Certified error bounds for uncertain elliptic equations

Arnold Neumaier

Fakultät für Mathematik, Universität Wien, Nordbergstr. 15, A-1090 Wien, Austria

Abstract

In many applications, partial differential equations depend on parameters which are only approximately known. Using tools from functional analysis and global optimization, methods are presented for obtaining certificates for rigorous and realistic error bounds on the solution of linear elliptic partial differential equations in arbitrary domains, either in an energy norm, or of key functionals of the solutions, given an approximate solution. Uncertainty in the parameters specifying the partial differential equations can be taken into account, either in a worst case setting, or given limited probabilistic information in terms of clouds.

Key words: linear elliptic partial differential equations, rigorous error bounds, verification, a posteriori error estimation, dual weighted residual (DWR), parametric, uncertainty propagation, clouds, limited probabilistic information
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1 Overview

In most practical applications, partial differential equations to be solved are only an approximate model of the real life situation they are intended to represent. In many cases, the modeling errors can be accounted for by adding parameters (constants or functions) to the model, and specifying the uncertainty in these parameters. Thus while one solves the equations only for a particular nominal value of the parameters (or a limited set of values defining specific scenarios), one is interested in how key quantities computed from the solution vary over the full set of allowed values for the parameters.

Email address: Arnold.Neumaier@univie.ac.at (Arnold Neumaier).
URL: http://www.mat.univie.ac.at/~neum/ (Arnold Neumaier).

The results in [19,31] show that is it now feasible to get realistic worst case error bounds for uncertain linear systems of equations with thousands of variables and uncertain parameters. However, to apply the techniques to partial differential equations, one needs to cope not only with the uncertainty due to parameters in the equations but also with the errors introduced by the discretization. In this paper we discuss an approach that, for linear, uniformly elliptic partial differential equations, provides a rigorous solution to this problem, tractable numerically at least for bounding a few linear or quadratic response functionals.

We begin in Section 2 by specifying the abstract setting for our investigations, and prove the basic norm inequalities needed for the later analysis. In particular, we present computable bounds for the inverse of linear operators, the main tool needed for the rigorous error analysis of linear systems of equations given in Section 3. Like in the dual weighted residual (DWR) method (Becker & Rannacher [4]), our error bounds for response functionals have the quadratic approximation property (so that they are asymptotically optimal), but in contrast to DWR, our bounds are rigorous and also capture the higher order contributions to the error. Section 4 shows how to put linear elliptic partial differential equations into our abstract framework.

Section 5 shows how to obtain, using global optimization techniques, bounds that not only cover the errors in solving the differential equations but also the errors caused by the uncertainty in the parameters. This provides reliable tools for the assessment of uncertainty in the solution of elliptic partial differential equations. Our bounds are independent of the way the approximations are obtained, hence can be used to independently verify the quality of an approximation computed by an arbitrary solver. The bounds not only account for discretization errors but also for other numerical errors introduced through numerical integration and boundary aproximations.

In the final Section 6, we discuss how to represent model uncertainty in terms of so-called clouds, cf. Neumaier [29]. Clouds describe the rough shapes of typical samples of various size, without fixing the details of the distribution. While a probabilistic reliability analysis requires the exact knowledge of the multivariate probability distribution of the uncetainty, a requirement which is nearly impossible to validate in case of many uncertain parameters, clouds use only probabilistic information readily available in practice.

Related work. Among the rigorous error bounds for linear elliptic equations, the work by Nakao [20,21] and Plum [35] is mathematically rigorous in that it also accounts for roundoff errors. Plum [36] and Yamamoto et al. [46] also discuss error bounds in the parameter-dependent case. The other work on rigorous error bounds I am aware of ignores rounding error issues, i.e., it assumes exact arithmetic in the computations. Work by Repin et al. (see, e.g.,

[39,40]) and KOROTOV et al. (see, e.g., [12]) contains aposteriori error bounds of a similar nature (but more complicated) as those presented in Section 3 for the case without uncertainty. Of a different type are the aposteriori bounds by the group of PERAIRE (e.g., [32,41,42]). They make use of the finite element structure and a piecewise polynomial form of the coefficients to derive their error bounds, again for the case without uncertainty. BERTSIMAS & CARAMANIS [6] use a semidefinite optimization approach, applicable for problems with polynomial coefficients only.

There is also a lot of work on approximate error estimation in the context of adaptive finite element methods. We only mention the book [1] by AINSWORTH & ODEN and the survey [4] by BECKER & RANNACHER, which contain numerous other references.

For work on bounding the errors under uncertainty, see, e.g., AINSWORTH & ODEN [1], BABUŠKA & STROBOULIS [3], BABUŠKA et al. [2]. While there are obvious analogies to what is done here, they start with a Taylor series expansion in the uncertainty, resulting in a complicated analysis and complicated bounds which are often pessimistic if bounded rigorously.

2 Norm inequalities

We begin by specifying the abstract setting for our investigations and prove the basic norm inequalities needed for the later analysis. In contrast to standard treatments which involve constants that are difficult to obtain for a general domain, all our assumptions can be verified rigorously by computer.

In this section, θ is a fixed parameter vector. In Section 5, we shall consider θ as an uncertain vector and study the dependence of our results on θ, to account for the uncertainty in mathematical modeling. Section 6 then shows how to incorporate probabilisitc information about θ.

