# Certified Rapid Solution of Partial Differential Equations for Real-Time Parameter Estimation and Optimization*

***M.A. Grepl*** [†], ***N.C. Nguyen*** [†‡], ***K. Veroy*** [†], ***A.T. Patera*** [†], ***and G.R. Liu*** [‡]

## 1 Introduction

Engineering analysis requires the prediction of selected "outputs" $s$ relevant to ultimate component and system performance; typical outputs include critical stresses or strains, flowrates or pressure drops, and various measures of temperature and heat flux. These outputs are functions of "inputs" $\mu$ that serve to identify a particular configuration of the component or system; typical inputs reflect geometry, properties, and boundary conditions and loads.

In many cases, the input-output function is best articulated as a (say) linear functional $\ell$ of a field variable $u(\mu)$ that is the solution to an input-parametrized partial differential equation (PDE); typical field variables and associated PDEs include temperature and steady/unsteady conduction, displacement and equilibrium elasticity/Helmholtz, and velocity and steady incompressible Navier-Stokes. System behavior is thus described by an input-output relation $s(\mu) = \ell(u(\mu))$ the evaluation of which requires solution of the underlying PDE.

*Invited paper submitted to Volume on 2nd Sandia Workshop on PDE-Constrained Optimization: Toward Real-Time and Online PDE-Constrained Optimization. This work was supported by DARPA and AFOSR under Grants F49620-03-1-0356 and FA9550-05-1-0114, by DARPA and GEAE under Grant F49620-03-1-0439, and by the Singapore-MIT Alliance.

[†] MIT, Rm 3-264, 77 Massachusetts Ave, Cambridge, MA 02139

[‡] National University of Singapore, 10 Kent Ridge Crescent, Singapore 117576

Our focus is on "deployed" systems — components or processes *in operation* in the field — and associated "Assess-Act" scenarios. In the Assess stage we pursue robust parameter estimation (inverse) procedures that map measured-observable outputs to (all) possible system-characteristic and environment-state inputs. In the subsequent Act stage we then pursue adaptive design (optimization) procedures that map mission-objective outputs to best control-variable inputs. The computational requirements on the PDE-induced evaluation $\mu \to s$ are formidable: the response must be *real-time* — we must "Assess-Act" *immediately*; and the outputs must be rigorously *certified* — we must "Assess-Act" *safely* and *feasibly* [24].

We describe here a method for real-time certified evaluation of PDE input-output relations; the two ingredients are reduced-basis (RB) approximation [2, 8, 10, 13, 19, 23, 25, 27] and *a posteriori* error estimation [19, 22, 29, 36, 37, 38]. We first describe the approach for elliptic linear second-order PDEs — Sections 2–5; we then consider extensions to certain nonlinear (incompressible Navier-Stokes) and parabolic (heat) equations — Sections 6 and 7, respectively.

## 2 Abstract Statement: Elliptic Linear Equations

We first consider the "exact" (superscript e) problem: given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, we evaluate $s^{\mathrm{e}}(\mu) = \ell(u^{\mathrm{e}}(\mu))$, where $u^{\mathrm{e}}(\mu)$ satisfies the weak form of our $\mu$-parametrized PDE, $a(u^{\mathrm{e}}(\mu), v; \mu) = f(v)$, $\forall\, v \in X^{\mathrm{e}}$. Here $\mu$ and $\mathcal{D}$ are the input and (closed) input domain, respectively; $u^{\mathrm{e}}(\mu)$ is our field variable; $X^{\mathrm{e}}$ is a Hilbert space with inner product $(w, v)$ and associated norm $\|w\| = \sqrt{(w,w)}$; and $a(\cdot,\cdot;\mu)$ and $f(\cdot)$, $\ell(\cdot)$ are $X^{\mathrm{e}}$-continuous bilinear and linear functionals, respectively.

Our interest here is in second-order PDEs, and thus $(H_0^1(\Omega))^\nu \subset X^{\mathrm{e}} \subset (H^1(\Omega))^\nu$: here $\Omega \subset \mathbb{R}^d$ is our spatial domain; $\nu = 1$ for a scalar field variable and $\nu = d$ for a vector field variable; and $H^1(\Omega)$ (respectively, $H_0^1(\Omega)$) is the usual Hilbert space of derivative square-integrable functions (respectively, derivative square-integrable functions that vanish on the domain boundary, $\partial\Omega$) [30]. The associated inner product $(\cdot,\cdot)$ is a $\mu$-independent continuous coercive symmetric bilinear form over $X^{\mathrm{e}}$ that perforce induces an $(H^1(\Omega))^\nu$-equivalent norm $\|\cdot\|$.

We next introduce $X$ (typically, $X \subset X^{\mathrm{e}}$), a reference finite element approximation space of finite dimension $\mathcal{N}$. Our reference (or "truth") finite element approximation $u(\mu) \in X$ is then defined by $a(u(\mu), v; \mu) = f(v)$, $\forall\, v \in X$: $u(\mu) \in X$ is a calculable surrogate for $u^{\mathrm{e}}(\mu)$ upon which we will build our RB approximation and with respect to which we will evaluate the RB error; $u(\mu)$ also serves as the "classical alternative" relative to which we will assess the efficiency of our approach. We assume that $\|u^{\mathrm{e}}(\mu) - u(\mu)\|$ is suitably small and hence that $\mathcal{N}$ is typically very large; our formulation must be both *stable* and *efficient* as $\mathcal{N} \to \infty$.

We shall make two crucial hypotheses. The first hypothesis is related to well-posedness, and is often verified only *a posteriori*. We assume that the inf-sup parameter, $\beta(\mu) \equiv \inf_{w \in X} \sup_{v \in X} [a(w, v; \mu)/(\|w\|\|v\|)]$, is strictly positive: $\beta(\mu) \geq \beta_0 > 0$, $\forall\, \mu \in \mathcal{D}$. The second hypothesis is related primarily to numerical efficiency, and is typically verified *a priori*. We assume that $a$ is *affine* in the parameter $\mu$: $a(w, v; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu) a^q(w, v)$, for $q = 1, \ldots, Q$ parameter-*dependent* functions

$\Theta^q(\mu) : \mathcal{D} \to \mathbb{R}$ and parameter-*independent* continuous bilinear forms $a^q(w, v)$. The affine assumption may in fact be relaxed [5].

## 3 Reduced-Basis Approximation

The reduced-basis (RB) approximation was first introduced in the late 1970s in the context of nonlinear structural analysis [2, 23] and subsequently abstracted and analyzed [8, 27] and extended [10, 13, 25] to a much larger class of parametrized partial differential equations. We first introduce nested samples $S_N \equiv \{\mu_1 \in \mathcal{D}, \ldots, \mu_N \in \mathcal{D}\}$, $1 \le N \le N_{\max}$, and associated nested "Lagrangian" RB spaces $W_N \equiv \operatorname{span}\{\zeta_n(\mu_n) \equiv u(\mu_n),\ 1 \le n \le N\}$, $1 \le N \le N_{\max}$. Our RB approximation is then: given $\mu \in \mathcal{D}$, evaluate $s_N(\mu) = \ell(u_N(\mu))$, where $u_N(\mu)$ satisfies $a(u_N(\mu), v; \mu) = f(v)$, $\forall\, v \in W_N$. We consider here only Galerkin projection.

In essence, $W_N$ comprises "snapshots" on the parametrically induced manifold $\mathcal{M} \equiv \{u(\mu) \,|\, \mu \in \mathcal{D}\} \subset X$. It is clear that $\mathcal{M}$ is very *low-dimensional*; furthermore, it can be shown under our hypotheses — we consider the equations for the sensitivity derivatives and invoke stability and continuity — that $\mathcal{M}$ is very *smooth*. We thus anticipate that $u_N(\mu) \to u(\mu)$ very rapidly, and hence that — at least for modest $P$ — we may choose $N \ll \mathcal{N}$. Many numerical examples justify this expectation (see Sections 5, 6, and 7); and, in certain simple cases, exponential convergence can be proven [20]. We emphasize that the deployed context requires global reduced-basis approximations that are *uniformly* (rapidly) convergent over the entire parameter domain $\mathcal{D}$; proper choice of the parameter samples $S_N$ is thus crucial (see Section 4).

We now represent $u_N(\mu)$ as $u_N(\mu) = \sum_{j \in \mathbb{N}} u_{N\,j}(\mu)\zeta_j$, where $\mathbb{N} \equiv \{1, \ldots, N\}$, and $\mathbb{N}_{\max} \equiv \{1, \ldots, N_{\max}\}$. Our RB output may then be expressed as $s_N(\mu) = \sum_{j \in \mathbb{N}} u_{N\,j}(\mu)\ell(\zeta_j)$, where — we now invoke our affine assumption — the $u_{N\,j}(\mu)$, $1 \le j \le N$, satisfy the $N \times N$ linear algebraic system

$$\sum_{j \in \mathbb{N}} \Big\{ \sum_{q \in \mathbb{Q}} \Theta^q(\mu) a^q(\zeta_j, \zeta_i) \Big\} u_{N\,j}(\mu) = f(\zeta_i), \quad \forall\, i \in \mathbb{N}\ , \tag{1}$$

where $\mathbb{Q} \equiv \{1, \ldots, Q\}$. (In practice we replace the $\zeta_j$, $1 \le j \le N$, with a $(\cdot,\cdot)$-orthonormalized system; the algebraic stiffness matrix is then well-conditioned.) It is clear from (1) that we may pursue an offline-online computational strategy [3, 13, 19, 29] ideally suited to the deployed real-time context.

In the *offline* stage — performed *once* — we first solve for the $\zeta_i$, $\forall\, i \in \mathbb{N}_{\max}$; we then form *and store* $f(\zeta_i), \ell(\zeta_i)$, $\forall\, i \in \mathbb{N}_{\max}$, and $a^q(\zeta_j, \zeta_i)$, $\forall\, (i, j) \in \mathbb{N}^2_{\max}$, $\forall\, q \in \mathbb{Q}$. In the online stage — performed many times, for each new $\mu$ "in the field" — we first assemble and subsequently invert the (full) $N \times N$ "stiffness" matrix $\sum_{q \in \mathbb{Q}} \Theta^q(\mu) a^q(\zeta_j, \zeta_i)$ to obtain the $u_{N\,j}(\mu)$, $1 \le j \le N$ — at cost $O(QN^2) + O(N^3)$; we then evaluate the sum $\sum_{j \in \mathbb{N}} u_{N\,j}(\mu)\ell(\zeta_j)$ to obtain $s_N(\mu)$ — at cost $O(N)$. The online complexity is *independent* of $\mathcal{N}$, and hence — given that $N \ll \mathcal{N}$ — we shall realize extremely rapid "deployed" response.

