Computer-Aided Design 43 (2011) 1402–1412

Contents lists available at SciVerse ScienceDirect

Computer-Aided Design

journal homepage: www.elsevier.com/locate/cad

Estimating the effects of removing negative features on engineering analysis

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ARTICLE INFO

Keywords:
Modification sensitivity
Design sensitivity
Engineering analysis error
Large design changes
DWR

ABSTRACT

This paper provides a general framework for the quantitative estimation of the effects of removing negative features on engineering analysis, or *modification sensitivity* for short. There are two main applications: (i) when defeaturing models so that finite element analysis may be carried out more quickly and with lower memory requirements, and (ii) when performing iterative design based on finite element analysis. Our approach can handle large as well as small features, and features with Neumann/natural boundary conditions prescribed on them; previous methods have difficulties in handling such cases.

Estimation of the modification sensitivity is achieved by reformulating it as a modeling error caused by use of different mathematical models to describe the same engineering analysis problem. Results are obtained using the dual weighted residual (DWR) method in combination with a heuristic assumption of small variation of the dual solution after defeaturing. The final derived sensitivity estimator is expressed in terms of the difference of local boundary integrations over the feature boundary, which can be explicitly evaluated using solutions defined on the defeatured model.

The algorithm's performance is demonstrated using a Poisson equation. Comparisons to results obtained by previous approaches indicate that it is both accurate and computationally efficient.

1. Introduction

Computational simulations, or engineering analyses, predict the physical behavior of a designed engineering component under various boundary constraints and external loadings. They allow engineers to investigate, visualize, and test various physical and mechanical properties and operations on a designed object before constructing a real physical prototype, shortening the design cycle. Engineering analysis is generally performed using finite element (FE) analysis on a mesh derived by discretizing a CAD model.

Such simulation-based design typically involves a process of repeated design changes which modify a designed model by adding or removing design features, or adjusting geometric parameters of features, to meet ultimate design objectives of functionality, manufacturability, aesthetics, and so on. A design objective is typically measured using local quantities of engineering interest [1], such as pointwise displacements or average temperatures over a region; global values are not able to provide specific enough information about the model. Each time a design change is made, for example, by adding a feature to the model, the engineering analysis problem must be solved again for the modified model in order to obtain these target local quantities. See Fig. 1(a). Such repeated analyses can be very expensive if the model's geometry is complex or a sophisticated or accurate analysis is required.

The overall computational efficiency can be much improved if the previous computational results for the prior design stage can be reutilized for the modified model. This idea can be put into practice by estimating differences between local quantities in the prior and current design, allowing decisions on design changes to be made. See Fig. 1(b). In some cases these changes may be small and local, but, in other cases, relatively large features may be added to or removed from a model. The approach reported here can handle cases where large negative features (with prescribed Neumann or natural boundary conditions) are removed—previous work has considered smaller, more local shape changes. (A companion paper also considers the case of positive features, but these require rather more heuristic methods [2]). In summary, we consider how to estimate the effects of removing large design features on the results of engineering analysis, measured in terms of changes in a particular quantity of engineering interest, in other words, the *modification sensitivity* for that quantity and model.

The problem of modification sensitivity estimation also arises when performing model simplification for analysis. Here, the aim is to remove design features that have little impact on the results of analysis, allowing the analysis to be performed more quickly on a simpler model. Irrelevant geometric details can significantly increase the time and computational complexity

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doi:10.1016/j.cad.2011.08.013

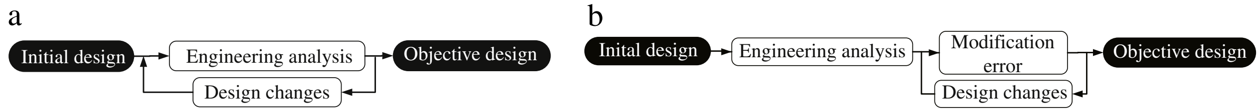
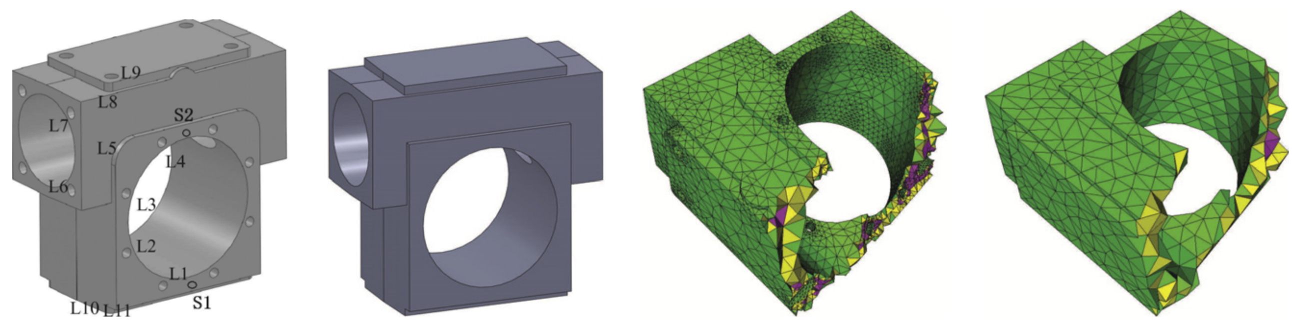


Fig. 1. Different strategies for simulation-based design. (a) Repeated engineering analysis is required for each design change; (b) using modification sensitivity estimation, only one step of engineering analysis is required for all model modifications.



(a) Original CAD model. (b) Defeatured CAD model. (c) Mesh for original model with 86 030 elements. (d) Mesh for defeatured model with 3990 elements.

Fig. 2. Suppressing features (36 holes, 8 blends, and 2 extrusions) from the fully featured model in (a) leaves the defeatured model in (b). It needs fewer mesh elements to represent it to the desired accuracy.

both for the meshing process and the FE analysis performed on it [3,4]. Worse, they may even lead to mesh generation failure [3] or ill-conditioned computations [5] that may produce inaccurate analysis results. In extreme cases, the fully featured problem may be too complex for an engineering analysis to be tractable, and model simplification is essential in such cases. Consider, for example, Fig. 2. Finite element analysis requires both geometric adaptivity and smooth mesh size transitions, leading to a mesh with far more elements for the fully featured model than for a corresponding defeatured model. The benefits of suppressing features come at a cost of somewhat different results of the analysis. Understanding such modification sensitivity is essential to ensure that a desired analysis accuracy can still be met after defeaturing.

As noted, this paper focuses on the modification sensitivity estimation of the case of removing *negative* features (of Neumann/natural boundary conditions) within the model's interior or along its boundary. This problem is of particular relevance in plate or shell analysis [6], where design changes are usually made within the material of the model. Estimating sensitivity to the creation of such negative features is also important in classical topological optimization [7], although that topic focuses on negative features of infinitesimal size while this paper focuses on negative features of possibly large size, which can be in the model's interior or on its boundary.

The general framework provided in this paper for estimating the effects of removing negative features on engineering analysis is based on reformulating the modification sensitivity, originally caused by a geometric difference, as a *modeling error*, caused by the use of different partial differential equations (PDEs) to mathematically model a physical phenomenon over the same geometric model. Estimating this modeling error is achieved using the *dual weighted residual* (DWR) method, originally developed in [8,9], in combination with a heuristic assumption that the difference between the dual solutions of the fully featured model and the defeatured model is small. This results in the derived modification sensitivity being expressed in the form of a local integration over the feature's boundary, which can be explicitly evaluated using engineering analysis results from the defeatured model.

The remainder of the paper is organized as follows. Related work is discussed in Section 2. The problem studied in this paper is defined more precisely in Section 3. Estimating the modification sensitivity using the DWR method is described in Section 4. The computational efficiency and accuracy of our approach and related approaches are discussed in Section 5, while numerical experiments are presented in Section 6. Conclusions are drawn in Section 7.

