Using Adjoint Solutions to Estimate Errors in Global Quantities

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Adjoint solutions are widely used in computational electromagnetics to provide sensitivities of global quantities to variation in design parameters. They can also be used to provide estimates of the discretization error in these quantities. Electrostatic force and capacitance are considered. Results are obtained for two test problems, using different meshes and different polynomial orders of hierarchal, tetrahedral finite elements. The estimates track the true errors well over a wide range. Furthermore, the estimates are good enough that, when added to the computed quantities, they reduce the error in those quantities, often substantially.

Index Terms—**Capacitance, electromagnetic analysis, error analysis, finite-element methods (FEMs), force.**

I. Introduction

COMPUTATIONAL methods are routinely used to find global quantities for electromagnetic devices. Unfortunately, the values obtained are rarely exact, because of discretization error. Though it is important for a designer to have an estimate of this error, there has been relatively little published on estimators for global quantities. Complementary variational principles offer one approach, but this is relatively expensive and seems not to have been explored except for the case of energy, for which rigorous bounds are available [1]. An earlier estimator for force error [2] was based on a virtual movement of a ring of nodes surrounding the body concerned. A more general method for arbitrary global quantities makes use of adjoint fields [3], but so far its application in electromagnetics has been limited to linear functionals in microwave problems, e.g., [4]. In this paper, the adjoint solution is used to estimate errors in quasistatic quantities that are nonlinear functionals of the field, e.g., electrostatic force and capacitance.

II. Estimating the Error in F

Consider a global quantity, $F(\mathbf{u})$, that is a functional of the field $\mathbf{u}$ within a device. Let $\mathbf{E}_e$ be the exact field and let $\mathbf{E}$ be a computational approximation to it, lying in a linear space H. We assume that $\mathbf{E}$ is the field in H satisfying

$$a(\mathbf{E},\mathbf{w}) = b(\mathbf{w}) \quad \forall \mathbf{w} \in H \tag{1}$$

where a is a symmetric bilinear form and b is a linear functional. Using $\mathbf{E}$ instead of $\mathbf{E}_e$ will give a value of F that is in error by $\Delta F = F(\mathbf{E}_e) - F(\mathbf{E})$, but if $\mathbf{E}$ is close to $\mathbf{E}_e$, this can be approximated by a functional linear in $\mathbf{E}_e - \mathbf{E}$

$$\Delta F \cong l(\mathbf{E}_e - \mathbf{E}) \tag{2}$$

where $l(\mathbf{u})$ is the first variation of F at $\mathbf{E}$: $\delta F(\mathbf{E},\mathbf{u})$. If we have a good enough approximation for $\mathbf{E}_e$ (Section III), we can use this equation to estimate the error in F.

There is another functional c that can be used instead. It is defined by

$$c(\mathbf{u}) \equiv l(\mathbf{u}) - a(\mathbf{E}_a,\mathbf{u}) \tag{3}$$

where $\mathbf{E}_a$ is the adjoint solution, the function in H satisfying

$$a(\mathbf{E}_a,\mathbf{w}) = l(\mathbf{w}) \quad \forall \mathbf{w} \in H. \tag{4}$$

We are justified in using c instead of l to get our estimate for ΔF because, for the exact field, we have

$$l(\mathbf{E}_e - \mathbf{E}) = c(\mathbf{E}_e). \tag{5}$$

When $\mathbf{E}_e$ is approximated, it can be shown that c, unlike l, is insensitive to the part of the error in the approximation that lies in H. Specifically, for any $\mathbf{h}$ in H

$$c(\mathbf{h}) = 0. \tag{6}$$

This makes c more accurate than l. Of course, it requires the solution to the adjoint (4). Fortunately, this solution is one that may already be computed for another purpose: It allows us to find the sensitivity of F to a geometric parameter g using the formula [5]

$$\frac{dF}{dg} = \frac{\partial F}{\partial g} + \frac{\partial b}{\partial g}(\mathbf{E}_a) - \frac{\partial a}{\partial g}(\mathbf{E},\mathbf{E}_a). \tag{7}$$