Let $\mathbb{U}$ be a (real or complex) Hilbert space with inner product written as u^*v, and let $W(\theta)$ be a θ-dependent bounded, positive definite Hermitian operator on $\mathbb{U}$ with bounded inverse. Then $\mathbb{U}$ is also a Hilbert space for the inner product $(u,v)_\theta := u^*W(\theta)v$ and the induced norm

$$|u|_\theta := \sqrt{u^*W(\theta)u}. \tag{1}$$

Let $\mathbb{H}$ be another Hilbert spaces with inner product written as a^*b, and let $M(\theta)$ be a θ-dependent bounded, positive definite Hermitian operator on $\mathbb{H}$ with bounded inverse. Then $\mathbb{H}$ is also a Hilbert space for the inner products

$(a,b)^{\pm}_{\theta} := a^* M(\theta)^{\pm 1} b$ and the induced norms

$$|b|^{\pm}_{\theta} := \sqrt{b^* M(\theta)^{\pm 1} b}, \tag{2}$$

and we have

$$|a^* b| \leq |a|^{-}_{\theta} |b|^{+}_{\theta}, \tag{3}$$

Let U be a subspace of $\mathbb{U}$ consisting of smooth functions, and let the differential operator $L : U \to \mathbb{H}$ be an injective continuous linear operator mapping U into $\mathbb{H}$. We define the Hilbert space $\mathbb{U}_\theta$ as the closure of the space of all $u \in U$ with finite **energy norm**

$$\|u\|_\theta := |Lu|^{+}_{\theta}; \tag{4}$$

This is indeed a norm since L was assumed to be injective. L extends by continuity to a linear mapping from $\mathbb{U}_\theta$ to $\mathbb{H}$. Clearly, $\mathbb{U}_\theta \subseteq \mathbb{U} \subseteq \mathbb{U}^*_\theta$, where $\mathbb{U}^*_\theta$ denotes the space dual to $\mathbb{U}_\theta$ in the topology of $\mathbb{U}$. We write $f^* u$ for the image of $u \in \mathbb{U}_\theta$ under $f \in \mathbb{U}^*_\theta$. The dual L^* of L is a linear mapping from $\mathbb{H}$ to $\mathbb{U}^*_\theta$; indeed, for any $b \in \mathbb{H}$, $L^* b$ is bounded since $|(L^* b)^* u| = |b^* L u| \leq |b|^{-}_{\theta} |Lu|^{+}_{\theta} = |b|^{-}_{\theta} \|u\|_\theta$, giving

$$\|L^* b\|^*_\theta \leq |b|^{-}_{\theta} \quad \text{for } b \in \mathbb{H}. \tag{5}$$

In the following, we usually suppress the dependence of W, M, etc. on θ.

Theorem 1 *The linear operator*

$$S := L^* M L \tag{6}$$

maps $\mathbb{U}_\theta$ to $\mathbb{U}^*_\theta$ and is Hermitian, positive definite, and invertible. For $r \in \mathbb{U}^*_\theta$ and $u \in \mathbb{U}_\theta$, we have

$$|r^* u| \leq \|r\|^*_\theta \|u\|_\theta. \tag{7}$$

$$\|r\|^*_\theta = \|S^{-1} r\|_\theta = \sqrt{r^* S^{-1} r}. \tag{8}$$

Moreover, if $r_0 \in \mathbb{U}^*_\theta$, $f \in \mathbb{H}$ then, for any $\tilde{f} \in \mathbb{H}$,

$$\|r_0 + L^* f\|^*_\theta \leq \|r_0 + L^* \tilde{f}\|^*_\theta + |f - \tilde{f}|^{-}_{\theta}. \tag{9}$$

Proof. (i) S is Hermitian and positive semidefinite, since M is. Since

$$\|u\|_\theta^2 = (|Lu|_\theta^+)^2 = (Lu)^* MLu = u^* Su, \tag{10}$$

$Su = 0$ implies $\|u\|_\theta = 0$, hence $u = 0$; thus S is injective and positive definite. By the representation theorem of Riesz (see, e.g., Theorem 5.7 in [10]), one can find for all $f \in \mathbb{U}_\theta^*$ a $u \in \mathbb{U}_\theta$ such that $f^* v = (Lu)^* M(Lv)$ for all $v \in \mathbb{U}_\theta$. Since $(Lu)^* M(Lv) = u^* L^* MLv = u^* Sv = (Su)^* v$, the resulting u satisfies $Su = f$. Thus S is surjective, hence invertible.

(ii) (7) is a general property of the dual norm.

(iii) If $r \in \mathbb{U}_\theta^*$ and $v := S^{-1} r$, the Cauchy-Schwarz inequality implies that $|r^* u| = |v^* Su| \le \|v\|_\theta \|u\|_\theta$, and equality holds for $u = v$. Hence $\|r\|_\theta^* = \sup\{|r^* u| / \|u\|_\theta \mid u \neq 0\} = \|v\|_\theta = \|S^{-1} r\|_\theta$. This proves the first equality in (8), and the second equality follows from (10).

(iv) We have $\|r_0 + L^* f\|_\theta^* = \|(r_0 + L^* \tilde{f}) + L^*(f - \tilde{f})\|_\theta^* \le \|r_0 + L^* \tilde{f}\|_\theta^* + \|L^*(f - \tilde{f})\|_\theta^*$. By (5), the second term is bounded by $|f - \tilde{f}|_\theta^-$. □

Since working with S^{-1} is not computationally feasible, it is important that the dual norm can be bounded in terms of the simpler norm $|\cdot|_\theta^+$.

Theorem 2 *If $\beta > 0$ and $LWL^* - \beta^2 M^{-1}$ is positive semidefinite then*

$$\|r\|_\theta^* \le \beta^{-1} |r|_\theta \quad \textit{for } r \in \mathbb{U}. \tag{11}$$

In particular, this holds if $E := LK + K^* L^* - K^* W^{-1} K - \beta^2 M^{-1}$ is positive semidefinite for some linear operator $K : \mathbb{H} \to \mathbb{U}_\theta$.