2. Related work

Unlike the well-studied analysis error estimates for FE approximation [10], the problem of estimating modification sensitivity is rarely studied, and it was stated to be an open problem in a recent survey on physically based model simplification [11]. Previous research work closely related to this topic includes studies on design sensitivity, feature sensitivity, and reanalysis techniques.

Design sensitivity analysis computes the derivatives of model response quantities with respect to design variables, and plays a critical role in design optimization. Given sufficiently small model modifications, shape sensitivity analysis [12] allows designers to compute the change in local quantities of interest when a model boundary is perturbed, based on infinitesimal changes, while topological sensitivity analysis [7,13] computes the change when an infinitesimal circular hole is created within an existing geometry. Extensions of topological sensitivity analysis to arbitrarily shaped features are given in [14,15]. Explicit analytical expressions have also been derived for, for example, the case of a classical Poisson equation [16]. Recently, a practical, efficient numerical approach was proposed by Gopalakrishnan and Suresh [17] and Turevsky et al. [18,19] for estimating the topological sensitivity (called *feature sensitivity* there) to the creation of an arbitrarily shaped small internal hole. However, design sensitivity analysis and its variants are essentially dependent on asymptotic expansions of target functionals, which strongly limits the nature of permissible sizes and locations of the features involved. They are hard to apply directly to the problem of large design changes we consider here.

Our sensitivity estimator is achieved by extending the DWR method. The DWR method was originally developed by Becker and Rannacher [8,20] to estimate the goal-oriented FE approximation error for a broad class of nonlinear problems. It was then extended by Oden and Prudhomme [9] to modeling error estimation. This prior work only considers problems in which the underlying geometry over which the analysis is performed, and the associated boundary conditions, remain unchanged before and after approximation. Recently, Cnossen [21] considered the possibility of applying the DWR method to fluid-flow problems in which varying boundary conditions may be used with fixed geometry. We go further and consider utilizing the DWR method for quite general geometric design changes, extending this previous work.

All the above-mentioned approaches consider goal-oriented modification sensitivity estimation. There are also heuristic approaches studying modification sensitivity in terms of global energy differences [22]. However, an essential starting step is that a cut boundary has to be selected around the suppressed feature to allow for local computation, and there is no obvious simple approach for doing so.

Another approach for estimating modification sensitivity is based on reanalysis techniques [6,23], which link small geometric modifications of a model to variations in its associated stiffness matrix. However, modifying large design features may drastically change this matrix. Moreover, for successful implementation of reanalysis techniques, steps of model preparation, meshing, and nodal mapping are required, which are non-trivial problems in their own right.

3. Problem statement

We now further explain and define the problem of estimating the effects of removing negative features on engineering analysis, i.e., modification sensitivity.

In our problem, we assume that we have a general engineering analysis problem defined over two different models, which for simplicity we call the *fully featured model* and a *defeatured model*. An engineering analysis problem concerning, for example, heat transfer or elasticity analysis, is generally described by one or more partial differential equations (PDEs) plus certain prescribed boundary conditions, e.g. external loadings or fixed temperatures. Performing engineering analysis on a model requires computing the field solutions of the corresponding boundary value PDE problem over the model, typically using FE methods.

The *fully featured model* might be a model before feature suppression when performing model simplification, or it might be a modified model with one or more added negative features in a simulation-based design scenario. It typically has a complex geometry, and its PDE solutions are very hard to compute or even intractable. The *defeatured model* might be a simplified model after removing features, or, in a design scenario, a simpler model before one or more negative features have been added to the design. Typically it has much simpler geometry, and its PDE solutions are much easier to determine (or may even be provided). Since only negative features are considered here, the fully featured model is contained within the volume of the defeatured model.

The negative features to be suppressed are assumed to be given in advance. This paper mainly focuses on estimating the effects of removing such a single negative feature on engineering analysis. A general approach to utilizing the results to help simplify complex models is not a trivial task, and it will be addressed in our future work.

Geometric differences between the fully featured model and the defeatured model perturb the underlying solutions to the analysis problems defined over these models, and affects values of the local quantities of interest. Our objective is to quantitatively estimate the modification sensitivity in terms of changes of local quantities of interest due to the geometric difference between the fully featured model and the defeatured model; we wish to do so without explicitly solving the analysis problem for the fully featured model.

A mathematical formulation is now given. The problem is first analyzed for the case of removing a single negative feature; its extension to multiple features will be discussed at the end of this section. As illustrated in Fig. 3, we have a fully featured model $\Omega - \omega$ and a defeatured model Ω, where $\omega \subset \Omega$ is a negative feature to be suppressed, provided by the user or other software. The engineering analysis problem over Ω or $\Omega - \omega$ is defined as follows. First, we define the solution u over $\Omega - \omega$ to be the solution to the following PDE problem:

$$\begin{cases} Lu = f & \text{in } \Omega - \omega, \\ Au = a & \text{on } \partial\Omega, \\ Bu = b & \text{on } \partial\omega, \end{cases} \tag{1}$$

where $\partial\Omega$ or $\partial\omega$ denotes the boundary of Ω or ω, and L, A, and B are abstract linear or nonlinear differential operators governing the physical phenomenon within the model interior, bounded by $\partial\Omega$ and $\partial\omega$. The problem and boundary conditions are further characterized by f, a, and b. For the particular problem studied in this paper, Neumann or homogeneous Dirichlet boundary conditions are assumed over boundary $\partial\Omega$, and Neumann boundary conditions are assumed over feature boundary $\partial\omega$.

Suppressing feature ω from model $\Omega - \omega$ leads to a new PDE problem with solution u_0 satisfying

$$\begin{cases} Lu_0 = f & \text{in } \Omega, \\ Au_0 = a & \text{on } \partial\Omega. \end{cases} \tag{2}$$

Note that the boundary conditions prescribed over feature ω in Eq. (1) disappear, due the removal of feature ω.

Typically, the analyst wishes to know certain results of the analysis such as average local stresses or temperatures. Such quantities of engineering interest may be defined in terms of an integral over a local region $S \subset \Omega - \omega$:

$$Q(u) = \int_S l(u)\, \mathrm{d}\Omega, \tag{3}$$

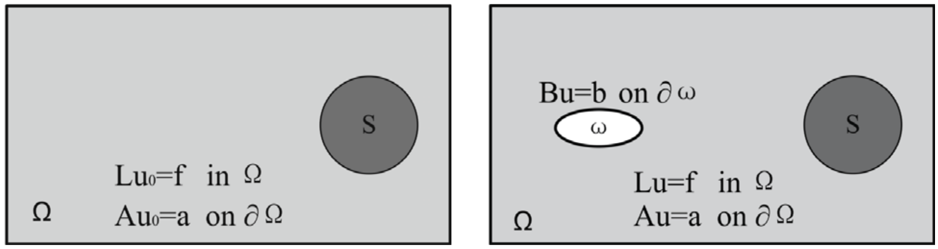
where $q(\cdot)$ is a linear or nonlinear bounded functional defined over the solution space.

The geometric difference between Ω and $\Omega - \omega$ causes the corresponding solutions u_0 and u to differ, which in turn affects the quantities of interest $Q(u_0)$ and $Q(u)$. The estimated effect on the engineering analysis results of removing a design feature, i.e., the *modification sensitivity*, is then given by

$$e(\Omega, \Omega - \omega) = Q(u) - Q(u_0). \tag{4}$$

We assume that the solution u_0 is known, and we wish to avoid explicitly computing u.