III. Approximating the Exact Solution

One way of generating an approximation to $\mathbf{E}_e$ would be to solve the computational problem again with a much larger number of basis functions. The result, while not exact, would be considerably more accurate than $\mathbf{E}$ and could be used to give a reasonable estimate of the error in $F(\mathbf{E})$, using the theory of the previous section. However, it is undesirable to solve a much larger computational problem. Instead, we use an approximation of the form

$$\bar{\mathbf{E}}_e = \mathbf{E} + \Delta\bar{\mathbf{E}} \tag{8}$$

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where $\Delta\bar{\mathbf{E}}$ is a linear combination of the new basis functions added. To find $\Delta\bar{\mathbf{E}}$, (1) is applied in the larger space, but with the original degrees of freedom *frozen*, i.e.

$$a(\Delta\bar{\mathbf{E}}, \Delta\mathbf{w}) = b(\Delta\mathbf{w}) - a(\mathbf{E}\Delta\mathbf{w}) \tag{9}$$

for all $\Delta\mathbf{w}$ that are linear combinations of the new basis functions. Even (9) is too big, because it is a matrix problem equal in size to the number of new basis functions, which generally exceeds the original problem size. An approximate solution to (9) is found by setting the off-diagonal terms of the matrix to zero.

The new basis functions could be generated in different ways, depending on the computational method being used. For the results in Section IV, they were generated by increasing by one the polynomial order of each hierarchal finite element.

IV. Alternative: No Adjoint Needed

If error estimates are needed for several global quantities, based on a single solution $\mathbf{E}$, the approach described in Section II would require a separate adjoint solution for each. If these adjoint solutions are not already available because they are needed to obtain sensitivities, the cost of error estimation can become high. Fortunately, there is an alternative to the adjoint approach, requiring just one additional solution no matter how many global quantities are involved. Further, the estimates produced by this approach are identical to the errors produced by the adjoint approach.

Suppose we have an approximation $\bar{\mathbf{E}}_e$, e.g., obtained by the method of the previous section. Then the adjoint theory of Section II tells us that a good estimate of the error in F is $c(\bar{\mathbf{E}}_e)$, and that this is more accurate than $l(\bar{\mathbf{E}}_e - \mathbf{E})$. However, it is possible to "correct" $\bar{\mathbf{E}}_e$ to obtain a new approximation $\hat{\mathbf{E}}_e$ with the property

$$l(\hat{\mathbf{E}}_e - \mathbf{E}) = c(\bar{\mathbf{E}}_e). \tag{10}$$

Once $\hat{\mathbf{E}}_e$ is found, the functional l can be used instead of c and no adjoints are needed. The new approximation is

$$\hat{\mathbf{E}}_e = \bar{\mathbf{E}}_e + \mathbf{e} \tag{11}$$

where $\mathbf{e}$ is the field in H satisfying

$$a(\mathbf{e}, \mathbf{w}) = -a(\bar{\mathbf{E}}_e - \mathbf{E}, \mathbf{w}) \quad \forall \mathbf{w} \in H. \tag{12}$$

Solving (12) takes as much work as finding one adjoint solution, but it only needs to be done once, independently of the number of error estimates needed.

V. Examples: Capacitance and Force

Consider the problem of finding the static electric field in a volume Ω of air around a number of conductors at specified potentials. For this problem, a and b are

$$a(\mathbf{u}, \mathbf{w}) = \varepsilon_o \int_\Omega \mathbf{u} \cdot \mathbf{w}\, d\Omega \quad b(\mathbf{w}) = -\varepsilon_o \int_\Omega \mathbf{E}_o \cdot \mathbf{w}\, d\Omega \tag{13}$$

and the space H is a discrete space of fields that are irrotational and have path integrals of zero between every pair of conductors, i.e., H corresponds to the case of all conductors grounded. The field $\mathbf{E}_o$ is any irrotational field matching the specified potentials applied to the conductors.

