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A SIMPLE METHOD FOR IMPROVING THE ACCURACY AND CONVERGENCE OF FEM COMPUTATIONS

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In the paper, a simple method for improving the convergence rate and accuracy of finite-element computations is presented. It is based on a discrete formulation of the problems on certain types of superelements and uses the formal-series technique. It makes possible a uniform treatment of problems with corner singularities and an improvement of accuracy in ordinary FEM computations, without any increase in the dimensionality of the problem.

1. Introduction

The accuracy of approximate solutions for boundary-value problems is of prime importance in every case, but there are circumstances, when it takes on a special value. One of such instances is shape optimization, where the gradient of the goal functional depends on derivatives of state variables, and therefore is very sensitive to the rate of convergence of approximation. The quality of approximation depends in turn on several factors, in particular:

- suitability of shape functions;
- the existence of singularities, which limit the rate of convergence and may cause significant errors even far from their origins, as we shall see in one of the examples.

In this paper, we present a uniform approach to both sources of error. The method is quite general and may be used in finite-element computations for partial differential equations or systems of any order (2-nd, 4-th or higher if it makes sense), but we shall concentrate here on the second-order examples and plane problems.

Let us imagine a bounded star-shaped domain Ω_s, having the centre at $0 \in \mathbb{R}^2$. The examples are shown in Fig. 1, where the centre is marked with a small circle. Assume for simplicity that they are already polygons. Next we construct from the outer boundary Γ_0 the consecutive cuts of these domains by similarity transformation, $\Gamma_i = r^i \cdot \Gamma_0$, where $0 < r < 1$. Between Γ_i and Γ_{i+1} lay the ring-like parts of Ω_s, denoted by Ω_i. These rings are also similar, and sum up to the whole Ω_s.

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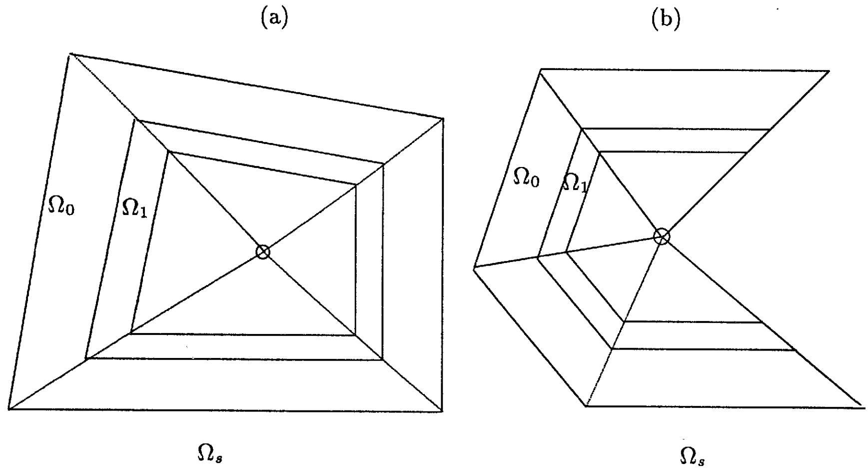

Fig. 1. Two types of domains (superelements): nonsingular (a) and with a singular point (b).

Our goal is to solve the elasticity or Laplace equations in such a domain using the finite-element method. For simplicity we assume here *the absence of volume forces or sources*. Let the parts between cross-sections k and $k+1$ be discretized with some kind of elements. We shall denote by u_k the vector of all the nodal values of the solution corresponding to the k-th cross-section. Now the elastic energy of the whole body after discretization can be written as

$$E = \sum_{k=0}^{\infty} E_k(u_k, u_{k+1}) \tag{1}$$

where E_k denotes the energy of the k-th ring. Let us concentrate on E_0. By eliminating internal nodes between sections Γ^0 and Γ^1, i.e. treating the rings as superelements, we get

$$E_0(u_0, u_1) = \frac{1}{2}[u_0^T, u_1^T] \cdot M \cdot \begin{bmatrix} u_0 \\ u_1 \end{bmatrix} \tag{2}$$

where the $2n\times 2n$ symmetric stiffness matrix M ($n = dim\ u_k$) has the form

$$M = \begin{bmatrix} A_1 & B \\ B^T & A_2 \end{bmatrix} \tag{3}$$

Observe that the $n\times n$ matrices A_1 and A_2 are symmetric and positive definite.