We now consider what happens for a model containing multiple features, and how to determine the modification sensitivity when a single feature or multiple features are removed. The ideas are explained most simply in terms of two features, but they generalize to multiple features. Suppose that model $M = \Omega - \omega_1 - \omega_2$ is a complex fully featured model containing two negative features ω_1, ω_2. These two features can always be assumed to be *disjoint* in their interior, as we can replace ω_1 with $\omega_1 - (\omega_1 \cap \omega_2)$ if they are not. The effect on the quantity of interest due to interactions between them has to be considered in the cases of multiple features. If ω_1 and ω_2 are not physically dependent (normally meaning they are not geometrically intersecting or very close), the two features can be processed separately to estimate their associated modification sensitivities. Furthermore, for each feature, say ω_1, two different sensitivity estimation calculations can be performed (i) taking the fully featured and defeatured models as $\Omega - \omega_1$ and Ω, that is, the sensitivity is computed as



(a) Defeatured model Ω. (b) Fully featured model $\Omega - \omega$.

Fig. 3. Engineering analysis problems for fully featured and defeatured geometric models.

$e(\Omega, \Omega - \omega_1)$, and (ii) taking them as $(\Omega - \omega_2) - \omega_1$ and $\Omega - \omega_2$, that is, the sensitivity is computed as $e(\Omega - \omega_2, (\Omega - \omega_2) - \omega_1)$. If there are no feature interactions, the two calculations produce the same result. Note, however, that the former strategy involves the same defeatured model Ω for different features ω_1 and ω_2 and has a defeatured model of greater geometric simplicity. For a complex engineering part with hundreds of features, the former will be much cheaper computationally, and so it is the strategy used in our experimental implementations in Section 6. On the other hand, if ω_1 and ω_2 are physically dependent, they should be taken to be a single high-level feature composed of multiple subfeatures, and a corresponding modification sensitivity estimate should be computed.

4. Modification sensitivity estimation using the DWR method

Estimation of the modification sensitivity defined by Eq. (4) is ultimately achieved by reformulating it as the modeling error between two different weak formulations. The modeling error is then estimated using the *dual weighted residual* (DWR) method [9]. Details are now given below.

4.1. The DWR method in modeling error estimation

We now introduce the use of the DWR method for modeling error estimation. Following common practice, the convention $N(\cdot;\cdot)$ is used to indicate a function linear in all arguments that follow the semicolon but possibly nonlinear for preceding arguments.

The problem of estimating the modeling error is defined for the following two abstract nonlinear problems expressed in weak form: find solutions u, u_0 such that

$$N(u; v) = F(v) \quad \forall v \in V, \tag{5}$$

and

$$N_0(u_0; v) = F_0(v) \quad \forall v \in V, \tag{6}$$

where $N(\cdot;\cdot), N_0(\cdot;\cdot)$ are semilinear forms defined on a Banach space V, and $F(\cdot), F_0(\cdot)$ are linear functionals on V. We assume that each equation admits a unique solution for either u or u_0.

Suppose that, for the above two different modeling equations, solution u_0 provides an approximation to solution u. For a particular quantity of interest $Q(u)$ as in Eq. (3), the problem of *modeling error estimation* is to evaluate $Q(u) - Q(u_0)$ without explicitly solving u from Eq. (5).

To do so, that is, to formulate such an auxiliary problem, we consider an *adjoint problem* with respect to the *prime problem*, following [1]. The prime problem in Eq. (5) has the following adjoint problem: find solution $p \in V$ such that

$$N'(u; q, p) = Q'(u; q) \quad \forall q \in V, \tag{7}$$

where $N'(u; q, p)$ and $Q'(u; q)$ are Gâteaux derivatives [9]. The corresponding adjoint problem for Eq. (6) is: find solution $p_0 \in V$ such that

$$N_0'(u_0; q, p_0) = Q'(u_0; q) \quad \forall q \in V. \tag{8}$$

Defining the residual functional to characterize the degree to which u_0 fails to satisfy the problem in Eq. (5) as

$$\mathcal{R}(u_0; v) = F(v) - N(u_0; v), \quad v \in V, \tag{9}$$

the following theorem is given in [9] for estimating the modeling error by dropping higher-order remainder terms.

Theorem 1 ([9]). *When $u - u_0$, $p - p_0$ are small, any approximation (u_0, p_0) of the solutions (u, p) of Eq. (7) gives an a posteriori error estimate of*

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p_0) + \mathcal{R}(u_0; p - p_0).$$

4.2. Conversion from modeling error to modification sensitivity

Based on the result in Theorem 1, we now give a general framework for modification sensitivity estimation. Let u, u_0 denote solutions of Eqs. (1) and (2) defined respectively on $\Omega - \omega$ and Ω, and p, p_0 denote their respective adjoint solutions defined as in Eqs. (7) and (8).

As the fully featured model is contained in the defeatured model, that is $\Omega - \omega \subset \Omega$, the part of the solution u_0 defined over geometry $\Omega - \omega$ is well defined, and is denoted by

$$\bar{u}_0 = u_0|_{\Omega-\omega}. \tag{10}$$

The solution $\bar{u}_0$ can seen as the solution of another engineering analysis problem defined over model $\Omega - \omega$ with particular Neumann conditions prescribed over the internal boundary $\partial\omega$: find $\bar{u}_0$ such that

$$\begin{cases} L\bar{u}_0 = f & \text{in } \Omega - \omega, \\ A\bar{u}_0 = a & \text{on } \partial\Omega, \\ \bar{B}\bar{u}_0 = \bar{b} & \text{on } \partial\omega, \end{cases} \tag{11}$$

where the last term $\bar{B}\bar{u}_0 = \bar{b}$ in this case corresponds to

$$\frac{\partial \bar{u}_0}{\partial n} = \frac{\partial u_0}{\partial n}. \tag{12}$$

Generally, the term $\bar{B}\bar{u}_0 = \bar{b}$ is different from the last equation of Eq. (1), that is, $Bu = b$, and it is this difference which is essentially the source of the modification sensitivity studied in this paper.

Let the corresponding abstract weak forms for Eqs. (1) and (11) be expressed as follows: find solutions $u, \bar{u}_0 \in V$ such that

$$N(u; v) = F(v) \quad \forall v \in V, \tag{13}$$

and

$$N_0(\bar{u}_0; v) = F_0(v) \quad \forall v \in V, \tag{14}$$

i.e., u and $\bar{u}_0$ are solutions of two different modeling equations, Eqs. (13) and (14), respectively.

Now, it is clear from Eq. (12) that

$$Q(u) - Q(u_0) = Q(u) - Q(\bar{u}_0). \tag{15}$$

The left-hand side of the equation, $Q(u) - Q(u_0)$, is the modification sensitivity defined over two different geometries $\Omega, \Omega - \omega$ considered here. The right-hand side of the equation, $Q(u) - Q(\bar{u}_0)$, is the modeling error defined over the same geometry $\Omega - \omega$ caused by two different weak formulations, that is, Eqs. (13) and (14). Their equality allows us to use the result in Theorem 1 to convert from modeling error estimation to modification sensitivity estimation.

Note that, when applying the DWR method to modeling error estimation, the solution and test spaces for Eqs. (7) and (8) have to be the same Banach space V. This is generally not satisfied for general boundary settings, but is satisfied for the particular boundary conditions stated in Eq. (1), that is, the solution and test spaces of Eqs. (1), (11), and their associated adjoint problems are the same. Thus, based on Theorem 1, and noticing that $\bar{u}_0 = u_0$ over $\Omega - \omega$, the following lemma can be given for modification sensitivity estimation.

Lemma 1. *The modification sensitivity in Eq. (4) is given as*

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p), \tag{16}$$

where u_0 is the solution to Eq. (2), and p is the adjoint solution to Eq. (1).

4.3. Modification sensitivity estimate

In this section, the sensitivity expression in Eq. (16) is further simplified to ultimately give a computable modification sensitivity estimate in the form of local boundary integrations.

