Output Bound Approximations for Partial Differential Equations; Application to the Incompressible Navier–Stokes Equations*

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Abstract. We describe an *a posteriori* finite element procedure for the efficient computation of lower and upper estimators for functional outputs of semilinear elliptic partial differential equations. The general theory is presented, and earlier applications of the procedure to a variety of different problems—including the Poisson equation, the advection-diffusion equation, elasticity problems, the Helmholtz equation, the Burgers equation, and eigenvalue problems—are reviewed. The method is then extended to treat incompressible flow problems, and numerical results are presented for a problem of natural convection in a complex enclosure.

1 Introduction and Motivation

In typical design problems, engineers are rarely interested in the entire field solution; only some selected characteristic metrics—or outputs—of the system are relevant. As an example, we consider the problem of cooling electronic components in a computer by natural convection of air in the enclosure represented in Fig. 1(a), where the temperature θ is fixed on boundary Γ_0, a heat flux q is imposed on segments Γ_1, Γ_2, and Γ_3, and $\partial\Omega \setminus \cup_{i=0}^{3}\Gamma_i$ is isolated. Such model is often the core of a design optimization problem—in the above example, we suppose that, given an input heat flux q, we wish to determine whether the mean temperature over Γ_1, $s = \int_{\Gamma_1} \theta \, ds$, is within an acceptable design interval, $\mathcal{I}_{\rm des} = [s_{\rm lo}, s_{\rm up}]$. In practice, many different fluxes q must be tested, so there is a premium on efficiency. Much more complex design questions can also be addressed.

In a classical finite element design approach, the output of interest is evaluated from an approximate solution of the original problem. In the problem of cooling electronic components, Fig. 1(a), we first evaluate the output of interest $s_\delta = S(\boldsymbol{u}_\delta, p_\delta, \theta_\delta)$ from an approximate field solution $(\boldsymbol{u}_\delta, p_\delta, \theta_\delta)$—here $\boldsymbol{u}_\delta$ is the velocity field, p_δ is the pressure field, θ_δ is the temperature field, and δ denotes the diameter of the discretization mesh $\mathcal{T}_\delta$. One then verifies whether $s_\delta \in \mathcal{I}_{\rm des}$, and the heat flux q is accepted or rejected accordingly. The shortcoming of the classical approach resides in the choice of the discretization mesh $\mathcal{T}_\delta$. If one chooses an "optimistic" relatively coarse

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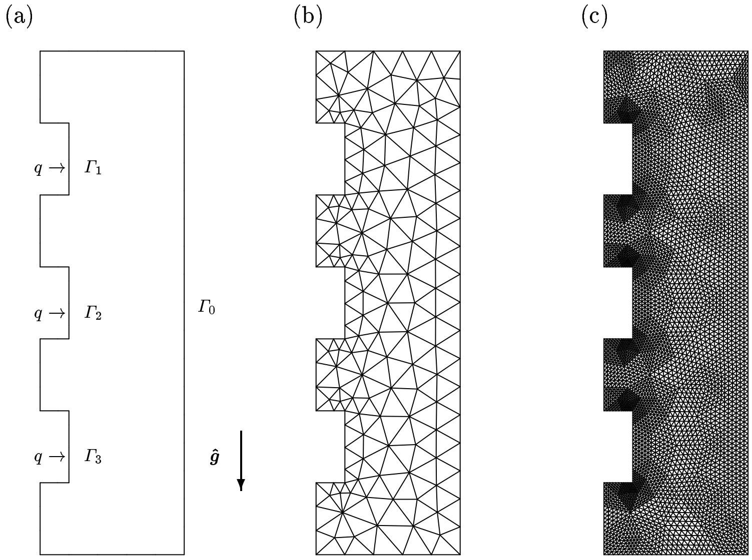

Fig. 1. (a): Domain Ω. (b): "Optimistic" coarse mesh, $\mathcal{T}_H$. (c): "Conservative" fine mesh, $\mathcal{T}_h$.

mesh $\mathcal{T}_H$, Fig. 1(b), the calculation is *inexpensive* but also *uncertain* since neither $s_H \in \mathcal{I}_{\text{des}} \Rightarrow s \in \mathcal{I}_{\text{des}}$ nor $s_H \notin \mathcal{I}_{\text{des}} \Rightarrow s \notin \mathcal{I}_{\text{des}}$. If, instead, one chooses a "conservative" sufficiently fine mesh $\mathcal{T}_h$, Fig. 1(c), then $s_h \approx s$ with reasonable *certainty*, but s_h is now very *expensive* to compute.

The purpose of this paper is to present a new approach which offers great promise in reconciling these conflicting requirements. We propose to construct a pair of output bound approximations, the estimators s_H^+ and s_H^-, computed predominantly on the mesh $\mathcal{T}_H$ and with the following attributes.

A1 As $H \rightarrow h$, we have $s_H^+ \rightarrow s_h$ from above and $s_H^- \rightarrow s_h$ from below $\forall H \leq H^*$. Here H^* is an unknown threshold discretization parameter; a detailed discussion of H^* will be given shortly; note that, for linear coercive problems, $H^* = \infty$.

A2 If we define the (half) bound gap $\Delta_H = \frac{1}{2}(s_H^+ - s_H^-)$, we have $\Delta_H \leq \eta |s_H - s_h|$ as $H \rightarrow h$, with η independent of H. This property guarantees the optimal convergence rate and sharpness of the bounds, provided the effectivity factor η is not too large.

A3 The bound gap Δ_H admits elemental decomposition $\Delta_H = \sum_{T_H \in \mathcal{T}_H} \Delta_{T_H}$, with $\Delta_{T_H} \geq 0$, for all elements T_H in $\mathcal{T}_H$; this will serve for adaptive refinement.

A4 The work required to evaluate s_H^+ and s_H^- is substantially smaller that the work necessary for the computation s_h, provided $H \ll h$.

Note that attribute A2 is important not only for efficiency, but also to ensure the "well-posedness" of the estimator formulation when $H^* < \infty$.

In our illustrative example, Fig. 1(a), the bound-based design would proceed as follows. Given a heat flux q, we choose an initial mesh $\mathcal{T}_H$, and we compute s_H^+ and s_H^-. Next, we define $\mathcal{I}_{\rm b} = [s_H^-, s_H^+]$; according to attribute A1 (provided $H \leq H^*$), if $\mathcal{I}_{\rm b} \in \mathcal{I}_{\rm des}$, we can accept q; if $\mathcal{I}_{\rm b} \in \mathbb{R} \backslash \mathcal{I}_{\rm des}$, we can reject q; otherwise, we use property A2, that is, we narrow the bound gap by taking a finer mesh (a smaller H), and we then repeat the procedure. In the latter case, attribute A3 is important as it allows us to optimally refine the mesh through an adaptive procedure. Attribute A4 ensures that the complete procedure is much less expensive than directly computing s_h.