## 4 A Posteriori Error Estimation

We first "presume" $\tilde{\beta}(\mu)$, a (to-be-constructed) positive lower bound for the inf-sup parameter, $\beta(\mu)$: $\beta(\mu) \geq \tilde{\beta}(\mu) \geq \tilde{\beta}_0 > 0$, $\forall\, \mu \in \mathcal{D}$. We next introduce the dual norm of the residual: $\varepsilon_N(\mu) \equiv \sup_{v \in X}[R(v;\mu)/\|v\|\,]$, where $R(v;\mu) \equiv f(v) - a(u_N(\mu), v; \mu)$, $\forall\, v \in X$.

We may now define our error estimator, $\Delta_N(\mu) \equiv \varepsilon_N(\mu)/\tilde{\beta}(\mu)$, and associated effectivity, $\eta_N(\mu) \equiv [\Delta_N(\mu)/\|u(\mu) - u_N(\mu)\|]$. We can then readily demonstrate [29, 38] that

$$1 \leq \eta_N(\mu) \leq \gamma(\mu)/\tilde{\beta}(\mu), \quad \forall\, \mu \in \mathcal{D},\ \forall\, N \in \mathbb{N}_{\max}, \tag{2}$$

where $\gamma(\mu) \equiv \sup_{w \in X} \sup_{v \in X}[a(w,v;\mu)/(\|w\|\|v\|)]$ is our continuity "constant." The left inequality states that $\Delta_N(\mu)$ is a *rigorous* upper bound for $\|u(\mu) - u_N(\mu)\|$; the right inequality states that $\Delta_N(\mu)$ is a (reasonably) *sharp* upper bound.

We may also develop bounds for the error in the output; we consider here the special "compliance" case in which $\ell = f$ and $a$ is symmetric — more general functionals $\ell$ and nonsymmetric $a$ require adjoint techniques [29]. We first define our output error estimator, $\Delta_N^s(\mu) \equiv \varepsilon_N^2(\mu)/\tilde{\beta}(\mu)$, which scales as the *square* of the dual norm of the residual, $\varepsilon_N(\mu)$. We can then demonstrate [22, 29, 38] that $1 \leq \Delta_N^s(\mu)/|s(\mu) - s_N(\mu)|$, $\forall \mu \in \mathcal{D}, \forall N \in \mathbb{N}_{\max}$ — $\Delta_N^s(\mu)$ is a rigorous upper bound for $|s(\mu) - s_N(\mu)|$; we may further prove [29] in the coercive case that $\Delta_N^s(\mu)/|s(\mu) - s_N(\mu)| \leq \gamma(\mu)/\tilde{\beta}(\mu)$ — $\Delta_N^s(\mu)$ is a (reasonably) sharp upper bound.

It remains to develop appropriate constructions and associated offline-online computational procedures for the efficient calculation of $\varepsilon_N(\mu)$ and $\tilde{\beta}(\mu)$. To begin, we consider the former [19, 22, 29]: we invoke duality, our reduced-basis expansion, the affine parametric dependence of $a$, and linear superposition to express

$$\varepsilon_N^2(\mu) = (\mathcal{C},\mathcal{C}) + \sum_{q \in \mathbb{Q}} \sum_{n \in \mathbb{N}} \Theta^q(\mu) u_{N\,n}(\mu) \{2(\mathcal{C}, \mathcal{L}_n^q) + \sum_{q' \in \mathbb{Q}} \sum_{n' \in \mathbb{N}} \Theta^{q'}(\mu) u_{N\,n'}(\mu) (\mathcal{L}_n^q, \mathcal{L}_{n'}^{q'})\},$$

where $\mathcal{C} \in X$ and $\mathcal{L}_n^q \in X$, $\forall\, n \in \mathbb{N}$, $\forall\, q \in \mathbb{Q}$ satisfy the *parameter-independent* Poisson(-like) problems $(\mathcal{C}, v) = f(v)$, $\forall\, v \in X$ and $(\mathcal{L}_n^q, v) = -a^q(\zeta_n, v)$, $\forall\, v \in X$.

An efficient offline-online decomposition may now be identified. In the offline stage — performed only once — we first solve for $\mathcal{C}$ and $\mathcal{L}_n^q$, $\forall\, n \in \mathbb{N}_{\max}$, $\forall\, q \in \mathbb{Q}$; we then form *and store* the associated parameter-independent inner products $(\mathcal{C},\mathcal{C}), (\mathcal{C},\mathcal{L}_n^q), (\mathcal{L}_n^q, \mathcal{L}_{n'}^{q'})$, $\forall\, (n,n') \in \mathbb{N}_{\max}^2$, $\forall\, (q,q') \in \mathbb{Q}^2$. In the online stage — performed many times, for each new value of $\mu$ "in the field" — we simply evaluate the $\varepsilon_N^2(\mu)$ sum in terms of $\Theta^q(\mu)$, $u_{N\,n}(\mu)$, and the precomputed inner products — at cost $O(Q^2N^2)$. The online cost is *independent* of $\mathcal{N}$ and, for $Q$ not too large, commensurate with the online cost to evaluate $s_N(\mu)$.

Finally, we turn to the development of our lower bound $\tilde{\beta}(\mu)$ for the inf-sup "constant" $\beta(\mu)$. For simplicity, we consider here the particular case $P = 1$, $Q = 2$, $\Theta^1(\mu) = 1$, and $\Theta^2(\mu) = \mu$, such that $a(w,v;\mu) \equiv a^1(w,v) + \mu a^2(w,v)$; we further suppose that $\mathcal{D}$ is convex. The more difficult general case, in which $P > 1$ and the $\Theta^q(\mu)$, $1 \leq q \leq Q$, are general functions of $\mu$, is considered in [22] and illustrated in subsequent sections of the present paper. As our point of departure, we note that $\beta(\mu) \equiv \inf_{v \in X} \sqrt{b(v,v;\mu)/\|v\|^2}$, where $b(w,v;\mu) = (T^\mu w, T^\mu v)$, $\forall\, w, v \in X$, and $w \in X \to T^\mu w \in X$ is defined as $(T^\mu w, v) = a(w,v;\mu)$, $\forall\, v \in X$.

Next, given any $\overline{\mu} \in \mathcal{D}$, we introduce $t(w,v;\mu;\overline{\mu}) \equiv b(w,v;\overline{\mu}) + (\mu - \overline{\mu})[a^2(w, T^{\overline{\mu}} v) + a^2(v, T^{\overline{\mu}} w)]$ and $\mathcal{D}^{\overline{\mu}} \equiv \{\mu \in \mathcal{D} \,|\, t(v,v;\mu;\overline{\mu}) \geq 0\}$. We may then define $\tau(\mu;\overline{\mu}) \equiv \inf_{v \in X} \sqrt{t(v,v;\mu;\overline{\mu})/\|v\|^2}$, $\forall\, \mu \in \mathcal{D}^{\overline{\mu}}$. Our function $\tau(\mu;\overline{\mu})$ enjoys three properties: $(i)$ $\beta(\mu) \geq \tau(\mu;\overline{\mu}) \geq 0$, $\forall\, \mu \in \mathcal{D}^{\overline{\mu}}$; $(ii)$ $\tau(\mu;\overline{\mu})$ is concave in $\mu$ over the convex domain $\mathcal{D}^{\overline{\mu}}$; and $(iii)$ $\tau(\mu;\overline{\mu})$ is "tangent" to $\beta(\mu)$ at $\mu = \overline{\mu}$. (To make property $(iii)$ rigorous we must in general consider non-smooth analysis and also possibly a continuous spectrum as $\mathcal{N} \to \infty$.)

We can now develop our inf-sup lower bound $\tilde{\beta} : \mathcal{D} \to \mathbb{R}$. We first specifiy a constant $\overline{\epsilon} \in \,]0,1[\,$. We then introduce a sample $E_J \equiv \{\overline{\mu}_1 \in \mathcal{D}, \ldots, \overline{\mu}_J \in \mathcal{D}\}$ and associated set of polytopes $C_J \equiv \{\mathcal{P}_1 \subset \mathcal{D}^{\overline{\mu}_1}, \ldots, \mathcal{P}_J \subset \mathcal{D}^{\overline{\mu}_J}\}$ that satisfy $(a)$ a "Positivity Condition," $\tau(\mu;\overline{\mu}_j) \geq \overline{\epsilon}\, \beta(\overline{\mu}_j)$, $\forall \mu \in \mathcal{P}_j, 1 \leq j \leq J$, and $(b)$ a "Coverage Condition," $\mathcal{D} \subset \cup_{j=1}^{J} \mathcal{P}_j$; we may now define (and compute) our lower bound as

$$\tilde{\beta}(\mu) \equiv \max_{\{j \in \{1,\ldots,J\} \,|\, \mu \in \mathcal{P}_j\}} \overline{\epsilon}\, \beta(\overline{\mu}_j). \tag{3}$$

(We can also develop piecewise *linear* approximations, though — as discussed further in Section 5 — our inf-sup lower bound need not be highly accurate.) It is readily demonstrated that $\tilde{\beta}(\mu)$ has the requisite theoretical and computational attributes: $\beta(\mu) \geq \tilde{\beta}(\mu) \geq \overline{\epsilon}\,\beta_0 > 0$, $\forall\, \mu \in \mathcal{D}$; and the online complexity $\mu \to \tilde{\beta}(\mu)$ depends only on $J$ — we need only find the maximum of the pre-tabulated $\beta(\overline{\mu}_j)$, $1 \leq j \leq J$, and multiply by $\overline{\epsilon}$ — which in turn depends only on $P$ and $Q$ and *not* on $\mathcal{N}$. Properties $(i)$, $(ii)$, and $(iii)$ permit us to parlay relatively few expensive (offline) evaluations into a very inexpensive global (online) lower bound.

We further elaborate on two points: verfication of the "Positivity Condition"; and choice of $\overline{\epsilon}$. As regards the former, the key ingredient is the concavity of $\tau(\mu;\overline{\mu}_j)$ in $\mu$: we need only confirm that $\tau(\cdot;\overline{\mu}_j) \geq \overline{\epsilon}\beta(\overline{\mu}_j)$ at the two endpoints of $\mathcal{P}_j$ to conclude that $\tau(\mu;\overline{\mu}_j) \geq \overline{\epsilon}\beta(\overline{\mu}_j)$, $\forall \mu \in \mathcal{P}_j$. (It thus follows, since $\beta(\mu) \geq \tau(\mu;\overline{\mu}_j)$, $\forall \mu \in \mathcal{P}_j$, that $\beta(\mu) \geq \overline{\epsilon}\beta(\overline{\mu}_j)$, $\forall \mu \in \mathcal{P}_j$ — this proves the lower bound, (3).) As regards the choice of $\overline{\epsilon}$, there is clearly a trade-off between good effectivity and computational effort: the larger we choose $\overline{\epsilon}$, the better our lower bound and hence the better (lower) our effectivity, $\eta_N(\mu)$ — but at the expense of more regions and hence larger $J$.