The simplified estimator is mainly derived by further investigation of the weak form of solution u, i.e., Eq. (13), and using the fact that u_0 is a solution to Eq. (2). Specifically, by performing integration by parts, the weak form Eq. (13) can be expressed as a sum of an interior integration over $\Omega - \omega$, and boundary integrations over the out boundary $\partial\Omega$ and the inner boundary $\partial\omega$. Then, Eq. (16) is derived by replacing u by u_0 in the corresponding residual form (9). By further noticing that u and u_0 share the same governing equation in the model interior $\Omega - \omega$ and over the outer boundary $\partial\Omega$, the estimator in Eq. (16) can be ultimately simplified as a difference between two local boundary integrations over the feature boundary $\partial\omega$. Solid mathematical expressions are given below.

This section uses the notation that, given two general vectors w, v, their inner product over a region S is

$$(w, v)|_S = \int_S w \cdot v \, \mathrm{d}V.$$

Let the general expression of performing integration by parts for $(Lw, v)|_{\Omega-\omega}$ be

$$(Lw, v)|_{\Omega-\omega} = H_{\partial\Omega}(w, v) + h_{\partial\omega}(w, v) - L^*(w, v)|_{\Omega-\omega}, \tag{17}$$

where L is the abstract differential operator in Eq. (1), and $H_{\partial\Omega}(w, v)$ and $h_{\partial\omega}(\cdot, \cdot), L^*$ are functionals defined over $V \times V$ expressed in forms of integrations over boundaries $\partial\Omega$, $\partial\omega$, and $\Omega - \omega$.

Now, consider replacing w in Eq. (17) by the particular solution u from Eq. (1). Evaluating the specific boundary conditions defined by $Au = a$ over the boundary $\partial\Omega$ for $H_{\partial\Omega}(w, v)$, we get a functional $\bar{H}_{\partial\Omega}(u, v)$. Similarly, evaluating boundary conditions $Bu = b$ defined over $\partial\omega$ for $h_{\partial\omega}(w, v)$, we get another functional $\bar{h}_{\partial\omega}(u, v)$. This leads to the corresponding weak formulation of Eq. (1):

$$(Lu, v)|_{\Omega-\omega} = \bar{H}_{\partial\Omega}(u, v) + \bar{h}_{\partial\omega}(u, v) - L^*(u, v)|_{\Omega-\omega}. \tag{18}$$

The difference between functionals $h_{\partial\omega}$ and $\bar{h}_{\partial\omega}$ comes from the fact that the boundary conditions over $\partial\omega$ are explicitly evaluated in $\bar{h}_{\partial\omega}$ or while not in $h_{\partial\omega}$. For example, if a Neumann boundary condition $\frac{\partial u}{\partial n} = g$ is prescribed over $\partial\omega$, we should have $h_{\partial\omega}(u, v) = \frac{\partial u}{\partial n} v$ and $\bar{h}_{\partial\omega}(u, v) = gv$. The two expressions are the same for the specific u, but are different for another different solution u_0, that is, $h_{\partial\omega}(u_0, v) = \frac{\partial u_0}{\partial n} v$ and $\bar{h}_{\partial\omega}(u_0, v) = gv$, which are generally different. The same fact holds for functionals $H_{\partial\Omega}$ and $\bar{H}_{\partial\Omega}$.

Using the above notation, the sensitivity estimation term $\mathcal{R}(u_0; p)$ in Eq. (16) can now be further simplified.

Theorem 2. *The modification sensitivity defined in Eq. (4) can be expressed as a difference between two local boundary integrations over the feature boundary $\partial\omega$:*

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p) = \bar{h}_{\partial\omega}(u_0, p) - h_{\partial\omega}(u_0, p), \tag{19}$$

where $h_{\partial\omega}(u_0, p)$ and $\bar{h}_{\partial\omega}(u_0, p)$ are defined as above.

Proof. See the Appendix. □

This theorem states that the modification sensitivity is essentially due to the difference of the PDE solutions along the boundary $\partial\omega$ before and after removing feature ω.

Compared to the expression based on volume integration in Eq. (16), the sensitivity expression in Eq. (19) is simpler. However, Eq. (19) still involves the solution p, which is defined over the geometry $\Omega - \omega$ and is assumed to be unavailable. In order to derive a computable sensitivity estimate, we further divide p into p_0 and $\varepsilon_0 = p - p_0$. From the linearity of $\mathcal{R}(u_0; p)$, we have

$$Q(u) - Q(u_0) \approx \bar{h}_{\partial\omega}(u_0, p_0) - h_{\partial\omega}(u_0, p_0) + (\bar{h}_{\partial\omega}(u_0, \varepsilon_0) - h_{\partial\omega}(u_0, \varepsilon_0)). \tag{20}$$

The first term, $\bar{h}_{\partial\omega}(u_0, p_0) - h_{\partial\omega}(u_0, p_0)$, can be directly evaluated from the prime and adjoint solutions u_0, p_0 defined over the defeatured model Ω. The second term, $\bar{h}_{\partial\omega}(u_0, \varepsilon_0) - h_{\partial\omega}(u_0, \varepsilon_0)$, is, however, dependent on the solution adjoint error $\varepsilon_0 = p - p_0$ or p defined over the feature boundary $\partial\omega$, and is not available.

This unavailable term can be further approximated by its exterior solution [24], i.e., the solution to the same analysis problem defined over geometry $R^n - \omega$ (n is the dimensionality of the model being analyzed), using the same boundary conditions as those for the solution u_0 over feature boundary $\partial\omega$. Alternatively, it can be bounded using values based on global energy norm estimates of the primal and adjoint problems [1]. The first estimation strategy requires solution of a further analysis problem, and has specific requirements on the size and location of the target feature. The second approach, on the other hand, involves complex computations.

For the particular problem of modification sensitivity estimation of *large* features, due to the locality of the adjoint problems in Eq. (7), in terms of its source term and boundary terms, the difference between solutions p and p_0 is typically negligible compared with the term $\mathcal{R}(u_0; p_0)$, and may be simply discarded. This is stated in the following result.

The modification sensitivity defined by Eq. (4) can be approximated by the difference of local boundary integrations:

$$Q(u) - Q(u_0) \approx \bar{h}_{\partial\omega}(u_0, p_0) - h_{\partial\omega}(u_0, p_0), \tag{21}$$

where u_0, p_0 are prime and adjoint solutions of Eq. (2), and $h_{\partial\omega}(u_0, p_0)$ and $\bar{h}_{\partial\omega}(u_0, p_0)$ are boundary integration terms over the feature boundary $\partial\omega$ defined by Eqs. (17) and (18).

The above result lacks rigorous proof of validity of dropping the term with respect to $R(u_0, p - p_0)$. We hope to verify this in our future work. Various examples, including those shown in Section 6, demonstrate the accuracy of Eq. (21) for modification sensitivity estimation.

In practical implementations, the solutions u_0 and p_0 are derived using FE methods from a very dense mesh generated from the defeatured model Ω ignoring any FE approximation error. Based on these values, the modification sensitivity can be easily evaluated based on Eq. (21).

5. Computational efficiency and accuracy

In this section, we use a classical Poisson equation to compare the computational efficiency and accuracy of the proposed approach with other methods: direct FE analysis, feature sensitivity [18], and topological sensitivity [16,13].

Poisson's equation is often encountered in heat and mass transfer theory, elasticity, and other areas of mechanics and physics. Let the fully featured and defeatured models respectively be $\Omega - \omega$ and Ω. The prime solution u_0 for the defeatured model is: find u_0 such that

$$\begin{cases} -\mathrm{div}(\nabla u_0) = f & \text{in } \Omega, \\ u_0 = 0 & \text{on } \Gamma_D, \\ \nabla u_0 \cdot n = h & \text{on } \Gamma_N, \end{cases} \tag{22}$$

where Γ_D, Γ_N are Dirichlet and Neumann boundaries, which taken together make up $\partial\Omega$; n is a unit outward normal vector to Γ_N.

