;Gr): X\times X\to\mathbb{R}$ is given by

$$g(w,v;Gr)\equiv a_0(w,v)+\tfrac{1}{2}\,a_1(w,w,v)-Gr\,F(v) \tag{1}$$

where $a_0(w,v)\equiv\int_\Omega v_{i,j}w_{i,j}$ (bilinear), $a_1(w,z,v)\equiv-\int_\Omega v_{i,j}\,(w_iz_j+w_jz_i)$ (trilinear), and $F(v)\equiv\frac{1}{4}\int_\Omega x_1v_2$ (linear bounded).‡ For our output we take $s^{\mathrm{e}}(Gr)=L(u^{\mathrm{e}}(Gr))$, where $L(v)=|\Omega_m|^{-1}\int_{\Omega_m}v_2$; here; $\Omega_m=]0.85,1.15[\times]0.42,0.58[$ is a small measurement region of area $|\Omega_m|=4.7\times10^{-2}$.

We next introduce a 'truth' finite element approximation space§ $Y\subset X$ of dimension $\mathcal{N}$ (with inner product and norm inherited from X). Our 'truth' approximation is then given by $u(Gr)\in Y$, $s(Gr)\in\mathbb{R}$, where $g(u(Gr),v;Gr)=0$, $\forall v\in Y$, and $s(Gr)=L(u(Gr))$. We shall build our RB projection upon (and measure our RB error with respect to) this *discrete* truth approximation; we thus assume that $\mathcal{N}$ is sufficiently large that $\|u(Gr)-u^{\mathrm{e}}(Gr)\|_X$ and $|s(Gr)-s^{\mathrm{e}}(Gr)|$ is acceptably small for all $Gr\in\mathscr{D}$ (see Reference [22] for relevant *a posteriori* error estimation procedures). Clearly, our formulation must be *stable* and *efficient* as $\mathcal{N}\to\infty$.

For given $z\in Y$, we define the derivative bilinear form $\mathrm{d}g(\cdot,\cdot;z): Y\times Y\to\mathbb{R}$ as

$$\mathrm{d}g(w,v;z)\equiv a_0(w,v)+a_1(w,z,v) \tag{2}$$

such that

$$g(z+w,v;Gr)=g(z,v;Gr)+\mathrm{d}g(w,v;z)+\tfrac{1}{2}\,a_1(w,w,v) \tag{3}$$

The inf–sup parameter and continuity constant are then given by $\beta(z)\equiv\inf_{w\in Y}\sup_{v\in Y}\mathrm{d}g(w,v;z)/\|w\|_Y\|v\|_Y$ and $\gamma(z)\equiv\sup_{w\in Y}\sup_{v\in Y}\mathrm{d}g(w,v;z)/\|w\|_Y\|v\|_Y$, respectively. We note from the Hölder inequality that

$$|a_1(w,z,v)|\leqslant\rho^2\|w\|_Y\|z\|_Y\|v\|_Y \tag{4}$$

and hence that $\gamma(z)\leqslant 1+\rho^2\|z\|_Y$; here,

$$\rho\equiv\sqrt{2}\,\sup_{v\in Y}\|v\|_{L^4(\Omega)}/\|v\|_Y \tag{5}$$

is a Sobolev embedding constant [15, 16] and $\|v\|_{L^p(\Omega)}\equiv(\int_\Omega(v_iv_i)^{p/2})^{1/p}$.

We shall make two (verifiable) hypotheses on the form of our problem and associated solutions. The first hypothesis, H-I, is affine parameter-dependence: $g(w,v;Gr)=\sum_{q=1}^{Q}\Theta_q(Gr)$

‡We choose the scaling of Reference [20]; the alternative scaling of Reference [21] may enjoy some conditioning advantages [1].

§We choose Y to be the (discretely) incompressible space of dimension $\mathcal{N}=4762$ derived from a Taylor–Hood P_2-P_1 approximation space [8] with 5538 velocity and 776 pressure degrees-of-freedom.

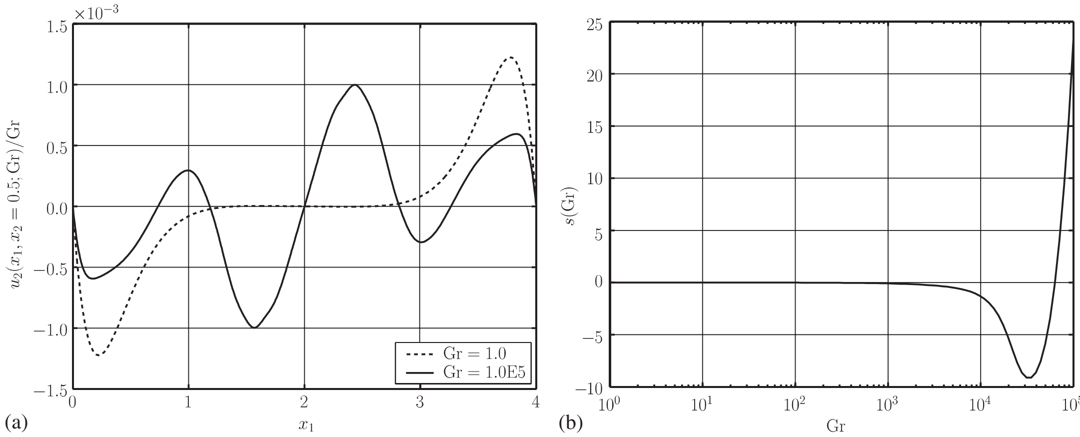

Figure 1. Plots of: (a) velocity profiles for $Gr = 1.0$ and 1.0×10^5; and (b) the output $s(Gr)$.

$g_q(w, v)$, where $\Theta_q : \mathscr{D} \to \mathbb{R}$ and $g_q : Y \times Y \to \mathbb{R}$, $q = 1, \ldots, Q$, are *Gr-dependent* functions and *Gr-independent* forms, respectively. For our particular problem it is very simple to verify H-I *a priori*: $Q = 2$. Our second hypothesis, H-II, is related to well-posedness: our manifold $\{u(Gr) | Gr \in \mathscr{D}\}$ is a nonsingular (isolated) solution branch; thus $\beta(u(Gr)) \geqslant \beta_0 > 0$, $\forall Gr \in \mathscr{D}$. We can verify H-II *a posteriori*.

Our truth solutions confirm the flow behaviour previously reported for this model natural-convection problem [20, 21]. For low *Gr* the flow is single-cell; at higher Gr the flow *smoothly evolves* to a three-cell pattern [20, 21]—the three-cell pattern is 'clearly identifiable' only for $Gr \geqslant 5.0 \times 10^4$. For lower *Gr* the flow is essentially Stokes; significant inertial behaviour is first evinced at $Gr = 10^4$. We show in Figure 1(a) $u_2(x_1 \in [0, 4], x_2 = \frac{1}{2}; Gr)/Gr$ for $Gr = 1$ and $Gr = 10^5$; and in Figure 1(b) we present $s(Gr)$ for $Gr \in [1, 10^5]$. The output—chosen to reflect the one-cell to three-cell transition—is not too remarkable, with deviations from the Stokes limit only for $Gr \in [10^4, 10^5]$¶ (see Reference [1] for a more interesting $Pr \neq 0$ Nusselt output).

3. REDUCED-BASIS APPROXIMATION

3.1. Formulation

We first introduce positive integers $N \leqslant N_{\max}$ and associated index sets $\mathbb{N} \equiv \{1, \ldots, N\}$ and $\mathbb{N}_{\max} \equiv \{1, \ldots, N_{\max}\}$. Then, given prescribed parameter points $Gr^n \in \mathscr{D}$, $1 \leqslant n \leqslant N_{\max}$, we introduce nested parameter samples $S_N \equiv \{Gr^1, \ldots, Gr^N\}$ and associated nested Lagrangian [7] RB spaces $W_N \equiv \mathrm{span}\{\zeta_n \equiv u(Gr^n), 1 \leqslant n \leqslant N\}$ for $1 \leqslant N \leqslant N_{\max}$. (In practice, the basis functions are Gram–Schmidt orthogonalized with respect to $(\cdot, \cdot)_Y$.)