As an illustrative example of our inf-sup lower bound construction we consider the Helmholtz-elasticity crack problem of the next section for $\mu = (\omega^2 \in [2.5, 5.0],\ z = 1.0,\ L = 0.2)$ — the crack location, $z$, and crack length, $L$, are fixed, and only the frequency squared, $\omega^2$, is permitted to vary — and material damping coefficient $d_m = 0.1$. We find that a sample $E_{J=3}$ suffices to satisfy our Positivity and Coverage Conditions for $\overline{\epsilon} = 0.4$. We present in Figure 1(a) $\beta(\mu)$; $\tau(\mu;\overline{\mu}_j)$ for $\mu \in \mathcal{D}^{\overline{\mu}_j}, 1 \leq j \leq J$; and our lower bound (3). We note that $\beta(\mu)$ is not concave (or convex) or even quasi-concave, and hence $\tau(\mu;\overline{\mu})$ is a necessary intermediary in the construction of our lower bound.

In conclusion, we can calculate a rigorous and sharp upper bound for $|s(\mu) - s_N(\mu)|$, $\Delta_N^s(\mu) \equiv \varepsilon_N^2(\mu)/\tilde{\beta}(\mu)$, with online complexity *independent* of $\mathcal{N}$. These inexpensive error bounds serve most crucially in the deployed stage — to choose optimal $N$, to confirm the desired accuracy, to establish strict feasibility, and to control sub-optimality. However, the bounds may also be gainfully enlisted in the

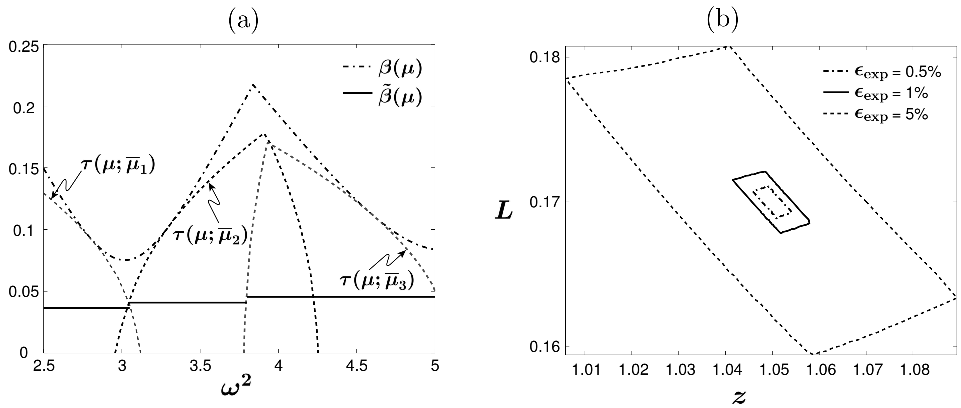


**Figure 1.** *Helmholtz-elasticity example:* (a) *Plots of* $\beta(\mu)$*;* $\tau(\mu;\overline{\mu}_j)$ *for* $\mu \in \mathcal{D}^{\overline{\mu}_j}, 1 \le j \le J$*; and* $\tilde{\beta}(\mu)$*.* (b) *Crack parameter uncertainty region* $\mathcal{R}$ *for* RB *Model* I *with* $N^{\mathrm{I}} = 25$.

pre-deployed stage — to construct optimal samples $S_N$ [22, 38]: Given $\Xi^F$, a very fine random sample over the parameter space $\mathcal{D}$ of size $n_{\mathrm{F}} \gg 1$, and an initial sample $S_1^{\mathrm{opt}} = \mu_1^*$, we [ DO $N = 2, ..., N_{\max}$; $\mu_N^* = \arg\max_{\mu \in \Xi^F} \Delta_{N-1}^s(\mu)$; $S_N^{\mathrm{opt}} = S_{N-1}^{\mathrm{opt}} \cup \mu_N^*$; END ]. Since the marginal cost to evaluate the error bound $\Delta_N^s(\mu)$ is small (online), our input sample $\Xi^F$ can be large, and the maximization problem for $\mu_N^*$ may be solved directly — by calculating $\Delta_{N-1}^s(\mu)$ for all $\mu \in \Xi^F$. (Multi-start gradient-based search techniques can also be exploited to effectively determine the true maximum of the (clearly oscillatory) error bound $\Delta_N^s(\mu)$ over $\mathcal{D}$.) Note that in contrast to POD economization procedures [33], *we never form the rejected snapshots*: our inexpensive bound $\Delta_N^s(\mu)$ serves as a (good) surrogate for the actual error.

## 5 Assess-Act Example: Helmholtz-Elasticity

We apply the RB method here to a Helmholtz-elasticity equation often encountered in solid mechanics: inverse analyses based on the Helmholtz-elasticity PDE can gainfully serve in non-destructive evaluation (NDE) procedures for crack characterization [11, 16, 18] and damage assessment [14, 17]. The RB method significantly improves the efficiency of these inverse procedures — accelerating the *many* evaluations [15] of the PDE outputs.

We consider a two-dimensional thin plate with a horizontal crack at the (say) interface of two lamina: the (original) domain $\Omega^{\mathrm{o}}(z, L) \subset \mathbb{R}^2$ is defined as $[0, 2] \times [0, 1] \setminus \Gamma_{\mathrm{C}}^{\mathrm{o}}$, where $\Gamma_{\mathrm{C}}^{\mathrm{o}} \equiv \{x_1 \in [z - L/2, z + L/2], x_2 = 1/2\}$ defines the idealized crack. The left surface of the plate is secured; the top and bottom boundaries are stress-free; and the right boundary is subject to a vertical oscillatory uniform force of frequency $\omega$. We model the plate as plane-stress linear isotropic elastic with (scaled) density unity, Young's modulus unity, and Poisson ratio 0.25; the latter determine the (parameter-independent) constitutive tensor $E_{ijk\ell}$. Our input is $\mu \equiv (\mu_{(1)}, \mu_{(2)}, \mu_{(3)}) \equiv (\omega^2, z, L)$; our output is the (oscillatory) amplitude of the average vertical displacement on the right edge of the plate.

The governing equation for the displacement $u^{\rm o}(x^{\rm o}; \mu) \in X^{\rm o}(\mu)$ is $a^{\rm o}(u^{\rm o}(\mu), v; \mu) = f^{\rm o}(v), \forall v \in X^{\rm o}(\mu)$, where $X^{\rm o}(\mu)$ is a quadratic finite element truth approximation subspace (of dimension $\mathcal{N} = 14{,}662$) of $X^{\rm e}(\mu) = \{v \in (H^1(\Omega^{\rm o}(z, L)))^2 \,|\, v|_{x_1^{\rm o}=0} = 0\,\}$; here $a^{\rm o}(w, v; \mu) \equiv \int_{\Omega^{\rm o}(z,L)} w_{i,j} E_{ijk\ell} v_{k,\ell} - \omega^2 w_i v_i$ ($v_{i,j}$ denotes $\partial v_i / \partial x_j$ and repeated physical indices imply summation), and $f^{\rm o}(v) \equiv \int_{x_1^{\rm o}=2} v_2$. The crack surface is hence modeled extremely simplistically — as a stress-free boundary; note that no crack-tip element is needed as the output of interest is far from the crack. The output $s^{\rm o}(\mu)$ is given by $s^{\rm o}(\mu) = \ell(u^{\rm o}(\mu))$, where $\ell^{\rm o}(v) = f^{\rm o}(v)$; we are thus "in compliance." (For the damped example of Section 4 we suitably complexify our field variable and space and replace $E_{ijk\ell}$ with a very simple "hysteretic" Kelvin model [4] $E_{ijk\ell}(1 + \sqrt{-1} d_m)$; here $d_m$ is a material damping constant.)

We now map $\Omega^{\rm o}(z, L)$ via a continuous piecewise-affine transformation to a fixed domain $\Omega$. This new problem can now be cast precisely in the desired abstract form of Section 2, in which $\Omega$, $X$, and $(w, v)$ are independent of the parameter $\mu$: as required, all parameter dependence now enters through the bilinear and linear forms. Furthermore, it is readily demonstrated that our affine assumption applies for $Q = 10$; the $\Theta^q(\mu)$ are of the form $\mu_{(1)}^{y_1} \mu_{(2)}^{y_2} \mu_{(3)}^{y_3}$ for exponents $y_1 = 0$ or 1, $y_2 = -1, 0$, or 1, and $y_3 = -1, 0$, or 1. See [22] for a detailed description of the $\Theta^q(\mu)$, $a^q(w, v)$, $1 \le q \le Q$, and the "bound conditioner" $(\cdot, \cdot)$.

We shall consider two different models. In Model I, relevant to the Assess stage, we consider the parameter domain $\mathcal{D}^{\rm I} \equiv [3.2, 4.8] \times \mathcal{D}^{z,L}$, where $\mathcal{D}^{z,L} \equiv [0.9, 1.1] \times [0.15, 0.25]$. Note that $\mathcal{D}^{\rm I}$ does not contain any resonances, and hence $\beta(\mu)$ is bounded away from zero; however, $\omega^2 = 3.2$ and $\omega^2 = 4.8$ — the two frequency extremes of our parameter domain — are quite close to corresponding natural frequencies, and hence the problem is distinctly non-coercive. In Model II, relevant to the Act stage, we consider the parameter domain $\mathcal{D}^{\rm II} \equiv [\omega^2 = 0] \times \mathcal{D}^{z,L}$, where — as in Model I — $\mathcal{D}^{z,L} \equiv [0.9, 1.1] \times [0.15, 0.25]$. Note that Model II is essentially steady linear elasticity and thus the problem is coercive and relatively easy; we shall hence focus our attention on Model I.