For $\Omega - \omega$, we wish to find the solution u such that

$$\begin{cases} -\mathrm{div}(\nabla u) = f & \text{in } \Omega - \omega, \\ u = 0 & \text{on } \Gamma_D, \\ \nabla u \cdot n = h & \text{on } \Gamma_N, \\ \nabla u \cdot n = g & \text{on } \omega, \end{cases} \tag{23}$$

where $\Gamma_D \cup \Gamma_N = \partial\Omega$.

The equivalent weak form for Eq. (23) is: find $u \in V$ such that

$$N(u, v) = F(v), \quad v \in V,$$

where

$$N(u, v) = \int_{\Omega-\omega} \nabla u \cdot \nabla v \, \mathrm{d}\Omega - \int_{\partial\Omega_N} hv \, \mathrm{d}\Gamma - \int_{\partial\omega} gv \, \mathrm{d}\Gamma,$$

$$F(v) = \int_{\Omega-\omega} fv \, \mathrm{d}\Omega,$$

and $V = \{v \in H^1(\Omega) : v|\Gamma_D = 0\}$.

In the following, we use P_C for the center of the smallest ball that encloses the internal feature ω, and

$$\tilde{p}_0 = p_0|_{P_C}, \qquad \nabla\tilde{u}_0 = \nabla u_0|_{P_C}, \qquad \nabla\tilde{p}_0 = \nabla p_0|_{P_C}. \tag{24}$$

To make a comparison with other approaches, we first summarize below related methods for estimating modification sensitivity, including direct FE analysis (FEA), topological sensitivity analysis (TSA), and feature sensitivity analysis (FSA).

(1) *FE analysis*. The difference between $Q(u)$ and $Q(u_0)$ is evaluated directly by computing the field solutions u, u_0 from Eqs. (1) and (2). We ignore any discrete FE approximation errors, and use the resulting value as the ground truth when comparing other approaches.

(2) *Topological sensitivity analysis* [14,16,13]. Explicit expressions are determined for the modification sensitivity for the cases of an internal circular or elliptic hole within an existing geometry.

For a circular hole ω of radius ϵ,

$$Q(u) = Q(u_0) + t(\epsilon) D_T Q, \tag{25}$$

where

$$t(\epsilon) = -2\pi\epsilon; \qquad D_T Q = g\tilde{p}_0, \quad \text{when } g \neq 0;$$

Table 1
Comparison of computational requirements of FEA, TSA, FSA, and our proposed approach for modification sensitivity estimation.

	FE analysis		Integration		
	Fine	Coarse	Exterior	Volume	Boundary
TSA		✓			
Ours		✓			✓
FSA		✓	✓		✓
FEA	✓	✓		✓	

or

$$t(\epsilon) = -\pi\epsilon^2; \qquad D_T Q = 2\nabla\tilde{u}_0 \cdot \nabla\tilde{p}_0 - f\tilde{p}_0, \quad \text{when } g = 0.$$

Here, g represents the external loadings prescribed on boundary $\partial\omega$. We call this the *TSA-Circle* result for short.

Similarly, for an ellipse with semi-axes a and b parallel to the main axes of the coordinate system, we have [14]

$$Q(u) = Q(u_0) + ab\pi(\nabla\tilde{u}_0^T T_\omega \nabla\tilde{p}_0 - f\tilde{p}_0), \tag{26}$$

where T_ω is defined as

$$T_\omega = \begin{pmatrix} 1 + a/b & 0 \\ 0 & 1 + b/a \end{pmatrix}.$$

We call this the *TSA-Ellipse* result for short.

(3) *Feature sensitivity analysis* [18]. Feature sensitivity describes the first-order change of a quantity of interest when an arbitrarily shaped small hole free of external loadings is created within a geometry. The corresponding computation is

$$Q(u) = Q(u_0) + \int_{\partial\omega} (V \cdot n)(F_1 + F_2) \, \mathrm{d}s,$$

where

$$F_1 = \frac{f\tilde{p}_0 - (\nabla\tilde{u}_0 + \nabla u_E) \cdot (\nabla\tilde{p}_0 + \nabla p_E)}{2},$$

$$F_2 = fp_E/3, \qquad V = P - P_C,$$

and u_E and p_E are the corresponding prime and adjoint exterior solutions defined over geometry $R^n - \omega$, $n = 2, 3$, taking the boundary conditions as those of the solution u_0 over feature boundary $\partial\omega$.

Estimating modification sensitivity using the different approaches listed above involves solving different PDE problems, for example, over the defeatured model Ω, the fully featured model $\Omega - \omega$, or the exterior geometry $R^2 - \omega$, and involves volume or boundary integrations for value evaluations. The requirements are summarized in Table 1.

Basically, solving the field problem over the fully featured model using FE analysis is most time consuming. This is followed in sequence by solving the field problems for the defeatured model, and for the exterior geometry. Solving the prime and adjoint problems using FE methods involves the same stiffness matrix, and solving both is not much more work than solving just one of them using the direct triangular decomposition method. Integration is generally much cheaper than FE analysis, and boundary integration is generally cheaper than volume integration. As can be seen from the summary in Table 1, the efficiencies of these related methods are, in increasing order, TSA, our approach, FSA, and direct FEA.

We now consider the accuracy of each method. Both TSA and FSA use pointwise values to approximate field values within a suppressed feature based on Eq. (24). This is in contrast to our modification sensitivity estimate, where prime and adjoint solutions u_0, p_0 are used directly without any approximation, and thus it is expected to be more accurate than TSA and FSA, particularly for features of large sizes. On the other hand, as we discard the terms involving ε_0 in Eq. (20), our method may in principle be less accurate than TSA or FSA for features of sufficiently small size. However, the goal of our paper is to be able to handle features of relatively large size; our experimental results in the next section demonstrate that this potential issue is not a problem in practice. Finally, we note that FSA is typically more effective than TSA for arbitrarily shaped features at the cost of additional computations of an auxiliary exterior problem, but both are equally as accurate as TSA-Circle for circular features or TSA-Ellipse for elliptic features.

Our experimental results in the next section agree with these analyses on efficiency and accuracy. Note all the proposed modification sensitivity analysis is applicable to arbitrary-shape negative features either in the model's interior or along its boundary, while the TSA or FSA is generally only application for negative features of sufficiently small size far away from the outer boundary.

6. Numerical experimental results

Our framework for estimating modification sensitivity has been implemented on a 2.8 GHz dual quad-core processor with 4 GB RAM using COMSOL [25], a commercial finite-element-based CAD/CAE system. We both demonstrate the efficiency and accuracy of our approach, and provide comparisons with those obtained using FEA, TSA, and FSA. The Poisson equation described in Section 5 is taken as a concrete example problem for analysis.

In all examples, unless otherwise stated, the quantity of interest is defined as the average of the solution u over a local region $S \in \Omega - \omega$:

$$Q(u) = \int_S u \, \mathrm{d}\Omega \bigg/ \int_S \mathrm{d}\Omega. \tag{27}$$

Here, when considering accuracy, we use *effectivity* to assess the results. The effectivity of a sensitivity estimator is usually measured in terms of an *effectivity index*, which can be defined as the ratio between the estimated sensitivity e and the exact value E; that is,

$$I = e/E. \tag{28}$$

When using a global energy norm, effectivity indices between 0.5 and 2.0 are often characterized as being reasonable values to achieve in the error estimation literature. However, for goal-oriented error estimation of the kind considered in this paper, it is generally very difficult or expensive to obtain highly accurate error estimates [26]. In practice, effectivity indices up to 10 can still be useful [27]. We leave readers to form their own judgements.

6.1. Effectivity testing

We first consider our method's effectivity under changes of shape of a design feature, and of the boundary conditions prescribed over its boundary.