The estimator formulation may be viewed as an implicit Aubin-Nitsche construction. The method is indebted to, but considerably generalizes, earlier finite element *a posteriori* error estimation techniques in that we obtain quantitative constant-free bounds—contrary to earlier explicit techniques [4]—for the output of interest—contrary to earlier implicit techniques [7,3,2]. Finally, some aspects of the method are also analogous to certain domain decomposition techniques [14,6].

2 Bound Procedure: Semi-Linear Elliptic Equations

2.1 Abstract Procedure

We consider here the problem: Find $u \in Y$ such that

$$\mathcal{A}(u, v) = 0, \quad \forall v \in Y,$$

where Y is a Hilbert space, and $\mathcal{A} : Y \times Y \to \mathbb{R}$ is a general form linear in the second argument. We further assume that we are interested in an output $s = S(u)$, where $S : Y \to \mathbb{R}$ is a prescribed output functional.

We next assume that we are given two finite element subspaces: Y_H, the coarse space, and Y_h, the fine space; we require $Y_H \subset Y_h \subset Y$. The associated coarse-space and fine-space approximations, u_H and u_h, exhibit complementary advantages and disadvantages. The fine-space solution, $u_h \in Y_h$, which satisfies the discrete problem

$$\mathcal{A}(u_h, v) = 0, \quad \forall v \in Y_h, \tag{1}$$

yields a very good approximation, $S(u_h)$, of the exact output s; nevertheless, the effort required to obtain u_h will typically be prohibitive. In contrast, the coarse-space solution, $u_H \in Y_H$, which satisfies the discrete problem

$$\mathcal{A}(u_H, v) = 0, \quad \forall v \in Y_H,$$

can be obtained with relatively modest computational effort; nevertheless the fidelity of the corresponding approximate output, $S(u_H)$, is no longer assured.

Prior to the description of the bound procedure, we need to introduce the following definitions and form expansions. We first define $\mathcal{E}(w,v) = \mathcal{A}(u_H + w, v) - \mathcal{A}(u_H, v)$. We next expand $\mathcal{E}(w,v) = E(w,v) + F(w,w,v) + G(w,v)$, where $E(w,v)$ is a bilinear form, $F(w_1,w_2,v)$ is a trilinear form (symmetric in w_1 and w_2), and $G(w,v)$ is the remainder, linear in v. A similar decomposition applied to the output functional yields $S(u_h + v) = S(u_H) + L(v) + M(v,v) + N(v)$, where $L(v)$ is linear, $M(v_1,v_2)$ is (symmetric) bilinear, and $N(v)$ is the remainder. We then decompose the symmetric part of $E(w,v)$, $E^s(w,v) = \frac{1}{2}(E(w,v) + E(v,w))$, into two components, $E^s(w,v) = E^s_c(w,v) + E^s_a(w,v)$, where $E^s_c(w,v)$ is positive semi-definite, that is $E^s_c(v,v) \geq 0, \forall v \in Y$. Finally, we introduce the "broken" spaces, $\hat{Y}_H \subset \hat{Y}_h \subset \hat{Y}$, such that $Y = \{v \in \hat{Y} \,|\, B(v,q) = 0, \forall q \in Z\}$, $Y_h = \{v \in \hat{Y}_h \,|\, B(v,q) = 0, \forall q \in Z\}$, and $Y_H = \{v \in \hat{Y}_H \,|\, B(v,q) = 0, \forall q \in Z_H\}$. Here $Z_H \subset Z$ are additional Hilbert spaces and $B : \hat{Y} \times Z \to \mathbb{R}$ is a bilinear form. The bound procedure then proceeds in five steps:

1. Compute $u_H \in Y_H$ as the solution of the primal problem
$$\mathcal{A}(u_H, v) = 0, \quad \forall v \in Y_H.$$
We then define the primal residual as $\mathcal{R}^{\mathrm{pr}}(v) = -\mathcal{A}(u_H, v), \forall v \in \hat{Y}$.
2. Compute the output adjoint $\psi_H \in Y_H$ as the solution of the dual problem
$$E(v, \psi_H) = -L(v), \quad \forall v \in Y_H. \tag{2}$$
We then define the dual residual as $\mathcal{R}^{\mathrm{du}}(v) = -L(v) - E(v,\psi_H), \forall v \in \hat{Y}$.
3. Compute the hybrid fluxes, $\sigma_H^{\mathrm{pr}} \in Z_H$ and $\sigma_H^{\mathrm{du}} \in Z_H$, which satisfy the equations
$$B(v, \sigma_H^{\mathrm{pr}}) = \mathcal{R}^{\mathrm{pr}}(v), \forall v \in \hat{Y}_H, \quad \text{and} \quad B(v, \sigma_H^{\mathrm{du}}) = \mathcal{R}^{\mathrm{du}}(v), \forall v \in \hat{Y}_H.$$
4. Compute the "reconstructed" errors, $\hat{e}^{\mathrm{pr}} \in \hat{Y}_h$ and $\hat{e}^{\mathrm{du}} \in \hat{Y}_h$,
$$2E^s_c(\hat{e}^{\mathrm{pr}}, v) = \mathcal{R}^{\mathrm{pr}}(v) - B(v, \sigma_H^{\mathrm{pr}}), \quad \forall v \in \hat{Y}_h, \tag{3}$$
$$2E^s_c(\hat{e}^{\mathrm{du}}, v) = \mathcal{R}^{\mathrm{du}}(v) - B(v, \sigma_H^{\mathrm{du}}), \quad \forall v \in \hat{Y}_h. \tag{4}$$
5. Evaluate the lower and upper bound approximations: $s_H^{\pm} = S(u_H) \pm \kappa E^s_c(\hat{e}^{\pm}, \hat{e}^{\pm})$, where $\kappa \in \mathbb{R}_+$ and $\hat{e}^{\pm} = \hat{e}^{\mathrm{pr}} \mp \frac{1}{\kappa}\hat{e}^{\mathrm{du}}$. The choice of κ will affect the bound gap $\Delta_H = \frac{1}{2}(s_H^+ - s_H^-) = \kappa E^s_c(\hat{e}^{\mathrm{pr}}, \hat{e}^{\mathrm{pr}}) + \frac{1}{\kappa} E^s_c(\hat{e}^{\mathrm{du}}, \hat{e}^{\mathrm{du}})$. Since $\hat{e}^{\mathrm{pr}}$ and $\hat{e}^{\mathrm{du}}$ do not depend on κ, we can readily find the κ which minimizes the bound gap,
$$\kappa^* = \sqrt{\frac{E^s_c(\hat{e}^{\mathrm{du}}, \hat{e}^{\mathrm{du}})}{E^s_c(\hat{e}^{\mathrm{pr}}, \hat{e}^{\mathrm{pr}})}}, \tag{5}$$
yielding the optimized bounds $s_H^{\pm} = S(u_H) - 2E^s_c(\hat{e}^{\mathrm{pr}}, \hat{e}^{\mathrm{du}}) \pm \Delta_H$, with $\Delta_H = 2\sqrt{E^s_c(\hat{e}^{\mathrm{pr}}, \hat{e}^{\mathrm{pr}}) E^s_c(\hat{e}^{\mathrm{du}}, \hat{e}^{\mathrm{du}})}$.