¶To achieve high accuracy and in particular rigorous error bounds we must approximate $u(Gr)$ and only *then* $s(Gr) = L(u(Gr))$; the relatively complex parametric dependence of the former (Figure 1(a)), not the relatively simple parametric dependence of the latter (Figure 1(b)), thus determines the difficulty of the RB task.

The RB (Galerkin) approximation $u_N(Gr)\in W_N$, $s_N(Gr)\in\mathbb{R}$, then satisfies $g(u_N(Gr), v; Gr)=0$, $\forall v\in W_N$, $s_N(Gr)=L(u_N(Gr))$. The critical observation is that the solution $u(Gr)$ resides on a *one-dimensional smooth* manifold. (The regularity of the velocity field in Gr may be deduced from the equations for the sensitivity derivatives; the stability and continuity properties of $\mathrm{d}g$ are crucial.) Thus, by restricting attention to this parametrically-induced manifold, we can very accurately approximate $u(Gr)$, $\forall Gr\in\mathcal{D}$, by a space of dimension $N\ll\mathcal{N}$. We confirm this conjecture empirically in Section 5.

3.2. Offline–online decomposition

The critical computational kernel—and dominant computational complexity—is the inner Newton iteration for $u_N(Gr)$. We pursue an offline–online computational procedure [4, 9, 19, 23]; detailed development for the (analogous) Burgers equation is described in Reference [17] and for Navier–Stokes in Reference [1], and we thus restrict ourselves here to a brief summary.

In the *offline* stage, performed once, we (i) solve for the RB functions ζ_n, $\forall n\in\mathbb{N}_{\max}$, at cost $O(N_{\max}\mathcal{N}^{\cdot\mathrm{NS}})$—here $\cdot$NS refers to a scaling exponent (>1) associated with the truth approximation Navier–Stokes solution procedure, and (ii) form the parameter-independent matrices and vectors required by the Newton kernel, at dominant cost (exploiting sparsity) $O(N_{\max}^3\mathcal{N})$. In the *online* stage—performed many times, for each new value of Gr—we simply assemble and invert the requisite (dense) $N\times N$ Jacobian, at total cost $O(N^3)$.[||] The online complexity is *independent of* $\mathcal{N}$, yielding extremely fast deployed response.

3.3. A dual problem

We shall also need a dual problem [18, 24, 25] associated with our output functional L. Towards that end, we first introduce an adjoint $\psi^N(Gr)\in Y$ satisfying the linear problem

$$\mathrm{d}g(\varphi,\psi^N(Gr);u_N(Gr)+\tfrac{1}{2}\,e^N(Gr))=-L(\varphi),\quad \forall\varphi\in Y \tag{6}$$

where $u_N(Gr)\in W_N$ is our RB approximation of Section 3.1 and $e^N(Gr)\equiv u(Gr)-u_N(Gr)$; well-posedness is discussed in Section 4.1.1. We may now readily demonstrate (under the assumption that $u_N(Gr)$ and $\psi^N(Gr)$ exist)

Lemma 1
For any $\chi\in Y$, $s(Gr)-s_N(Gr)=g(u_N(Gr),\chi;Gr)+g(u_N(Gr),\psi^N(Gr)-\chi;Gr)$.

Proof
The proof is a particular case of a more general result for adjoint approximations for nonlinear problems [25]. We note that $-L(e^N(Gr))=\mathrm{d}g(e^N(Gr),\psi^N(Gr);u_N(Gr)+\frac{1}{2}\,e^N(Gr))=a_0(e^N(Gr),\psi^N(Gr))+a_1(e^N(Gr),u_N(Gr)+\frac{1}{2}\,e^N(Gr),\psi^N(Gr))=a_0(u(Gr)-u_N(Gr),\psi^N(Gr))+a_1(u(Gr)-u_N(Gr),\frac{1}{2}(u(Gr)+u_N(Gr)),\psi^N(Gr))$; but by symmetry of a_1 with respect to

[||]As an example of *assembly*, we consider the representative Jacobian term $a_1(\delta u_N,\bar{u}_N,\zeta_i)=\sum_{j=1}^{N}\sum_{k=1}^{N}\bar{u}_{N\,k}a_1(\zeta_j,\zeta_k,\zeta_i)\delta u_{N\,j}$, $1\leqslant i\leqslant N$ $(*)$; here $\bar{u}_N=\sum_{k=1}^{N}\bar{u}_{N\,k}\zeta_k$ and $\delta u_N=\sum_{j=1}^{N}\delta u_{N\,j}\zeta_j$ are the previous iterate and current update, respectively. In the *offline* stage we form and store $a_1(\zeta_j,\zeta_k,\zeta_i)$, $1\leqslant i,j,k\leqslant N_{\max}$; in the *online* stage we perform the $\bar{u}_N$, δu_N-weighted sum $(*)$—at cost $O(N^3)$.

the first two arguments, $a_1(u(Gr)-u_N(Gr), \frac{1}{2}(u(Gr)+u_N(Gr)), \psi^N(Gr)) = \frac{1}{2}\, a_1(u(Gr), u(Gr), \psi^N(Gr)) - \frac{1}{2}\, a_1(u_N(Gr), u_N(Gr), \psi^N(Gr))$; hence $-L(e^N(Gr)) = GrF(\psi^N(Gr)) - [a_0(u_N(Gr), \psi^N(Gr)) + \frac{1}{2}\, a_1(u_N(Gr), u_N(Gr), \psi^N(Gr))] = -g(u_N(Gr), \psi^N(Gr); Gr)$. The result then follows from linearity of $g(w, v; Gr)$ in v. □

Lemma 1 shall be important in developing our *a posteriori* output error estimators.

To construct our output error estimators we shall also require an RB adjoint approximation: Given prescribed parameter points $Gr^{\mathrm{du},n} \in \mathscr{D}$, $1 \leqslant n \leqslant N^{\mathrm{du}}_{\max}$, we introduce nested parameter samples $S^{\mathrm{du}}_{N^{\mathrm{du}}} \equiv \{Gr^{\mathrm{du},1}, \ldots, Gr^{\mathrm{du},N^{\mathrm{du}}}\}$ and associated nested RB spaces $W^{\mathrm{du}}_{N^{\mathrm{du}}} \equiv \mathrm{span}\{\xi_n \equiv \psi^{N_{\max}}(Gr^{\mathrm{du},n}),\ 1 \leqslant n \leqslant N^{\mathrm{du}}\}$ for $1 \leqslant N^{\mathrm{du}} \leqslant N^{\mathrm{du}}_{\max}$; $\psi^N_{N^{\mathrm{du}}}(Gr) \in W^{\mathrm{du}}_{N^{\mathrm{du}}}$ then satisfies $\mathrm{d}g(\varphi, \psi^N_{N^{\mathrm{du}}}(Gr); u_N(Gr)) = -L(\varphi)$, $\forall \varphi \in W^{\mathrm{du}}_{N^{\mathrm{du}}}$. This RB dual problem readily admits an offline–online decomposition; the online effort to compute $\psi^N_{N^{\mathrm{du}}}(Gr)$ will typically be *considerably less* than the online effort to compute $u_N(Gr)$, since the former is equivalent to a *single* Newton iteration of the latter.

4. *A POSTERIORI* ERROR ESTIMATION

We first motivate the need for *a posteriori* error estimation. Given a RB solution $u_N(Gr)$, many questions can arise: Is there even a solution $u(Gr)$ near $u_N(Gr)$?; Is $|s(Gr) - s_N(Gr)| \leqslant \varepsilon^s_{\mathrm{tol}}$ (the maximum acceptable error)?; Is $s(Gr) \leqslant C_{\mathrm{constraint}}$ (say, a feasibility condition in a design optimization)? If these questions cannot be answered, we may propose the wrong—and potentially unsafe or infeasible—action in the deployed context. A fourth question is also important: Is N *too* large, $|s(Gr) - s_N(Gr)| \ll \varepsilon^s_{\mathrm{tol}}$, with an associated steep N^3 efficiency penalty? In this case, an overly conservative approximation may jeopardize the real-time response and associated action. Finally, we may also consider the efficiency of the samples S_N and associated RB spaces W_N: Do we satisfy our global 'acceptable error level' condition, $|s(Gr) - s_N(Gr)| \leqslant \varepsilon^s_{\mathrm{tol}}$, $\forall Gr \in \mathscr{D}$, for (close to) the smallest possible value of N?