We first present basic numerical results. For our reduced-basis spaces we pursue the optimal sampling strategy described in Section 4 for $N_{\max}^{\rm I} = 32$ (Model I) and $N_{\max}^{\rm II} = 6$ (Model II); for our inf-sup lower bound samples we choose $\bar{\epsilon} = 1/5$ which yields $J^{\rm I} = 84$ and $J^{\rm II} = 1$. We present in Table 1 $\Delta_{N,\max,\rm rel}$, $\eta_{N,\rm ave}$, $\Delta^s_{N,\max,\rm rel}$, and $\eta^s_{N,\rm ave}$ as a function of $N = N^{\rm I}$ for Model I. Here $\Delta_{N,\max,\rm rel}$ is the maximum over $\Xi_{\rm Test}$ of $\Delta_N(\mu)/\|u_{N_{\max}}(\mu)\|_{\max}$, $\eta_{N,\rm ave}$ is the average over $\Xi_{\rm Test}$ of $\Delta_N(\mu)/\|u(\mu) - u_N(\mu)\|$, $\Delta^s_{N,\max,\rm rel}$ is the maximum over $\Xi_{\rm Test}$ of $\Delta^s_N(\mu)/|s_{N_{\max}}(\mu)|_{\max}$, and $\eta^s_{N,\rm ave}$ is the average over $\Xi_{\rm Test}$ of $\Delta^s_N(\mu)/|s(\mu) - s_N(\mu)|$. Here $\Xi_{\rm Test} \in (\mathcal{D}^{\rm I})^{343}$ is a random parameter sample of size 343, $\|u_{N_{\max}}(\mu)\|_{\max} \equiv \max_{\mu \in \Xi_{\rm Test}} \|u_{N_{\max}}(\mu)\| = 2.0775$, and $|s_{N_{\max}}(\mu)|_{\max} \equiv \max_{\mu \in \Xi_{\rm Test}} |s_{N_{\max}}(\mu)| = 0.089966$. We observe that the RB approximation converges very rapidly, and that our rigorous error bounds are in fact quite sharp. The effectivities are not quite $O(1)$ primarily due to the relatively crude inf-sup lower bound. (Thanks to the rapid convergence of RB approximations, $O(10)$ effectivities do not significantly (adversely) affect efficiency.)

| $N$ | $\Delta_{N,\max,\mathrm{rel}}$ | $\eta_{N,\mathrm{ave}}$ | $\Delta^s_{N,\max,\mathrm{rel}}$ | $\eta^s_{N,\mathrm{ave}}$ |
|---|---|---|---|---|
| 10 | 6.19E-01 | 13.11 | 8.40E-01 | 22.50 |
| 15 | 5.76E-02 | 13.44 | 4.74E-03 | 17.22 |
| 20 | 1.58E-02 | 13.22 | 4.50E-04 | 15.44 |
| 25 | 5.69E-03 | 12.57 | 4.47E-05 | 14.50 |
| 30 | 1.32E-03 | 12.47 | 2.95E-06 | 14.27 |

**Table 1.** *Numerical results for Model I.*

Turning now to computational effort (again for Model I), for $N = N^{\mathrm{I}} = 25$ and any given $\mu$ (say, $(4.0, 1.0, 0.2)$) — for which the error in the reduced-basis output $s_N(\mu)$ relative to the truth (approximation) $s(\mu)$ is *certifiably* less than $\Delta^s_N(\mu)$ (say, $2.38 \times 10^{-7}$) — the Online Time to compute both $s_N(\mu)$ and $\Delta^s_N(\mu)$ is less than 1/330 the Time to directly calculate $s(\mu) = \ell(u(\mu))$. Clearly, the savings will be even larger for problems with more complex geometry and solution structure in particular in three space dimensions. Nevertheless, even for our current very modest example, the computational economies are very significant. (Note, however, that this comparison does not include the RB offline effort, and is hence meaningful only in the real-time context or in the limit of many evaluations.)

We now consider an Assess-Act scenario that illustrates the new capabilities enabled by rapid certified input-output evaluation [1]. We first consider the Assess stage (based on Model I): given experimental measurements in the form of intervals $[s(\omega_k^2, z^*, L^*)(1 - \epsilon_{\exp}),\ s(\omega_k^2, z^*, L^*)(1 + \epsilon_{\exp})]$, $1 \le k \le K$, we wish to determine a region $\mathcal{R} \in \mathcal{D}^{z,L}$ in which the true but unknown crack parameters, $(z^*,\ L^*)$, must reside. We first introduce $s^{\pm}_N(\mu) \equiv s_N(\mu) \pm \Delta^s_N(\mu)$, and recall that — thanks to our bound theorem (2) — $s(\mu) \in [s^-_N(\mu), s^+_N(\mu)]$. We may then define

$$\mathcal{R} \equiv \big\{(z,L) \in \mathcal{D}^{z,L} \,|\, [s^-_N(\omega_k^2, z, L), s^+_N(\omega_k^2, z, L)] \cap [s(\omega_k^2, z^*, L^*) \\ (1 - \epsilon_{\exp}), s(\omega_k^2, z^*, L^*)(1 + \epsilon_{\exp})] \neq \emptyset, 1 \le k \le K\big\};$$

clearly, we have accommodated both *numerical* and *experimental* error and uncertainty (within our model assumptions), and hence $(z^*, L^*) \in \mathcal{R}$.

In Figure 1(b) we present $\mathcal{R}$ for $K = 2$ and ($\omega_1^2 = 3.2$, $\omega_2^2 = 4.8$) for $\epsilon_{\exp} = 0.5\%, 1\%, 5\%$. (In actual practice, we first find one point in $\mathcal{R}$; we then conduct a binary chop at different angles to map out the boundary of $\mathcal{R}$.) As expected, as $\epsilon_{\exp}$ decreases, $\mathcal{R}$ shrinks towards the exact (synthetic) value, $z^* = 1.05, L^* = 0.17$. Note that in this example for our RB Model I we choose $N^{\mathrm{I}} = 25$, and it is hence clear from Table 1 that the RB error contributes negligibly to the uncertainty region $\mathcal{R}$; we could hence achieve even faster parameter estimation response — at little cost in precision — by decreasing $N^{\mathrm{I}}$.

Most importantly, for any finite $\epsilon_{\exp}$, $\mathcal{R}$ *rigorously captures the uncertainty* in our assessment of the crack parameters without *a priori* regularization hypotheses

[7]. The crucial new ingredient is reliable fast evaluations that permit us to conduct a much more extensive search over parameter space; for a given $\epsilon_{\rm exp}$, $\mathcal{R}$ may be generated online in less than 51 seconds (even for $N^{\rm I} = 25$) on a Pentium 1.6 GHz laptop. Our search over possible crack parameters will certainly never be truly exhaustive, and hence there may be small undiscovered "pockets of possibility" in $\mathcal{D}^{z,L}$; however, we have clearly reduced the uncertainty relative to more conventional approaches. (Of course, our procedure can also only *characterize* cracks within the specified low-dimensional parametrization; however, more general null hypotheses can be constructed to *detect* model deviation.)

Finally, we consider the Act stage (based on Model II). We presume here that the component must withstand an in-service steady force (normalized to unity) such that the deflection $s(0, z^*, L^*)$ in the "next mission" does not exceed a specified value $s_{\max}$. Of course, in practice, we will not be privy to $(z^*, L^*)$. To address this difficulty we first define $s^+_{\mathcal{R}} \equiv \max_{(z,L)\in\mathcal{R}} s^+_N(0, z, L)$, where $s^+_N(0, z, L) = s_N(0, z, L) + \Delta^s_N(0, z, L)$; our corresponding "go/no-go" criterion is then given by $s^+_{\mathcal{R}} \leq s_{\max}$. It is readily observed that $s^+_{\mathcal{R}}$ rigorously accommodates both experimental (crack) and numerical uncertainty — $s(0, z^*, L^*) \leq s^+_{\mathcal{R}}$ — and that the associated go/no-go discriminator is hence *fail-safe*. Furthermore, as $\epsilon_{\rm exp}$ tends to zero and $N^{\rm I}$ and $N^{\rm II}$ increase, $s^+_{\mathcal{R}}$ will tend to $s(0, z^*, L^*)$; indeed, for $\epsilon_{\rm exp} = 1\%$ and $N^{\rm I} = 25$, $N^{\rm II} = 6$, $[s^+_{\mathcal{R}} - s(0, z^*, L^*)]/|s(0, z^*, L^*)| = 4.73\text{E-}05$. In summary, in real-time, we can both Assess the current state of the crack and subsequently Act to ensure the safety (or optimality) of the next "sortie."

# 6 Incompressible Navier-Stokes Equations

To illustrate the difficulties that arise in the treatment of nonlinear problems we consider a particular example [36]: the steady incompressible Navier-Stokes equations — Pr(andtl) = 0 natural convection in an enclosure [31, 34].

Our formulation of Section 2 is still applicable (except $a$ is no longer bilinear): $\mu \equiv \mathrm{Gr} \equiv$ Grashof number; $\mathcal{D} \equiv [1.0, 1.0\text{E}5]$; $u^{\rm e}(\mu) = (u^{\rm e}_1(\mu), u^{\rm e}_2(\mu))$ is the velocity field; $\Omega = [0, 4] \times [0, 1]$; $X^{\rm e} = \{(H^1_0(\Omega))^2 \,|\, \nabla \cdot v = 0\}$; $(w, v) = \int_\Omega w_{i,j} v_{i,j}$; $a(w, v) = a_0(w, v) + \frac{1}{2} a_1(w, w, v)$, where $a_0(w, v) \equiv \int_\Omega w_{i,j}\, v_{i,j}$ and $a_1(w, z, v) \equiv -\int_\Omega (w_i z_j + w_j z_i)\, v_{i,j}$ are the viscous and convective terms, respectively; $f(v; \mu) = \mu f_0(v) = \mu \int_\Omega \left(1 - \frac{1}{4} x_1\right) v_2$ is the buoyancy contribution; and $\ell(v) \equiv 2 \int_{\Gamma_0} v_1(x) dx_2$ (for $\Gamma_0 = \{x_1 = 2, x_2 \in [0.5; 1]\}$) measures the flowrate. (Note that the pressure does not appear explicitly since we pose the problem over divergence-free velocity fields.)

We next introduce $X$, a reference finite element approximation space. Our reference (or "truth") finite element approximation $u(\mu) \in X$ is then defined by $a(u(\mu), v) = f(v; \mu)$, $\forall\, v \in X$. As before, $u(\mu)$ is a surrogate for $u^{\rm e}(\mu)$ upon which we build our RB approximation, and relative to which we measure our RB error. Here $X$ is the space (of dimension $\mathcal{N} = 2{,}786$) of discretely divergence-free functions associated with a classical Taylor-Hood $\mathbb{P}_2 - \mathbb{P}_1$ finite element approximation [10]. (For future reference, we also define $\widetilde{X}$, the full Taylor-Hood velocity space.)

The derivative of $a$ plays a central role: here $da(w, v; z) \equiv a_0(w, v) + a_1(w, z, v)$ satisfies $a(z+w, v) = a(z, v) + da(w, v; z) + \frac{1}{2} a_1(w, w, v)$. It is readily shown [36] that

$da(w,v;z) \le \gamma(z)\|w\|\|v\|$ for $\gamma(z) = 1 + \rho^2\|z\|$; here $\rho \equiv \sqrt{2}\sup_{v\in\widetilde{X}} \|v\|_{L^4(\Omega)}/\|v\|$ is a Sobolev embedding constant [35], and $\|v\|_{L^p(\Omega)} \equiv (\int_\Omega (w_i w_i)^{p/2})^{1/p}$. We shall further assume [36] — and verify *a posteriori* — that $\{u(\mu)\,|\,\mu \in \mathcal{D}\}$ is a non-singular (isolated) solution branch: $\beta(u(\mu)) \ge \beta_0 > 0$, $\forall\, \mu \in \mathcal{D}$, where $\beta(z) \equiv \inf_{w\in X} \sup_{v\in X} da(w,v;z)/\|w\|\|v\|$ is the inf-sup parameter relevant to our nonlinear problem. Numerical simulations [31, 34] demonstrate that the flow *smoothly evolves* from a single-cell structure for the lower Gr in $\mathcal{D}$ to an inertia-dominated three-cell structure for the higher Gr in $\mathcal{D}$.

