Optimization of finite element grids by direct energy search

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(Received March 1976)

One of the possible approaches to the reduction of computational costs in finite element analysis is the selection of 'optimal grids', which produce the 'best' answers, in the sense of minimizing a discretization error measure, for a fixed level of computational effort. The grid optimization problem is studied in the case of grids of similar topology having a fixed number of degrees of freedom per node. A general formulation based on weighted-residual error measures is specialized to field problems associated with a positive-definite energy functional, the minimization of which, with respect to variable node locations, is adopted as a grid optimality criterion. The problem is then embedded in the framework of the general non-linear programming problem, and desirable computational features of candidate search algorithms are described.

Introduction

The problem of reducing the cost of analysing a continuous problem through a finite element discretization technique can be attacked from three different angles: (M) *model selection*—choose an appropriate variational or quasi-variational principle associated with the governing field equations, and select finite element base functions that produce 'best' answers in the sense of minimizing a discretization error measure e_M for a fixed level of computational effort; (G) *grid optimization*—assume that (M) has been resolved in favour of a specific formulation and finite element model. Then select a grid* that minimizes a discretization error measure e_G (which often coincides with e_M) for a fixed level of computational effort; (S) *solution technique selection*—assume that (M) and (G) have been resolved in favour of a specific model and grid, respectively. Then select a solution algorithm that minimizes the number of operations required to process the discrete system of equations.

None of the preceding aspects of the cost reduction problem has been solved to date. The level and quantity of research, however, varies substantially according to the particular area considered.

Approach (M) pertains to basic finite element technology. There has been virtually no effort devoted to tackle the model-selection problem from the stated viewpoint, as the number of optimization variables is enormous. Moreover, there is little agreement on how to characterize 'best answers', and on uniform procedures for systematic evaluation of the computational effort.

Approach (G) pertains to the field of automated grid selection techniques. There has been little research in this area, but a general plan of attack on the problem is beginning to emerge.

Much of the ongoing research is devoted to approach (S), which pertains to the 'sparse matrix technology' branch of numerical analysis. New sparse equation-solving strategies under study promise to reduce substantially the computational effort in certain classes of problems, such as three-dimensional continua, but implementation in a production scale will probably have to wait several years.

This paper is concerned with a restricted form of approach (G), in which the number of degrees of freedom per node and the grid topology remain invariant during the grid selection process. Under those assumptions, the computational effort remains constant if the number of nodes is fixed, and grid optimization reduces to the more manageable problem of optimal node distribution.

*The term 'grid' is used to signify the set of node points associated with a discrete finite element model, and the system of degrees of freedom selected at the node points. The term 'mesh' refers to the partition of a domain into elementary subdomains by lines or surfaces defined by the node set.

Formulation of the node distribution problem

A fruitful approach to the problem of automated selection of optimal finite element grids of specified topology is based on the idea of minimizing a discretization error measure with respect to the node locations. This idea is presented in this section in a formal context so as to provide a general foundation to future investigations; the approach is later specialized to a class of field problems and an energy-norm measure.

Consider a bounded spatial domain D with boundary B in the real m-dimensional space R^m, over which a static field problem is posed:

$$Lu = f \tag{1}$$

where L is a linear or non-linear operator, f is a prescribed forcing function, and u is the unknown solution. The problem (1) is complemented by suitable boundary conditions (BC) on B.

The solution of problem (1) is approximated by a trial- or base-function expansion:

$$u(\boldsymbol{x}) \approx v(\boldsymbol{x}) = \boldsymbol{\Phi}(\boldsymbol{x})^T \boldsymbol{q} \tag{2}$$

where column vector $\boldsymbol{\Phi}$ collects the N_q base functions $\phi_j(\boldsymbol{x})$ and vector $\boldsymbol{q}$ the associated generalized coordinates or degrees of freedom q_j; $\boldsymbol{x}$ denotes the array of spatial coordinates $(x_1, \ldots x_m)$ and superscript T denotes matrix transposition. The determination of the coefficients q_j can be examined within the general framework of weighted-residual methods[1]:

$$e_w(u) = (r, w) = (Lu - f, w) = 0 \tag{3}$$

where w is a prescribed weight function, $r = Lu - f$ is the residual associated with problem (1), and the inner-product notation $(\ldots)$ stands for the domain integral:

$$(u, v) = \int_D uv \, \mathrm{d}R^m \tag{4}$$

Specific choices of the weight function produce the Galerkin, least-square, collocation, subdomain, and adjoint formulations[2,3].