We have shown in earlier papers [13,11] that, if we define $e = u_h - u_H$,

$$s_H^{\pm} = S(u_h) \pm D^{\pm} \pm I^{\pm}, \tag{6}$$

with

$$\begin{aligned} D^{\pm} &= \kappa^* E_c^s(e - \hat{e}^{\pm}, e - \hat{e}^{\pm}), \\ I^{\pm} &= \kappa^* E_a^s(e, e) \mp F(e, e, \psi_H) \mp M(e, e) + \kappa^* F(e, e, e) \\ &\quad \mp G(e, \psi_H) \mp N(e) + \kappa^* G(e, e). \end{aligned} \tag{7}$$

Here $D^{\pm} \geq 0$ is a positive semi-definite term and $I^{\pm}$ is an indefinite term. The essential point is that, for a large and important class of problems—semilinear elliptic partial differential equations—,there exists a splitting, $E^s = E_c^s + E_a^s$, such that, relative to $D^{\pm}$, the corrections in $I^{\pm}$ involve weaker norms or higher power of the error e; therefore, $D^{\pm}$ dominates all other deviations of $s_H^{\pm}$ from $S(u_h)$ for H sufficiently small ($H < H^*$). We conclude that s_H^- and s_H^+ approach $S(u_h)$ from below and above, respectively. Note that for linear coercive problems $I^{\pm} = 0$, and we obtain bounds for all H ($H^* = \infty$).

2.2 Basic Spaces

We now introduce different concrete functional spaces which will serve as building blocks for defining the spaces Y, Y_H, Y_h, $\hat{Y}$, $\hat{Y}_H$, $\hat{Y}_h$, Z, and Z_H in the instantiations of the general procedure.

Let $\Omega \in \mathbb{R}^d$ ($d = 1, 2$) be open with Lipschitz boundary. We first set $X = H_0^1(\Omega)$ [1], and we define the finite element spaces

$$X_\delta^{(p)} = \{v \in X \mid v|_{T_\delta} \in \mathbb{P}_p(T_\delta), \forall T_\delta \in \mathcal{T}_\delta\},$$

where $\delta = h$ or H, $p = 1, 2$, $\mathcal{T}_h$ and $\mathcal{T}_H$ are two triangulations chosen such that $X_H^{(p)} \subset X_h^{(p)}$ ($\mathcal{T}_h$ is a refinement of $\mathcal{T}_H$), T_δ denotes an element in $\mathcal{T}_\delta$, and $\mathbb{P}_p(T_\delta)$ is the space of all polynomials of degree $\leq p$ defined on T_δ. We next define the "broken" spaces

$$\hat{X} = \{v \in L^2(\Omega) \mid v|_{T_H} \in H^1(T_H), \forall T_H \in \mathcal{T}_H\},$$

and, for $\delta = h$ or H,

$$\hat{X}_\delta^{(p)} = \{v \in L^2(\Omega) \mid v|_{T_H} \in H^1(T_H), \forall T_H \in \mathcal{T}_H;\ v|_{T_\delta} \in \mathbb{P}_p(T_\delta), \forall T_\delta \in \mathcal{T}_\delta\}.$$

Note that $v \in \hat{X}$ may be discontinuous over $\partial T_H, \forall T_H \in \mathcal{T}_H$. The "broken" meshes corresponding to the spaces $\hat{X}_H$ and $\hat{X}_h$ are represented in Figs. 2(a) and (b).

Given the set of edges γ of $\mathcal{T}_H$, $\Gamma(\mathcal{T}_H)$, we define the hybrid flux spaces $Q = L^2(\Gamma(\mathcal{T}_H))$, and

$$Q_H^{(p)} = \{v \in Q \mid v|_\gamma \in \mathbb{P}_p(\gamma), \forall \gamma \in \Gamma(\mathcal{T}_H)\}.$$

(Note that for $\Omega \subset \mathbb{R}^1, v|_\gamma \in \mathbb{R}$.) Finally, we define the continuity form, $b : \hat{X} \times Q \to \mathbb{R}$

$$b(v,\tau) = \sum_{\gamma \in \Gamma(\mathcal{T}_H)} \int_\gamma [v]_\gamma \tau|_\gamma \, ds,$$

where $[v]_\gamma$ denotes the jump in v across γ when $\gamma \in \Omega$ and the trace of v when $\gamma \in \partial\Omega$. For this definition of $b(v,\tau)$ the following equivalence conditions are satisfied: $X = \{v \in \hat{X} \mid b(v,\tau) = 0, \forall \tau \in Q\}$, and $X_H = \{v \in \hat{X}_H \mid b(v,\tau) = 0, \forall \tau \in Q_H\}$.

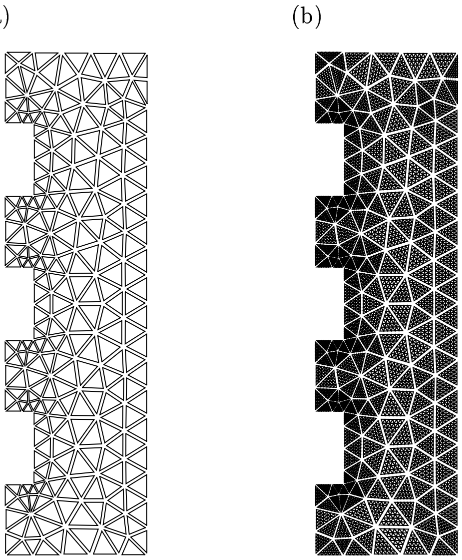

Fig. 2. (a): Space $\hat{X}_H$. (b) Space $\hat{X}_h$.