Now suppose that there are just two conductors. If the potential difference between them is 1 V, the capacitance between them is just twice the electric stored energy. To find the capacitance, then, the quantity of interest is the energy

$$F(\mathbf{u}) = \frac{\varepsilon_o}{2} \int_\Omega (\mathbf{u} + \mathbf{E}_o)^2\, d\Omega. \tag{14}$$

From this, the functional l is given by

$$l(\mathbf{u}) = \delta F(\mathbf{E} + \mathbf{E}_o, \mathbf{u}) = \varepsilon_o \int_\Omega (\mathbf{E} + \mathbf{E}_o) \cdot \mathbf{u}\, d\Omega. \tag{15}$$

From (1) and (13), it is clear that $l(\mathbf{w}) = 0$ for $\mathbf{w}$ in H; so, from (5), the adjoint solution in this case is zero.

The net electrostatic force on conductor A can be extracted from the field in a number of ways, but, here, we use

$$\mathbf{F}(\mathbf{u}) = \varepsilon_o \int_\Omega \left\{ (\mathbf{u} + \mathbf{E}_o)^2 \frac{\nabla\gamma}{2} - (\mathbf{u} + \mathbf{E}_o) \cdot \nabla\gamma(\mathbf{u} + \mathbf{E}_o) \right\} d\Omega \tag{16}$$

where γ is a scalar taking the value 1 on conductor A and 0 on all other conductors. This is the "g-function" result of [6]; it can be obtained from the principle of virtual work [2]. Both F and l are vectors in this case; l is given by

$$\mathbf{l}(\mathbf{u}) = \varepsilon_o \int_\Omega \{(\mathbf{E} + \mathbf{E}_o) \cdot \mathbf{u}\nabla\gamma - \mathbf{u} \cdot \nabla\gamma(\mathbf{E} + \mathbf{E}_o) - (\mathbf{E} + \mathbf{E}_o) \cdot \nabla\gamma\mathbf{u}\} d\Omega. \tag{17}$$

Note that each component of the force needs its own adjoint solution, unless the method of Section IV is used.

VI. Results

A. Square Wires

Fig. 1 shows the square cross sections of three identical conducting wires, together with part of the surface of the tetrahedral mesh used to analyze the problem. Conductors A and B are close, and there is, consequently, a large force developed on each. Conductor C is further away, with a much smaller force.

The wires are assumed to be infinitely long, so the problem is really two dimensional (2-D). However, it was solved with tetrahedral finite elements, taking a 5-mm section along the z axis as the volume for analysis. In the x–y plane, virtual boundaries were placed roughly 200-mm away from the wires, to truncate the domain. Two meshes were used: a coarse mesh, as shown in Fig. 1, with 1450 tetrahedra; and a fine mesh, with 2599 tetrahedra. Since 2-D analysis is possible in this case, the reference forces were obtained with a commercial 2-D finite element code,

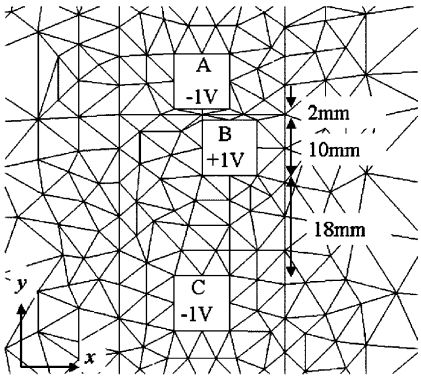

Fig. 1. Three square wires with applied potentials.

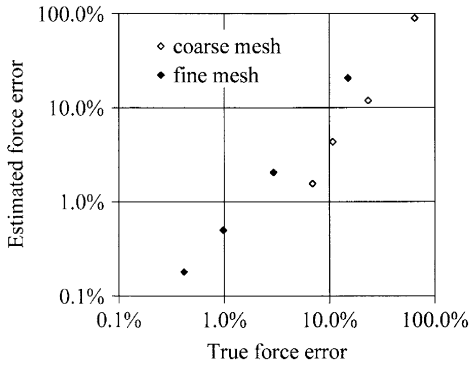

Fig. 2. Magnitude of the estimated error in the net force on conductor A (Fig. 1), plotted against the true magnitude of the error.