Proof. Let $r \in \mathbb{U}$ and put $u := S^{-1} r$, $v := MLu$. By assumption, we have $v^* M^{-1} v = (MLu)^* M^{-1} MLu = u^* L^* MLu = u^* Su = r^* S^{-1} r$ and $L^* v = L^* MLu = Su = r$, hence $0 \le v^*(LWL^* - \beta^2 M^{-1}) v = v^* LWL^* v - \beta^2 v^* M^{-1} v = r^* Wr - \beta^2 r^* S^{-1} r$. Therefore $\beta^2 r^* S^{-1} r \le r^* Wr$, giving $\beta \|r\|_\theta^* = \sqrt{\beta^2 r^* S^{-1} r} \le \sqrt{r^* Wr} = |r|_\theta$. The result follows since the operator $LWL^* - \beta^2 M^{-1} = E + (L^* - W^{-1} K)^* W (L^* - W^{-1} K)$ is positive semidefinite if E is. □

In the applications (cf. Section 4), W, M, K are multiplication operators over a domain Ω, and L is a first order differential operator. In this case, E is also a multiplication operator; the derivatives cancel by integration by parts. Thus checking positive semidefiniteness reduces to a purely algebraic problem tractable by means of semidefinite programming (see, e.g., Kočvara &

STINGL [15]) or interval analysis (see, e.g., NEUMAIER [26, end of Section 2] and [30, Theorem 11.1]).

Now let $A : \mathbb{U}_\theta \to \mathbb{U}_\theta^*$ be a bounded linear operator, so that there is a $\theta > 0$ such that $\|Au\|_\theta^* \le \tau\|u\|_\theta$ for $u \in \mathbb{U}_\theta$. By squaring, this is found to be equivalent to the assumption that $\tau^2 S - A^* S^{-1} A$ is positive semidefinite. For example, $\tau = 1$ if $A = S$. A numerical value for τ is nowhere required; the boundedness assumption is needed in the following results only to guarantee invertibility of A.

Theorem 3 *If $\sigma > 0$ and $B^*A + A^*B - B^*SB - \sigma^2 S$ is positive semidefinite for some linear operator B mapping $\mathbb{U}_\theta$ into itself then A is invertible and*

$$\|Au\|_\theta^* \ge \sigma\|u\|_\theta \quad \textit{for } u \in \mathbb{U}_\theta, \tag{12}$$

$$\|A^{-1}r\|_\theta \le \sigma^{-1}\|r\|_\theta^* \quad \textit{for } r \in \mathbb{U}_\theta^*, \tag{13}$$

$$|s^* A^{-1} r| \le \sigma^{-1}\|s\|_\theta^*\|r\|_\theta^* \quad \textit{for } r, s \in \mathbb{U}_\theta^*. \tag{14}$$

Proof. Since $(Au - SBu)^* S^{-1}(Au - SBu) = (\|Au - SBu\|_\theta^*)^2 \ge 0$, the assumption implies

$$\begin{aligned} 0 &\le u^*(B^*A + A^*B - B^*SB - \sigma^2 S)u \\ &= u^*(A^*S^{-1}A - \sigma^2 S)u - (Au - SBu)^* S^{-1}(Au - SBu) \\ &\le u^*(A^*S^{-1}A - \sigma^2 S)u = (Au)^* S^{-1}(Au) - \sigma^2 u^* S u, \end{aligned}$$

whence $\|Au\|_\theta^* = \sqrt{(Au)^* S^{-1}(Au)} \ge \sqrt{\sigma^2 u^* S u} = \sigma\|u\|_\theta$, giving (12). Now the Lax-Milgram theorem (see, e.g., Theorem 5.8 in [10]) implies the invertibility of $S^{-1}A$, and since $A^{-1} = (S^{-1}A)^{-1}S^{-1}$, that of A. Putting $u = A^{-1}f$, we find $\sigma\|A^{-1}r\|_\theta \le \|r\|_\theta^*$, giving (13). Finally, $|s^*A^{-1}r| \le \|s\|_\theta^*\|A^{-1}r\|_\theta \le \sigma^{-1}\|s\|_\theta^*\|r\|_\theta^*$, giving (14). □

In the special case where

$$A = L^*ML + N^*L - L^*N \tag{15}$$

for some linear mapping N from $\mathbb{U}$ to $\mathbb{H}$, we have $A^* = L^*ML - N^*L + L^*N$, hence $A + A^* = 2S$, and the hypothesis of the theorem holds with $\sigma = 1$ and the identity operator B. The hypothesis of the theorem can also be verified in more general cases: For elliptic second order A, we may assume without loss of generality that both L and $A - S$ are first order differential operators and M is a multiplication operator. For $0 < \gamma < 1$ and the choice $\sigma = \sqrt{1 - \gamma^2}$,

$B = 1+\gamma Q$ with a multiplication operator Q satisfying $Q^*Q = 1$, the operator $B^*A + A^*B - B^*SB - \sigma^2 S$ reduces to a multiplication operator. (Use that the commutators of A and A^* with B and B^* are first order differential operators, and that a Hermitian first order operator is a multiplication operator.) Thus verification can proceed as discussed after Theorem 2.

3 Error analysis of linear systems

We now apply the tools obtained above to the rigorous error analysis of linear systems of equations. A numerical method for solving $Au = f$ usually only produces an approximate solution u_0. The error in the θ-norm, and the error of a linear functional g^*u of the solution u can be bounded in terms of dual norms.