In short, the essentially *ad hoc* nature of RB discretizations, the strongly superlinear scaling (with N) of the RB online complexity, and the particular needs of deployed real-time systems demand rigorous and quantitative *a posteriori* error estimators.

4.1. *Brezzi–Rappaz–Raviart theory*

4.1.1. Energy bounds. We first define the dual norm of the residual, $\varepsilon_N(Gr) \equiv \sup_{v \in Y} g(u_N(Gr), v; Gr)/\|v\|_Y$, and the inf–sup and continuity constants associated with the derivative at $u_N(Gr)$, $\beta_N(Gr) \equiv \beta(u_N(Gr))$ and $\gamma_N(Gr) \equiv \gamma(u_N(Gr))$, respectively. We further introduce a *lower bound* for $\beta_N(Gr)$ (to be developed in Section 4.2.3), $\tilde{\beta}_N(Gr)$: we require $0 \leqslant \tilde{\beta}_N(Gr) \leqslant \beta_N(Gr)$, $\forall Gr \in \mathscr{D}$.

We next introduce the key parameters required by the BRR theory [11–13]. First, we define a proximity indicator (a 'non-dimensional' measure of the residual), $\tau_N(Gr) \equiv 2\rho^2 \varepsilon_N(Gr)/\tilde{\beta}^2_N(Gr)$. Second, we define our bound for the error in the Y norm as

$$\Delta_N(Gr) \equiv \tilde{\beta}_N(Gr)\rho^{-2}\left(1 - \sqrt{1 - \tau_N(Gr)}\right) \tag{7}$$

We can now state [12, 14].

Proposition 2.1
For $\tau_N(Gr)<1$, there exists a unique solution $u(Gr)\in\mathscr{B}(u_N(Gr),\tilde{\beta}_N(Gr)/\rho^2)$, where $\mathscr{B}(z,r)\equiv\{y\in Y \mid \|y-z\|_Y<r\}$; furthermore, $\|u(Gr)-u_N(Gr)\|_Y\leqslant\Delta_N(Gr)$.

Proof
Our demonstration is only a very minor variation on the proof given in Reference [12, Theorem 2.1]; we simply specialize the general result to our particular problem [17]. (Note also that our context is *finite-dimensional*—since our bounds are with respect to the truth approximation—and hence various hypotheses simplify.) We first note from (1), (2), and (4) that

$$g(w^2,v;Gr)-g(w^1,v;Gr)=\int_0^1 \mathrm{d}g(w^2-w^1,v;w^1+t(w^2-w^1))\,\mathrm{d}t \tag{8}$$

and

$$|\mathrm{d}g(w,v;z^2)-\mathrm{d}g(w,v;z^1)|=|a_1(w,z^2-z^1,v)|\leqslant\rho^2\|w\|_Y\|v\|_Y\|z^2-z^1\|_Y \tag{9}$$

We next introduce the operator $H^{Gr}(w)$, $w\in Y\to H^{Gr}(w)\in Y$, defined as

$$\mathrm{d}g(H^{Gr}(w),v;u_N(Gr))=\mathrm{d}g(w,v;u_N(Gr))-g(w,v;Gr),\quad \forall v\in Y \tag{10}$$

note (10) is well-posed for all $w\in Y$ (*finite-dimensional*) thanks to our hypothesis $\tau_N(Gr)<1$ and hence $\beta_N(Gr)>0$. A fixed point of $H^{Gr}(w)$, $H^{Gr}(w^*)=w^*$, implies a zero of g, $g(w^*,v;Gr)=0$, $\forall v\in Y$.

We now consider $w^1\in\overline{\mathscr{B}}(u_N(Gr);\alpha)$, $w^2\in\overline{\mathscr{B}}(u_N(Gr);\alpha)$. It follows from (8)–(10) that $\|H^{Gr}(w^2)-H^{Gr}(w^1)\|_Y\leqslant(\rho^2\alpha/\tilde{\beta}_N(Gr))\|w^2-w^1\|_Y$; hence $\|H^{Gr}(w^2)-H^{Gr}(w^1)\|_Y<\|w^2-w^1\|_Y$ for all $\alpha\in[0,\tilde{\beta}_N(Gr)/\rho^2[$. We can further prove that, for $w\in\overline{\mathscr{B}}(u_N(Gr),\alpha)$,

$$\begin{aligned}\|H^{Gr}(w)-u_N(Gr)\|_Y &\leqslant \tilde{\beta}_N(Gr)^{-1}\left(\varepsilon_N(Gr)+\int_0^1 \rho^2\|t(w-u_N(Gr))\|_Y\|w-u_N(Gr)\|_Y\,\mathrm{d}t\right)\\ &\leqslant \tilde{\beta}_N(Gr)^{-1}\left(\varepsilon_N(Gr)+\tfrac{1}{2}\rho^2\alpha^2\right)\end{aligned}$$

hence $H^{Gr}(w)$ maps $\overline{\mathscr{B}}(u_N(Gr),\alpha)$ into itself for all $\alpha\in[\Delta_N(Gr),\tilde{\beta}_N(Gr)\rho^{-2}(1+\sqrt{1-\tau_N(Gr)})]$. We can thus conclude from the contraction mapping theorem that for all $\alpha\in[\Delta_N(Gr),\tilde{\beta}_N(Gr)\rho^{-2}[$ there exists a unique solution $u(Gr)\in\overline{\mathscr{B}}(u_N(Gr),\alpha)$ satisfying $g(u(Gr),v;Gr)=0$, $\forall v\in Y$. This completes the proof. □

We may also now readily prove

Corollary 2.2
For $\tau_N(Gr)\leqslant\frac{1}{2}$, $\beta(u(Gr))\geqslant\tilde{\beta}_N(Gr)/\sqrt{2}$.

Proof
It follows directly from Theorem 2.1 and Equation (1.2) of Reference [12] that, for $\tilde{\beta}_N(Gr)^{-1}\rho^2\|u(Gr)-u_N(Gr)\|_Y<1$, $\beta(u(Gr))\geqslant\tilde{\beta}_N(Gr)-\rho^2\|u(Gr)-u_N(Gr)\|_Y$. However, from

our Proposition 2.1 and (7) (for $\tau_N(Gr) \leqslant \frac{1}{2}$) $\rho^2 \|u(Gr) - u_N(Gr)\|_Y \leqslant \tilde{\beta}_N(Gr)(1 - \sqrt{\frac{1}{2}})$; thus $\beta(u(Gr)) \geqslant \tilde{\beta}_N(Gr)(1 - (1 - \sqrt{\frac{1}{2}})) = \tilde{\beta}_N(Gr)/\sqrt{2}$. □

Corollary 2.2 is essential in confirming Hypothesis H-II, providing a sufficient (though not necessary) condition for the well-posedness of the truth approximation. (Corollary 2.2 also demonstrates existence and uniqueness of $\psi^N(Gr)$ of (6) for $\tau_N(Gr) < 1$.)

Finally, we may bound the effectivity $\eta_N(Gr) \equiv \Delta_N(Gr)/\|e^N(Gr)\|_Y$ (recall $e^N(Gr) \equiv u(Gr) - u_N(Gr)$) in

Corollary 2.3
For $\tau_N(Gr) \leqslant \frac{1}{2}$, $\eta_N(Gr) \leqslant 4\kappa_N(Gr)$, where $\kappa_N(Gr) \equiv \gamma_N(Gr)/\tilde{\beta}_N(Gr)$.