We may directly apply the RB formulation of Section 3 to the incompressible Navier-Stokes equations [13, 25, 36]. The most significant new issue is (efficient) calculation of the nonlinear terms. We consider the inner Newton update: given a current iterate $\overline{u}_N(\mu) = \sum_{n=1}^N \overline{u}_{N\,n}(\mu)\,\zeta_n$, we must find an increment $\delta u_N \in W_N$ such that $da(\delta u_N, v; \overline{u}_N) = R(v;\mu)$, $\forall\, v \in W_N$; here $R(v;\mu) \equiv f(v;\mu) - a(u_N(\mu), v)$, $\forall\, v \in X$ is the residual. The associated algebraic equations are thus

$$\sum_{j=1}^N \left\{a_0(\zeta_j,\zeta_i) + \sum_{n=1}^N \overline{u}_{N\,n}(\mu) a_1(\zeta_j,\zeta_n,\zeta_i)\right\}\delta u_{N\,j}$$
$$= \mu f_0(\zeta_i) - \sum_{j=1}^N \left\{a_0(\zeta_j,\zeta_i) + \tfrac{1}{2}\sum_{n=1}^N \overline{u}_{N\,n}(\mu) a_1(\zeta_j,\zeta_n,\zeta_i)\right\}\overline{u}_{N\,j}(\mu),\ \forall\, i \in \mathbb{N},$$

where we recall that $f(v;\mu) = \mu f_0(v)$ and $\mu \equiv \mathrm{Gr}$.

We can directly apply the offline-online procedure described in Section 3 for linear problems, except now we must perform summations both over the affine parameter dependence (rather trivial here) *and* over the reduced-basis coefficients (of the current Newton iterate, $\overline{u}_N(\mu)$). In the online stage — for given new $\mu$ — at each Newton iteration $\overline{u}_N(\mu) \to \delta u_N$ we first assemble the right-hand side (residual) — at cost $O(N^3)$; we then form and invert the left-hand side (Jacobian) — at cost $O(N^3)$. The complexity of the online stage is independent of $\mathcal{N}$; furthermore, for our quadratic nonlinearity, there is little increased cost relative to the linear case. Unfortunately, for a $p^{\text{th}}$-order nonlinearity, the online cost for the residual assembly and Jacobian formation will scale as $O(N^{p+1})$, and thus standard Galerkin projections are viable only for $p = 2$ or at most $p = 3$ [38]. Fortunately, for larger $p$ and non-polynomial nonlinearities — and for non-affine parameter dependence [5] — quite effective collocation-like alternatives are available.

Turning now to *a posteriori* error estimation, we first "presume" $\tilde{\beta}_N(\mu)$, a (to-be-constructed) positive lower bound for the inf-sup parameter $\beta_N(\mu) \equiv \beta(u_N(\mu))$: $\beta_N(\mu) \ge \tilde{\beta}_N(\mu) \ge 0$, $\forall\, \mu \in \mathcal{D}$. We next recall the dual norm of the residual, $\varepsilon_N(\mu) \equiv \sup_{v\in X} R(v;\mu)/\|v\|$, and introduce $\tau_N(\mu) \equiv 2\rho^2\varepsilon_N(\mu)/\tilde{\beta}_N^2(\mu)$, where $\rho$ is our $L^4(\Omega)$-$\widetilde{X}$ embedding constant. Finally, we define $N^*(\mu)$ such that $\tau_N(\mu) < 1$ for $N \ge N^*(\mu)$; we require $N^*(\mu) \le N_{\max}$, $\forall\, \mu \in \mathcal{D}$. (The latter is a condition on $N_{\max}$ that reflects both the convergence rate of the RB approximation and the quality of our inf-sup lower bound.)

We may now define our error estimator: for $N \ge N^*(\mu)$, $\Delta_N(\mu) \equiv (\tilde{\beta}_N(\mu)/\rho^2)$ $(1 - \sqrt{1 - \tau_N(\mu)})$; note that, as $\varepsilon_N(\mu) \to 0$, $\Delta_N(\mu)$ tends to the "linear case" $\varepsilon_N(\mu)/\tilde{\beta}_N(\mu)$. Our main result is then: Given any $\mu \in \mathcal{D}$, for all $N \ge N^*(\mu)$, there exists a unique (truth approximation) solution $u(\mu) \in X$ in the ball $\mathcal{B}(u_N(\mu), \tilde{\beta}_N(\mu)/\rho^2) \equiv \{z \in X \mid \|z - u_N(\mu)\| < \tilde{\beta}_N(\mu)/\rho^2\}$; furthermore, $\|u(\mu) - u_N(\mu)\| \leq \Delta_N(\mu)$. The proof [36, 37] is a slight specialization of the abstract "Brezzi-Rappaz-Raviart" result [6, 12]; we can further provide several corollaries related to $(i)$ the well-posedness of the truth approximation, and $(ii)$ the effectivity of our error bound [36]. (We may also develop bounds for the output of interest [36].)

The real challenge is computational: how can we compute $\varepsilon_N(\mu)$, $\rho$, and $\tilde{\beta}_N(\mu)$? (Note that, armed with these quantities, we can evaluate $\tau_N(\mu)$ and hence verify $N \geq N^*(\mu)$.) The reduced-basis context is in fact a rare opportunity to render the Brezzi-Rappaz-Raviart theory *completely quantitative*. To begin, we consider $\varepsilon_N(\mu)$: as for the linear case, we invoke duality, our reduced-basis expansion, the affine parameter dependence of $a$ (and $f$), and linear superposition to express

$$\varepsilon_N^2(\mu) = \mu^2(\mathcal{C},\mathcal{C}) + \sum_{n=1}^{N} u_{N\,n}(\mu)\big\{2\mu(\mathcal{C},\mathcal{L}_n) + \sum_{n'=1}^{N} u_{N\,n'}(\mu)\big\{2\mu(\mathcal{C},\mathcal{Q}_{n\,n'}) + (\mathcal{L}_n,\mathcal{L}_{n'}) + \sum_{n''=1}^{N} u_{N\,n''}(\mu)\,\big\{2(\mathcal{L}_n,\mathcal{Q}_{n'n''}) + \sum_{n'''=1}^{N} u_{N\,n'''}(\mu)\,(\mathcal{Q}_{n\,n'},\mathcal{Q}_{n''n'''})\big\}\big\}\big\}\;, \quad (4)$$

where $(\mathcal{C}, v) = f(v)$, $\forall\, v \in X$, $(\mathcal{L}_n, v) = -a_0(\zeta_n, v)$, $\forall\, v \in X$, $\forall\, n \in \mathbb{N}$, and $(\mathcal{Q}_{n\,n'}, v) = -\frac{1}{2}a_1(\zeta_n, \zeta_{n'}, v)$, $\forall\, v \in X$, $\forall\, (n, n') \in \mathbb{N}^2$; the latter are again simple (vector) Poisson problems.

We can now readily adapt the offline-online procedure developed in the linear case [36, 37]. In the online stage — for each new $\mu$ — we perform the sum (4) in terms of the *pre*-formed and *stored* inner products (for example, $(\mathcal{Q}_{nn'}, \mathcal{Q}_{n''n'''})$, $1 \leq n, n', n'', n''' \leq N$) and the RB coefficients $u_{N\,n}(\mu)$, $1 \leq n \leq N$ — at cost $O(N^4)$. Although the $N^4$ scaling, which arises due to the trilinear term in the residual, is certainly unpleasant, the error bound is calculated only once: in actual practice, the additional online cost attributable to the dual norm of the residual is not too large. Unfortunately, for a $p^{\text{th}}$-order nonlinearity, the online evaluation of $\varepsilon_N(\mu)$ scales as $O(N^{2p})$, and our approach is thus viable only for $p = 2$. Fortunately, for larger $p$ and non-polynomial nonlinearities — and for non-affine parameter dependence [5] — collocation-like alternatives are available; however, in general, there will be some *loss of rigor* in our error estimation.

We next turn to the calculation of $\rho$. The critical observation is that $\rho$ is the supremum of a "Rayleigh-quotient." Thus $\rho$ is related to the smallest multiplier of an associated Euler-Lagrange nonlinear eigenproblem [35]: $(\hat{\lambda}, \hat{\psi}) \in (\mathbb{R}_+, \widetilde{X})$ satisfies $(\hat{\psi}, v) = 2\hat{\lambda}^2 \int_\Omega \hat{\psi}_j \hat{\psi}_j \hat{\psi}_i v_i$, $\forall\, v \in \widetilde{X}$, for $\|\hat{\psi}\|^4_{L^4(\Omega)} = 1$; the ground state is denoted $(\hat{\lambda}_{\min}, \hat{\psi}_{\min})$, and $\rho = \hat{\lambda}^{-1}_{\min}$. In practice, it may be difficult to isolate the ground state, and we thus consider a homotopy procedure.

Towards that end, we first introduce a parametrized generalization of the Euler-Lagrange equation: given $\alpha \in [0, 1]$, $(\lambda(\alpha), \psi(\alpha)) \in (\mathbb{R}_+, \widetilde{X})$ satisfies $(\psi(\alpha), v) = 2\lambda^2(\alpha)[\alpha \int_\Omega \psi_j(\alpha)\psi_j(\alpha)\psi_i(\alpha)v_i + (1 - \alpha)\int_\Omega \psi_i(\alpha)v_i]$, $\forall\, v \in \widetilde{X}$, for normalization $\alpha\|\psi(\alpha)\|^4_{L^4(\Omega)} + (1-\alpha)\|\psi(\alpha)\|^2_{L^2(\Omega)} = 1$; the ground state is denoted $(\lambda_{\min}(\alpha), \psi_{\min}(\alpha))$, and $\rho = \lambda^{-1}_{\min}(1)$. We may now apply standard Newton continuation methods to proceed from the known ground state at $\alpha = 0$ — $(\lambda_{\min}(0), \psi_{\min}(0))$ is the lowest eigenpair of a simple (vector) "Laplacian" linear eigenproblem — to the ground state of interest at $\alpha = 1$; for sufficiently small increments in $\alpha$, we will remain on the desired (lowest-energy) branch. For our particular domain, we find (offline) $\rho = 0.4416$; since $\rho$ is $\mu$-independent, no online computation is required.

Finally, as regards the inf-sup lower bound, $\tilde{\beta}_N(\mu)$, we may directly apply appropriate extensions [22, 36] of the procedure developed in Section 5. The nonlinear case does present a new difficulty: the parameter dependence of the (linearized) operator is now induced by the reduced-basis solution $u_N(\mu)$ — in our case, through the $a_1(w, u_N(\mu), v)$ term — and hence is *not known a priori*. Fortunately, since $u_N(\mu) \to u(\mu)$ we may develop a "universal" lower bound for sufficiently large $N$; the complications are thus largely practical in nature. (For our particular problem, $J = 34$ — the sample is relatively small despite the rather large range in Grashof.)