Now comes the crutial observation. Assume that Ω_i has been triangulated and the linear finite elements have been used. Then the matrix M is proportional to the area of the ring, i.e. r^2, and inversely proportional to the squares of the lengths of the sides of triangles, since the discretized gradient of u computed in terms of nodal values is inversely proportional to r. As a result, M is the same for all rings, and E_k have the same form for all k.

Using the above notation we may write the energy of the whole Ω_s as

$$E = \frac{1}{2} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ \vdots \end{bmatrix}^T \cdot \begin{bmatrix} A_1 & B & & & \\ B^T & A & B & & \\ & B^T & A & B & \\ & & B^T & \ddots & \\ & & & & \ddots \end{bmatrix} \cdot \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ \vdots \\ \vdots \end{bmatrix} \tag{4}$$

where $A = A_1 + A_2$. If we could express E as a function of a u_0 only, $E = E(u_0)$, then it would be possible to write down the whole energy in terms of a finite number of nodal values.

For the sake of simplicity we shall conduct all the subsequent reasoning in the case of *homogeneous* equations with *constant coefficients* and containing only *the main part* of the elliptic differential operator. However, as mentioned later, the method may be extended to non-homogeneous equations with variable coefficients as well. The differential operators of lower order may be treated as disturbances.

The above cosiderations are related to the problem of representing the infinite body, which has received some attention in the FEM literature. The relation results from the fact that a star-shaped domain can be always transformed by inversion to an external one. In (Givoli, 1992; Grote and Keller, 1994) use is made of the exact analytic solutions in certain kinds of infinite domains in order to get substitute boundary conditions. Here we treat the problem from the beginning in its discrete formulation and use the energetic approach. In (Sharau, 1994) a completely different method is used, depending on treating the infinite body as a certain kind of elastic support. The method presented here may be proved to be correct (convergent), but of course it has also some limitations.

2. Problem Formulation

Let us return to the expression for E, (4), and solve the elasticity equations in the whole right part imposing the boundary conditions on u_0. The neccessary condition for the minimum of energy takes the form

$$M_\infty \cdot u_\infty = \begin{bmatrix} A & B & & & \\ B^T & A & B & & \\ & B^T & A & B & \\ & & B^T & \ddots & \\ & & & & \ddots \end{bmatrix} \cdot \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} -B^T \\ 0 \\ 0 \\ \vdots \\ \vdots \end{bmatrix} \cdot u_0 \tag{5}$$

As a result, after putting $u_i = Q_i u_0, \ i = 1, 2, \ldots$, we must solve the matrix equation of infinite order

$$M_\infty \cdot Q_\infty = \begin{bmatrix} A & B & & & \\ B^T & A & B & & \\ & B^T & A & B & \\ & & B^T & \ddots & \\ & & & & \ddots \end{bmatrix} \cdot \begin{bmatrix} Q_1 \\ Q_2 \\ Q_3 \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} -B^T \\ 0 \\ 0 \\ \vdots \\ \vdots \end{bmatrix} \tag{6}$$

where $Q_1, Q_2, \ldots$ have dimensions $n \times n$.

It is well known (Cooke, 1950) that such systems may have infinitely many solutions. Therefore we impose the physical condition that the consecutive energy terms (2) diminish, or the requirement that the neccessary condition gives a minimum, not a saddle point or maximum of the elastic energy. As it will turn out, this makes the solution unique.

If we could obtain the expression for Q_i in the multiplicative form, $Q_i = Q^i$, then, taking into account that $u_k = Q_k u_0 = Q^k u_0$, the energy on the whole domain takes the form

$$\begin{aligned} E(u_k, u_{k+1}) &= \frac{1}{2}(u_k^T A_1 u_k + u_{k+1}^T B^T u_k + u_k^T B u_{k+1} + u_{k+1}^T A_2 u_{k+1}) \\ &= \frac{1}{2} u_0^T (Q^T)^k \cdot [A_1 + Q^T B^T + BQ + Q^T A_2 Q] \cdot Q^k u_0 \end{aligned} \tag{7}$$

Hence, assuming the convergence of the infinite sum, the whole E may be computed as

$$E = \frac{1}{2} u_0^T \cdot S \cdot u_0$$

where

$$S = \sum_{k=0}^{\infty} (Q^T)^k \cdot R \cdot Q^k, \quad R = A_1 + Q^T B^T + BQ + Q^T A_2 Q$$

The series for S can be, as we shall see later, computed exactly in a closed form.