Proof
We first note from standard duality arguments that $\varepsilon_N(Gr) = \|\hat{e}^N(Gr)\|_Y$, where $\hat{e}^N(Gr) \in Y$ satisfies

$$(\hat{e}^N(Gr), v)_Y = -g(u_N(Gr), v; Gr), \quad \forall v \in Y \tag{11}$$

It then follows from (3) for $z = u_N(Gr)$ and $w \equiv e^N(Gr)$ that $g(u(Gr), v; Gr) = g(u_N(Gr), v; Gr) + \mathrm{d}g(e^N(Gr), v; u_N(Gr)) + \frac{1}{2} a_1(e^N(Gr), e^N(Gr), v)$, and hence $\|\hat{e}^N(Gr)\|_Y \leqslant \gamma_N(Gr)\|e^N(Gr)\|_Y + \frac{1}{2}\rho^2\|e^N(Gr)\|_Y^2$. We now bound (for $\tau_N(Gr) < 1$) $\|e^N(Gr)\|_Y \leqslant \Delta_N(Gr)$ and (from (7)) $\Delta_N(Gr) \leqslant 2\varepsilon_N(Gr)/\tilde{\beta}_N(Gr)$ to deduce that $\frac{1}{2}\Delta_N(Gr) \leqslant \gamma_N(Gr)\tilde{\beta}_N(Gr)^{-1}$ $\|e^N(Gr)\|_Y + \rho^2\varepsilon_N(Gr)\tilde{\beta}_N(Gr)^{-2}\Delta_N(Gr)$. However, from our assumption on $\tau_N(Gr)$, we obtain $\rho^2\varepsilon_N(Gr)/\tilde{\beta}_N^2(Gr) = \frac{1}{2}\tau_N(Gr) \leqslant \frac{1}{4}$; the desired result directly follows. □

Corollary 2.3, which provides a lower bound for $\|e^N(Gr)\|_Y$, relates to the sharpness of $\Delta_N(Gr)$; in Section 5 we provide a more quantitative discussion.

4.1.2. Output bounds. We first introduce the adjoint (or dual) residual, $R^{\mathrm{du},N}_{N^{\mathrm{du}}}(\varphi; Gr) \equiv -L(\varphi) - \mathrm{d}g(\varphi, \psi^N_{N^{\mathrm{du}}}(Gr); u_N(Gr))$, $\forall \varphi \in Y$; the adjoint residual dual norm $\varepsilon^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr) \equiv \sup_{\varphi \in Y} R^{\mathrm{du},N}_{N^{\mathrm{du}}}(\varphi; Gr)/\|\varphi\|_Y$; and, for $\tau_N(Gr) < 1$, the adjoint error bound,

$$\Delta^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr) \equiv \frac{2\varepsilon^{\mathrm{du},N}_{N^{\mathrm{du}}}}{\tilde{\beta}_N(Gr)(1 + \sqrt{1 - \tau_N(Gr)})} + \frac{1 - \sqrt{1 - \tau_N(Gr)}}{1 + \sqrt{1 - \tau_N(Gr)}}\|\psi^N_{N^{\mathrm{du}}}(Gr)\|_Y \tag{12}$$

Our output error bound is then given by $\Delta^s_{N,N^{\mathrm{du}}}(Gr) \equiv \|L\|_{Y'}\Delta_N(Gr)$ for $N^{\mathrm{du}} = 0$ (a notational convenience), and

$$\Delta^s_{N,N^{\mathrm{du}}}(Gr) = |g(u_N(Gr), \psi^N_{N^{\mathrm{du}}}(Gr); Gr)| + \varepsilon_N(Gr)\Delta^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr) \tag{13}$$

for $1 \leqslant N^{\mathrm{du}} \leqslant N^{\mathrm{du}}_{\max}$; here $\|L\|_{Y'} \equiv \sup_{\varphi \in Y} L(\varphi)/\|\varphi\|_Y$ is independent of *Gr*. (The only new computational ingredients are $\varepsilon^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr)$, $\|\psi^N_{N^{\mathrm{du}}}(Gr)\|_Y$, and $|g(u_N(Gr), \psi^N_{N^{\mathrm{du}}}(Gr); Gr)|$.)

We may now prove

Lemma 3.1
For $\tau_N(Gr) < 1$, $\|\psi^N(Gr) - \psi^N_{N^{\mathrm{du}}}(Gr)\|_Y \leqslant \Delta^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr)$.

Proof
We note that $\psi^N(Gr) - \psi^N_{N^{\mathrm{du}}}(Gr)$ satisfies $\mathrm{d}g(\varphi, \psi^N(Gr) - \psi^N_{N^{\mathrm{du}}}(Gr); u_N(Gr)) = R^{\mathrm{du},N}_{N^{\mathrm{du}}}(\varphi; Gr) - \frac{1}{2}\, a_1(\varphi, e^N(Gr), \psi^N(Gr) - \psi^N_{N^{\mathrm{du}}}(Gr)) - \frac{1}{2}\, a_1(\varphi, e^N(Gr), \psi^N_{N^{\mathrm{du}}}(Gr))$; the result then follows from (4), Proposition 2.1, (7), and (12). □

And thus

Proposition 3.2
For $\tau_N(Gr) < 1$, $|s(Gr) - s_N(Gr)| \leqslant \Delta^s_{N,N^{\mathrm{du}}}(Gr)$.

Proof
For $N^{\mathrm{du}} = 0$ we invoke continuity of L and Proposition 2.1; for $N^{\mathrm{du}} > 0$ we invoke Lemma 1 (for $\chi = \psi^N_{N^{\mathrm{du}}}(Gr)$), Cauchy–Schwarz, Lemma 3.1, and (13). □

In Section 5 we shall investigate the effectivity of this output error bound.

4.2. Construction of error estimators

The framework described above is essentially the nonlinear extension of the much simpler linear *a posteriori* error estimator result $\|u(Gr) - u_N(Gr)\|_Y \leqslant \varepsilon_N(Gr)/\tilde{\beta}_N(Gr)$ [19]—to which our non-linear error estimator, $\Delta_N(Gr)$, reduces in the limit that $\varepsilon_N(Gr)$ tends to zero. The challenge, as in the linear case [18, 19], is the development of calculable, predictive error estimators: error estimators that are quantitative, rigorous, sharp, and inexpensive—online complexity independent of $\mathcal{N}$.

4.2.1. The dual norm of the residual(s). We now consider the calculation of $\varepsilon_N(Gr) = \|\hat{e}^N(Gr)\|_Y$. We first note from (11) that $\hat{e}^N(Gr) \in Y$ satisfies

$$(\hat{e}^N(Gr), v)_Y = GrF(v) - \sum_n a_0(\zeta_n, v) u_{N\,n}(Gr) - \sum_n \sum_{n'} \frac{1}{2}\, a_1(\zeta_n, \zeta_{n'}, v) u_{N\,n}(Gr) u_{N\,n'}(Gr), \quad \forall v \in Y \tag{14}$$

where $\sum_m$ with no upper limit explicitly provided shall denote $\sum_{m=1}^N$. (We recall that $u_N(Gr)$ may be expressed as $\sum_n u_{N\,n}(Gr)\zeta_n$.) It follows from linearity that $\hat{e}^N(Gr) = Gr\,\hat{z}^0 + \sum_n \hat{z}^1_n u_{N\,n}(Gr) + \sum_n \sum_{n'} \hat{z}^2_{nn'} u_{N\,n}(Gr) u_{N\,n'}(Gr)$, where $\hat{z}^0 \in Y$ satisfies $(\hat{z}^0, v)_Y = F(v)$, $\forall v \in Y$, $\hat{z}^1_n \in Y$ satisfies $(\hat{z}^1_n, v)_Y = -a_0(\zeta_n, v)$, $\forall v \in Y$, $\forall n \in \mathbb{N}_{\max}$, and $\hat{z}^2_{nn'} \in Y$ satisfies $(\hat{z}^2_{nn'}, v)_Y = -\frac{1}{2}\, a_1(\zeta_n, \zeta_{n'}, v)$, $\forall v \in Y$, $\forall n, n' \in \mathbb{N}^2_{\max}$. We thus obtain

$$\begin{aligned} \|\hat{e}^N(Gr)\|^2_Y = Gr^2(\hat{z}^0, \hat{z}^0)_Y + \sum_n u_{N\,n}(Gr) \Bigg\{ & 2Gr(\hat{z}^0, \hat{z}^1_n)_Y + \sum_{n'} u_{N\,n'}(Gr) \Bigg\{ 2Gr(\hat{z}^0, \hat{z}^2_{nn'})_Y \\ & + (\hat{z}^1_n, \hat{z}^1_{n'})_Y + \sum_{n''} u_{N\,n''}(Gr) \Bigg\{ 2(\hat{z}^1_n, \hat{z}^2_{n'\,n''})_Y \\ & + \sum_{n'''} u_{N\,n'''}(Gr) \Bigg\{ (\hat{z}^2_{nn'}, \hat{z}^2_{n''n'''})_Y \Bigg\} \Bigg\} \Bigg\} \Bigg\} \end{aligned} \tag{15}$$

which is a nested quadruple sum.