2.3 Instantiations

Linear Coercive. Our first example is the Poisson equation with homogeneous Dirichlet boundary conditions: $-\nabla^2 u = f$ in $\Omega, u|_{\partial\Omega} = 0$. We shall start by the identification of the various abstract spaces and forms of the general formulation: $\mathcal{A}(w,v) = \int_\Omega \nabla w \cdot \nabla v - fv \, dA$, $Y = X$, $\mathcal{E} = E = E_c^s(w,v) = \int_\Omega \nabla w \cdot \nabla v \, dA$, $F = G = 0$, $Y_\delta = X_\delta^{(1)}$, $\hat{Y}_\delta = \hat{X}_\delta^{(1)}$, $Z_H = Q_H^{(1)}$, and $B = b$. Next, we review the different steps of the bound procedure. Steps 1 and 2 (coarse primal and dual equilibria) are straightforward. For the hybrid flux equilibration, Step 3, we adopt (and adapt) the procedure developed in the context of energy-norm implicit Neumann subproblem indicators [7]. The solvability of the hybrid flux equations follows the equilibria obtained in Steps 1 and 2 [17]. This construction of equilibrated hybrid fluxes ensures the solvability of the local Neumann subproblems for the error reconstruction in Step 4. Then the optimal lower and upper bounds are computed in Step 5. The bound error expression, Eqs. (6) and (7), reads $s_H^{\pm} = S(u_h) \pm \kappa^* \int_\Omega |\nabla(e - \hat{e}^{\pm})|^2 \, dA$.

The advection-diffusion equation is an example of nonsymmetric linear coercive problem: $-\nu\nabla^2 u + U \cdot \nabla u = f$ in $\Omega, u|_{\partial\Omega} = 0$, $\nu > 0$, and $\nabla \cdot U = 0$ in Ω. The following identification shows that nonsymmetric problems fall readily into the formalism: $\mathcal{A}(w,v) = \int_\Omega \nabla w \cdot \nabla v + (U \cdot \nabla w)v - fv \, dA$, $Y = X$, $\mathcal{E} = E(w,v) = \int_\Omega \nabla w \cdot \nabla v + (U \cdot \nabla w)v \, dA$, $F = G = 0$, $E^s = E_c^s(w,v) = \int_\Omega \nabla w \cdot \nabla v \, dA$, $Y_\delta = X_\delta^{(1)}$, $\hat{Y}_\delta = \hat{X}_\delta^{(1)}$, $Z_H = Q_H^{(1)}$, and $B = b$. The identification yields the bound error expression $s_H^{\pm} = S(u_h) \pm \kappa^* \int_\Omega |\nabla(e - \hat{e}^{\pm})|^2 \, dA$, identical to that for the Poisson problem.

We now illustrate the use of product spaces, which permits extension to vector-valued problems and, as will be seen later, to "many-field" problems like natural convection. We treat the linear two-dimensional elasticity system,

$$-\frac{\partial}{\partial x_j}(E_{ijkl}\frac{\partial u_k}{\partial x_l}) = f_i \text{ in } \Omega, \quad u_i|_{\partial\Omega} = 0,$$

where E_{ijkl} is the elasticity constitutive tensor. For this problem the spaces are defined by the following products: $Y = X \times X$, $Y_\delta = X_\delta^{(1)} \times X_\delta^{(1)}$, $\hat{Y}_\delta = \hat{X}_\delta^{(1)} \times \hat{X}_\delta^{(1)}$, and $Z_H = Q_H^{(1)} \times Q_H^{(1)}$. The forms are given by

$$\mathcal{A}(\boldsymbol{w},\boldsymbol{v}) = \int_\Omega E_{ijkl}\frac{\partial w_k}{\partial x_l}\frac{\partial v_i}{\partial x_j} - f_i v_i \, dA,$$
$$\mathcal{E} = E = E_c^s(\boldsymbol{w},\boldsymbol{v}) = \int_\Omega E_{ijkl}\frac{\partial w_k}{\partial x_l}\frac{\partial v_i}{\partial x_j} \, dA,$$

$F = G = 0$, and $B(\boldsymbol{v},\boldsymbol{\tau}) = b(v_i,\tau_i)$. The bound error expression reads

$$s_H^{\pm} = S(u_h) \pm \kappa^* \int_\Omega E_{ijkl}\frac{\partial(e_i - \hat{e}_i^{\pm})}{\partial x_j}\frac{\partial(e_k - \hat{e}_k^{\pm})}{\partial x_l} \, dA.$$

Advection-diffusion and elasticity results are presented in [17]. Different outputs, such as the average of the field variable over parts of the domain (advection-diffusion), or the averaged force or displacement over parts of the domain boundary, are considered. The results demonstrate the convergence of the upper and lower bounds from above and below, $s_H^{\pm}/s_h \to 1$, the optimality of the convergence rate, $|s_H^{\pm}/s_h - 1| \propto CH^2$ ($\mathbb{P}_1$ elements), and, for a mesh that barely resolves the solution, $|s_H^{\pm}/s_h - 1| \approx 10\%$. In [19], the local bound gap contributions are used in an adaptive mesh refinement strategy.

The procedure is easily generalized to treat other examples of linear coercive problems such as stabilized linear advection (a hyperbolic problem, in fact) [11].

Linear Noncoercive. We consider the Helmholtz equation with homogeneous Dirichlet boundary conditions: $-\nabla^2 u - k^2 u = f$ in $\Omega, u|_{\partial\Omega} = 0$. The identification of spaces and forms yields $\mathcal{A}(w,v) = \int_\Omega \nabla w \cdot \nabla v - k^2 wv - fv\, dA$, $Y = X$, $\mathcal{E} = E = E^s(w,v) = \int_\Omega \nabla w \cdot \nabla v - k^2 wv\, dA$, $F = G = 0$, $E^s_c(w,v) = \int_\Omega \nabla w \cdot \nabla v\, dA$, $E^s_a(w,v) = -k^2 \int_\Omega wv\, dA$, $Y_\delta = X^{(1)}_\delta$, $\hat{Y}_\delta = \hat{X}^{(1)}_\delta$, $Z_H = Q^{(1)}_H$, and $B = b$. Another variant of the method for the Helmholtz equation is found in [18]. The complex Helmholtz problem in two-dimensional exterior domains (scattering wave problem) has been treated in [22]; other examples of linear noncoercive problems include the calculation of bound approximations for sensitivity derivatives [8].

Nonlinear Noncoercive. We now discuss the nonlinear Burgers equation (in one space dimension): $-\nu u_{xx} + uu_x = f$ in $\Omega =]0,1[$, with $u(0) = 0 = u(1) = 0$; here $\nu > 0$ is the viscosity. This equation leads to the form $\mathcal{A}(w,v) = \int_0^1 \nu w_x v_x + w w_x v - fv\, dx$. For this problem, we consider the following (nonlinear) output: $S(v) = \int_0^1 \nu v_x \chi_x - \frac{1}{2} v^2 \chi_x\, dx$, where $\chi \in C^1(\Omega)$ is such that $\chi(0) = 0, \chi(1) = 1$. For u sufficiently smooth, we have $S(u) = \nu u_x(1)$. We define the functional spaces as $Y = X$, $Y_\delta = X^{(1)}_\delta$, $\hat{Y}_\delta = \hat{X}^{(1)}_\delta$, and $Z_H = Q^{(1)}_H$. We can now proceed with the form expansions: $E(w,v) = \int_0^1 \nu w_x v_x - u_H w v_x\, dx$, $F(w_1,w_2,v) = -\frac{1}{2}\int_0^1 w_1 w_2 v_x\, dx$, $G(w) = 0$, $L(w) = \int_0^1 \nu w_x \chi_x - w u_H \chi_x\, dx$, $M(w_1,w_2) = -\frac{1}{2}\int_0^1 w_1 w_2 \chi_x\, dx$, and $N(w) = 0$. The coercive splitting yields $E^s_c(w,v) = \int_0^1 \nu w_x v_x\, dx$ and $E^s_a(w,v) = \frac{1}{2}\int_0^1 (u_H)_x wv\, dx$. Another variant of the method is found in [18]. Other results on the Burgers equation with adaptivity are presented in [11].