3. Formal-Series Approach

In this section we shall solve eqn. (6) by embedding the problem into the framework of operations on infinite series, see e.g. (Stanley, 1986). Let us establish the correspondence between the infinite vector $f_\infty = [f_1, f_2, \ldots]^T$ and the formal power series:

$$f(x) = \sum_{i=1}^{\infty} f_i \frac{x^{i-1}}{(i-1)!} \tag{8}$$

Differentiating this series gives

$$Df(x) = \sum_{i=2}^{\infty} f_i \frac{x^{i-2}}{(i-2)!}$$

or, in vector representation,

$$f_\infty = [f_1, f_2, \ldots]^T, \quad Df_\infty = [f_2, f_3, \ldots]^T \tag{9}$$

This shows that the differentiation may be represented as multiplication by the matrix

$$Df_\infty = \begin{bmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & 0 & 1 & \\ & & & \ddots & \ddots \end{bmatrix} \cdot f_\infty \tag{10}$$

and similarly for integration. Let us notice that M_∞ has a block structure, i.e. every n-th row repeats itself after shifting n places to the right. Therefore we must introduce a whole vector of functions

$$w^k(x) = \sum_{j=1}^{\infty} w_j^k \frac{x^{j-1}}{(j-1)!}, \qquad k = 1, \ldots, n \tag{11}$$

and write $u_i = [w_i^1, \ldots, w_i^n]^T$, so that

$$u(x) = \begin{bmatrix} w^1(x) \\ \vdots \\ w^n(x) \end{bmatrix} = \sum_{i=1}^{\infty} u_i \frac{x^{i-1}}{(i-1)!} \tag{12}$$

If we neglect the first n rows, the system (6) is equivalent to

$$B^T \cdot \int u + A \cdot u + B \cdot Du = 0$$

and putting $\bar{u} = \int u$ gives finally the differential equation

$$B \cdot \bar{u}'' + A \cdot \bar{u}' + B^T \cdot \bar{u} = 0$$

The solution must have the form $\bar{u} = r_\lambda \cdot e^{\lambda x}$, where $\dim r_\lambda = n$. Furthermore, λ is the root of the $2n$-th order characteristic polynomial

$$\det(B \cdot \lambda^2 + A \cdot \lambda + B^T) = 0 \tag{13}$$

and r_λ should be the right eigenvector:

$$(B \cdot \lambda^2 + A \cdot \lambda + B^T) \cdot r_\lambda = 0$$

In general, (13) has $2n$ roots. However, from the particular form of (13) it follows that these roots occur in pairs, $(\lambda_i, 1/\lambda_i)$, $i = 1, \ldots n$. Let us eliminate at this point the roots with absolute values greater than 1, and consider (after rearranging) only $\lambda_1, \ldots, \lambda_n$. The corresponding solutions have the form

$$\bar{u} = c_{1,1} r_{\lambda_1} \exp(\lambda_1 x) + c_{2,1} r_{\lambda_2} \exp(\lambda_2 x) + \ldots + c_{n,1} r_{\lambda_n} \exp(\lambda_n x) \tag{14}$$

The constants $c_{1,1}, \ldots, c_{n,1}$ are chosen in such a way that the first n rows of (6) are satisfied. Let us notice, however, that eqn. (6) has n right-hand sides. That is why we have double subscripts here: $c_{p,q}$ denotes the p-th constant corresponding to the q-th column on the right.