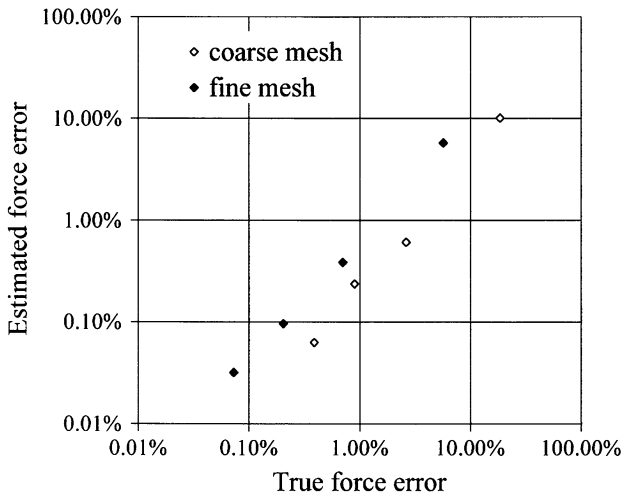

Fig. 3. Magnitude of the estimated error in the net force on conductor C (Fig. 1), plotted against the true magnitude of the error.

ElecNet [7], using 2892 triangular elements of order 4 (23 310 degrees of freedom).

An estimate for the force error vector $\Delta\mathbf{F}$ was obtained for the force on conductor A, using the methods described above. The true force error vector was also calculated, using the reference force. Fig. 2 shows the magnitude of the estimated error plotted against the magnitude of the true error. The four points for the coarse mesh correspond to four different polynomial orders of the finite elements (1 through 4); similarly for the four points for the fine mesh. Fig. 3 shows the same quantities for the

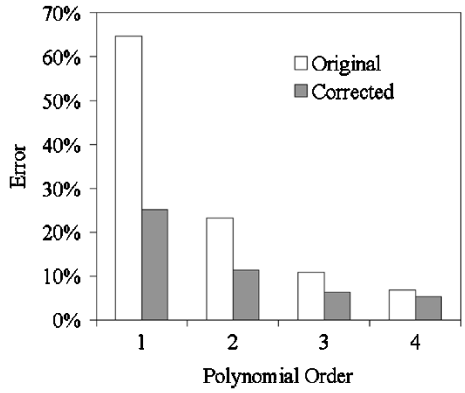

Fig. 4. True magnitude of the error in the net force on conductor A, for the original computed force and for the same force after correcting it by adding the vector error estimate. Coarse mesh.

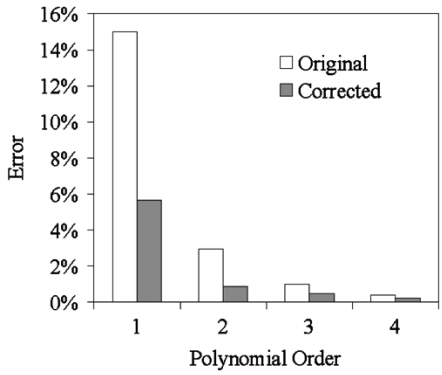

Fig. 5. True magnitude of the error in the net force on conductor A, for the original computed force and for the same force after correcting it by adding the vector error estimate. Fine mesh.

force on conductor C, which is about 50 times smaller. In both cases, the estimates tracks the true force error over a wide range. The estimator is noticeably more accurate on the fine mesh.

The estimate of $\Delta\mathbf{F}$ is not only good in magnitude, but also in direction. This is best shown by adding the vector estimate to the computed force to give another, corrected, force. Figs. 4 and 5 show that the corrected force has a smaller true error than the original computed force for all four polynomial orders on both the coarse and fine meshes. This would obviously not be the case if the direction of $\Delta\mathbf{F}$ was very wrong, even if its magnitude was correct. The error estimate has another use, then: By adding it to the computed quantity, some reduction in error is possible.