We now apply the framework to the symmetric eigenvalue problem: $-\nabla^2 u = \lambda u$ in $\Omega, u|_{\partial\Omega} = 0$. We first define $Y = X \times \mathbb{R}$, $Y_\delta = X^{(1)}_\delta \times \mathbb{R}$, $\hat{Y}_\delta = \hat{X}^{(1)}_\delta \times \mathbb{R}$, and $Z_H = Q^{(1)}_H$. We then write the form $\mathcal{A}((w,\mu),(v,\alpha)) = \int_\Omega \nabla w \cdot \nabla v - \mu wv + \alpha w^2\, dA - \alpha$. This forms leads to $\mathcal{E} = E + F$, $G = 0$, $E((w,\mu),(v,\alpha)) = \int_\Omega \nabla w \cdot \nabla v - \lambda_H wv - \mu u_H v + 2\alpha u_H w\, dA$, and $F((w,\mu)_1,(w,\mu)_2,(v,\alpha)) = \int_\Omega \alpha w_1 w_2 - \frac{1}{2}(\mu_1 w_2 v + \mu_2 w_1 v)\, dA$. The splitting is defined by $E^s_c = \int_\Omega \nabla w \cdot \nabla v\, dA$ and $E^s_a = \int_\Omega -\lambda_H wv + \frac{1}{2}(\mu u_H v + \alpha u_H w)\, dA$. The eigenvalue problem is treated in [13].

2.4 Discussion of Attributes

Attribute A1. For coercive linear problems, in view of Eqs. (6) and (7), bounds are obtained uniformly for all H. An alternative proof and interpretation can be obtained by a duality argument [16,17,19].

For noncoercive problems, we require an additional hypothesis—a variation on the standard Aubin-Nitsche relationship between the L^2 and H^1 discretization error—which applies generally to second-order equations that satisfy a Gårding inequality [20]. More precisely, we assume that there exists three positive constants, C^1_D, C^2_D and C_I, such that (say for the lower bound and $\mathbb{P}_1$ elements) $C^1_D H^2 \le D^- \le C^2_D H^2$ and $|I^-| \le C_I H^4$; then,

$s_H^- = s_h - D^- - I^- \leq s_h - C_D^1 H^2 + C_I H^4 \leq s_h$, for $H \leq H*$ where $H^* = \sqrt{C_D^1/C_I}$. (A weaker hypothesis is introduced in [21].)

We now show that the noncoercive examples presented above fulfill this hypothesis. For the Helmholtz equation, we have $s_H^\pm = S(u_h) \pm D^\pm \pm I^\pm$, where $D^\pm = \kappa^* E_c^s(e - \hat{e}^\pm, e - \hat{e}^\pm) = \kappa^* \int_\Omega |\nabla(e - \hat{e}^\pm)|^2 \, dA$, and $I^\pm = \kappa^* E_a(e,e) = -\kappa^* k^2 \int_\Omega e^2 \, dA$. We see that $|\kappa^* E_a(e,e)| \leq C\|e\|_{L^2}^2$ vanishes as $O(H^4)$—much faster than $\kappa^* E_c^s(e - \hat{e}^\pm, e - \hat{e}^\pm)$, which should tend to zero as $O(H^2)$. It then follows that s_H^- and s_H^+ will approach $S(u_h)$ from below and above for H sufficiently small, $H < H^*$.

For the Burgers equation, we first note that $F(e,e,e) = 0$; therefore, we find $s_H^\pm = S(u_h) \pm \kappa^* \int_0^1 \nu(e_x - \hat{e}_x^\pm)^2 \, dx + \frac{1}{2}\int_0^1 (\pm\kappa^* u_H + \psi_H + \chi)_x e^2 \, dx$. Again, we see that the indefinite terms appear only in the weaker norm, and should be dominated by the gradient as H becomes small. Note that for both the Burgers equation and the Helmholtz equation the singular-perturbation prefactor (ν and k^{-2}, respectively) unfortunately favors the indefinite terms; nevertheless, the corresponding numerical singular-perturbation parameter (for instance, the grid Peclet number) will be small as soon as the coarse space even roughly resolves the structure of the solution, and thus the bound property will be preserved except perhaps on very crude meshes.

If we consider the eigenvalue problem with the output being the eigenvalue $S(v,\alpha) = \alpha$ (see [13] for the more general case), we have $s_H^\pm = \lambda_h \pm \kappa^* \int_\Omega |\nabla(e - \hat{e}^\pm)|^2 \, dA \mp \kappa^* \lambda_H \int_\Omega e^2 \, dA$. Since $\kappa^* \int_\Omega |\nabla(e - \hat{e}^\pm)|^2 \, dA$ is $O(H^2)$ and since from a priori results [23] we know that $\|e\|_{L^2}^2 = O(H^4)$; the estimators $s_H^\pm$ will approach λ_h from above and below as $H \to h$. In all cases studied in [13], upper and lower bounds are obtained, except in one case for a very coarse discretization. As expected, the convergence rate is $O(H^2)$ (for $\mathbb{P}_1$ elements).

We conclude that, even if H^* is not known *a priori*, bounds are obtained once the solution is marginally resolved. In numerical examples, we have almost always observed $H^* = \infty$, and thus the uncertainty associated with H^* is not an important practical issue, though it constitutes a real theoretical issue. Finally, H^* is a threshold parameter (bounds are obtained for all $H < H^*$); therefore, even if H^* is not known, the method present a significant advantage over previous explicit *a posteriori* estimation procedures in which estimators involve unknown constants and functions.

There is another source of uncertainty associated with the choice of the fine mesh $\mathcal{T}_h$, which should be selected fine enough to ensure that $|s - s_h|$ is negligible (recall that s is the exact solution). In practice, the mesh $\mathcal{T}_h$ is chosen conservatively by estimating *a priori* the size of the smallest structure anticipated and ensuring that $\mathcal{T}_h$ provides for an accurate representation of such structures.