Let us now introduce the following notation:

$$R_\lambda = [r_{\lambda_1}, \ldots, r_{\lambda_n}], \quad C = [c_{j,k}]_{j,k=1,\ldots,n}, \quad \Lambda = \mathrm{diag}[\lambda_1, \ldots, \lambda_n]$$

It may be proved by replacing the exponential functions in (14) with equivalent infinite series and taking into account the definitions of coefficients in the formal series, that the solution of (6) takes the form

$$Q_1 = R_\lambda \cdot \Lambda \cdot C, \;\; Q_2 = R_\lambda \cdot \Lambda^2 \cdot C, \ldots, \; Q_n = R_\lambda \cdot \Lambda^n \cdot C$$

The choice of the matrix of constants C must ensure the fulfilment of the first block of equations, which leads to the formula $C = R_\lambda^{-1}$. More precisely, from

$$AQ_1 + BQ_2 + B^T = 0,$$

$$B^T Q_1 + AQ_2 + BQ_3 = 0$$

one obtains the matrix equation

$$(AR_\lambda \Lambda + BR_\lambda \Lambda^2) \cdot (I - CR_\lambda) \cdot \Lambda C = 0$$

and $\det(C) \neq 0$ because $\det(B) \neq 0$. In consequence, we get, as was required,

$$Q_1 = Q = R_\lambda \cdot \Lambda \cdot R_\lambda^{-1}, \quad Q_i = Q^i = R_\lambda \cdot \Lambda^i \cdot R_\lambda^{-1}, \quad i = 1, 2, \ldots$$

In general, there may appear $\lambda = 1$, which corresponds to the constant solution. For the scalar Laplace equation it must have multiplicity 2, with only one eigenvector. For the elasticity system, there exist pairs consisting of eigenvalue $\lambda = 1$ and an eigenvector responsible for constant displacements in 2 or 3 independent directions. However, they do not contribute to the energy, so the convergence of the energy series is assured by the next eigenvalue strictly less than 1.

We may also prove that, after regrouping the terms, the matrix S takes on the simple form:

$$S = A_1 + BQ$$

4. Three-Dimensional Case

Let us consider the three-dimensional domains, where the layers $\Omega_1, \Omega_2, \ldots$ are cut out from the 3-D body by the outer surface transformed by similarity with origin at 0. The derivatives of discretized functions still contain terms proportional to $1/r$, but the volumes of elements are proportional to r^3, so as a result

$$E_i = \frac{1}{2}[(u_i^h)^T, (u_{i+1}^h)^T] \cdot (r^{i-1}M) \cdot \begin{bmatrix} u_i^h \\ u_{i+1}^h \end{bmatrix}, \quad i = 1, 2, \ldots \tag{15}$$

with M having the form as in (3). Hence the system $M_\infty \cdot Q_\infty = B_\infty$ becomes

$$\begin{bmatrix} A_2 + rA_1 & rB & 0 & \cdots \\ rB^T & rA_2 + r^2A_1 & r^2B & \cdots \\ 0 & r^2B^T & r^2A_2 + r^3A_1 & r^3B \\ \ddots & \ddots & \ddots & \ddots \end{bmatrix} Q_\infty = \begin{bmatrix} -B^T \\ 0 \\ 0 \\ \vdots \end{bmatrix} \tag{16}$$

The rows do not repeat here exactly, so the solution requires some scaling. Let I be the $n \times n$ identity matrix, and define

$$P = \operatorname{diag}[r^{-1/2}I, r^{-1}I, \ldots, r^{-i/2}I, \ldots]$$

Then (16) may be rewritten (the diagonal infinite matrix is invertible) as

$$(P^{-1} \cdot \tilde{M}_\infty \cdot P^{-1}) \cdot Q_\infty = B_\infty$$

where $\tilde{M}_\infty = P \cdot M_\infty \cdot P$. Moreover, the system $\tilde{M}_\infty \cdot \tilde{Q}_\infty = \tilde{B}_\infty$, where $\tilde{Q}_\infty = P^{-1}Q_\infty$, $\tilde{B}_\infty = PB_\infty$, has the form

$$\begin{bmatrix} \frac{1}{r}A_2 + A_1 & \frac{1}{\sqrt{r}}B & 0 & \cdots \\ \frac{1}{\sqrt{r}}B^T & \frac{1}{r}A_2 + A_1 & \frac{1}{\sqrt{r}}B & \cdots \\ 0 & \frac{1}{\sqrt{r}}B^T & \frac{1}{r}A_2 + A_1 & \cdots \\ & & \ddots & \ddots \\ & & & \ddots \end{bmatrix} \tilde{Q}_\infty = \begin{bmatrix} \frac{-1}{\sqrt{r}}B^T \\ 0 \\ 0 \\ \vdots \\ \vdots \end{bmatrix} \tag{17}$$

which falls into the framework of our method, with eigenvalue problem (13)

$$\det[\lambda^2 \frac{1}{\sqrt{r}}B + \lambda(\frac{1}{r}A_2 + A_1) + \frac{1}{\sqrt{r}}B^T] = 0 \tag{18}$$