Theorem 4 *Under the hypothesis of Theorem 3, let $r = f - Au_0$, Then, for any approximation $u_0 \in \mathbb{U}_\theta$ of the solution u of $Au = f$, we have:*

(i) (Estimate in the energy norm)

$$\|u - u_0\|_\theta \le \sigma^{-1}\|r\|_\theta^*. \tag{16}$$

(ii) (First order error) If $g \in \mathbb{U}_\theta^*$ then

$$|g^*u - g^*u_0| \le \sigma^{-1}\|g\|_\theta^*\|r\|_\theta^*. \tag{17}$$

(iii) (Second order error) If $v_0 \in \mathbb{U}_\theta$ and $s = g - A^*v_0$ then

$$|g^*u - g^*u_0 - v_0^*r| = |s^*A^{-1}r| \le \sigma^{-1}\|s\|_\theta^*\|r\|_\theta^*. \tag{18}$$

$$g^*u - g^*u_0 \in [\gamma - \delta, \gamma + \delta], \quad \gamma = v_0^*r,\ \delta = \sigma^{-1}\|s\|_\theta^*\|r\|_\theta^*. \tag{19}$$

Proof. The error $u - u_0$ satisfies $A(u - u_0) = Au - Au_0 = f - Au_0 = r$. Now (i) follows since $\|u - u_0\|_\theta = \|A^{-1}r\|_\theta \le \sigma^{-1}\|r\|_\theta^*$ by (13). (ii) follows from (i) since $|g^*u - g^*u_0| = |g^*(u - u_0)| = |g^*A^{-1}r| \le \|g\|_\theta^*\|r\|_\theta^*$ by (14). Finally, (iii) follows from $g^*(u-u_0) = (A^*v_0+s)^*(u-u_0) = (v_0^*A+s^*)A^{-1}r = v_0^*r+s^*A^{-1}r$ and (14). □

The bound (iii) vanishes if v_0 equals the solution v of the **dual problem** $A^*v = g$; hence we have $g^*u = g^*u_0 + v^*r$. Thus, to get good error bounds, v_0 should be chosen as an approximation to the solution of the dual problem. Note that the second order nature of the bounds in (iii) implies that it is

generally sufficient to solve the dual problem to a lower accuracy than the primal problem, since the dominant contribution to the error in g^*u_0 comes from the correction v_0^*r which is of first order.

In the dual weighted residual (DWR) method ((Becker & Rannacher [4])), often used for approximate error estimation in adaptive finite element methods, v_0 is referred to as the dual weight; the approximate error estimation simply consists in ignoring the second order correction $s^*A^{-1}r$. Thus, as in DWR, our error bounds for response functionals have the quadratic approximation property (so that they are asymptotically optimal), but in contrast to DWR, our bounds are rigorous and also capture the higher order contributions to the error.

Note that if $\delta < |\gamma|$ then the quotient

$$q := (|\gamma| + \delta)/(|\gamma| - \delta) \tag{20}$$

is a computable bound for the **efficiency index** $(|\gamma| + \delta)/|g^*u - g^*u_0|$, and therefore allows a check on the accuracy (rather than the size) of the bound. To assess the quality of the bound, we assume that u_0 has been found to an accuracy of $O(\varepsilon)$, and v_0 to an accuracy of $O(\varepsilon_0)$, as measured by the dual norm of the residuals. Then $g^*u = g^*u_0 + O(\varepsilon)$. In typical cases, where the error $g^*u - g^*u_0$ is not $o(\varepsilon)$, we find $q = 1 + O(\varepsilon_0)$, indicating an asymptotically excellent quality of the bound. In the other case, when $g^*u - g^*u_0 = o(\varepsilon)$, the computed bound is also $o(\varepsilon)$, hence better than typical. These statements hold independent of the value of σ used, and they remain true when the dual norm is estimated using Theorem 2, as long as $|r|_\theta^+ = O(\varepsilon)$ and $|s|_\theta^+ = O(\varepsilon_0)$. Thus the influence of an underestimated σ or an overestimate in (11) is relatively harmless, although a gross under- or overestimation of course degrades the value of δ and hence delays the onset of the asymptotic behavior.

To avoid numerical computations with singular functions for general right hand sides, we now proceed in a more detailed manner, using the easily computable norm $\|f\|$ on the subspace $\mathbb{U}$ of $\mathbb{U}_\theta^*$. For simplicity, we assume that A has the form (15) and take $\sigma = 1$, in accordance with the remark after Theorem 3; more general situations are treated similarly. Since the right hand sides are not necessarily in $\mathbb{U}$, we assume that they are decomposed in the form

$$f = f' + L^*f'', \quad g = g' + L^*g'', \tag{21}$$

where f', g' are functions in $\mathbb{U}$, and f'', g'' are functions in $\mathbb{H}$. (Primes don't denote differentiation.) By definition of the dual space, this is always possible with $f' = g' = 0$, but often more natural splittings are directly available, while

the splittings with $f' = g' = 0$ might be nontrivial to find. Clearly, f'', g'' are determined by f, g only up to the addition of a function from the space

$$\mathbb{B} := \{b \in \mathbb{H} \mid L^*b \in \mathbb{U}\} \tag{22}$$

of smooth functions in $\mathbb{H}$. Under these assumptions, we can bound the solution of the equation $Au = f$ using Theorem 4, provided we can bound the residuals r and s. The primal residual $r = f' + L^*f'' - Au_0$ can be written as $r = (f' - N^*Lu_0 + L^*b) + L^*(f'' - MLu_0 + Nu_0 - b)$, for arbitrary $b \in \mathbb{H}$, and by (11) and (5), we have, for smooth $b \in \mathbb{B}$,

$$\|r\|_\theta^* \le \beta^{-1}|f' - N^*Lu_0 + L^*b|_\theta + |f'' - MLu_0 + Nu_0 - b|_\theta^-. \tag{23}$$

Note that we need the smoothness requirement $b \in \mathbb{B}$, i.e., $L^*b \in \mathbb{U}$, in order that the θ-norm can be evaluated. A good choice is therefore obtained by smoothing the expression $f'' - MLu_0 + Nu_0 \approx b \in \mathbb{B}$. Similarly, the dual residual $s = g' + L^*g'' - A^*v_0$ can be written as $s = (g' + N^*Lv_0 + L^*c) + L^*(g'' - MLv_0 - Nv_0 - c)$ for arbitrary $c \in \mathbb{H}$, giving, for $c \in \mathbb{B}$,

$$\|s\|_\theta^* \le \beta^{-1}|g' + N^*Lv_0 + L^*c|_\theta + |g'' - MLv_0 - Nv_0 - c|_\theta^-. \tag{24}$$

Now c should be chosen by smoothing $g'' - MLv_0 - Nv_0 \approx c \in \mathbb{B}$. All bound calculations are thus reduced to finding an approximate (fine grid) solution of the primal problem, the low resolution (coarse grid) solution of a dual problem (if the functional of interest is not just the error in the energy norm), the calculation of four residual functions (on the fine grid), two applications of smoothing fine grid data, and the integrations necessary to compute the norms. Typically, therefore, the work should not be much higher than that for the computation of the approximation alone.