The offline–online decomposition is now clear. In the *offline* stage, performed once, we (i) solve for the $\hat{z}^0$, $\hat{z}^1_n$, $\forall n \in \mathbb{N}_{\max}$, and $\hat{z}^2_{nn'}$, $\forall n, n' \in \mathbb{N}^2_{\max}$, at dominant cost $O(N^2_{\max}\mathcal{N}^{\cdot \mathrm{Po}})$—here $\cdot$Po refers to a scaling exponent (>1) associated with the (divergence-free) truth-approximation Poisson solution procedure, and then (ii) form the relevant parameter-independent inner products, $(\hat{z}^0, \hat{z}^0)_Y, \ldots, (\hat{z}^2_{nn'}, \hat{z}^2_{n''n'''})_Y$, $\forall n, n', n'', n''' \in \mathbb{N}^4_{\max}$, at dominant cost (exploiting sparsity) $O(N^4_{\max}\mathcal{N})$. In the *online* stage—performed many times, for each new value of Gr—we simply evaluate the requisite quadruple sum, (15), at dominant cost $O(N^4)$. The online complexity is *independent of* $\mathcal{N}$: although the N^4 scaling is less than pleasant, in practice N is quite small; furthermore, this calculation is invoked only once (in contrast to the Newton kernel). We may develop a similar procedure for the dual norm of the adjoint residual, $\varepsilon^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr)$; the online complexity is $O(N^2(N^{\mathrm{du}})^2)$, independent of $\mathcal{N}$.

4.2.2. The Sobolev constant. In actual practice, and solely for simplicity, we compute an *upper bound* for the Sobolev constant ρ, replacing (the divergence-free space) Y with $\tilde{Y} \equiv [(H^1_0(\Omega))^2]_{\mathrm{truth}}$; in order to avoid excessive nomenclature, we simply redefine $\rho \equiv \sqrt{2}\, \sup_{v \in \tilde{Y}} \|v\|_{L^4(\Omega)}/\|v\|_Y$. As our point of departure, we note [15, 16] that $\rho = (2/\hat{\lambda}_{\min})^{1/2}$, where $(\hat{\lambda}, \hat{\phi}) \in (\mathbb{R}_+, \tilde{Y})$ satisfies the Euler–Lagrange equation $(\hat{\phi}, v)_Y = \hat{\lambda} \int_\Omega \hat{\phi}_j \hat{\phi}_j \hat{\phi}_i v_i$, $\forall v \in \tilde{Y}$, $\|\hat{\phi}\|^4_{L^4(\Omega)} = 1$, and $(\hat{\lambda}_{\min}, \hat{\phi}_{\min})$ denotes the ground state. To solve this non-linear eigenproblem, and in particular to ensure that we realize the ground state, we pursue a homotopy procedure.

Towards that end, we introduce $\alpha \in [0, 1]$ and associated increment $\Delta\alpha < 1$: $(\lambda(\alpha), \phi(\alpha)) \in (\mathbb{R}_+, \tilde{Y})$ then satisfies

$$(\phi(\alpha), v)_Y = \lambda(\alpha)\left(\alpha \int_\Omega \phi_j(\alpha)\phi_j(\alpha)\phi_i(\alpha)v_i + (1-\alpha)\int_\Omega \phi_i(\alpha)v_i\right), \quad \forall v \in \tilde{Y}$$

$$\alpha\|\phi\|^4_{L^4(\Omega)} + (1-\alpha)\|\phi\|^2_{L^2(\Omega)} = 1 \tag{16}$$

$(\lambda_{\min}(\alpha), \phi_{\min}(\alpha))$ shall denote the ground state. We observe that $(\lambda_{\min}(1), \phi_{\min}(1)) = (\hat{\lambda}_{\min}, \hat{\phi}_{\min})$, and that $(\lambda_{\min}(0), \phi_{\min}(0))$ is the lowest eigenpair of a standard (vector) Laplacian eigenproblem. Our homotopy procedure is simple: we first set $\alpha^{\mathrm{old}} = 0$ and find $(\lambda_{\min}(0), \phi_{\min}(0))$ by standard techniques; then, until $\alpha^{\mathrm{new}} = 1$, we set $\alpha^{\mathrm{new}} \leftarrow \alpha^{\mathrm{old}} + \Delta\alpha$, solve (16) for $(\lambda_{\min}(\alpha^{\mathrm{new}}), \phi_{\min}(\alpha^{\mathrm{new}}))$ by Newton iteration initialized to $(\lambda_{\min}(\alpha^{\mathrm{old}}), \phi_{\min}(\alpha^{\mathrm{old}}))$, and update $\alpha^{\mathrm{old}} \leftarrow \alpha^{\mathrm{new}}$. For our particular domain, we find (offline) $\rho = 0.4416$; since ρ is parameter-independent, no online computation is required.

4.2.3. The inf–sup lower bound. We now consider the construction of $\tilde{\beta}_N(Gr)$, a lower bound for $\beta_N(Gr)$. We note that, in contrast to ρ, $\beta_N(Gr)$ *must* be calculated with respect to the divergence-free space Y.

We first define, for given $Gr \in \mathscr{D}$, the linear operator $w \in Y \to T^{Gr}_N w \in Y$ as $(T^{Gr}_N w, v)_Y = \mathrm{d}g(w, v; u_N(Gr))$, $\forall v \in Y$. We then define, for $t \in \mathbb{R}$ and given $\overline{Gr}$,

$$\begin{aligned}\mathscr{T}(w, v; t; \overline{Gr}) \equiv{}& (T^{\overline{Gr}}_{N_{\max}} w, T^{\overline{Gr}}_{N_{\max}} v)_Y \\ &+ t[a_1(w, u'_{N_{\max}}(\overline{Gr}), T^{\overline{Gr}}_{N_{\max}} v) + a_1(v, u'_{N_{\max}}(\overline{Gr}), T^{\overline{Gr}}_{N_{\max}} w)]\end{aligned} \tag{17}$$

where $u'_{N_{\max}}(\overline{Gr})(=\mathrm{d}u_{N_{\max}}(\overline{Gr})/\mathrm{d}Gr)\in W_{N_{\max}}$ satisfies $\mathrm{d}g(u'_{N_{\max}}(\overline{Gr}),v;u_{N_{\max}}(\overline{Gr}))=F(v)$, $\forall v\in W_{N_{\max}}$. Next, for $t\in\mathbb{R}$ and given $\overline{Gr}$, we introduce $\mathscr{F}(t;\overline{Gr})\equiv\inf_{v\in Y}\mathscr{T}(v,v;t;\overline{Gr})/\|v\|_Y^2$, and $\delta_N(t;\overline{Gr})\equiv\rho^2\|u_N(\overline{Gr}+t)-u_{N_{\max}}(\overline{Gr})-tu'_{N_{\max}}(\overline{Gr})\|_Y$. Then

Lemma 4.1
The function $\mathscr{F}(t;\overline{Gr})$ is concave in t. Hence, given $t_1<t_2$, for all $t\in[t_1,t_2]$, $\mathscr{F}(t;\overline{Gr})\geqslant\min\{\mathscr{F}(t_1;\ \overline{Gr}),\mathscr{F}(t_2;\ \overline{Gr})\}$.

Proof
We define $\alpha=(t_2-t)/(t_2-t_1)\in[0,1]$ such that $t=\alpha t_1+(1-\alpha)t_2$. It follows from (17) that $\mathscr{T}(v,v;t;\overline{Gr})=\alpha\mathscr{T}(v,v;t_1;\overline{Gr})+(1-\alpha)\mathscr{T}(v,v;t_2;\overline{Gr})$ and hence $\mathscr{F}(t;\overline{Gr})=\inf_{v\in Y}(\alpha\mathscr{T}(v,v;t_1;\overline{Gr})+(1-\alpha)\mathscr{T}(v,v;t_2;\overline{Gr}))/\|v\|_Y^2\geqslant\alpha\mathscr{F}(t_1;\overline{Gr})+(1-\alpha)\mathscr{F}(t_2;\overline{Gr})\geqslant\min\{\mathscr{F}(t_1;\overline{Gr}),\mathscr{F}(t_2;\overline{Gr})\}$. □

We shall also need

Lemma 4.2
For given $Gr\in\mathscr{D}$, $\overline{Gr}\in\mathscr{D}$, and $t\equiv Gr-\overline{Gr}$, the inf–sup parameter satisfies $\beta_N(Gr)\geqslant-\delta_N(t;\overline{Gr})+\sqrt{\max\{\mathscr{F}(t;\overline{Gr}),\delta_N^2(t;\overline{Gr})\}}\geqslant 0$.