In a finite element discretization technique, the domain D is replaced by the union of finite element subdomains, over which the base functions ϕ_j are defined in piecewise fashion. The degrees of freedom q_i are selected as values of u, and perhaps their derivatives, at an appropriate set of N nodes. Insertion of that assumption into equation (3) leads to an algebraic system of the form:

$$\boldsymbol{A}\boldsymbol{q} = \boldsymbol{b} \tag{5}$$

which is complemented by suitable discrete counterparts of the continuous BC.

Let $\boldsymbol{q}^*$ denote a solution of (5) and $v^* = v(\boldsymbol{q}^*) = \boldsymbol{\Phi}^T\boldsymbol{q}^*$ the finite element solution (2) over D. Define an *a posteriori* weighted error measure

$$e_w^*(v) = (Lv^* - f, w^*) \tag{6}$$

where the weighting function w^* is often (but not necessarily) identical to the weight function w in equation (3). If the number of degrees of freedom per node N_q/N is fixed, an optimal grid will be characterized by the following condition:

an optimal n*-node grid minimizes* $|e_w^*|$ *for a fixed* N

The characterization of an optimal grid is seen to depend on three factors: (a) the field problem being solved, i.e., equation (1). Different forcing functions f would in general lead to different optimal node placements. Moreover, if the problem is time-dependent, the optimal spatial grid can be expected to be a function of time; (b) the selection of the quasi-variational principle (3) to produce the discrete system (5); (c) the selection of the discretization error measure (6), which quantifies the accuracy of the approximate solution.

The user of a finite element programme is generally expected to provide an initial grid G_0. A computational procedure by which the programme can 'move' nodes of the initial grid to generate a sequence of 'improved' grids $G_1, G_2, \ldots$, which have progressively smaller discretization errors, is called a *node distribution procedure*. The displacement of the nodes to new locations may be viewed as a pseudo-dynamical process. The motion of the nodes is subject to certain kinematic constraints discussed later; once those constraints are adjoined in terms of appropriate equality and/or inequality conditions, the node distribution problem can be formally expressed as a non-linear programming problem.

Historical background

The selection of 'adequate' finite element idealizations has attracted the attention of many investigators since the method gained widespread acceptance in the early sixties. There is presently abundant literature on procedures for setting up finite element models, although much of the material is buried in relatively inaccessible user's manuals. Most of that literature is concerned with computerized procedures for generating regular grids, usually complemented by empirical mesh-layout principles such as 'use a finer grid in regions of expected high solution gradients'.

Empirical guidelines intend to convey, in engineering-oriented terms, the importance of judicious selection of weight functions in the error expression (6), but are of little help to the average user facing the task of preparing a complex two- or three-dimensional discrete model. There are many problems in which optimal mesh-layout rules cannot be invoked with any certainty until a fairly accurate solution is available; however, critical design features such as stress concentrations may be masked by a poor choice of the initial model. Analysis flowtime restrictions and high computational costs may also preclude extensive modifications of the original model.

The general approach to mesh optimization has received scant attention in the technical literature. The prevalent feeling among programme developers is that the cost of obtaining an optimal grid by computer-directed search techniques would far exceed the cost of re-analysing the problem with manually improved models. That objection is certainly valid if the mesh optimization problem is attacked *in extenso*. There are two important computational difficulties associated with the approach based on the minimization of the error expression (6): (1) the calculation of the residual integrals may be extremely difficult if the trial functions ϕ_j are not in the domain of the operator L,

as is often the case in finite element analysis†; (2) a very small error norm e_w^* may be produced by fortuitous cancellation of the weighted residual integral despite the fact that v^* is a poor approximation to u. This possibility can only be avoided by selecting a weight function w^* that renders equation (6) non-negative in the residual (as in the least-square method, where $w^* = \partial \boldsymbol{r}(v)/\partial \boldsymbol{q}$).

Jensen[4] has studied the optimal placement of nodes in two-dimensional domains within the framework of both classical and variational finite-difference formulations. Nodes are distributed according to a *nodal density function*, which is initially specified by the user (e.g., through direct CRT input in interactive work), and recalculated by the programme on the basis of estimates of the local discretization error.