The above bounds may also be used for bounding from above sufficiently nice nonlinear functionals $\mu(u)$ of the solution. This may be relevant in applications, e.g., to guarantee that a safety constraint $\mu(u) \le \overline{\mu}$ is satisfied. To avoid a detailed nonlinear analysis we assume that

$$c(u) := \gamma(Lu)^*MLu - \mu(u) \quad \text{is convex in } u \tag{25}$$

for a suitable constant $\gamma \ge 0$. Convexity implies $c(u) \ge c(u_0) + c'(u_0)(u - u_0)$. Inserting the definition of $c(u)$, a short calculation gives

$$\mu(u) \le \mu(u_0) + \mu'(u_0)(u - u_0) + \gamma\|u - u_0\|_\theta^2,$$

which can be bounded by the above formulas. For example, if we have an approximation $w \approx Lu$, we can represent its error $e := |Lu - w|_\theta^+$ by

$$\begin{aligned} e^2 &= (|(Lu_0 - w) - L(u - u_0)|_\theta^+)^2 \\ &= (|Lu_0 - w|_\theta^+)^2 - 2\,\mathrm{Re}(Lu_0 - w)^* ML(u - u_0) + (|L(u - u_0)|_\theta^+)^2 \\ &= (|Lu_0 - w|_\theta^+)^2 - 2\,\mathrm{Re}\, g^*(u - u_0) + \|u - u_0\|_\theta^2, \end{aligned}$$

where $g = L^*M(Lu_0 - w)$. All terms in the right hand side can be computed or bounded by the theorem.

As the bounds in [12,39,40], the above bounds are independent of the way the approximations are obtained. Hence they can be used to independently verify the quality of an approximation computed by an arbitrary solver. The bounds not only account for discretization errors but also for other numerical errors introduced through numerical integration and boundary approximations.

Of course, the numerical errors made in evaluating the bounds themselves remain unaccounted. For a fully rigorous implementation in the mathematical sense, one would also need to bound these errors. Because of the aposteriori nature of our bounds, an error control is needed *only* for the evaluation of the bounds (23), (24), and (18); the approximations u_0, v_0, r and s may be arbitrary and hence can be computed without error control. Thus the error control can be restricted to fairly simple arithmetic operations and to numerical integration. In both cases, the tools from interval analysis (see [18,28] for introductions, [25] for an in depth treatment, and [8,33,34] for circular interval arithmetic for numerical integration) apply without serious complications when the data are assumed to be given exactly. Indeed, Nakao [20,21] and Plum [35] rigorously solve linear elliptic equations with interval methods.

The dangers of excessive overestimation inherent in naive applications of interval techniques come up, however, when the data are uncertain, and care is needed to get reliable and realistic bounds in this case. We do this below (in Section 5) by resorting to global optimization rather than applying interval methods directly. Of course, mathematically rigorous global optimization [13,16,30] also involves the use of interval techniques, but these are hidden from naive users who simply need to feed a global optimization package with a symbolic description of their problem.

4 Linear elliptic partial differential equations

This section shows how to represent linear scalar elliptic partial differential equations in our abstract framework. Systems of linear elliptic partial differential equations and linear elliptic partial differential equations on manifolds can be handled in an analogous way. Here we take our spaces to be real vector spaces. All objects in this section may depend on θ, although this dependence is not written explicitly.

Let $\Omega \subseteq \mathbb{R}^d$ be a nonempty and open domain with boundary $\Gamma = \partial\Omega$. Let $U = C^1(\overline{\Omega})$ be the space of continuous real-valued functions on $\overline{\Omega}$ which are continuously differentiable in Ω. We assume that Ω is a regular domain, i.e., that there is at almost all $x \in \Gamma$ an outer normal $\mathbf{n}(x) \in \mathbb{R}^d$ such that

$$\int_\Omega dx\, \nabla u(x) = \int_\Gamma d\sigma(x)\mathbf{n}(x)u(x) \quad \text{for } u \in U, \tag{26}$$

where $d\sigma$ is the Lebesgue measure on Γ. The space U is naturally embedded in $\mathbb{U} := L^2(\Omega) \oplus L^2(\Gamma)$ via the identification $u = (u|_\Omega, u|_\Gamma)$ for $u \in U$. In general, we write u_Ω and u_Γ for the projection of $u \in \mathbb{U}$ to $L^2(\Omega)$ and $L^2(\Gamma)$, respectively. Then the inner product in $\mathbb{U}$ is

$$u^* v = \int_\Omega dx\, u_\Omega(x)v_\Omega(x) + \int_\Gamma d\sigma(x)u_\Gamma(x)v_\Gamma(x).$$

We put $\mathbb{H} = \mathbb{U} \oplus L^2(\Omega)^d$, and write b_0 and $\mathbf{b} = (b_1, \ldots, b_d)^T$ for the projection of $b = \binom{b_0}{\mathbf{b}}$ to $\mathbb{U}$ and $L^2(\Omega)^d$, respectively. Then the inner product in $\mathbb{H}$ is

$$a^* b = a_0^* b_0 + \mathbf{a}^*\mathbf{b} = a_0^* b_0 + \sum_{k=1}^d \int_\Omega dx\, a_k(x)b_k(x).$$