B. Parallel Plates

Consider two flat, square, conducting plates, each 5-mm thick and 40 mm on a side (Fig. 6). The plates are parallel and 10-mm apart, with an electrostatic potential difference maintained between them. The three-dimensional FEM was applied to one eighth of the geometry (using symmetry) to find the capacitance between the plates, and the force of attraction between them. The capacitance and force computed with a very fine mesh at order 4 were taken as the true values.

Figs. 7 and 8 plot the magnitude of the estimated error in the force and capacitance, respectively, versus the magnitude of the true error, for various unstructured meshes (3646 to 23 114

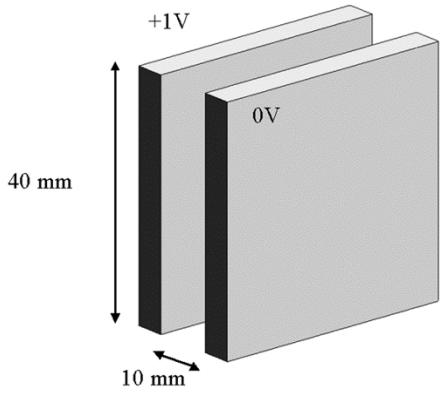

Fig. 6. Two flat, square, conducting plates with a potential difference of 1 V applied between them.

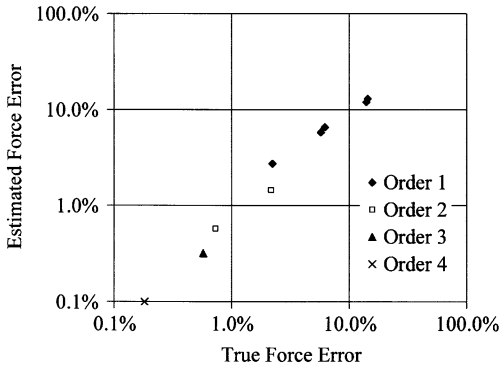

Fig. 7. Magnitude of the estimated error in the net force of attraction between the plates (Fig. 6), plotted against the true magnitude of the error.

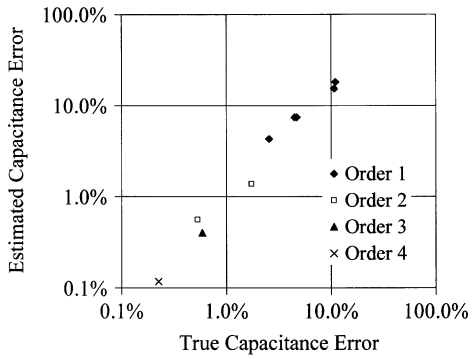

Fig. 8. Magnitude of the estimated error in the capacitance between the plates (Fig. 6), plotted against the true magnitude of the error.

tetrahedra) and polynomial orders. Again, the estimators track the errors reasonably well over a wide range.

Fig. 9 demonstrates that not just the magnitude, but also the sign of the estimate in the capacitance error is correct. By adding the estimate, a considerable reduction in error can be achieved.

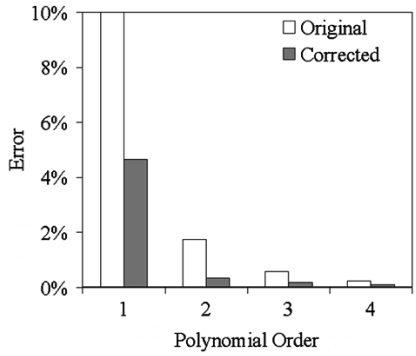

Fig. 9. True magnitude of the error in capacitance between the plates (Fig. 6), for the original computed capacitance and for the same capacitance after correcting it by adding the error estimate. Four orders on the same mesh.

VII. Conclusion

A general method for estimating errors in global quantities has been presented. If adjoint solutions are already being computed for other purposes (e.g., to find sensitivities), they may be used to find the estimates; otherwise, a single additional solution of the same size as the original is sufficient to estimate errors in all global quantities. The results for electrostatic force and capacitance show that the estimates are reliable. In fact, they are good enough in both magnitude and direction to provide improved values for the global quantities.

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