In the first simple two-dimensional (2D) example, the model is an axis-aligned rectangle centred at (0, 0), containing a single feature, an internal elliptic hole ω (see Fig. 4). The hole is also centered at (0, 0) and has semi-axes of a and $a/2$ for various values of a. The local circular region of interest within which we wish to estimate the average solution is centered at $(0.7, 0.2)$ and has radius 0.1. The corresponding parameters of the Poisson equation in Eq. (23) are set as $f = 1$ and $u = 0$ along the outer boundary, and $\partial u/\partial n = g$. The effectivity of the modification sensitivity estimator was tested under variations of the feature sizes a, locations, and external loadings g, as will be explained later. The quantity of interest is defined via Eq. (27).

The modification sensitivity was computed using the proposed method for varying internal feature sizes, locations, and boundary

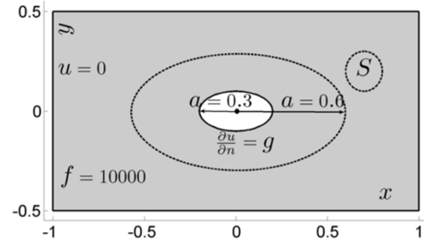


Fig. 4. Removing an internal elliptical hole from a rectangular block.

conditions. In the first test, a was changed from 0.1 to 0.6. The resulting effectivity indices are plotted in Fig. 5(a); they range between 1.0 and 1.12, demonstrating that the method is highly effective in modification sensitivity estimation for various feature sizes.

Note that, when $a = 0.6$, the internal feature ω (plotted with the dashed line in Fig. 4) is large, occupying over a quarter of the area of the rectangular block, dominating it. This dominance of ω can be observed in Fig. 5(b), where $I_Q = (Q(u) - Q(u_0))/Q(u_0)$ is plotted with variation of a to show relative variation in the solution. The change to the average values in S caused by including ω can be as much as a factor of 5 compared to the value computed from the defeatured model. Such cases are not atypical of real design problems, and are not handled well by previous approaches.

Our method's effectivity was also tested under variations of both the elliptic feature's size and center: a was varied from 0.1 to 0.6, and the x-coordinate of the center was varied from 0 to 0.2, leaving the y-coordinate unchanged. A comparison between the estimated sensitivity and the exact value $Q(u) - Q(u_0)$ is plotted in Fig. 6(a), and the effectivity index surface is also plotted in Fig. 6(b). The values of the indices are all around 1.0, again showing the algorithm to be highly effective under these variations.

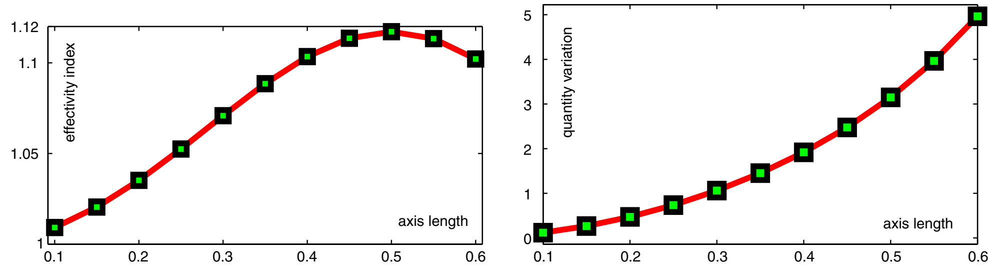
The proposed method can also handle the case when a non-homogeneous Neumann condition is prescribed on the internal feature ω. For the example in Fig. 4, the Neumann boundary term g was randomly set to $2^i(i-1)r$ for a random number $0 < r < 1$ and test number $i = 1, 2, \ldots, 11$. The applied g values and corresponding effectivity indices are shown in Fig. 7. Again, our algorithm is shown to be highly effective.

6.2. Comparison with topological sensitivity and feature sensitivity

We next compare the effectivity and efficiency of our method with direct FEA, TSA, and FSA. The direct FE analysis results were taken as the ground truth for the other approaches. TSA testing considered two different strategies: Eq. (25) for a circular hole (TSA-Circle), and Eq. (26) for an elliptic hole (TSA-Ellipse).

This test used the example in Fig. 8 of an internal elliptic hole ω with semi-major axis and semi-minor axis respectively a and $a/2$; values of a are explained shortly. This example was taken from [18] with a slight modification: for the Poisson equation as defined in Eq. (23), the source term was given the value $f = 20$, instead of 1, to cause bigger values of modification sensitivity. Outer boundary conditions are depicted in Fig. 8; the boundary for the internal elliptic hole was set free. When applying TSA-Circle, a spherical hole with the same cross-section was used as the internal feature instead of this elliptic feature. The quantity of interest is defined via Eq. (27).

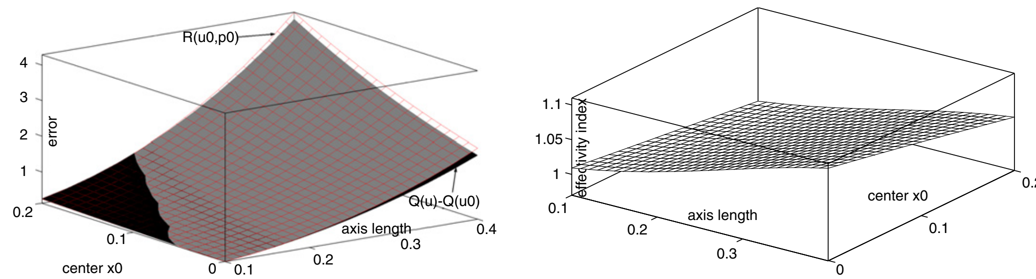
In this example, the semi-major axis a was varied between 0.05 and 0.095. The computed quantities of interest and the effectivity indices for the results obtained by different approaches are summarized and compared in Figs. 9 and 10. The estimated quantity obtained using each approach was defined as $Q(u_0) + e$ for the solution u_0 over the defeatured model, plus the estimated



(a) Effectivity index.

(b) Variation of local quantity as the ratio $(Q(u) - Q(u_0))/Q(u_0)$.

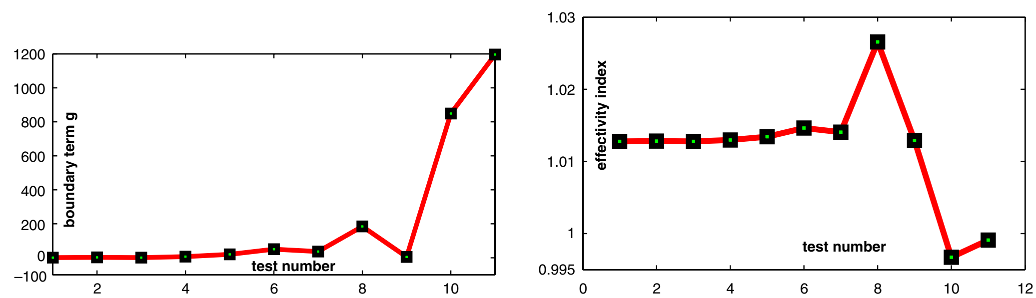
Fig. 5. Effectivity with varying internal feature size in Fig. 4.



(a) Comparison between $R(u_0; p_0)$ and $Q(u) - Q(u_0)$.

(b) Effectivity index surface.

Fig. 6. Performance under variations of the internal feature size and center location for the example in Fig. 4.



(a) Value of g.

(b) Effectivity index.

Fig. 7. Performance under variations of Neumann boundary term g on the internal feature for the example in Fig. 4.

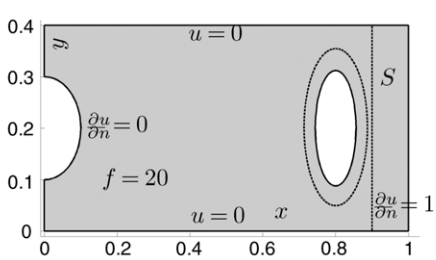


Fig. 8. Example used to compare methods, from [18].