Attribute A2. The bounds produced by the procedure are sharp. The bound gap converges at an optimal rate: $\Delta_H \leq CH^2$ (proved for linear coercive and certain noncoercive equations, for $\mathbb{P}_1$ elements, in [12]), and the the effectivity factor, $\eta = \Delta_H/|s_h - s_H|$, has been measured for various applications, typically $1 \le \eta \le 10$.

Attribute A3. Since the cost of computing the bounds is essentially a function of the number of elements T_H in $\mathcal{T}_H$, it is desirable to construct optimized triangulations that maximize the bound accuracy (minimize the bound gap) for a given number of degrees of freedom. As shown in [19], the bound gap Δ_H can be expressed as a sum of local elemental positive contributions: $\Delta_H = \sum_{T_H \in \mathcal{T}_H} \Delta_{T_H}$, with $\Delta_{T_H} \ge 0$. We can, therefore, implement a simple adaptive strategy. Starting from an initial grid, $\mathcal{T}_H^0$, with bound gap Δ_H^0, we generate a sequence of triangulations $\{\mathcal{T}_H^k, k = 1, 2, ...\}$ with corresponding bound gaps $\{\Delta_H^k, k = 1, 2, ...\}$, such that each triangulation $\mathcal{T}_H^k$ is obtained by refinement of the selected triangles T_H^{k-1} such that $\Delta_{T_H}^{k-1} > \alpha \max_{T_H} \Delta_{T_H}^{k-1}$, for a specified parameter $0 < \alpha < 1$. The approach ensures that, for a sufficiently large k, $\Delta_H^k \le \Delta_{\mathrm{targ}}$, where $\Delta_{\mathrm{targ}} > 0$ is a gap target.

Attribute A4. We recall that u_h and $S(u_h)$ are the field variable and the output that are effectively indistinguishable from the truth—and correspondingly expensive. Our lower and upper bounds are only interesting if they can be obtained at considerably less expense than computation of $S(u_h)$—and preferably at only slightly greater expense than computation of $S(u_H)$, the coarse approximation. From our definitions of $X_h^{(p)}$ and $\hat{X}_h^{(p)}$ and the identifications of Y_h and $\hat{Y}_h$ for the different semilinear elliptic problems considered in Section 2.3, we see that Eqs. (3) and (4) correspond to many local, uncoupled, small, Neumann subproblems, whereas Eq. (1) corresponds to a single, large, global problem. It follows that Eqs. (3) and (4) present a smaller bandwidth—yielding substantial savings in both memory and computational time of direct solution strategies—and a smaller condition number—yielding faster convergence in iterative methods. In addition, Eqs. (3) and (4) are symmetric, positive-definite, and completely decoupled—the latter enabling straightforward parallel implementations. Furthermore, for nonlinear equations, the dual problem, Eq. (2), and the subproblems, Eqs. (3) and (4), are linear, leading to extra savings compared to the original fine mesh problem. Relative savings are reduced as the global solver improves.

3 Output Bounds for Incompressible Flow Problems

We first consider the Stokes equations

$$-\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) + \frac{\partial p}{\partial x_i} = f_i \quad \text{in } \Omega,$$

$$\frac{\partial u_i}{\partial x_i} = 0 \quad \text{in } \Omega, \quad u_i|_{\partial\Omega} = 0,$$

where $\boldsymbol{f}$ is a prescribed function, $\boldsymbol{u}$ is the velocity field, and p is the pressure field. We define the function spaces $X = H_0^1(\Omega) \times H_0^1(\Omega)$, $Y = X \times L^2(\Omega)/\mathbb{R}$, and $\mathcal{A}((\boldsymbol{w},r),(\boldsymbol{v},q)) : Y \times Y \to \mathbb{R}$,

$$\mathcal{A}((\boldsymbol{w},r),(\boldsymbol{v},q)) = \int_\Omega \left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right)\frac{\partial v_i}{\partial x_j} - p\frac{\partial v_i}{\partial x_i} - f_i v_i - q\frac{\partial w_i}{\partial x_i}\, dA.$$

Then the weak formulation of the Stokes problem is: Find $(\boldsymbol{u},p) \in Y$ such that

$$\mathcal{A}((\boldsymbol{u},p),(\boldsymbol{v},q)) = 0, \quad \forall(\boldsymbol{v},q) \in Y.$$

We also specify an output functional $S : Y \to \mathbb{R}$, and, as usual, two discretization meshes $\mathcal{T}_\delta$, $\delta = h, H$—$\mathcal{T}_h$ being a refinement of $\mathcal{T}_H$. We choose the Crouzeix-Raviart finite element spaces for the velocity and the pressure [5],

$$\begin{aligned} X_\delta^{(2+)} &= \{\boldsymbol{v} \in H_0^1(\Omega) \times H_0^1(\Omega) \,|\, v_i|_{T_\delta} \in \mathbb{P}_2(T_\delta) \oplus B_3(T_\delta), \forall T_\delta \in \mathcal{T}_\delta\}, \\ M_\delta &= \{p \in L^2(\Omega)/\mathbb{R} \,|\, p|_{T_\delta} \in \mathbb{P}_1(T_\delta), \forall T_\delta \in \mathcal{T}_\delta\}, \end{aligned}$$

where $B_3(T_\delta)$ denotes the space of bubble functions of degree 3 on T_δ. The "broken" spaces $\hat{X}_\delta^{2+}$ and $\hat{M}_\delta$ are obtained as usual by relaxing the continuity across the edges of the coarse mesh. Note that, since the pressure is discontinuous across element boundaries, we have $M_\delta = \hat{M}_\delta$. Then, we set $Y_\delta = X_\delta^{(2+)} \times M_\delta$ and $\hat{Y}_\delta = \hat{X}_\delta^{(2+)} \times \hat{M}_\delta$. Finally, we define the hybrid flux spaces $Z_H = Q_H^{(2)} \times Q_H^{(2)}$ and the bilinear form $B(\boldsymbol{v},\boldsymbol{\tau}) = b(v_i,\tau_i)$.