Oliveira[5] proposed that nodes pertaining to a compatible (energy-bounding) finite element discretization of a linear structural system be distributed so as to minimize the total potential energy of the discrete system, and showed that nodes of such 'energy-optimized' grids would fall along iso-energetic contours, i.e., lines or surfaces of equal energy density; however, no computational procedures for generating such grids were discussed. The total energy minimization (*TEM*) optimality criterion is restricted to a class of self-adjoint field problems and a special type of finite elements, but it has significant computational advantages when applicable, as both of the numerical difficulties noted for the general approach are avoided.

McNeice and Marcal[6] applied the *TEM* criterion to the manual improvement of one- and two-dimensional finite element grids involving a small number of free optimization variables.

Grid optimization by energy minimization

We restrict our attention in the sequel to the case in which the operator L in equation (1) is linear, positive definite, and self-adjoint, as is the case in elastic structural analysis. The selection of the weight function $w = \delta u$ in equation (2) leads to the Galerkin form‡:

$$(Lu - f, \delta u) = 0 \tag{7}$$

which is equivalent to the variational statement:

$$\min E(u) = \min_u (\tfrac{1}{2}Lu - f, u) \tag{8}$$

The functional $E(u)$ will be called the *total energy*, because it possesses such meaning in the applications. The integrand of equation (8):

$$d(u) = \tfrac{1}{2}uLu - fu = d_I(u) - d_E(u) \tag{9}$$

represents the *energy density*, whose components d_I and d_E are the internal and external energy density, respectively.

A finite discretization of equation (1) is said to be *compatible*, *conforming* or *energy-bounding*, if the assumed finite element base functions satisfy minimal continuity requirements associated with the admissible solutions of the equivalent variational problem (8). The total energy $E_v(v)$ associated with any admissible discrete solution (2) satisfies the energy inequality[7]:

$$E_v(v) \geqslant \min_u E(u) = E_{\min} \tag{10}$$

The discretization error in the energy norm (8) is:

$$e_E(v) = E_v(v) - E_{\min} \geqslant 0 \tag{11}$$

Note that equation (11) is a very convenient global error measure on account of the following advantages: (a) it is non-negative definite, therefore precluding the possibility of fortuitous error cancellation; (b) E_v can be calculated directly from the discrete solution vector $\boldsymbol{q}$ (cf. equation (14)); local-residual manipulations are then avoided; (c) convergence of $e_E(v)$ to zero is sufficient to guarantee mean-square convergence of the approximate solution v to u, as the following bound holds[8]:

$$\|v - u\|_2^2 = (v - u, v - u) \leqslant \lambda_{\min}^{-2} e_E(v) \tag{12}$$

where $\lambda_{\min}$ denotes the smaller eigenvalue of $Lu = \lambda u$ (which is real and positive on account of the positive-definiteness assumption on L).

Optimal node placement

Let $\boldsymbol{X}$ denote the vector of node location coordinates:

$$\boldsymbol{X} = (x_j^i), \quad \text{for} \quad i = 1, \ldots N \quad \text{and} \quad j = 1, \ldots m \tag{13}$$

The set $\boldsymbol{X}$ defines the geometry of the finite element grid $G(\boldsymbol{X})$ over D. The total energy E_v of the discrete problem can be considered to be a function of both $\boldsymbol{q}$ (the degree-of-freedom vector) and $\boldsymbol{X}$:

$$E_v(\boldsymbol{q}, \boldsymbol{X}) = \tfrac{1}{2}\boldsymbol{q}^T\boldsymbol{A}(\boldsymbol{X})\boldsymbol{q} - \boldsymbol{b}(\boldsymbol{X})^T\boldsymbol{q} \tag{14}$$

Minimization of E_v with respect to $\boldsymbol{q}$ while keeping $\boldsymbol{X}$ (the grid) constant yields the (linear) Ritz–Galerkin system (5) whose solution $\boldsymbol{q}^*$ is $\boldsymbol{A}^{-1}\boldsymbol{b}$. Substitution of $\boldsymbol{q}^*$ into equation (14) gives the total energy as a function of $\boldsymbol{X}$ alone:

$$\begin{aligned} E_v^*(\boldsymbol{X}) &= E_v(\boldsymbol{A}^{-1}\boldsymbol{b}, \boldsymbol{X}) = -\tfrac{1}{2}\boldsymbol{q}^*(\boldsymbol{X})\boldsymbol{b}(\boldsymbol{X}) \\ &= -\tfrac{1}{2}\boldsymbol{b}^T(\boldsymbol{X})\boldsymbol{A}^{-1}(\boldsymbol{X})\boldsymbol{b}(\boldsymbol{X}) \end{aligned} \tag{15}$$

