

# Numerical methods in the engineering practice. A mathematical introduction with an approach to their evaluation

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## ABSTRACT

In a recent paper the general form of partial differential equations that governs most of the engineering problems have been put forward together and a brief historical outline of FD, FE, BE and DEMs has been given.

Questions related to comparison of the BEMs with others have been formulated, some answers have been attempted.

Now the discussion is carried on further centred on BEM versus FEM.

## 1. INTRODUCTION

In a recent paper (Martins,1995) it has been shown that the differentials equations which govern most of the engineering problems in continuum mechanics are of the form:

$$A \frac{\partial^2 u}{\partial t^2} + B \frac{\partial^2 u}{\partial x \partial t} + C \frac{\partial^2 u}{\partial x^2} = F(t, x, u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x}). \quad (1.1)$$

The correspondent homogeneous Eqn. is

$$L[u] \equiv A \frac{\partial^2 u}{\partial t^2} + B \frac{\partial^2 u}{\partial x \partial t} + C \frac{\partial^2 u}{\partial x^2} = 0 \quad (1.2)$$

In this equation A, B, C are given constants if the material is homogeneous. The value of the discriminant

$$k = B^2 - 4AC \quad (1.3)$$

gives the type of Eqn [1.2].

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If  $k < 0$ , Eqn[1.2] is of elliptic type; If  $k > 0$ , Eqn[1.2] is of hyperbolic type; and if  $k = 0$ , Eqn[1.2] is of parabolic type (Weinberger, 1970)

If A, B and C are scalar constants, Eqn[1.2] governs scalar potential problems (steady and unsteady irrotational flow, heat exchange and transfer, diffusion and convection, electrostatics, flow through porous media, etc.).

After change of coordinates, for the elliptic type Eqn[1.2] takes the form (Laplace)

$$\frac{\partial^2 u}{\partial \xi^2} + \frac{\partial^2 u}{\partial \zeta^2} = 0 \quad (1.4)$$

For the hyperbolic type Eqn[1.2] takes the form:

$$\frac{\partial^2 u}{\partial \xi \partial \zeta} = 0 \quad (1.5)$$

For the parabolic type Eqn[1.2] takes the form:

$$\frac{\partial^2 u}{\partial \zeta^2} = 0 \quad (1.6)$$

Vectorial Problems:

The differential Eqn[1.1] can be generalised to “vectorial” forms considering the instead one function  $u$  we have a vector of  $n$  components. Usually, these components are either 3 displacements or velocities in Solid or Fluid Mechanics.

In these cases A, B and C are matrices of coefficients, eventually constants, representing the properties of the medium.

These differential equations represent “constraints” of the variables in space and time in the domains. Initial (at time  $t=0$ ) on the domain, and on the boundary there are conditions to be satisfied (Dirichelet’s, Newman’s or mixed conditions), giving altogether “boundary value problems”. These conditions are data, which are also “constraints” for the problem of finding values for the field variables in the domain and some complementary values for the variables and/or its derivatives at the boundary.

In general, each type of boundary value problem has its specific method of numerical solution. However, since the value of the discriminant depends on A, B, C which in turn are related to material properties, it follows that the type of problem may change if the materials properties change from one zone to the other of the domain. This is one first difficulty to get a proper numerical solution in non-homogeneous media.

It should be noted that the general form the Eqn[1.1] has a second member which may be a function  $F(x, t, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t})$  not only of  $x$  and  $t$ , but also of the dependent variable  $u$  and its first order derivatives  $\frac{\partial u}{\partial x}$  and  $\frac{\partial u}{\partial t}$ .

If  $F$  is linear in  $u$ ,  $\frac{\partial u}{\partial t}$  and  $\frac{\partial u}{\partial x}$ , the whole equation is still linear, but if  $F$  is non-linear in those variables, the equation is said “quasi linear”, since still is linear in the higher derivatives.

It should be notice that, if there are derivatives  $\frac{\partial u}{\partial t}$  and  $\frac{\partial u}{\partial x}$ , the whole equation is of mixed type, i.e., elliptic and hyperbolic at the same time, for example, and according to the values of the coefficients  $A$ ,  $B$ ,  $C$  and those of  $\frac{\partial u}{\partial t}$  and  $\frac{\partial u}{\partial x}$  in  $F$  (supposed to be linear) either the elliptic component or the hyperbolic component may prevail. This circumstance should be taken into account in the numerical solution.

Also, if  $F$  is not linear in  $u$ ,  $\frac{\partial u}{\partial t}$  and/or  $\frac{\partial u}{\partial x}$ , the solution of the problem may not be unique, creating difficulties in the numerical solution.

Even if in equation  $F$  is function of  $t$  and  $x$ , only, the corresponding boundary value problem will be a “well posed problem” only if the following conditions are satisfied (e.g. Weinberger, 1970):

i ) The function  $F$  and the functions  $f(x)$  and  $g(x)$  corresponding to initial conditions.

$$u(x,0) = f(x) \text{ and } \frac{\partial u}{\partial t}(x,0) = g(x), \quad 0 < x < 1, t = 0$$

are “regular enough”.