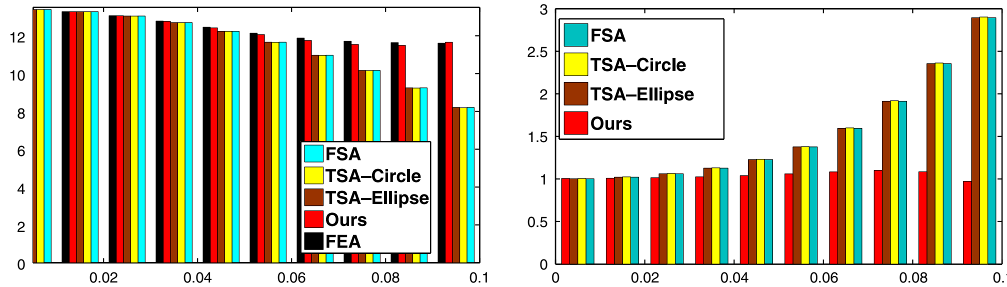
sensitivity e. The bar plots in Fig. 9 show values of the local quantity of interest and the effectivity index obtained by each approach for each test case; the curve plots in Fig. 10 demonstrate their global variation.

Fig. 9(a) shows that the estimated quantity using our approach was always very close to the benchmark results computed using direct FE analysis, for all values of a. FSA, TSA-Circle, and TSA-Ellipse, however, behave differently—as the value of a increases, the estimated quantities drastically move away from the benchmark value. Overall variations of the quantities can easily be seen in Fig. 10(a) and (b).

We note that the estimates obtained with TSA-Ellipse and FSA always agreed over the whole range of a. The former, however, is cheaper to compute as it does not involve solving other auxiliary exterior problems. They are slightly closer to the benchmark FEA results than estimates using TSA-Circle. (Outcomes reported in [18] only compare their approach to TSA-Circle without considering the more accurate TSA-Ellipse).

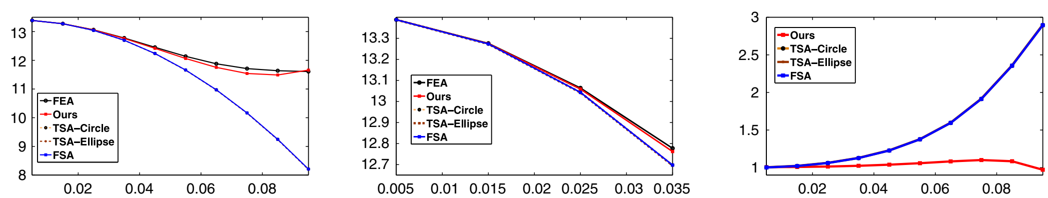
The corresponding effectivity indices are also compared in Fig. 9(b). Over the whole range of a, the effectivity of our estimate was always around 1. This was in contrast to results of other approaches, which ranged from 1 to 3. Overall variations of the effectivity indices can easily be seen in Fig. 10(c) and (d). This further demonstrates the superior accuracy of our method in estimating modification sensitivity, even for large design changes, unlike previous methods.

In detail (see Fig. 10(b) and (d)), when the feature size was relatively small, with a ranging from 0.005 to 0.035, the computed quantity of interest was very close to the benchmark FEA results for all approaches. In particular, when parameter a is very close to 0.005, TSA-Ellipse and FSA perform slightly better than our approach, which can be explained by the fact that we have discarded the term $\bar{h}_{\partial\omega}(u_0, \varepsilon_0) - h_{\partial\omega}(u_0, \varepsilon_0)$ in Eq. (19). These results demonstrate the minor effects on sensitivity estimation of doing so.

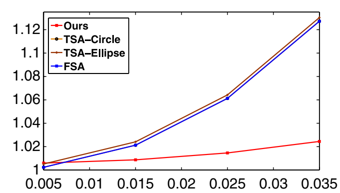


(a) Local quantity of interest: average of u over S. (b) Effectivity index.

Fig. 9. Modification sensitivity estimates using FEA, TSA, FSA, and our method for the model in Fig. 8.



(a) Local quantity of interest: average u over S. (b) Close-up of local quantity of interest: average of u over S. (c) Effectivity index.



(d) Close-up of effectivity index.

Fig. 10. Modification sensitivity estimates using FEA, TSA, FSA, and our method for the model in Fig. 8.

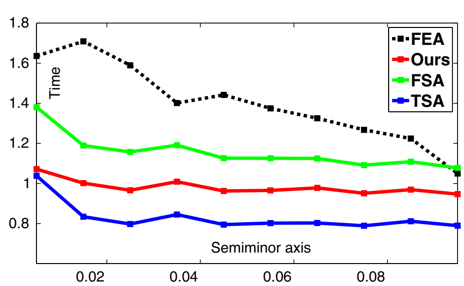


Fig. 11. Time taken by FEA, TSA, FSA, and our method for the model in Fig. 8.

Computation times for this problem, for each method, are given in Fig. 11. As can be seen, the topological sensitivity method was quickest, then our method, then feature sensitivity, and finally direct FE analysis. This is consistent with our discussion in Section 5.

6.3. Three-dimensional example

We now consider how our method performed on a somewhat more realistic three-dimensional (3D) example $\mathcal{M}$ with 11 candidate features labeled $L_1, \ldots, L_{11}$, shown in Fig. 2(a). L_{10} and L_{11} are respectively a blind hole and a blend on the bottom. We note that features typically appear on the boundaries of 3D models, unlike 2D models, where they are generally in the interior, which means that approaches like TSA or FSA are typically unsuitable. In comparison, our method can be directly applied to 3D models without modification.

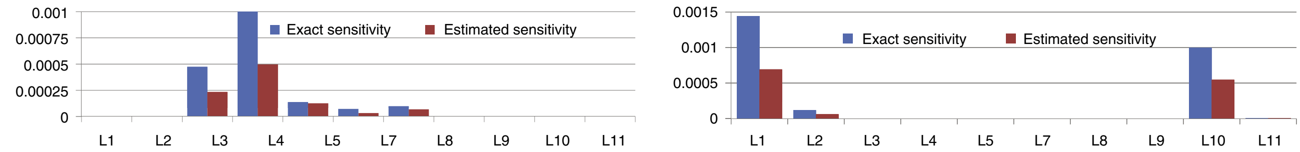
The corresponding parameters of the Poisson equation in Eq. (23) were set as follows: the source term was set to $f = 1$, $u = 0$ along the planar regions on the model's left and right sides, and the condition $\partial u/\partial n = -1$ was set over the central large cylindrical region. The quantities of interest $Q_1(u)$ and $Q_2(u)$, defined via Eq. (27), were measured over two different regions S_1 and S_2 shown in Fig. 2(a). We denote $\mathcal{M}_0 = \mathcal{M} + \cup_{i=1}^{11} L_i$ as the fully defeatured model for later use.

We aim to simplify model $\mathcal{M}$ by suppressing certain features from $\mathcal{L} = \{L_1, \ldots, L_{11}\}$ so that changes between the field solutions u_0^i of the final simplified model $\mathcal{M}_m^i$, $i = 1, 2$, and solutions u of the fully featured model $\mathcal{M}$ are under certain sensitivity control.

Thus, the corresponding modification sensitivity was first computed to estimate the effects of removing each single feature L_i, $i = 1, \ldots, 11$, from model $\mathcal{M}$, that is, $e(\mathcal{M}, \mathcal{M} + L_i)$; see its definition in Eq. (4). For the reason given in Section 6, for these 11 features with little interaction, we instead computed sensitivity $e(\mathcal{M}_0 - L_i, \mathcal{M}_0)$, which is approximately equal to $e(\mathcal{M}, \mathcal{M} + L_i)$ but much cheaper to compute; our experimental results also demonstrate their close approximation, not further shown here.

In order to demonstrate the effectivity of the modification sensitivity estimation, comparison between the estimated modification sensitivities with the benchmark sensitivities obtained using direct FE analysis for the local quantities defined over S_1 and S_2 are shown in Fig. 12(a) and (b); values are recorded as 0 when below 10^{-6}. The associated effectivity indices for regions S_1 and S_2 are plotted in Fig. 13.