Proof
We first define $\sigma(w)\equiv\|T_N^{Gr}w\|_Y/\|w\|_Y$ and express $T_N^{Gr}w=T_{N_{\max}}^{\overline{Gr}}w+(T_N^{Gr}w-T_{N_{\max}}^{\overline{Gr}}w)$ to obtain

$$\sigma^2(w)=\{\|T_{N_{\max}}^{\overline{Gr}}w\|_Y^2+\|T_N^{Gr}w-T_{N_{\max}}^{\overline{Gr}}w\|_Y^2+2(T_{N_{\max}}^{\overline{Gr}}w,T_N^{Gr}w-T_{N_{\max}}^{\overline{Gr}}w)_Y\}/\|w\|_Y^2 \tag{18}$$

We next note that, for $t=Gr-\overline{Gr}$,

$$\begin{aligned}(T_{N_{\max}}^{\overline{Gr}}w,T_N^{Gr}w-T_{N_{\max}}^{\overline{Gr}}w)_Y&=a_1(w,u_N(Gr)-u_{N_{\max}}(\overline{Gr}),T_{N_{\max}}^{\overline{Gr}}w)=ta_1(w,u'_{N_{\max}}(\overline{Gr}),T_{N_{\max}}^{\overline{Gr}}w)\\&\quad+a_1(w,u_N(Gr)-u_{N_{\max}}(\overline{Gr})-tu'_{N_{\max}}(\overline{Gr}),T_{N_{\max}}^{\overline{Gr}}w)\end{aligned} \tag{19}$$

furthermore, from (4)

$$\begin{aligned}&|a_1(w,u_N(Gr)-u_{N_{\max}}(\overline{Gr})-tu'_{N_{\max}}(\overline{Gr}),T_{N_{\max}}^{\overline{Gr}}w)|\\&\quad\leqslant\delta_N(t;\overline{Gr})\|w\|_Y\|T_{N_{\max}}^{\overline{Gr}}w\|_Y\\&\quad\leqslant\delta_N(t;\overline{Gr})\|w\|_Y(\|T_N^{Gr}w\|_Y+\|T_{N_{\max}}^{\overline{Gr}}w-T_N^{Gr}w\|_Y)\\&\quad\leqslant\delta_N(t;\overline{Gr})\sigma(w)\|w\|_Y^2+\tfrac{1}{2}\,\delta_N^2(t;\overline{Gr})\|w\|_Y^2+\tfrac{1}{2}\|T_{N_{\max}}^{\overline{Gr}}w-T_N^{Gr}w\|_Y^2\end{aligned} \tag{20}$$

We conclude from (17)–(20) that $\sigma^2(w)\geqslant\mathscr{T}(w,w;t;\overline{Gr})/\|w\|_Y^2-2\delta_N(t;\overline{Gr})\sigma(w)-\delta_N^2(t;\overline{Gr})$; this quadratic inequality (recall $\sigma(w)\geqslant 0$) then yields $\sigma(w)\geqslant-\delta_N(t;\overline{Gr})+\sqrt{\max\{\mathscr{T}(w,w;t;\overline{Gr})/\|w\|_Y^2,\delta_N^2(t;\overline{Gr})\}}$. It is readily shown [19] that $\beta_N(Gr)=\inf_{w\in Y}\sigma(w)$, and hence $\beta_N(Gr)\geqslant-\delta_N(t;\overline{Gr})+\sqrt{\max\{\mathscr{F}(t;\overline{Gr}),\delta_N^2(t;\overline{Gr})\}}$. □

We may now construct our inf–sup lower bound, $\tilde{\beta}_N(Gr)$.

We first introduce a partition $\mathscr{P}_J \equiv \{\mathscr{R}^j \equiv]\overline{Gr}^j_-, \overline{Gr}^j_+[, 1 \leqslant j \leqslant J\}$ such that $\mathscr{R}^j \cap \mathscr{R}^{j'} = \emptyset$, $1 \leqslant j < j' \leqslant J$, and $\cup_{j=1}^J \overline{\mathscr{R}}^j = \mathscr{D}$; we further define $\log \overline{Gr}^j = \frac{1}{2}(\log \overline{Gr}^j_- + \log \overline{Gr}^j_+)$, $1 \leqslant j \leqslant J$. Then, for given $Gr \in \mathscr{D}$, our lower bound is

$$\tilde{\beta}_N(Gr) = -\delta_N(t; \overline{Gr}) + \sqrt{\max\{\min\{\mathscr{F}(0; \overline{Gr}), \mathscr{F}(t_*; \overline{Gr})\}, \delta_N^2(t; \overline{Gr})\}} \tag{21}$$

where $\overline{Gr} = \overline{Gr}^{\mathscr{I}Gr}$, $\overline{Gr}_\pm = \overline{Gr}_\pm^{\mathscr{I}Gr}$, $t = Gr - \overline{Gr}$, $t_\pm = \overline{Gr}_\pm - \overline{Gr}$, and $t_* = t_+$ (respectively, t_-) if $t \geqslant 0$ (respectively, $t < 0$); here $\mathscr{I}: \mathscr{D} \to \{1, \ldots, J\}$ is a mapping such that $Gr \in \overline{\mathscr{R}}^{\mathscr{I}Gr}$. We may then prove

Proposition 4.3
For all $Gr \in \mathscr{D}$, $\beta_N(Gr) \geqslant \tilde{\beta}_N(Gr) \geqslant 0$.

Proof
The result directly follows from Lemma 4.1, Lemma 4.2, and (21). □

Proposition 4.3 only guarantees a lower bound; to ensure a *good* lower bound, our partition must be sufficiently fine. We shall say that a partition $\mathscr{P}_J$ is ε_β-conforming if

$$\tilde{\beta}_{N_{\max}}(Gr) \geqslant \varepsilon_\beta \beta_{N_{\max}}(\overline{Gr}^{\mathscr{I}Gr})(>0), \quad \forall Gr \in \mathscr{D} \tag{22}$$

if (22) is not honoured for any $\varepsilon_\beta \in]0, 1[$ there will exist $Gr \in \mathscr{D}$ for which the hypothesis of Proposition 2.1, $\tau_N(Gr) < 1$, is not satisfied, and hence for which certification is impossible.

We now turn to the offline–online computational procedure. In the *offline* stage, performed once, we (i) tabulate $\mathscr{F}(0; \overline{Gr}^j) = (\beta^2_{N_{\max}}(\overline{Gr}^j))$ and $\mathscr{F}(\overline{Gr}^j_\pm - \overline{Gr}^j; \overline{Gr}^j)$, $1 \leqslant j \leqslant J$, at dominant cost $O(3J\mathscr{N}^{\cdot \mathrm{SV}})$**—here $\cdot$SV refers to a scaling exponent (>1) associated with the truth-approximation singular-value solution procedure, and (ii) form the δ_N-related parameter-independent inner products $(\zeta_n, \zeta_{n'})_Y$, $\forall n, n' \in \mathbb{N}^2_{\max}$, at dominant cost (exploiting sparsity) $O(N^2_{\max}\mathscr{N})$. The properties of $\mathscr{F}(Gr - \overline{Gr}; \overline{Gr})$ are crucial. First, $\mathscr{F}(Gr - \overline{Gr}; \overline{Gr})$ is concave in $Gr - \overline{Gr}$: hence, a *finite* number of expensive evaluations suffice to rigorously construct $\tilde{\beta}_N(Gr)$. Second, $\mathscr{F}(Gr - \overline{Gr}; \overline{Gr})$ is (sub-)tangent to $\beta^2_{N_{\max}}(Gr)$ at $Gr = \overline{Gr}$—the more pessimistic bounds such as ρ appear only in the *second-order* correction, $\delta_N(Gr - \overline{Gr}; \overline{Gr})$: hence, J will be 'small' (for example, relative to simpler continuity constructions [17]). In the *online* stage—performed many times, for each new value of Gr—we need only (i) find $\overline{Gr} = \mathscr{I}Gr$, at cost $O(\log J)$, and (ii) evaluate $\delta_N(Gr - \overline{Gr}; \overline{Gr})$, at dominant cost $O(N^2_{\max})$.