This implies the existence of a solution  $u(x,t)$ .

ii ) The solution is unique.

iii) Continuity. The different solutions  $u(x,t)$  corresponding to sets of data which differ in small quantities, must differ in small quantities also.

(Continuity implies uniqueness, but it is easier to show uniqueness).

Furthermore, for the problem to have a unique solution the matrices  $A$ ,  $B$  and  $C$  must be positive definite (Weinberger, 1970).

As particular cases of Eqn[1.1] under vectorial form, we have the system of differential equations that govern the displacements in the motion of the linear elastic body (e.g. Atkinson and Fox, 1980):

$$\mu (u_{j,ii} + u_{j,ii}) + \lambda u_{i,ij} + \rho_0 b_j = \rho_0 \frac{D^2 u_j}{Dt^2} \quad (1.7)$$

$$i, j = 1, 2, 3$$

where the repeated indices represent summation and the comma represents partial derivation.

$D$  stands for derivation in terms of material (Lagrange) coordinates.  $\mu$  and  $\lambda$  are the Lamé's constants,  $\rho_0$  the mass per unit volume of the material and  $b_j$  the components of the body forces.

If there is no motion Eqn[1.7] becomes (Novozhilov):

$$\mu \nabla^2 u_j + (\lambda + \mu) \frac{\partial e}{\partial x_j} + F_j = 0 \quad (1.8)$$

$$\text{where } e = \frac{\partial u_i}{\partial x_i} \text{ is the volume strain of the body} \quad (1.9)$$

$$\nabla^2 = \frac{\partial^2}{\partial(x_j, x_j)} \quad (1.10)$$

is the Laplace's operator.

$$\mu \equiv G = \frac{E}{2(1+\nu)} \quad \text{and} \quad \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \quad (1.11)$$

where E is the Young's Modulus and  $\nu$  the Poisson's ratio.

The system of Eqns[1.8] can be generalised for the porous linear elastic media with pore pressures  $p_w(x,y,z)$  under the form (Biot, 1944; Wilkins, 1964; Nemat Nasser and Chung, 1992). In the case of zero body force  $F_j$ :

$$G \nabla^2 u_j + \frac{G}{1-2\mu} \frac{\partial e}{\partial x_j} - \alpha \frac{\partial p_w}{\partial x_j} = 0 \quad (1.12)$$

and

$$k \nabla^2 p_w = \alpha \frac{\partial e}{\partial t} + \frac{1}{Q} \frac{\partial p_w}{\partial t} \quad (1.13)$$

where

$$\alpha = \frac{2(1+\nu) G}{3(1-2\nu) H}$$

and k the permeability of the porous media and G, H and Q elastic constants.

For a completely saturated porous material  $\alpha = 1$  and  $Q = \infty$  (Biot, 1944).

Eqns[1.12] and [1.13] can be further generalised for the case of the viscoelastic porous media with internal fluid flow (Biot, 1956)

These are only a few problems of Continuum Mechanics to be solved.

Discontinuum Mechanics is now rapidly developing with problems of Mechanics of Granular Materials, Block Mechanics and Mechanics of no tension or no-Compression Materials and Structures. Some of these problems and others in Continuum Mechanics lead to Operational Research solutions involving optimisation of functions of variables subjected to inequality constraints which can be of algebraic and/or differential type (differential inequalities) (Martins, 1985). Optimisation problems derive also from inverse (back analysis) problems, damage problems, etc.

Many of those problems are best solved by the "Discrete Element Method" (Cundall, 1971; Williams and Mustoe, 1993).

Also, some “evolution problems” lead to integral-differential equations of “parabolic” type (Wahlbin, in Light 1991, Zhang, 1990)

$$\frac{\partial u}{\partial t} + A(t)u + \int_0^t B(t, \sigma)u(\sigma)d\sigma = f(t) \quad t > 0, x \in \Omega \quad (1.14)$$

$$\begin{aligned} u &= 0 \text{ on } \partial \Omega \\ u(0) &= g(x) \end{aligned} \quad (1.15)$$

which govern transient fluid flow and deformation in elastic porous media (Habetler and Schiffman, 1970) and viscoelastic problems (Camino, 1988).

In Eqn[1.14]  $A(t)$  is a second order elliptic, symmetric, positive definite, linear (mostly) partial differential operator in space variables and  $B(t)$  is an at most second order partial differential operator, not necessarily elliptic.

The “hyperbolic” counterpart of Eqns[1.14] and [1.15] is :

$$\frac{\partial^2 u}{\partial t^2} + A(t)u + \int B(t, \sigma)u(\sigma)d\sigma = f(t) \quad (1.16)$$

but now with an initial boundary condition  $\frac{\partial u}{\partial t}(0) = h(x)$  (1.17)

added.

Oden et al. (1971) had dealt with this kind of problems.

The usual numerical methods, FE, BE and FDMs have cope with potential problems, both scalar and vectorial. However, so far, many of the kind of problems just referred have not yet been solved satisfactorily for cases with complex boundary conditions, inhomogeneities and non-linearities.