Now let c, $\mathbf{d}$ and G be a scalar, d-dimensional vector and symmetric $d \times d$ matrix function of Ω, respectively, with bounded, measurable coefficients. Then the linear operator $M = \begin{pmatrix} c & \mathbf{d}^T \\ \mathbf{d} & G \end{pmatrix}$ defined by

$$Mb := \begin{pmatrix} cb_0 + \mathbf{d}^T\mathbf{b} \\ \mathbf{d}b_0 + G\mathbf{b} \end{pmatrix} \quad \text{for } b \in \mathbb{H}$$

maps $\mathbb{H}$ into itself and satisfies $M^* = M$. The linear operators $N = \binom{p_0}{\mathbf{p}}$ and

$L = \binom{h}{\nabla}$ defined for $p \in \mathbb{H}$ and $h \in L^\infty(\Omega)$ by

$$Nu := \begin{pmatrix} p_0 u \\ \mathbf{p} u \end{pmatrix}, \quad Lu := \begin{pmatrix} hu \\ \nabla u \end{pmatrix} \quad \text{for } u \in U$$

map U to $\mathbb{H}$ and satisfy

$$N^* b = p_0 b_0 + \mathbf{p}^T \mathbf{b}, \quad L^* b = (b_{0\Omega} h|_\Omega - \nabla \cdot \mathbf{b},\ b_{0\Gamma} h|_\Gamma + \mathbf{n}^T \mathbf{b}) \quad \text{for } b \in \mathbb{H}.$$

The formula for L^* follows from

$$\int_\Omega dx\, \mathbf{b}^T \nabla u = \int_\Omega dx\, (-\nabla \cdot \mathbf{b}) u + \int_\Gamma d\sigma\, (\mathbf{n}^T \mathbf{b}) u \quad \text{for } u \in U, \mathbf{b} \in U^d, \qquad (27)$$

which is a simple consequence of Green's formula (26).

With these definitions and $A := L^* M L + N^* L - L^* N + c_0$, we have $Au = L^*(MLu - Nu) + N^* L u + c_0 u$, and since

$$MLu - Nu = \begin{pmatrix} \mathbf{d}^T \nabla u + (ch - p_0) u \\ G \nabla u + (\mathbf{d} h - \mathbf{p}) u \end{pmatrix}, \quad N^* L u + c_0 u = \mathbf{p}^T \nabla u + (p_0 h + c_0) u,$$

the equation $Au = f' + L^* f''$ (with $f' \in \mathbb{U}$ and $f'' \in \mathbb{H}$) describes the partial differential equation

$$-\nabla \cdot (G \nabla u + (\mathbf{d} h - \mathbf{p}) u) + (\mathbf{d} h + \mathbf{p})^T \nabla u + (ch^2 + c_0) u = f'_\Omega + f''_0 h - \nabla \cdot \mathbf{f}''$$

for $x \in \Omega$, with mixed boundary conditions

$$\mathbf{n} \cdot (G \nabla u + (\mathbf{d} h - \mathbf{p}) u) + (\mathbf{d} h + \mathbf{p})^T \nabla u + (ch^2 + c_0) u = f'_\Gamma + f''_0 h + \mathbf{n} \cdot \mathbf{f}''$$

for $x \in \Gamma$. (The terms involving p_0 cancel, hence we can put $p_0 = 0$.) This is the most general linear second order partial differential equation with mixed boundary conditions.

The adjoint problem is simply obtained by replacing N by $-N$ and hence $\mathbf{p}$ by $-\mathbf{p}$.

A is elliptic if and only if G is positive definite. In this case, we can make M positive definite, too, by replacing c with some $c_1 > \mathbf{d}^T G^{-1} \mathbf{d}$, compensating for this change by adjusting c_0 to $c_0 + (c - c_1) h^2$.

5 Bounds under uncertainty

In most practical applications, the partial differential equation to be solved is only an approximate model of the real life situation it is intended to represent. In many cases, the modeling errors can be represented by adding parameters (constants or functions) to the model, and specifying the uncertainty in these parameters. If we collect all uncertain parameters into a (possibly infinite-dimensional) vector θ, each admissible choice of θ defines a possible **scenario**. Thus while one solves the equations only for a particular nominal value of the parameters (or a limited set of values defining specific scenarios), one is interested in how the solution varies over the full set of admissible scenarios.

In this section, we assume that the uncertainty is specified deterministically by a condition $\theta \in \Theta_s$, where Θ_s is the region of uncertainty. (The label s becomes relevant in Section 6.) We employ global optimization techniques to obtain bounds that not only cover the errors in solving the differential equations but also the errors caused by the uncertainty in the parameters. This provides reliable tools for the assessment of uncertainty in the solution of elliptic partial differential equations. The problem to be solved, of the form

$$A(\theta)u = f(\theta) \quad \text{for some } \theta \in \Theta_s, \tag{28}$$

is assumed to be parameterized by θ. Thus the solution $u = u(\theta)$ depends on θ, and all computed approximations depend on θ, too. Therefore, the bounds derived in Section 3 will also depend on θ. For simplicity, we discuss here only the second-order error bounds (19), which now take the form

$$g^*u(\theta) - g^*u_0(\theta) \in [\gamma(\theta) - \delta(\theta), \gamma(\theta) + \delta(\theta)], \tag{29}$$
$$\gamma(\theta) = v_0(\theta)^* r(\theta), \quad \delta(\theta) = \sigma^{-1}\|s(\theta)\|_\theta^* \|r(\theta)\|_\theta^*,$$

where $r(\theta) = f(\theta) - A(\theta)u_0(\theta)$, $s(\theta) = g - A(\theta)^* v_0(\theta)$. Since the uncertainty region contains infinitely many scenarios, we need additional preparations to reduce the work to a finite and tractable amount. We compute an initial approximation $u_0 = u_0(\theta)$ for $u = u(\theta)$ by interpolation from approximate solutions u_l of (28) for a small number of scenarios $\theta_l \in \Theta$. In the simplest case, a single scenario $\theta_0 \in \Theta$ suffices, leading to a θ-independent approximation u_0; however, better results are obtained if sufficiently many scenarios are used to ensure that $u_0(\theta)$ captures the essential variation in θ, since the errors will then be smaller. In principle one can increase the number of scenarios used adaptively, until the error bounds obtained are satisfying.