We conclude with a brief discussion of the adaptive sampling procedure introduced in Section 4. In the nonlinear case a similar procedure may be pursued, but with two important differences. First, as already indicated, $\beta_N(\mu)$ and hence $\tilde{\beta}_N(\mu)$ will now depend on the reduced-basis solution $u_N(\mu)$; furthermore, $\beta_N(\mu)$ will only be meaningful for larger $N$. Thus in the sample construction stage we must replace $\tilde{\beta}_N(\mu)$ in $\Delta_N(\mu)$ with a simple but relevant surrogate — for example, a piecewise-constant (over $\mathcal{D}$) approximation to $\beta(u(\mu))$. Second, in the nonlinear context our error bound is conditional — a small solution to the error equation is only assured if $\tau_N(\mu) < 1$. Thus the greedy procedure must first select on $\arg\max_{\mu \in \Xi^F} \tau_N(\mu)$ — until $\tau_N(\mu) < 1$, $\forall\, \mu \in \Xi^F$ — and only subsequently select on $\arg\max_{\mu \in \Xi^F} \Delta_N(\mu)$; the resulting sample will ensure rapid convergence to a *certifiably* accurate solution.

In Table 2 we present $\Delta_{N,\,\mathrm{rel}}(\mu) \equiv \Delta_N(\mu)/\|u_{N_{\max}}(\mu)\|$ and $\eta_N(\mu) \equiv \Delta_N(\mu)/\|u(\mu) - u_N(\mu)\|$ as a function of $N$ for $\mu = \mathrm{Gr} = 1.0\mathrm{E}1$ (single-roll) and $\mu = \mathrm{Gr} = 8.5\mathrm{E}4$ (three-roll). The "*" indicates that $N < N^*(\mu)$ — $\tau_N(\mu) \geq 1$: no error bound is available. For $\mathrm{Gr} = 1.0\mathrm{E}1$, we find $N^*(\mu) = 1$, and hence we obtain error bounds for all $N$; the error bound tends to zero very rapidly; and the effectivity is $O(1)$ [22, 36]. For $\mathrm{Gr} = 8.5\mathrm{E}4$, we find $N^*(\mu) = 9$, and hence we obtain error bounds only for rather accurate approximations; however, the error bound still tends to zero rapidly with $N$ — our samples $S_N^{\mathrm{opt}}$ are constructed to provide uniform convergence; and the effectivity is still quite good. It is perhaps surprising that the Brezzi-Rappaz-Raviart theory, which is not really designed for quantitative service, indeed yields such sharp results; in fact, as $\varepsilon_N(\mu) \to 0$, the cruder bounds — in particular, $\rho$ — no longer play a role.

Finally, we note that the online cost (on a Pentium® M 1.6GHz processor) to predict $s_N(\mu)$ and $\Delta_N(\mu)$ (and a bound for the error in the output, $\Delta_N^s(\mu)$ [36]) is typically 10ms and 90ms, respectively — compared to order minutes for direct finite element calculation of $s(\mu) = \ell(u(\mu))$.

## 7 Parabolic Equations

We consider here the extension of the RB methods and associated *a posteriori* error estimators described in Sections 1-4 to *parabolic* PDEs — in particular, the heat equation; we shall "simply" treat time as an additional, albeit special, param-

|  | Gr = 1.0E1 |  |  | Gr = 8.5E4 |  |  |
|---|---|---|---|---|---|---|
| $N$ | $\tau_N$ | $\Delta_{N,\,\mathrm{rel}}$ | $\eta_N$ | $\tau_N$ | $\Delta_{N,\,\mathrm{rel}}$ | $\eta_N$ |
| 3 | 2.0 E−2 | 5.0 E−2 | 1.0 | $\infty$ | * | * |
| 6 | 1.2 E−2 | 3.0 E−2 | 1.0 | 2.8 E+1 | * | * |
| 9 | 4.4 E−3 | 1.1 E−2 | 1.0 | 5.2 E−1 | 1.5 E−4 | 14.1 |
| 12 | 2.7 E−6 | 6.8 E−6 | 1.0 | 5.8 E−1 | 1.7 E−4 | 20.5 |
| 15 | 3.0 E−7 | 7.6 E−7 | 1.0 | 1.9 E−2 | 4.6 E−6 | 17.6 |

**Table 2.** *Error bounds and effectivities for* Gr = 1.0E1 *and* Gr = 8.5E4.

eter [32]. For further details, we refer the reader to [9]. (There are many approaches to model reduction for initial-value problems: POD methods [33]; balanced-truncation techniques [21]; and even reduced-basis approaches [28]. However, in general, these frameworks do not accommodate parametric variation (or, typically, rigorous *a posteriori* error estimation).) For simplicity, we directly consider a $K$-level time-discrete framework (corresponding to Euler Backward discretization, although we can also readily treat higher-order schemes such as Crank-Nicolson) associated to the time interval $[0, t_f]$: we define $\mathbb{T} \equiv \{t^0, \ldots, t^K\}$, where $t^k = k\Delta t$, $0 \le k \le K$, and $\Delta t = t_f/K$; for notational convenience, we also introduce $\mathbb{K} = \{1, \ldots, K\}$. (Clearly, our results must be stable as $\Delta t \to 0,\ K \to \infty$.)

Given $\mu \in \mathcal{D} \subset \mathbb{R}^P$, we evaluate the (here, single) output $s(\mu, t^k) = \ell(u(\mu, t^k))$, $\forall\, k \in \mathbb{K}$, where $u(\mu, t^k) \in X$, $\forall\, k \in \mathbb{K}$, satisfies

$$\Delta t^{-1} m(u(\mu, t^k) - u(\mu, t^{k-1}), v) + a(u(\mu, t^k), v; \mu) = b(t^k) f(v), \quad \forall\, v \in X, \qquad (5)$$

with initial condition (say) $u(\mu, t^0) = 0$. Here $\mu$ and $\mathcal{D}$ are the input and input domain; $u(\mu, t^k)$, $\forall\, k \in \mathbb{K}$, is our field variable; $X \subset X^{\mathrm{e}}$ is our truth approximation subspace for $X^{\mathrm{e}}$ (and $(\cdot,\cdot)$, $\|\cdot\|$) defined in Section 2; $a(\cdot,\cdot;\mu)$ and $m(\cdot,\cdot)$ are $X^{\mathrm{e}}$-continuous and $L^2(\Omega)$-continuous symmetric bilinear forms, respectively; $f(\cdot)$, $\ell(\cdot)$ are $L^2(\Omega)$-continuous linear forms; and $b(t^k)$ is the (here, single) "control" input at time $t^k$.

We shall make the following assumptions. First, we require that $a$ and $m$ are independent of time — the system is thus linear time-invariant (LTI). Second, we assume that $a$ and $m$ are coercive: $0 < \alpha_0 \le \alpha(\mu) \equiv \inf_{v \in X}[a(v, v; \mu)/\|v\|^2]$ and $0 < \sigma_0 \le \inf_{v \in L^2(\Omega)}[m(v, v)/\|v\|^2_{L^2(\Omega)}]$. Third, we assume that $a$ depends affinely on $\mu$: $a(w, v; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu)\ a^q(w, v)$ for $q = 1, \ldots, Q$ parameter-*dependent* functions $\Theta^q(\mu) : \mathcal{D} \to \mathbb{R}$ and parameter-*independent* continuous bilinear forms $a^q(w, v)$. (For simplicity, we also assume that $m$, $f$, and $\ell$ are parameter-independent.)

To ensure rapid convergence of the reduced-basis output approximation we shall need a dual (or adjoint) problem which shall evolve backward in time. Invoking the LTI property, we can express the adjoint for the output at time $t^L$, $1 \le L \le K$, as $\psi^L(\mu, t^k) \equiv \Psi(\mu, t^{K-L+k})$, $1 \le k \le L$; here $\Psi(\mu, t^k) \in X$, $\forall\, k \in \mathbb{K}$, satisfies $\Delta t^{-1} m(v, \Psi(\mu, t^k) - \Psi(\mu, t^{k+1})) + a(v, \Psi(\mu, t^k); \mu) = 0$, $\forall v \in X$, with final condition $m(v, \Psi(\mu, t^{K+1})) \equiv \ell(v)$, $\forall\, v \in X$. In essence, thanks to the primal LTI property and the linearity of the output functional, the dual system is invariant to a shift in time of the final condition; thus, to obtain $\psi^L(\mu, t^k)$, $1 \leq k \leq L$, $\forall L \in \mathbb{K}$, we need only solve once for $\Psi(\mu, t^k)$, $\forall\, k \in \mathbb{K}$, and then appropriately translate the result — we do not need to solve $K$ separate dual problems [9].

We now introduce the nested samples $S^{\rm pr}_{N_{\rm pr}} = \{\tilde\mu^{\rm pr}_1, \ldots, \tilde\mu^{\rm pr}_{N_{\rm pr}}\}$, $1 \leq N_{\rm pr} \leq N_{\rm pr,max}$, and $S^{\rm du}_{N_{\rm du}} = \{\tilde\mu^{\rm du}_1, \ldots, \tilde\mu^{\rm du}_{N_{\rm du}}\}$, $1 \leq N_{\rm du} \leq N_{\rm du,max}$, where $\tilde\mu \equiv (\mu, t^k) \subset \widetilde{\mathcal{D}} \equiv \mathcal{D} \times \mathbb{T}$. Note the samples must now reside in the *parameter-time* space $\widetilde{D}$; we also introduce separate (and different) samples for the primal and dual problems. We then define the associated nested RB spaces $W^{\rm pr}_{N_{\rm pr}} = {\rm span}\{\zeta^{\rm pr}_n \equiv u(\tilde\mu^{\rm pr}_n = (\mu_n, t^{k_n})^{\rm pr}),\ 1 \leq n \leq N_{\rm pr}\}$, $1 \leq N_{\rm pr} \leq N_{\rm pr,max}$, and $W^{\rm du}_{N_{\rm du}} = {\rm span}\{\zeta^{\rm du}_n \equiv \Psi(\tilde\mu^{\rm du}_n = (\mu_n, t^{k_n})^{\rm du}),\ 1 \leq n \leq N_{\rm du}\}$, $1 \leq N_{\rm du} \leq N_{\rm du,max}$. Note that for the primal basis we choose — as justified by the LTI hypothesis — an impulse input: $b(t^k) = 1$ for $k = 1$, and $b(t^k) = 0$ for $2 \leq k \leq K$.