We now proceed with the usual form expansion; we have $E = E^s = E_c^s + E_a^s \equiv E_{c,V}^s$ where

$$\begin{aligned} E_c^s((\boldsymbol{w},r),(\boldsymbol{v},q)) &= \int_\Omega \left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right)\frac{\partial v_i}{\partial x_j}\, dA, \\ E_a^s((\boldsymbol{w},r),(\boldsymbol{v},q)) &= -\int_\Omega p\frac{\partial v_i}{\partial x_i} + q\frac{\partial w_i}{\partial x_i}\, dA. \end{aligned}$$

Here E_c^s is coercive over $H_0^1(\Omega) \times H_0^1(\Omega)$, and $E_{c,V}^s$ indicates that E^s is coercive if we take $\boldsymbol{w}$ and $\boldsymbol{v}$ in V, where

$$V = \{\boldsymbol{v} \in H_0^1(\Omega) \times H_0^1(\Omega) \,|\, \int_\Omega \frac{\partial v_i}{\partial x_i} q\, dA = 0, \forall q \in L^2(\Omega)\}.$$

We define $\boldsymbol{e} = \boldsymbol{u}_h - \boldsymbol{u}_H$ and $\epsilon = p_h - p_H$, and we consider Eqs. (6) and (7). We see that $E_a^s((\boldsymbol{e},\epsilon),(\boldsymbol{e},\epsilon)) = O(H^4)$ is not subdominant; therefore, bounds cannot be obtained for this problem by strictly following the general procedure. Nevertheless, uniform bounding properties are recovered for this problem if we replace, in Step 4 of the bound procedure, $(\boldsymbol{u}_H, p_h) \in Y_H$ by $(\tilde{\boldsymbol{u}}_H, \tilde{p}_H) \in Y_h$, where $\tilde{\boldsymbol{u}}_H$ is chosen such that

$$\int_\Omega \frac{\partial \tilde{u}_{H,i}}{\partial x_i} q\, dA = 0, \quad \forall q \in M_h.$$

An appropriate choice of $(\tilde{\boldsymbol{u}}_H, \tilde{p}_H)$ is to take the M_h-incompressible "Stokes projection" of $(\boldsymbol{u}_H, p_H)$ with the additional constraint that $\tilde{\boldsymbol{u}}_H|_{\partial T_H} = \boldsymbol{u}_H|_{\partial T_H}$. Since we use discontinuous pressure, these projections are elemental and, thus, inexpensive. With this new formulation, we have two possible strategies: either we use $E^s_{c,V}$, or we use E^s_c in the local Neumann subproblems. Since the former choice yields M_h-incompressible reconstructed errors, it is arguably more accurate. For earlier results on the Stokes problem, with a slightly different approach, see [15].

The extension of the above formulation to the Navier-Stokes equations,

$$
\begin{aligned}
-\frac{\partial}{\partial x_j}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)+u_j\frac{\partial u_i}{\partial x_j}+\frac{\partial p}{\partial x_i} &= f_i \quad \text{in } \Omega, \\
\frac{\partial u_i}{\partial x_i} &= 0 \quad \text{in } \Omega, \quad u_i|_{\partial\Omega}=0,
\end{aligned}
$$

is obtained if we define

$$
\mathcal{A}((\boldsymbol{w},r),(\boldsymbol{v},q)) = \int_\Omega \left(\frac{\partial w_i}{\partial x_j}+\frac{\partial w_j}{\partial x_i}\right)\frac{\partial v_i}{\partial x_j} - u_i u_j \frac{\partial v_i}{\partial x_j} - p\frac{\partial v_i}{\partial x_i} - f_i v_i - q\frac{\partial w_i}{\partial x_i}\, dA. \quad (8)
$$

The general form expansion combines the approaches for the Burgers equation and the Stokes equations. Again, to guarantee subdominance of the indefinite terms in Eqs. (6) and (7), we use the projection $(\tilde{\boldsymbol{u}}_H, \tilde{p}_H)$. To retain the solvability of the local Neumann subproblems, Eqs. (3) and (4), the nonlinear terms in the primal problem are written in their conservative form, and $(\tilde{\boldsymbol{u}}_H, \tilde{p}_H)$ must be replaced by $(\boldsymbol{u}_H, p_H)$ in the convective (L^2) parts of $\mathcal{R}^{\mathrm{du}}$. Optimal asymptotic bounds are obtained since the perturbations $\|\boldsymbol{u}_H - \tilde{\boldsymbol{u}}_H\|_{H^1}$, $\|\boldsymbol{u}_H - \tilde{\boldsymbol{u}}_H\|_{L^2}$, and $\|p_H - \tilde{p}_H\|$ can be shown to be sufficiently small.

The natural convection problem,

$$
\begin{aligned}
-\frac{\partial^2 u_i}{\partial x_j^2}+u_j\frac{\partial u_i}{\partial x_j}+\frac{\partial p}{\partial x_i} &= -\,\beta\theta\hat{g}_i \quad \text{in } \Omega, \\
\frac{\partial u_i}{\partial x_i} &= 0 \quad \text{in } \Omega, \\
-\frac{1}{\alpha}\frac{\partial^2 \theta}{\partial x_j^2}+u_j\frac{\partial \theta}{\partial x_j} &= 0 \quad \text{in } \Omega,
\end{aligned} \quad (9)
$$

where $\hat{\boldsymbol{g}}$ is the unit vector indicating the direction of gravity, α is the Prandtl number, β is the Grashof number, and θ is the temperature, requires us to incorporate the temperature equation in the formulation. This is readily achieved using a product space formulation since the indefinite error term due to the Boussinesq coupling in the bound error expression involves only weak norms. Moreover, the weak coupling allows us to introduce two parameters

κ_u and κ_θ; these parameters can be optimized independently (with relations similar to Eq. (5)), yielding sharper bounds. For a detailed presentation of the formulation for this problem, see [10].

We will now present numerical results for a simple natural convection test case. The geometry of the problem is shown in Fig. 3(a). The boundary conditions are $\boldsymbol{u}|_{\partial\Omega} = 0$, $\theta = 0$ on Γ_0, $\frac{\partial\theta}{\partial n} = 1$ on Γ_I, and $\frac{\partial\theta}{\partial n} = 0$ otherwise. The Prandtl number and the Grashof number are $\alpha = 1$ and $\beta = 30,000$. For this choice of parameters, the Nusselt number is $\mathrm{Nu} = 2.49$ ($\mathrm{Nu}^{-1} = \frac{1}{\Gamma_I}\int_{\Gamma_I} \theta\, ds$); for a pure conduction problem in this geometry, $\mathrm{Nu} = 1$, and thus $\mathrm{Nu} = 2.49$ indicates the existence of velocity and thermal boundary layers near Γ_I and Γ_0. The elements of the coarsest mesh, $\mathcal{T}_{H_0}$, (represented on Fig. 3(a)) are chosen so that the diameter of the mesh, H_0, is approximately the size of the thickness of the boundary layers.

Figures 3(b) and 3(c) show the convergence of the bounds for a nonlinear output,

$$S(u) = \int_\Omega |\boldsymbol{u}|^2\, dA,$$

corresponding to the kinetic energy of the flow. For this problem, bounds are always observed on all the meshes considered. In Fig. 3(b), we have represented the normalized lower and upper bounds s_H^+/s_h and s_H^-/s_h, and the normalized "coarse" mesh output, s_H/s_h, for different meshes $\mathcal{T}_H$. The mesh diameters vary from $H = H_0$ to $H = H_0/6$; $\mathcal{T}_h = \mathcal{T}_{H_0/6}$ is the fine mesh. Figure 3(c) demonstrates that the convergence rate of the bound gap is optimal, $O(H^4)$; the measured effectivity factor is $7.3 \le \eta \le 7.7$.