5. Superelements

Singular elements. Consider a discretized problem on some domain Ω_h (finite or infinite). Let p_0 be a point on $\partial\Omega_h$, where a geometrical singularity of the solution may occur (a reentrant corner, a change of the type of boundary conditions), belonging also to the nodes of triangulation. The standard way of dealing with such problems is to refine locally the discretization at the cost of increasing dimensionality (Grisvard, 1985). Our method suggests another approach. Let us create a star-shaped domain consisting of all triangles having p_0 as a vertex, see Fig. 1. Then we may treat this star as a superelement and construct a stiffness matrix for it using p_0 as a similarity origin. In this way, we have a mesh refinement without dimensionality increase. Moreover, the rate of convergence is the same as in the smooth case.

Improving accuracy. Let us consider the discretization consisting of convex quadrilaterals. Taking centres of these quadrilaterals as similarity origins, we may construct stiffness matrices in the same way as for superelements. Such an approach does not increase dimensionality, but, as shown by experiments, improves the accuracy in comparison with ordinary linear elements on triangles, also in the non-singular case.

Generalizations. As mentioned in the introduction, the method may be extended in two directions. If we assume piecewise constant over the superelements (quadrilaterals as in Fig. 1), coefficients approximating the real ones, the derivation does not require any change. Two approaches are possible:

1. Assuming constant forces (sources) over the superelements, we may also solve the infinite system, at the expense of much more complicated derivation.
2. Treating the solutions of the discrete (infinite) homogeneous system over the superelement as the shape functions (basis) in the FEM approximation. Such an approach is often used with continuous solutions. However, our method has the advantage that it does not require the knowledge of classical solutions. The right-hand side is of course also assumed piecewise constant over the superelement. This approach is used in numerical experiments and shows an increase in the accuracy.

6. Numerical Experiments

Corner singularity. In this case, the test domain constituted a unit circle with one quarter cut out. On the radii bounding the cut out part the homogeneous Neumann boundary conditions have been imposed. A well-known singular solution $u = r^{2/3} \cdot \cos(\frac{2}{3}\phi)$ has been used as a test function, see (Grisvard, 1985).

The discretization consisted of n evenly spaced radii and $[n/3]$ rings. We have computed two error indicators: the maximal error along the line $\Gamma = \{r = 0.5\}$ and the $L_2(\Gamma)$ convergence rate. The star mentioned in the last section consisted of all triangles having a vertex at 0. The results are summarized in Table 1. Since the convergence rate is computed for a projection on a line, theoretically it should be equal to 1.166... for the ordinary FEM and 1.5 for the FEM using local singular elements (Grisvard, 1985). As we see, our approach is as good as the second case. This example also demonstrates that singularity destroys convergence not only in its vicinity, but in other places, as well.

Tab. 1. Maximal error and convergence rate for corner singularity.

	n=6	n=12	n=24	$L_2(\Gamma)$-conv. rate
FEM	0.083	0.023	0.008	1.27
Series approach	0.057	0.012	0.003	1.60

Tab. 2. Maximal error and convergence rate for the homogeneous case.

	n=6	n=12	n=24	L_2-conv. rate
FEM	9.79	3.34	1.03	2.25
Series approach	4.76	1.49	0.45	2.22

Improving accuracy. Here the computational domain consisted of the square $[0,4]\times[0,4]$ divided into $n\times n$ subsquares. Each subsquare was replaced by the superelement as shown in Fig. 1(a). We have compared the performance of the ordinary linear finite element with our modified one for two cases:

a) Test function $u = \exp(x)\sin y$ satisfying the homogeneous Dirichlet equation. The results are in Table 2.

b) Test function $u = y^2 \exp(x)$ satisfying non-homogeneous Dirichlet equation. The results are in Table 3.

In both cases we have obtained the same rate of convergence as for the ordinary FEM, with twice better accuracy.

Tab. 3. Maximal error and convergence rate for the non-homogeneous case.

	n=6	n=12	n=24	L_2-conv. rate
FEM	0.246	0.072	0.021	2.18
Series approach	0.197	0.049	0.013	2.17

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