4.3. Sampling procedure

We first construct our primal samples and spaces, S_N and W_N, $1 \leqslant N \leqslant N_{\max}$; we then select our dual samples and spaces, $S^{\mathrm{du}}_{N^{\mathrm{du}}}$ and $W^{\mathrm{du}}_{N^{\mathrm{du}}}$, $1 \leqslant N^{\mathrm{du}} \leqslant N^{\mathrm{du}}_{\max}$. We pursue (very similar) greedy optimization procedures [1] for both the primal and dual; in the interest of brevity, we consider only the former here.

We first provide a random parameter test sample $\Xi_\mathrm{T} \in (\mathscr{D})^{n_\mathrm{T}}$ of size n_T, a 'smallest (energy) error tolerance' $\varepsilon_{\mathrm{tol,rel,min}}$, and an initial sample S_{N_0}; we further introduce—since $u_{N_{\max}}(Gr)$ is

**In practice, to determine an ε_β-conforming partition $\mathscr{P}_J$—that is, to find appropriate $Gr^j_\pm$, $1 \leqslant j \leqslant J$, such that (22) is satisfied for prescribed $\varepsilon_\beta \in]0, 1[$—we must perform additional singular value calculations.

of course not yet available—$\overline{\tau}_N(Gr)$ (respectively, $\overline{\Delta}_N(Gr)$) given by $\tau_N(Gr)$ (respectively, $\Delta_N(Gr)$) with $\tilde{\beta}_N(Gr)$ replaced by a crude surrogate, $\overline{\beta}(Gr)$. We now recurse: Given a sample S_N (initially, S_{N_0}), we calculate $Gr^* = \arg\max_{Gr \in \Xi_{\rm T}} \overline{\tau}_N(Gr)$ and $Gr^{**} = \arg\max_{Gr \in \Xi_{\rm T} | \overline{\tau}_N(Gr)<1} \overline{\Delta}_{N,\rm rel}(Gr)$, where $\overline{\Delta}_{N,\rm rel}(Gr) \equiv \overline{\Delta}_N(Gr)/\|u_N(Gr)\|_Y$; next, if $\overline{\tau}_N(Gr^*)>1$ (respectively, $\overline{\tau}_N(Gr^*)<1$) we set $Gr^{N+1}=Gr^*$ (respectively, $Gr^{N+1}=Gr^{**}$) and $S_{N+1}=S_N \cup Gr^{N+1}$; we then continue this process until $N=N_{\max}$ such that $\overline{\tau}_{N_{\max}}(Gr)<1$, $\forall Gr \in \Xi_{\rm T}$, and $\max_{Gr \in \Xi_{\rm T}} \overline{\Delta}_{N_{\max},\rm rel}(Gr) \leqslant \varepsilon_{\rm tol,rel,min}$. It is important to note that $\overline{\Delta}_N(Gr)$ is an accurate surrogate for the true error that can be calculated very efficiently—complexity independent of $\mathcal{N}$—in the limit of many queries: only the *selected* (expensive) snapshots must actually be computed; we may thus choose $n_{\rm T}$ large.

In summary, we can expect that our sequence of spaces W_N will provide rapidly certifiable (thanks to Gr^*) and rapidly convergent (thanks to Gr^{**}) approximations *uniformly over* $\mathcal{D}$.[††]

5. NUMERICAL RESULTS

We set $\varepsilon_{\rm tol,rel,min}=10^{-6}$ (see Section 4.3) and $\varepsilon_\beta=0.5$ (see (22)) to construct our RB (primal) sample and inf–sup partition, respectively; we obtain $N_{\max}=18$ and $J=39$. To present our numerical results we introduce a random test sample over $\mathcal{D}$, $\Xi_{\rm Test} \in (\mathcal{D})^{n_{\rm Test}}$ of size $n_{\rm Test}=25$ (note the sample is in lin(Gr), not log(Gr), and hence most of the points are in the difficult range $[10^4, 10^5]$); we further define 'Max_{Gr}' to be the maximum over all Gr in $\Xi_{\rm Test}$, and 'Avg_{Gr}' to be the average over all Gr in $\Xi_{\rm Test}$. We shall discard all results $(N, Gr) \in \mathbb{N}_{\max} \times \Xi_{\rm Test}$ for which our *a posteriori* bounds are contaminated by round-off error; our criterion is $(\|\hat{e}^N(Gr)\|_Y/\|u(Gr)\|_Y)^2 < 10 \times 10^{-16}$.

We first consider the 'energy' (or Y) norm. We present in Table I $e^N_{\max,\rm Rel} \equiv \text{Max}_{Gr}(\|e^N(Gr)\|_Y/\|u(Gr)\|_Y)$, $\tau_{N,\max} \equiv \text{Max}_{Gr}\tau_N(Gr)$, $\Delta_{N,\max,\rm Rel} \equiv \text{Max}_{Gr}\Delta_N(Gr)/\|u(Gr)\|_Y$, and $\overline{\eta}_N \equiv \text{Avg}_{Gr}\eta_N(Gr)$, as a function of N; we recall that $\eta_N(Gr) \equiv \Delta_N(Gr)/\|e^N(Gr)\|_Y$. We observe that the error decreases very rapidly; that the 'certifiability' hypothesis of Proposition 2.1, $\tau_N(Gr)<1$, is satisfied uniformly over $\Xi_{\rm Test}$ for $N \geqslant 10$; and that our error estimator (when applicable) is indeed a strict *and* reasonably sharp upper bound—even $\max_{N \in \mathbb{N}_{\max}} \text{Max}_{Gr}\eta_N(Gr)=25.7$ is well below the worst-case bound of Corollary 2.3.[‡‡] Note that for the rapidly convergent RB approximation, effectivities of $O(10)$ suffice: for a given accuracy $\varepsilon_{\rm tol}$, N' such that $\Delta_{N'}(Gr)=\varepsilon_{\rm tol}$—our *certifiably* sufficient approximation—is only slightly larger than N'' such that $\|e^{N''}(Gr)\|_Y=\varepsilon_{\rm tol}$—the *actually* sufficient approximation; the 'error in the error' can be large since the error itself decreases so quickly—this also justifies our relatively crude inf–sup lower bound.

It is perhaps surprising that the BRR theory—not specifically designed for quantitative application—indeed yields such sharp results. As already noted, as $\varepsilon_N(Gr) \to 0$, $\Delta_N(Gr) \sim$

[††]Nevertheless, our sampling procedure is not infallible, and hence it is possible that we encounter (online) a $Gr' \in \mathcal{D}$ for which $\Delta_N(Gr')$ is unacceptably large. In this event—note for purposes of rigor, sharpness, and efficiency we always evaluate $\Delta_N(Gr)$ online for each new 'deployed' Gr value considered—we would need to return to the offline stage and append Gr' to our sample. To avoid the latter, we typically choose $n_{\rm T}$ reasonably large and $\varepsilon_{\rm tol,rel,min}$ conservatively small.

[‡‡]Note $\beta_{N_{\max}}(Gr)$ is unity for $Gr \in [1, 10^4]$ and then smoothly decreases for $Gr \geqslant 10^4$ to 0.155 at $Gr=10^5$; $\gamma_{N_{\max}}$ is unity for low Gr and then increases with Gr for $Gr \geqslant 10^4$ to $\gamma_{N_{\max}}=8.75$ at $Gr=10^5$. Thus Corollary 2.3 predicts (say for $N=N_{\max}$) a worst-case effectivity of $4\gamma_N(Gr=10^5)/\tilde{\beta}_N(Gr=10^5)=229.1$.

Table I. Reduced-basis error, proximity measure, error bound, and effectivity as a function of N.