The dual problem will usually be solved only at a nominal scenario θ_0 in the center of the uncertainty set, since we do not expect to need a highly accurate

dual solution to get accurate bounds. (However, if uncertainties are large, a θ-dependent dual approximation may be important.)

With these preparations, we can now define the two quantities

$$\underline{e}_s := \min\{\gamma(\theta) - \delta(\theta) \mid \theta \in \Theta_s\}, \quad \overline{e}_s := \max\{\gamma(\theta) + \delta(\theta) \mid \theta \in \Theta_s\},$$

and find the desired rigorous error bounds

$$g^* u(\theta) - g^* u_0(\theta) \in [\underline{e}_s, \overline{e}_s] \quad \text{for all } \theta \in \Theta_s.$$

For safety tests, usually only an inequality for $g^* u(\theta)$ must be verified, and it sufficies to compute one of $\underline{e}_s, \overline{e}_s$.

The computation of $\underline{e}_s$ and $\overline{e}_s$ is a *global* optimization problem, since we really need the worst case to have a valid bound. If θ is not too high-dimensional, these global optimization problems are computational tractable. In particular, for polynomial dependence of the problem data on θ, the resulting optimization problem is purely algebraic if the number of uncertain variable is finite. Its coefficients can be determined analytically or by numerical integration, using the approximate solution of the primal and dual equation. Thus the error bounding process is completely decoupled from the PDE solver, and the work for the bounds is independent of the work spent in computing the approximations.

The resulting version of the optimization problem can be specified in an algebraic modeling language such as AMPL [9] and solved with a variety of modern solvers. Many of these are available online via the NEOS interface [24]. Thus even large uncertainties and strongly nonlinear dependence of the solution on the parameters can be handled reliably.

We note that if the input data depend continuously differentiably on θ then the bounds derived in Section 3 also depend continuously differentiably on the data (with a rare exception when a residual term in the norm vanishes exactly). Moreover, using automatic differentiation techniques [11], it is not difficult to transform a program calculating the desired bounds into a program that provides together with the bounds also the gradient with respect to the uncertain parameters. In the COCONUT system [7,43], this can even be done with intervals, and with slopes in place of the gradient. This makes it possible to get bounds which remain rigorous even in the presence of rounding errors.

If the uncertainties are small, the global optimization problem is likely to have only one local minimizer, in which case a local minimization is sufficient to locate it. We sacrifice the guarantee of knowing whether we indeed have the

global minimum, but have the advantage that a much larger suite of solvers is available.

If the uncertainties are large or the solution depends sensitively on the uncertainties (which happens near bifurcation points of the differential equation), it is recommended to use Lyapunov-Schmidt reduction techniques to separate a few dominant uncertainty degrees of freedom. This improves the conditioning of the linear systems to be solved and gives more detailed information about the near-singular structure. For details see [27].

In the present paper, we concentrated on bounding a single response functional $\mu(u)$ satisfying the assumption (25). Of course, everything also applies when a few such functionals must be analyzed. However, if the number of response functionals grows, this approach becomes inefficient. Recent work by the author and Andrzej Pownuk [31] in the context of the finite element analysis of truss structures (where the resulting linear equations have a similar structure as those coming from discretized partial differential equations) show that it is in principle possible to efficiently find realistic worst case bounds on thousands of uncertain parameters and response functions. It should be possible to combine the techniques used there with the present methods for handling discretization errors to get similar results also for differential equations.

6 Modeling probabilistic uncertainty by clouds

In most practical applications, the uncertainties in the problem description can be specified only approximately, and a worst case analysis is inappropriate since the worst case has an exceedingly small probability. Rather, one wants to get some information on the variation of the solution over the most likely scenarios.

To describe these scenarios, we shall use the concept of clouds. This is a new notion for handling uncertainty, recently introduced in Neumaier [29]. It allows the representation of incomplete stochastic information in a clearly understandable and computationally attractive way. Clouds describe the rough shapes of typical samples of various size, without fixing the details of the distribution.

In contrast to probabilistic reliability analysis (see, e.g., Rackwitz [38], Schueller [44,45]), which requires the exact knowledge of the multivariate probability distribution of the uncertainty, a requirement which is nearly impossible to validate in practice, clouds use only probabilistic information readily available in practice.

In contrast to fuzzy sets (see, e.g., MÖLLER & BEER [17] for large-scale uncertainty analysis in terms of fuzzy sets) whose operational meaning is also fuzzy, clouds have a well-defined operational semantics within probability theory, so that computations with clouds give reliable probabilistic information.

The use of clouds permits a worst case analysis without losing track of important probabilistic information. All computed probabilities are safeguarded against uncertainty in a way consistent with the limited information about probability distributions typically available in the multiparameter case.