We next present results obtained for the model problem, 1(a). More precisely, Eqs. (9) are solved in the domain Ω with the following boundary conditions: $\boldsymbol{u}|_{\partial\Omega} = 0$; $\theta = 0$ on segment Γ_0; $\frac{\partial\theta}{\partial n} = q$ on segments Γ_1, Γ_2, and Γ_3; $\frac{\partial\theta}{\partial n} = 0$ otherwise. The output of interest is $s = \frac{1}{|\Gamma_1|}\int_{\Gamma_1} \theta\, ds$. For this case the (nondimensional) flux $q = 1$, and the Prandtl and Grashof numbers are $\alpha = 1$ and $\beta = 50,000$; the resulting streamlines are shown in Fig. 4(a). In this example an automatic adaptive strategy is used to refine the grid and "optimally" narrow the bound gap. The effectiveness of the adaptive procedure is summarized in Table 1, in which $\mathcal{T}_H$, $\mathcal{T}_{H'}$, and $\mathcal{T}_{H''}$ denotes the successive adapted meshes corresponding to Figures 4(b), (c) and (d), respectively; the mesh $\mathcal{T}_{H/2}$ is a *uniform* refinement of $\mathcal{T}_H$. Table 1 shows that a reduction of the relative bound gap from $\approx 8\%$ for mesh $\mathcal{T}_H$ to $< 1\%$ for mesh $\mathcal{T}_{H''}$ is achieved by optimal refinement with a final mesh which contains only slightly more than twice the number of elements of the mesh $\mathcal{T}_H$.

In conclusion, for a problem of natural convection involving the full nonlinear incompressible Navier-Stokes and energy equation at moderate Reynolds number, we have obtained new finite element error indicators which are constant-free, accurate, relevant (providing bounds directly for the quantities of interest), and efficient; these estimators can greatly reduce the numerical uncertainty associated with the use of inexpensive meshes.

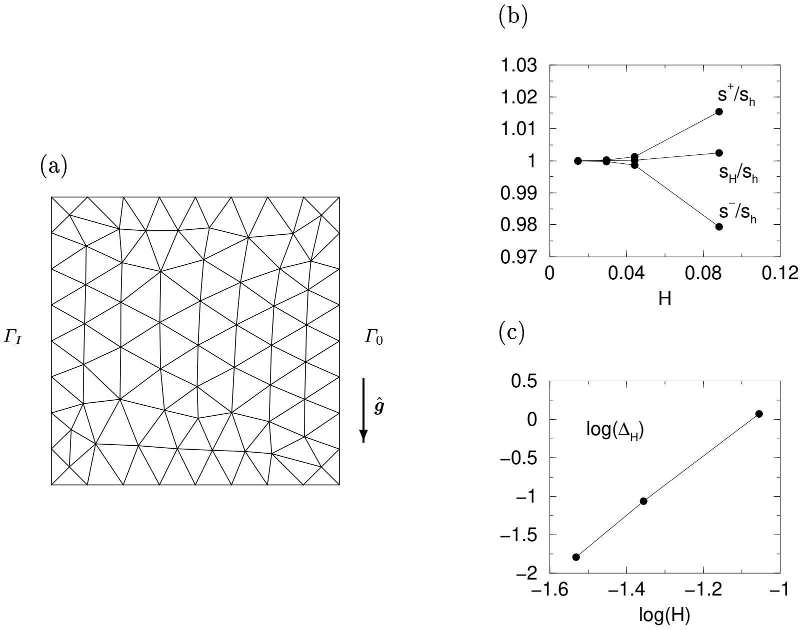

Fig. 3. Natural convection: first test case. (a) Domain and mesh $\mathcal{T}_{H_0}$. (b) Convergence of the bounds $s_H^{\pm}$. (c) Convergence of the bound gap Δ_H.

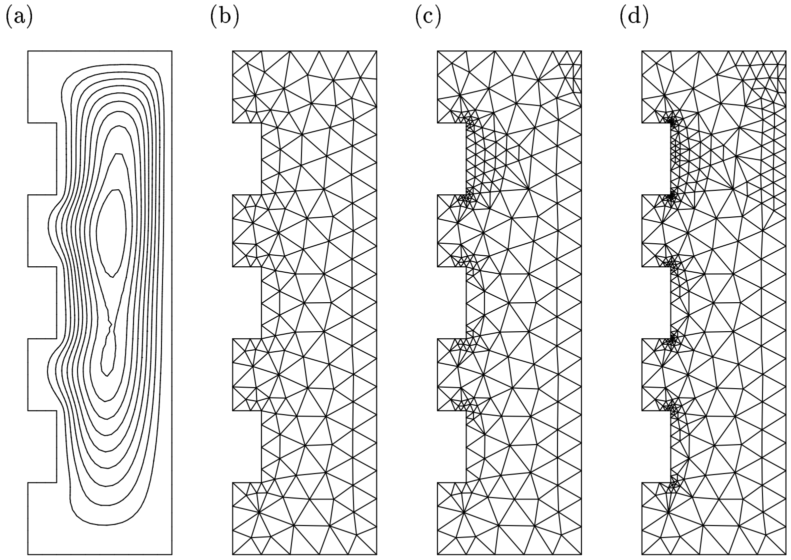

Fig. 4. Natural convection: model problem. (a) Streamlines. (b) Mesh $\mathcal{T}_H$. (c) Mesh $\mathcal{T}_{H'}$. (d) Mesh $\mathcal{T}_{H''}$.

	$\mathcal{T}_H$	$\mathcal{T}_{H'}$	$\mathcal{T}_{H''}$	$\mathcal{T}_{H/2}$
# of elements	264	416	628	1056
s^-	0.253	0.270	0.273	0.272
s^+	0.296	0.282	0.279	0.286
Δ_H	0.0212	0.0057	0.0026	0.0036

Table 1. Natural convection: model problem.

Finally, although the capabilities of the method have now been demonstrated in a variety of different contexts, some outstanding areas of investigation remain. In the application to incompressible fluid flow problems, the method should be extended to treat time-dependent problems [9], three-dimensional problems, and linear stability problems; the extension to compressible flow problems also presents interesting challenges. Moreover, recently, a new output bound result which generalizes the present approach has been formulated [21] that provides a framework for applications in iteration error estimation and control—stopping criteria for iterative solution methods for systems of linear equations, for instance. Finally, the efficiency of the method (its implementation on parallel computers) and its concrete use in design optimization of industrial (non-academic) systems should be demonstrated.

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