N	$e^N_{\max,\mathrm{Rel}}$	$\tau_{N,\max}$	$\Delta_{N,\max,\mathrm{Rel}}$	$\bar{\eta}_N$
2	4.36×10^{-1}	∞	—	—
4	1.51×10^{-1}	∞	—	—
6	4.51×10^{-2}	∞	—	—
8	3.31×10^{-2}	$4.68 \times 10^{+1}$	—	—
10	4.29×10^{-3}	5.44×10^{-1}	7.23×10^{-3}	7.00
12	2.32×10^{-3}	1.61×10^{-1}	3.52×10^{-3}	6.83
14	3.63×10^{-5}	1.08×10^{-1}	1.12×10^{-4}	7.43
16	8.23×10^{-6}	2.24×10^{-2}	1.54×10^{-5}	7.55
18	1.28×10^{-6}	1.73×10^{-2}	5.78×10^{-6}	10.06

Table II. Reduced-basis output error, error bound, and effectivity as a function of N for $N^{\mathrm{du}} = 0$, 10.

N	$e^s_{N,\max}$	$\Delta^s_{N,N^{\mathrm{du}}=0,\max}$	$\eta^s_{N,N^{\mathrm{du}}=0,\max}$	$\Delta^s_{N,N^{\mathrm{du}}=10,\max}$	$\eta^s_{N,N^{\mathrm{du}}=10,\max}$
10	8.57×10^{-3}	3.44×10^{-1}	$6.98 \times 10^{+3}$	2.1507×10^{-2}	$1.92 \times 10^{+2}$
12	1.39×10^{-3}	1.68×10^{-1}	$1.40 \times 10^{+3}$	4.7546×10^{-3}	$6.33 \times 10^{+0}$
14	4.09×10^{-4}	3.47×10^{-2}	$1.29 \times 10^{+3}$	5.0779×10^{-4}	$1.03 \times 10^{+1}$
16	1.44×10^{-5}	6.15×10^{-3}	$4.48 \times 10^{+4}$	3.6295×10^{-5}	$7.87 \times 10^{+0}$
18	1.16×10^{-5}	3.41×10^{-3}	$1.70 \times 10^{+3}$	2.2570×10^{-5}	$2.70 \times 10^{+0}$

$\varepsilon_N(Gr)/\tilde{\beta}_N(Gr)$, and thus the more pessimistic bounds (in particular, as reflected in ρ) are absent; nevertheless, as Gr increases, there is some degradation in the effectivity due to the increased strength of the nonlinearity relative to the dissipative terms. We also note that $\tau_N(Gr)$ *is* seriously impacted by the cruder estimates (such as ρ): even with our 'certification-oriented' samples, the hypothesis of Proposition 2.1 may force us to consider higher N than actually required for accuracy; this is particularly true as we consider the output error.

We now turn to the output error bounds. We define the output effectivity as $\eta^s_{N,N^{\mathrm{du}}}(Gr) \equiv \Delta^s_{N,N^{\mathrm{du}}}(Gr)/|s(Gr)-s_N(Gr)|$; we also recall (from Lemma 1 and (11)) that $|s(Gr)-s_N(Gr)| = |(\hat{e}^N(Gr),\psi^N(Gr))_Y|$. We present in Table II $e^s_{N,\max} \equiv \mathrm{Max}_{Gr}|s(Gr) - s_N(Gr)|$, $\Delta^s_{N,N^{\mathrm{du}}=0,\max}$, $\eta^s_{N,N^{\mathrm{du}}=0,\max}$, $\Delta^s_{N,N^{\mathrm{du}}=10,\max}$, and $\eta^s_{N,N^{\mathrm{du}}=10,\max}$ as a function of N; here, $\Delta^s_{N,N^{\mathrm{du}},\max} \equiv \mathrm{Max}_{Gr}\Delta^s_{N,N^{\mathrm{du}}}(Gr)$, and $\eta^s_{N,N^{\mathrm{du}},\max} \equiv \mathrm{Max}_{Gr}\eta^s_{N,N^{\mathrm{du}}}(Gr)$. The output converges quite rapidly.[§§]

[§§]We recall that adjoint techniques are typically applied to (i) develop effective *a posteriori* estimators, and (ii) (efficiently) increase the accuracy of the output [24]. In our case we focus on (i) since, in part due to the 'exponential' convergence of the RB approximation, and in part due to the $\tau_N(Gr) < 1$ condition, the accuracy of the uncorrected output is typically more than adequate. However, we can also pursue (ii): we define $\tilde{s}_{N,N^{\mathrm{du}}}(Gr) = s_N(Gr) + g(u_N(Gr), \psi^N_{N^{\mathrm{du}}}(Gr); Gr)$; then (from Lemma 1, (12), and Proposition 3.2) $|s(Gr) - \tilde{s}_{N,N^{\mathrm{du}}}(Gr)| \leqslant \varepsilon_N(Gr)\Delta^{\mathrm{du},N}_{N^{\mathrm{du}}}(Gr) \equiv \tilde{\Delta}^s_{N,N^{\mathrm{du}}}(Gr)$. For our problem (with rather different primal and dual solutions) we achieve increased accuracy for modest N^{du}—the error in $\tilde{s}_{N,N^{\mathrm{du}}}(Gr)$ is $O(10^{-6})$ at $N = 14$, $N^{\mathrm{du}} = 12$; however, the effectivity $\tilde{\Delta}^s_{N,N^{\mathrm{du}}}(Gr)/|s(Gr) - \tilde{s}_N(Gr)|$ is poor because we are again ignoring correlations, now between $\hat{e}^N(Gr)$ and the adjoint *error* $(\psi^N(Gr) - \psi^N_{N^{\mathrm{du}}}(Gr))$. In fact, we can develop procedures in which we devote some adjoint resources to improve accuracy and the remainder to control effectivity; but the optimal allocation of resources for given *certifiable* accuracy requires further deliberation.

The simple error bound $\Delta^s_{N,N^{\mathrm{du}}=0} \equiv \|L\|_{Y'}\Delta_N(Gr)$—though clearly computationally convenient, in particular for many outputs—ignores the correlation between $\hat{e}^N(Gr)$ and $\psi^N(Gr)$, and hence yields very poor effectivities; in contrast (for fixed N sufficiently large), $\Delta^s_{N,N^{\mathrm{du}}=10}(Gr)$ captures the correlation between $\hat{e}^N(Gr)$ and $\psi^N(Gr)$, and hence yields good effectivities (except for $N=10$, for which $\tau_N(Gr)$—and hence the second term in (12)—is not yet sufficiently small). For our particular problem, in which the primal and dual solutions are rather different, good effectivities are obtained with rather modest dual approximations—$N^{\mathrm{du}} < N$—that thus increase the online cost by *at most* a factor of two.

Finally, we note that the online cost to evaluate $s_N(Gr)$ and $\Delta_N(Gr)$, $\Delta^s_{N,N^{\mathrm{du}}}(Gr)$ for any new Gr is very small: first, because N (and N^{du}) is very small—thanks to (i) the good convergence properties of (S_N and hence) W_N and ($S^{\mathrm{du}}_{N^{\mathrm{du}}}$ and hence) $W^{\mathrm{du}}_{N^{\mathrm{du}}}$, and (ii) the rigorous and sharp 'stopping criterion' provided by $\Delta_N(Gr)$, $\Delta^s_{N,N^{\mathrm{du}}}(Gr)$; and second, because the marginal computational complexity to evaluate $s_N(Gr)$ and $\Delta_N(Gr)$, $\Delta^s_{N,N^{\mathrm{du}}}(Gr)$ depends only on N, N^{du} and *not* on $\mathcal{N}$—thanks to the offline/online computational decomposition. For our example, the online computation time (on a Pentium® M 1.6 GHz processor) for $Gr \in \Xi_{\mathrm{Test}}$ is typically 45 ms for $s_N(Gr)$, 20 ms for $\Delta_N(Gr)$, and an additional 10 ms for $\Delta^s_{N,N^{\mathrm{du}}}(Gr)$; the resulting computational savings relative to finite element approaches are significant, typically $O(100)$. Since the online computation time is independent of $\mathcal{N}$, the computational economies will be even more significant for more complex problems in particular in three space dimensions—without compromising rigorous certainty.

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