According to the estimated modification sensitivity $e(\mathcal{M}_0 - L_i, \mathcal{M}_0)$ for each feature L_i, features L_3 and L_4 have a large influence on the quantity defined over region S_1, showing that a suitable simplified model for this problem should keep these features, but delete other features, resulting in a simplified model $\mathcal{M}_m^1 = \mathcal{M}_0 - L_3 - L_4$. Similarly, a different simplified model $\mathcal{M}_m^2 = \mathcal{M}_0 - L_1 - L_{10}$ is suitable for the quantity defined over region S_2. Table 2 further



(a) Results for region S_1.

(b) Results for region S_2.

Fig. 12. The estimated modification sensitivity for each feature compared with that obtained using direct FE analysis, for the quantity defined over regions S_1 and S_2.

Table 2
Comparisons of the computational results for the fully featured model, the fully defeatured model, and the partially defeatured model obtained by our modification sensitivity estimate.

	R_1			R_2		
	$\mathcal{M}$	$\mathcal{M}_0$	$\mathcal{M}_m^1$	$\mathcal{M}$	$\mathcal{M}_0$	$\mathcal{M}_m^2$
Mesh elements	85 132	4512	20 762	85 132	4512	27 134
Running time (s)	5.90	0.26	1.232	5.90	0.26	1.732
Quantity ($\times 10^{-6}$)	4.01	3.80	3.99	4.02	3.69	3.99
Quantity difference ($\times 10^{-6}$)	0	0.21	0.02	0	0.33	0.03

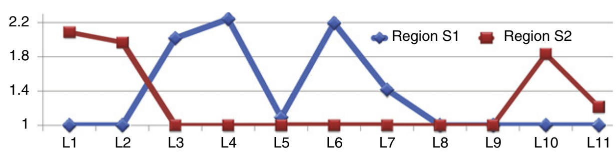


Fig. 13. Effectivity index curves for the quantities of interest defined over regions S_1 and S_2.

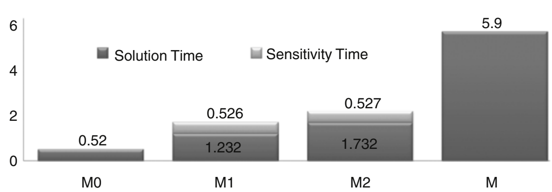


Fig. 14. Computational time in solving the analysis problem over the fully featured model M, the fully defeatured model M_0, and the partially defeatured models M_m^1 and M_m^2 (plus time of modification sensitivity estimations).

compares the two groups of models, $\mathcal{M}$, $\mathcal{M}_0$, $\mathcal{M}_m^1$, and $\mathcal{M}$, $\mathcal{M}_0$, $\mathcal{M}_m^2$, in terms of number of mesh elements, solution time, corresponding quantities, and difference of quantities from their exact values.

As can be observed from the results in Table 2, using the fully featured model $\mathcal{M}$ is most time consuming; it may even not be affordable for large and complex geometries. Simply using the fully defeatured model $\mathcal{M}_0$ significantly reduces the computational time but also leads to large analysis errors. As a trade-off, by keeping certain important features directed by the estimated modification sensitivities, a partially defeatured model $\mathcal{M}_m^1$ or $\mathcal{M}_m^2$ of intermediate complexity was obtained which both reduces the analysis complexity, and simultaneously maintains high analysis fidelity. The computational time for solving the analysis problem defined over models $\mathcal{M}$, $\mathcal{M}_0$ and $\mathcal{M}_m^1$, $\mathcal{M}_m^2$ (plus time of modification sensitivity estimations to guide their generations) is also compared in Fig. 14.

Note clearly that the final simplified model $\mathcal{M}_m^1$ or $\mathcal{M}_m^2$ was obtained using prime and adjoint solutions defined over the fully defeatured model $\mathcal{M}_0$, which only needs to be computed once for all features, and for all regions containing quantities of interest such as S_1 and S_2. This saves much computational time.

This example also shows that different local quantities of interest may require different simplified models to maintain certain analysis fidelity. Solely using geometry-based simplification criteria is an unsuitable approach.

7. Conclusions and future work

As can be observed from the experimental results, our novel method for estimating modification sensitivity is both accurate and efficient, even for large negative features. Such cases cannot be well handled by previous approaches such as topological sensitivity analysis or feature sensitivity analysis, which were mainly intended for design optimization, and focus on relatively small changes.

Our method has similar computational efficiency to topological sensitivity analysis, in that only prime and adjoint solutions of the defeatured model need to be computed for all non-interacting features, and it is less computationally expensive than the approach of feature sensitivity analysis, as the latter requires certain additional solutions to auxiliary exterior problems for each feature.

Moreover, due to use of the adjoint formulation, the error can be efficiently estimated with little extra effort when a feature changes in shape, size, location, or boundary conditions. Since repeated design changes are required in simulation-based design, and also as CAD models typically contain many different features at different locations and of different shapes, this will save much computational cost.

However, the approach here is limited to negative features with Neumann boundary conditions, where the fully featured model is contained within the defeatured model. A companion paper [2] considers its extension to positive features. The key issue involved in this extension is how to derive suitable boundary conditions outside the defeatured model so that the conversion from modification sensitivity to modeling error is still possible. We are also exploring applying Nitsche's method to handle cases of general features with prescribed Dirichlet boundary conditions.

Acknowledgments

We thank the reviewers for their comments, which have helped to improve the paper. This work described in this paper was partially supported by the NSF of China (60736019), the National Basic Research Program of China (2011CB302400), the 863 High Technology Plan of China (2008AA04Z115), and the Fundamental Research Funds for the Central Universities (1A5000*172210101[43]).

Appendix. Modification sensitivity estimators

From the definition of $N(u, v)$, we have

$$N(u, v) = (Lu, v)|_{\Omega-\omega} = \bar{H}_{\partial\Omega}(u, v) + \bar{h}_{\partial\omega}(u, v) - L^*(u, v)|_{\Omega-\omega}.$$

The residual $R(u_0; v)$ defined by Eq. (9) then becomes

$$R(u_0; v) = N(u_0; v) - F(v) = \bar{H}_{\partial\Omega}(u_0, v) + \bar{h}_{\partial\omega}(u_0, v) - L^*(u_0, v)|_{\Omega-\omega} - (f, v)|_{\Omega-\omega}. \tag{A.1}$$

On the other hand, directly evaluating $\boldsymbol{u}_0$ in Eq. (17) gives

$$L^*(u_0, v)|_{\Omega-\omega} = H_{\partial\Omega}(u_0, v) + h_{\partial\omega}(u_0, v) - (Lu_0, v)|_{\Omega-\omega}. \tag{A.2}$$

By observing that solutions u, u_0 share the same boundary conditions over the outer boundary $\partial\Omega$, we have

$$H_{\partial\Omega}(u_0, v) = \bar{H}_{\partial\Omega}(u_0, v).$$

Correspondingly, replacing Eq. (A.2) into Eq. (A.1), we get

$$R(u_0; v) = \bar{h}_{\partial\omega}(u_0, v) - h_{\partial\omega}(u_0, v) + (Lu_0, v)|_{\Omega-\omega} - (f, v)|_{\Omega-\omega}.$$

As u_0 is a solution to Eq. (2), or $Lu_0 = f$, this ultimately gives

$$R(u_0; v) = \bar{h}_{\partial\omega}(u_0, v) - h_{\partial\omega}(u_0, v). \tag{A.3}$$

Replacing v by p in Eq. (A.3), we have

$$Q(u) - Q(u_0) \approx \mathcal{R}(u_0; p) = \bar{h}_{\partial\omega}(u_0, p) - h_{\partial\omega}(u_0, p).$$

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