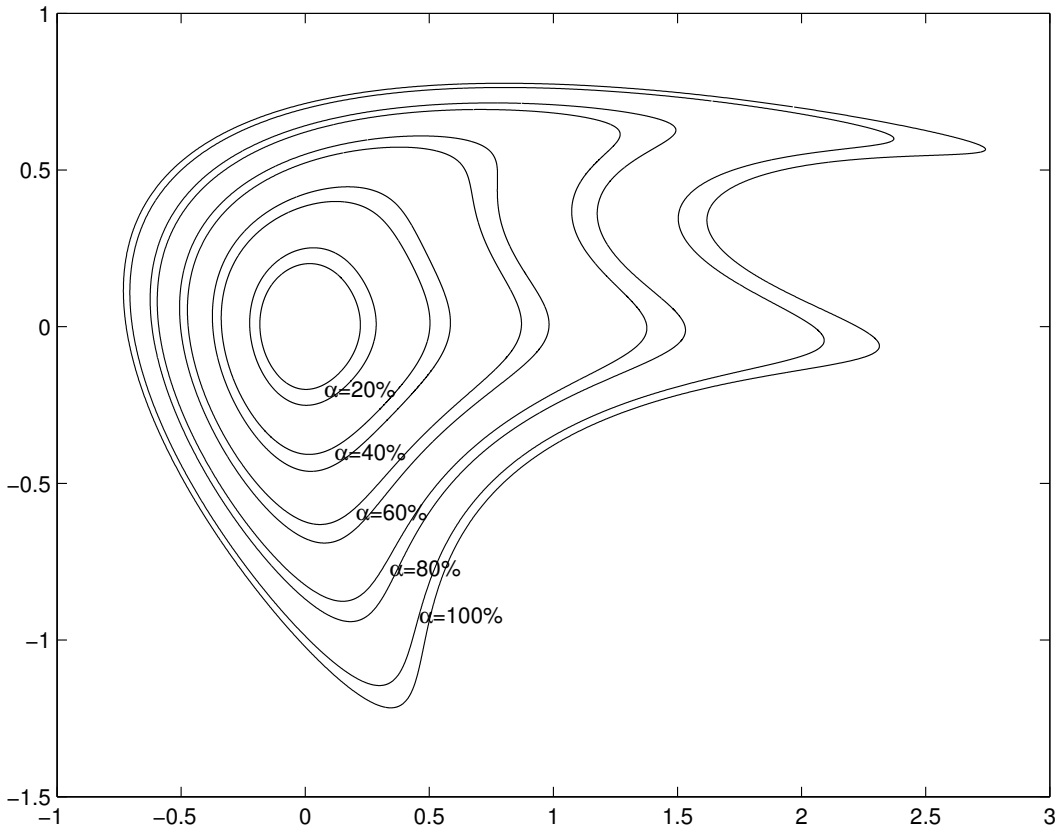

Fig. 1. A 2-dimensional cloud with inner and outer boundaries for the confidence levels

The special case of interest for large-scale models is a **confocal cloud** defined by a continuous **potential** V which assigns to each scenario θ a potential function $V(\theta)$ defining the shape of the cloud, and a **lower probability** $\underline{\alpha}(s)$ and an **upper probability** $\overline{\alpha}(s)$ defining the fuzzy boundary of the cloud. Writing $\Pr(A)$ for the probability of a statement A involving θ (which is now a random vector), the defining property of a cloud is that, for all s,

$$\underline{\alpha}(s) \le \Pr(V(\theta) < s) \le \Pr(V(\theta) \le s) \le \overline{\alpha}(s), \tag{30}$$

where $\underline{\alpha}$ and $\overline{\alpha}$ are strictly increasing continuous functions of s mapping the

range of V to $[0,1]$. In the notation of [29], this corresponds to the level function defined by $\underline{x}(\xi) = \underline{\alpha}(V(\xi))$, $\overline{x}(\xi) = \overline{\alpha}(V(\xi))$. For a given failure probability ε and $\alpha = 1-\varepsilon$, the so-called α**-cut** describes an inner region $\underline{C}_\alpha$ of α**-relevant** scenarios with $V(\theta) < \underline{s}_\varepsilon$ and a (generally larger) region $\overline{C}_\alpha$ of α**-reasonable** scenarios with $V(\theta) < \overline{s}_\varepsilon$, where $\overline{\alpha}(\underline{s}_\varepsilon) = 1-\varepsilon$ and $\underline{\alpha}(\overline{s}_\varepsilon) = 1-\varepsilon$. The conditions defining the cloud guarantee that $\underline{s}_\varepsilon \leq \overline{s}_\varepsilon$, and that there is a region C with $\underline{C}_\alpha \subseteq C \subseteq \overline{C}_\alpha$ containing a fraction of α from all scenarios considered possible.

To apply the techniques of the previous section, we define regions of uncertainty labelled by the potential value s representing the boundary of a level set in the cloud, $\Theta_s := \{\theta \mid V(\theta) \leq s\}$. Then the uncertainty is specified by a family of deterministic conditions $\theta \in \Theta_s$, where the probabilistic information is restricted to the interpretation of s and is given in the form $\Pr(\theta \in \Theta(s)) \in [\underline{\alpha}(s), \overline{\alpha}(s)]$.

The potential determines the shape of the cloud. In particular, potentials of the form $V(\theta) = \max_k |(\theta - \theta_0)_k|/r_k$ define confocal **rectangular clouds** (a sort of fuzzy boxes), $V(\theta) = \max_k |(A\theta - b)_k|$ defines confocal **polyhedral clouds**, and $V(\theta) = \|A\theta - b\|^2$ defines confocal **elliptic clouds** (a sort of fuzzy ellipsoids). An example of a confocal cloud with arbitrary shape is given in Figure 1.

The shape of the cloud can be easily adapted to uncertain probabilistic information. Frequently, high-dimensional probabilistic models are employed for uncertainty modeling because this is the only current way to draw conclusions from probabilistic uncertainty (e.g., by Monte Carlo simulation or a first or second order reliability method [38,45]). Such probability distributions usually reflect qualitative insight into the error structure. On the other hand, it is hardly possible to validate a particular probability distribution when the number of parameters are more than a handful – the amount of data needed for a statistically significant positive conclusion would be astronomical. However, we can take the negative loglikelihood of an estimated distribution as definition of the potential of a cloud, and then use the limited sample information available to construct a cumulative distribution function for the values of the potential. Together with error margins for the cumulative distribution function available from the Kolmogorov-Smirnov test (see, e.g., [37]), this provides reliable information in the form of a cloud.

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