Our RB approximation is then: given $\mu \in \mathcal{D}$, evaluate $s_N(\mu, t^k) = \ell(u_N(\mu, t^k)) + \sum_{k'=1}^{k} R^{\rm pr}(\Psi_N(\mu, t^{K-k+k'}); \mu, t^{k'})\ \Delta t$, $\forall\, k \in \mathbb{K}$, where (pr) $u_N(\mu, t^k) \in W^{\rm pr}_{N_{\rm pr}}$, $\forall\, k \in \mathbb{K}$, satisfies $\Delta t^{-1} m(u_N(\mu, t^k) - u_N(\mu, t^{k-1}), v) + a(u_N(\mu, t^k), v; \mu) = b(t^k)\, f(v)$, $\forall\, v \in W^{\rm pr}_{N_{\rm pr}}$, with initial condition $u_N(\mu, t^0) = 0$, and (du) $\Psi_N(\mu, t^k) \in W^{\rm du}_{N_{\rm du}}$, $\forall\, k \in \mathbb{K}$, satisfies $\Delta t^{-1} m(v, \Psi_N(\mu, t^k) - \Psi_N(\mu, t^{k+1})) + a(v, \Psi_N(\mu, t^k); \mu) = 0$, $\forall\, v \in W^{\rm du}_{N_{\rm du}}$, with final condition $m(v, \Psi_N(\mu, t^{K+1})) \equiv \ell(v)$, $\forall\, v \in W^{\rm du}_{N_{\rm du}}$. Here, $\forall\, k \in \mathbb{K}$, $R^{\rm pr}(v; \mu, t^k) \equiv b(t^k)\, f(v) - (\Delta t^{-1} m(u_N(\mu, t^k) - u_N(\mu, t^{k-1}), v) + a(u_N(\mu, t^k), v; \mu))$, $\forall\, v \in X$, is the primal residual. Note that we include a residual correction term (the inner product of the primal residual with the dual RB solution) in $s_N(\mu, t^k)$ to improve the accuracy of our output prediction [26] and to obtain the "square" effect in the convergence of the output bound. We could, of course, also increase the accuracy of $s_N(\mu, t^k)$ by improving the primal RB solution $u_N(\mu, t^k)$ (i.e., by increasing $N_{\rm pr}$); however, in the case of a single or relatively few outputs, the dual formulation is computationally advantageous.

The offline-online computational procedure is similar to the elliptic case of Section 3 but with the added complexity of the dual problem and the time dependence [9]. In the *online* stage, we first assemble the requisite RB "stiffness" matrices — at cost $O((N^2_{\rm pr} + N^2_{\rm du} + N_{\rm pr} N_{\rm du})Q)$; we then solve the primal and dual problems — at cost $O(N^3_{\rm pr} + N^3_{\rm du} + K(N^2_{\rm pr} + N^2_{\rm du}))$; and finally we evaluate the RB output approximation $s_N(\mu; t^k)$, $\forall\, k \in \mathbb{K}$ — at cost $O(K(K+1) N_{\rm pr} N_{\rm du})$. The online complexity is thus *independent* of $\mathcal{N}$, and in fact not too sensitive (for our LTI system) to $K$.

We now turn to *a posteriori* error estimation. We stress that the development of the error bounds is in no way limited to the RB approximation described here: we may consider "any" stable ODE or PDE system and any reduced-order model. To begin, we assume that we are given $\tilde\alpha(\mu) : \mathcal{D} \to \mathbb{R}_+$, a positive lower bound for the coercivity constant, $\alpha(\mu)$ : $\alpha(\mu) \geq \tilde\alpha(\mu) \geq \tilde\alpha_0 > 0$, $\forall\, \mu \in \mathcal{D}$. In our symmetric case $\alpha(\mu) = \beta(\mu)$ and thus $\tilde\alpha(\mu)$ can be constructed according to Section 4; in fact, thanks to coercivity, much simpler procedures typically suffice [29]. We next recall the dual norm of the primal and dual residuals: $\forall\, k \in \mathbb{K}$, $\varepsilon^{\rm pr}_{N_{\rm pr}}(\mu, t^k) \equiv \sup_{v \in X}[R^{\rm pr}(v; \mu, t^k)/\|v\|]$ and $\varepsilon^{\rm du}_{N_{\rm du}}(\mu, t^k) \equiv \sup_{v \in X}[R^{\rm du}(v; \mu, t^k)/\|v\|]$, where $\forall\, k \in \mathbb{K}$, $R^{\rm du}(v; \mu, t^k) \equiv -(\Delta t^{-1} m(v, \Psi_N(\mu, t^k)$

$- \Psi_N(\mu, t^{k+1})) + a(v, \Psi_N(\mu, t^k); \mu)), \forall\, v \in X$. Finally, we introduce the "spatio-temporal" energy norm, $|||v(\mu, t^k)|||^2 \equiv m(v(\mu, t^k), v(\mu, t^k)) + \sum_{k'=1}^{k} \Delta t\, a(v(\mu, t^{k'}), v(\mu, t^{k'}); \mu), \forall\, v \in X$.

We may now define our error estimators: $\forall\, \mu \in \mathcal{D}$, $\forall\, k \in \mathbb{K}$, $\Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^k) \equiv \tilde{\alpha}^{-\frac{1}{2}}(\mu)(\Delta t \sum_{k'=1}^{k} \varepsilon^{\rm pr}_{N_{\rm pr}}(\mu, t^{k'})^2)^{\frac{1}{2}}$; $\Delta^{\rm du}_{N_{\rm du}}(\mu, t^k) \equiv \tilde{\alpha}^{-\frac{1}{2}}(\mu)(\Delta t \sum_{k'=k}^{K} \varepsilon^{\rm du}_{N_{\rm du}}(\mu, t^{k'})^2)^{\frac{1}{2}}$; and

$$\Delta^s(\mu, t^k) \equiv \Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^k)\ \Delta^{\rm du}_{N_{\rm du}}(\mu, t^{K-k+1}). \tag{6}$$

We can then readily demonstrate that $|||u(\mu, t^k) - u_N(\mu, t^k)||| \le \Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^k)$ and $|s(\mu, t^k) - s_N(\mu, t^k)| \le \Delta^s(\mu, t^k)$, $\forall\, k \in \mathbb{K}$, $\forall\, \mu \in \mathcal{D}$, $1 \le N_{\rm pr} \le N_{\rm pr,max}$, $1 \le N_{\rm du} \le N_{\rm du,max}$ [9] — we obtain rigorous (and, as we shall see, rather sharp) upper bounds for the primal error, dual error, *and* output error. (Note that our particular form (6) assumes that $\Psi(\mu, t^{K+1})$ — here, $\mu$-independent — is a member of $W^{\rm du}_{N_{\rm du}}$; this requirement is readily relaxed.)

The offline-online procedure for the computation of $\Delta^s(\mu, t^k)$, $\forall\, k \in \mathbb{K}$ — in particular, for the calculation of the requisite primal and dual residual norms — is similar to the elliptic case of Section 4 but with the added complexity of the dual problem and the time dependence [9]. In particular, in the *online* stage — for any given new $\mu$ — we evaluate the $\varepsilon^{\rm pr}_{N_{\rm pr}}(\mu, t^k)^2$ and $\varepsilon^{\rm du}_{N_{\rm du}}(\mu, t^k)^2$ sums in terms of $\Theta^q(\mu)$, $u_{N\,n}(\mu, t^k)$, $\Psi_{N\,n'}(\mu, t^{k'})$ and the *precomputed* inner products — at cost $O(K(N^2_{\rm pr} + N^2_{\rm du})Q^2)$. Thus, all online calculations are indeed *independent* of $\mathcal{N}$.

We now turn to a particular numerical example. We consider the design of a heat shield (one cell of which is shown in Figure 2): the left boundary $\partial\Omega_{\rm out}$ is exposed to a temperature unity and Biot number $\mathrm{Bi}_{\rm out}$ "source" for $t \in [0, t_f]$; the right boundary as well as the top and bottom (symmetry) boundaries are insulated; and the internal boundaries $\partial\Omega_{\rm in}$ — corresponding to three square cooling channels — are exposed to a temperature zero and Biot number $\mathrm{Bi}_{\rm in}$ "sink." Our input parameter is hence $\mu \equiv (\mu_{(1)}, \mu_{(2)}) \equiv (\mathrm{Bi}_{\rm out}, \mathrm{Bi}_{\rm in}) \in \mathcal{D} \equiv [0.01, 0.5] \times [0.001, 0.1]$; our output is the average temperature of the structure — a surrogate for the maximum temperature of the (to-be-protected) right boundary for $t \in [0, \infty[$ .

The underlying PDE is the heat equation. The (appropriately non-dimensionalized) governing equation for the temperature $u(\mu, t^k) \in X$ is thus (5), where $X$ is a linear finite element truth approximation subspace (of dimension (exploiting symmetry) $\mathcal{N} = 1{,}396$) of $X^{\rm e} \equiv H^1(\Omega)$; $a(w, v; \mu) \equiv \int_\Omega \nabla w \cdot \nabla v + \mu_{(1)} \int_{\partial\Omega_{\rm out}} w\, v + \mu_{(2)} \int_{\partial\Omega_{\rm in}} w\, v$; $m(w, v) \equiv \int_\Omega w\, v$; $f(v; \mu) \equiv \mu_{(1)} \int_{\partial\Omega_{\rm out}} v$, which is now (affinely) parameter-dependent; $b(t^k) = 1, \forall k \in \mathbb{K}$; and $(w, v) \equiv \int_\Omega \nabla w \cdot \nabla v + 0.01 \int_{\partial\Omega_{\rm out}} w\, v + 0.001 \int_{\partial\Omega_{\rm in}} w\, v$ — hence we may choose $\tilde{\alpha}(\mu) = 1$. The output is given by $s(\mu, t^k) = \ell(u(\mu, t^k))$, where $\ell(v) \equiv |\Omega|^{-1} \int_\Omega v$.