The grid optimization process based on the discretization error measure (11) can now be stated as follows: minimize $E_v^*(\boldsymbol{X})$ with respect to the node location set $\boldsymbol{X}$, subject to certain geometric constraints in $\boldsymbol{X}$.†

Note that the actual calculation of e_E^* is not required. Given two grids $G(\boldsymbol{X}_1)$ and $G(\boldsymbol{X}_2)$, the latter is considered to better if $E_v^*(\boldsymbol{X}_2) < E_v^*(\boldsymbol{X}_1)$, a test that does not require knowledge of $E_{\min}$. The fact that an estimate of the exact solution is not required is an important computational advantage of the *TEM* criterion.

Grid optimization as a non-linear programming problem

A grid optimization procedure based on the direct minimization of $E_v^*(\boldsymbol{X})$ can be conveniently implemented within the framework of the general non-

†Delta and dipole functions then appear at interelement boundaries if L is a differential operator.

‡Also called the 'principle of virtual work' in structural analysis.

†The concept of 'least-energy grid' can be easily extended to eigenvalue problems.

linear programming problem‡ as follows:

1. The total energy function $E_v^*(\boldsymbol{X})$ becomes the object function.
2. The entries of $\boldsymbol{X}$ (nodal coordinates) become the optimization variables.
3. Equality constraints of the form $h_j(\boldsymbol{X}) = 0$ correspond to kinematic restrictions on the motion of the grid, namely: (a) nodes located on smooth boundary lines or physical interfaces must remain there; (b) nodes located at domain corners are fixed; (c) the analyst may specify additional constraints on node motions in order to reduce the number of optimization variables.
4. Inequality constraints of the form $g_j(\boldsymbol{X}) \geqslant 0$ result from conditions restricting the maximum local mesh distortion. This can be achieved by monitoring the Jacobian of the elemental volume (area, length) used in the numerical integration over the finite element subdomains while computing the entries of $\boldsymbol{A}$ and $\boldsymbol{b}$. The determinant of that Jacobian must remain positive everywhere to guard against loss of the one-to-one mapping between element and global coordinates. A grid that violates this constraint is said to be *infeasible*.

Minimization algorithm

The key computational features of the grid optimization scheme that govern the choice of minimization algorithm are: (I) the calculation of analytic derivatives of the energy function $E_v^*(\boldsymbol{X})$ with respect to the $\boldsymbol{X}$ variables is a hopeless task in the case of arbitrary two- and three-dimensional grids; (II) the optimization problem is usually of high dimensionality (more than 10 optimization variables is considered a high-dimensionality problem in the field of non-linear programming); (III) equality constraints on node motions can be trivially implemented by simple exclusion of optimization variables in many practical problems provided that the local coordinate axes are appropriately oriented at those node locations.

Property (I) forces the selection of a derivative-free minimization method, or at most a gradient method with finite-difference estimation of object function derivatives. Property (II) favours methods whose performance does not degrade drastically as the number of optimization variables increases. Finally, property (III) suggests that an unconstrained minimization technique with simple modifications to account for node motion and mesh distortion constraints could be used to assess the feasibility of the energy minimization technique in a series of test problems. (Unconstrained minimization algorithms are simpler to implement, check out and problem-adapt than methods developed to handle very general constraints.)

A later paper will report on a series of numerical experiments carried out with a non-linear programming implementation, discuss the implications of automated grid optimization in the synthesis of mesh-layout rules in sub-structures, and describe current research in simplified mesh optimality criteria based on a local (element-level) energy distribution rather than on a total-energy criterion. The latter topic is closely related to similar work in structural optimization.

‡The reader is reminded that non-linear programming is a branch of applied mathematics concerned with the minimization of a general multivariate function (the object or merit function) under arbitrary constraint conditions. Most applications of non-linear programming fall in the area of optimization problems. References 9–11 can be recommended as modern introductory treatments to the subject.

Acknowledgement

This research has been sponsored by the Air Force Office of Scientific Research/AFSC, United States Air Force, under Contract No. F44620-71-C-0109.

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