## 2. SOME KEY QUESTIONS

The main issue in this subject is to answer to the following questions:

- i. Why both FEMs, BEMs, FDMs and DEMs remain in use? If there was a method better than all the others to solve all kinds of engineering problems, that would be take over.
- ii. How many comparisons have been made so far between potentials (scalar or vectorial, i.e., displacements) and derivatives (fluxes or stresses) for the **same** points at boundary and at element sides and other points within the domain, calculated by the FEM, FEM and by the FDM, for the same physical problem with several discretization hypothesis?
- iii. How many error estimates comparisons for the calculated values by FEM, BEM and by FDM as indicated in ii. (not in terms of energy norms) have been done?

- iv. How does the calculation effort (time and cost) compares between the BEM, EM and the FDM, for various shapes of boundary and for various cases of singularities in the boundary geometry and in boundary conditions, to get the same accuracy.
- v. Are there specific problems where a method is the best for the solution of a given problem with an approximation just enough in the engineering practice? In the affirmative which are the problems better solved by each of the above methods?
- vi. Does the development of computer capabilities contribute to the coexistence of both methods or is a way for the prevailing of one of them?
- vii. Is there any way of relating the H and G matrices in the BEM Eqn  $Hu = Gq$  to the stiffness and flexibility matrices K and  $K^{-1}$  in the EM Eqn  $Ku=F$  for the same boundary points ?
- viii. Is it possible and easy to solve problems in nonhomogeneous (zoned) media with irregular shape domains sub-dividing them in sub-domains with regular shapes, and to cover each of these with circular domais and use for them particular solutions instead of the BEM fundamental solution which is not available for non-homogeneous media ?
- ix. Which is the best method to cope with Operational Research problems (Optimisation, inverse, sensitive analysis, etc.)?
- x. In what way each of those methods can be linked with the bifurcation and chaos theories? Does the development of these theories contributes to easier and/or more rigorous solution of the engineering problems? Which of these may first benefit of the recent development of those theories?

We do not have the velleity of giving answer to all these questions, but a number of them will be discussed, focusing the FE and the BEMs.

In relation to the first question it can be said that, broadly speaking, BEMs have advantage when all the dimensions of the domain are nearly the same, because the amount of data to be fed in the problem is much less in the case of the BEMs. However, due to the great development of pre-processors and post-processors the difference is becoming less relevant when there is need for graphical field representation of the values of the variables (mainly stresses or fluxes).

In relation to the second question we could not find in the literature one sole comparison done in that way. The same for the third to fifth questions. In relation to these what is usual is that most of the published comparisons between FE and BEM solutions refer mainly to the CUP time involved in the solutions and "accuracy" for very simple cases. Furthermore, error estimations are usually given in relation to the field variable (i.e., displacements for the case of elastostatics problems) and not of its derivatives (stress or fluxes in the case of scalar potential problems). Also, many of the error estimates are done for the energy norms and not for the stresses themselves. The important question would be to fix "a priori" the maximum acceptable error for a given engineering problem and to find the mesh refinement and type of element needed in both EM and BEM to reach such an accuracy and then compare the calculation effort necessary in each case.

On the other hand there is in literature a very small amount of comparisons between the stresses calculated at the same points by FEMs and by BEMs. Particularly important is to determinate the stress (or flux in the case of scalar potential problems) discontinuities at the boundaries of each element in the FEMs when the field variables are the displacements. The BEMs have no such discontinuities. However, in this case, the accuracy of the stresses calculated at any internal point are still dependent of the accuracy obtained for the elements of the matrices  $H$  and  $C$  in the final linear equation  $Hu = Bq$ .

In relation to question vi it seems that, in effect, computer rapid increase in capacity and speed of calculation make indifferent the use of BEM or EM, provide a safe and "robust" code is available.

In what refers question vii it can be said that such an exercise is possible removing the difficulty of  $F$  being a force and  $q$  being a traction and, therefore  $q$  needs to be integrated along the sides neighbouring each boundary node. This exercise would give a good insight in the relationships between BEM and FEM. It can be said that using the BEM a big FE can be created (Azeredo,1984).

Referring question viii it seems, in effect, to be possible, in the future, to solve by this method, problems of heterogeneous media in irregular domains (Arantes e Oliveira, 1965; Yasnitsky,1995).

Referring to question ix it seems that the EM has, so far, more published results than BEM for Operational Research (Optimisation) problems.

In relation to the last question a lot o research is needed in both methods to take advantage of the new theories of bifurcation and chaos in the solution of engineering problems. Perhaps coupling these and other numerical methods is the trend for the future.

(Zienkiewicz, Kelly and Bettess 1977, Brady and Wassying 1981, Varadarajan et al.1982, Li et al. 1986, Bossrit 1988, Stern and Taylor 1988, Von Storff 1989, Mang et al. 1989, Belytschko and Liu 1991, Lu, Belytschko and Liu 1991, Estorff and Antes 1991, Von Estorff 1992, Zhang et al. 1992, Zeng 1992, Lee 1993, Zeng and Zhao 1994)

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