We now present numerical results. Our "optimal" primal and dual samples are constructed (separately) by procedures similar to the greedy approach described for the elliptic case in Section 4 [9]: at each step (say, for the primal) we select the parameter value $\mu^*$ for which $\Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^K)$ is maximized; we then select the time $t^{k^*}$ for which $\varepsilon^{\rm pr}_{N_{\rm pr}}(\mu^*, t^k)$ is maximized. In Table 3 we present, as a function of $N_{\rm pr}$ $(= N_{\rm du})$, $\Delta^{\rm pr}_{\rm max,rel}$, $\overline{\eta}^{\rm pr}$, $\Delta^s_{\rm max,rel}$, and $\overline{\eta}^s$: $\Delta^{\rm pr}_{\rm max,rel}$ is the max-

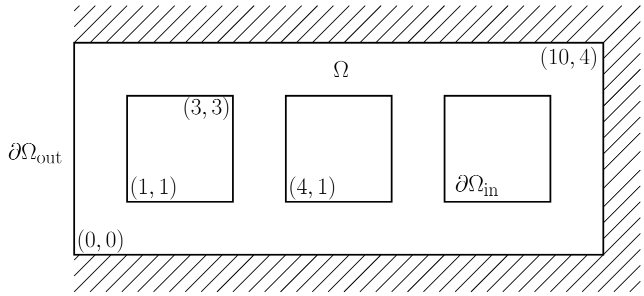


**Figure 2.** *One "cell" of the heat shield.*

| $N_{\rm pr}$ | $\Delta^{\rm pr}_{\rm max,rel}$ | $\overline{\eta}^{\rm pr}$ | $\Delta^{s}_{\rm max,rel}$ | $\overline{\eta}^{s}$ |
|---|---|---|---|---|
| 4 | 1.6 E−00 | 5.44 | 1.6 E−00 | 95.63 |
| 8 | 6.3 E−02 | 1.55 | 6.7 E−03 | 30.92 |
| 12 | 1.0 E−02 | 1.03 | 2.6 E−04 | 8.43 |
| 16 | 3.2 E−03 | 1.02 | 1.5 E−05 | 11.45 |
| 20 | 8.8 E−04 | 1.01 | 1.1 E−06 | 17.43 |

**Table 3.** *Convergence results for the heat equation.*

imum over $\Xi_{\rm Test}$ of $\Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^K)/|||u_N(\mu_u, t^K)|||$, $\overline{\eta}^{\rm pr}$ is the average over $\Xi_{\rm Test} \times \mathbb{T}$ of $\Delta^{\rm pr}_{N_{\rm pr}}(\mu, t^k)/|||u(\mu, t^k) - u_N(\mu, t^k)|||$, $\Delta^s_{\rm max,rel}$ is the maximum over $\Xi_{\rm Test}$ of $\Delta^s_N(\mu, t^K)/|s_N(\mu_s, t^K)|$, and $\overline{\eta}^s$ is the average over $\Xi_{\rm Test}$ of $\Delta^s_N(\mu, t_\eta(\mu))/|s(\mu, t_\eta(\mu)) - s_N(\mu, t_\eta(\mu))|$. Here $\Xi_{\rm Test} \in (\mathcal{D})^{400}$ is a random input sample of size 400; $\mu_u \equiv \arg\max_{\mu\in\Xi_{\rm Test}} |||u_{N_{\max}}(\mu, t^K)|||$, $\mu_s \equiv \arg\max_{\mu\in\Xi_{\rm Test}} |s_{N_{\max}}(\mu, t^K)|$ (note the output grows with time), and $t_\eta(\mu) \equiv \arg\max_{t^k\in\mathbb{T}} |s(\mu, t^k) - s_N(\mu, t^k)|$. The output converges rapidly, and the effectivities are reasonably good.

Finally, we note that the calculation of $s_N(\mu, t^k)$ and $\Delta^s_N(\mu, t^k)$, $\forall\, k \in \mathbb{K}$, is (say, for $N_{\rm pr} = N_{\rm du} = 12$) roughly 120 times faster than direct calculation of the truth approximation output $s(\mu, t^k) = \ell(u(\mu, t^k))$, $\forall\, k \in \mathbb{K}$. We may thus work with $s_N(\mu, t^k) + \Delta^s_N(\mu, t^k)$ as a *certifiably* conservative (upper bound) and accurate surrogate for the average temperature $s(\mu, t^k)$ in truly interactive design exercises.

# Bibliography


[1] S. Ali, *Real-time Optimal Parametric Design using the Assess-Predict-Optimize Strategy*, PhD thesis, Singapore-MIT Alliance, Nanyang Technological University, Singapore, 2003.

[2] B. O. Almroth, P. Stern, and F. A. Brogan, *Automatic choice of global shape functions in structural analysis*, AIAA Journal, 16 (1978), pp. 525–528.

[3] E. Balmes, *Parametric families of reduced finite element models: Theory and applications*, Mechanical Systems and Signal Processing, 10 (1996), pp. 381–394.

[4] E. Barkanov, *Transient response analysis of structures made from viscoelastic materials*, Int. J. Numer. Meth. Engng., 44 (1999), pp. 393–403.

[5] M. Barrault, N. C. Nguyen, Y. Maday, and A. T. Patera, *An "empirical interpolation" method: Application to efficient reduced-basis discretization of partial differential equations*, C. R. Acad. Sci. Paris, Série I., 339 (2004), pp. 667–672.

[6] G. Caloz and J. Rappaz, *Numerical analysis for nonlinear and bifurcation problems*, in Handbook of Numerical Analysis, Vol. V, P. Ciarlet and J. Lions, eds., Techniques of Scientific Computing (Part 2), Elsevier Science B.V., 1997, pp. 487–637.

[7] H. W. Engl, M. Hanke, and A. Neubauer, *Regularization of Inverse Problems*, Kluwer Academic, Dordrecht, 1996.

[8] J. P. Fink and W. C. Rheinboldt, *On the error behavior of the reduced basis technique for nonlinear finite element approximations*, Z. Angew. Math. Mech., 63 (1983), pp. 21–28.

[9] M. A. Grepl and A. T. Patera, *A Posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations*, M2AN (Math. Model. Numer. Anal.), 39 (2005), pp. 157–181.

[10] M. D. Gunzburger, *Finite Element Methods for Viscous Incompressible Flows: A Guide to Theory, Practice, and Algorithms*, Academic Press, Boston, 1989.

[11] S. I. Ishak, G. R. Liu, S. P. Lim, and H. M. Shang, *Locating and sizing of delamination in composite laminates using computational and experimental methods*, Composite Part B, 32 (2001), pp. 287–298.

[12] K. Ito and S. S. Ravindran, *A reduced basis method for control problems governed by PDEs*, in Control and Estimation of Distributed Parameter Systems, W. Desch, F. Kappel, and K. Kunisch, eds., Birkhäuser, 1998, pp. 153–168.

[13] ———, *A reduced-order method for simulation and control of fluid flows*, Journal of Computational Physics, 143 (1998), pp. 403–425.

[14] G. R. Liu and S. C. Chen, *Flaw detection in sandwich plates based on time-harmonic response using genetic algorithm*, Comput. Methods Appl. Mech. Engrg., 190 (2001), pp. 5505–5514.

[15] G. R. Liu, X. Han, and K. Y. Lam, *A combined genetic algorithm and non-linear least squares method for material characterization using elastic waves*, Comput. Methods Appl. Mech. Engrg., 191 (2002), pp. 1909–1921.

[16] G. R. Liu and K. Y. Lam, *Characterization of a horizontal crack in anisotropic laminated plates*, International Journal of Solids and Structures, 31 (1994), pp. 2965–2977.

[17] G. R. Liu, K. Y. Lam, and J. Tani, *Characterization of flaws in sandwich plates: Numerical experiment*, JSME International Journal (A), Japan, 38 (1995), pp. 554–562.

[18] G. R. Liu, Z. C. Xi, K. Y. Lam, and H. M. Shang, *A strip element method for analyzing wave scattering by a crack in an immersed composite laminate*, Journal of Applied Mechanics, 66 (1999), pp. 898–903.

[19] L. Machiels, Y. Maday, I. B. Oliveira, A. T. Patera, and D. V. Rovas, *Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems*, C. R. Acad. Sci. Paris, Série I, 331 (2000), pp. 153–158.

[20] Y. Maday, A. T. Patera, and G. Turinici, *Global* a priori *convergence theory for reduced-basis approximation of single-parameter symmetric coercive elliptic partial differential equations*, C. R. Acad. Sci. Paris, Série I, 335 (2002), pp. 289–294.

[21] B. Moore, *Principal component analysis in linear systems: Controllability, observability, and model reduction*, IEEE Transactions on Automatic Control, 26 (1981), pp. 17–32.

[22] N. C. Nguyen, K. Veroy, and A. T. Patera, *Certified real-time solution of parametrized partial differential equations*, in Handbook of Materials Modeling, S. Yip, ed., Springer, 2005, pp. 1523–1558.

[23] A. K. Noor and J. M. Peters, *Reduced basis technique for nonlinear analysis of structures*, AIAA Journal, 18 (1980), pp. 455–462.

[24] I. B. Oliveira and A. T. Patera, *Reduced-basis techniques for rapid reliable optimization of systems described by parametric partial differential equations. Submitted, Optimization and Engineering.*

[25] J. S. Peterson, *The reduced basis method for incompressible viscous flow calculations*, SIAM J. Sci. Stat. Comput., 10 (1989), pp. 777–786.

[26] N. Pierce and M. B. Giles, *Adjoint recovery of superconvergent functionals from pde approximations*, SIAM Review, 42 (2000), pp. 247–264.

[27] T. A. Porsching, *Estimation of the error in the reduced basis method solution of nonlinear equations*, Mathematics of Computation, 45 (1985), pp. 487–496.

[28] T. A. Porsching and M. L. Lee, *The reduced basis method for initial value problems*, SIAM Journal on Numerical Analysis, 24 (1987), pp. 1277–1287.

[29] C. Prud'homme, D. Rovas, K. Veroy, Y. Maday, A. T. Patera, and G. Turinici, *Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods*, Journal of Fluids Engineering, 124 (2002), pp. 70–80.

[30] A. Quarteroni and A. Valli, *Numerical Approximation of Partial Differential Equations*, Springer, 2nd ed., 1997.

[31] B. Roux, ed., *Numerical Simulation of Oscillatory Convection in Low-Pr Fluids: A GAMM Workshop*, vol. 27 of Notes on Numerical Fluids Mechanics, Vieweg, 1990.

[32] D. Rovas, *Reduced-Basis Output Bound Methods for Parametrized Partial Differential Equations*, PhD thesis, Massachusetts Institute of Technology, Cambridge, MA, October 2002.

[33] L. Sirovich, *Turbulence and the dynamics of coherent structures, part 1: Coherent structures*, Quarterly of Applied Mathematics, 45 (1987), pp. 561–571.

[34] A. C. Skeldon, D. S. Riley, and K. A. Cliffe, *Convection in a low Prandtl number fluid*, Journal of Crystal Growth, 162 (1996), pp. 95–106.

[35] G. Talenti, *Best constant in Sobolev inequality*, Ann. Mat. Pura Appl., 110 (1976), pp. 353–372.

[36] K. Veroy and A. T. Patera, *Certified real-time solution of the parametrized steady incompressible Navier-Stokes equations; Rigorous reduced-basis* a posteriori *error bounds*, International Journal for Numerical Methods in Fluids, 47 (2005), pp. 773–788.

[37] K. Veroy, C. Prud'homme, and A. T. Patera, *Reduced-basis approximation of the viscous Burgers equation: Rigorous* a posteriori *error bounds*, C. R. Acad. Sci. Paris, Série I, 337 (2003), pp. 619–624.

[38] K. Veroy, C. Prud'homme, D. V. Rovas, and A. T. Patera, A posteriori *error bounds for reduced-basis approximation of parametrized noncoercive and nonlinear elliptic partial differential equations (AIAA Paper 2003-3847)*, in Proceedings of the 16th AIAA Computational Fluid Dynamics Conference, June 2003.