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SOLUTION OF TRANSIENT DIFFUSIVE PROBLEMS USING THE DIRECT INTERPOLATION TECHNIQUE

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Abstract: The stability of the transient response of BEM (boundary element method) formulations, which use time-independent fundamental solutions, such as the double reciprocity formulation (DEM), is its greatest numerical difficulty. The coupling of direct integration schemes from the finite difference method with the boundary discretization model implies restrictions on the value of the time step. This means that such values are located within a limited range, and cannot be too large due to lack of consistency in the response, nor too small, as instability is produced. Recently, an alternative formulation called the direct interpolation method (MECID) was proposed, which uses the same radial interpolation functions as the MECDR, but approximating the entire core of the domain integral of the transient term. Since MECID has been shown to be more robust than MECDR, this work presents comparative simulations between the two formulations. The transient heat conduction problem was chosen due to its simplicity compared to dynamic problems. However, in these cases, restrictions related to the recommended range of integration interval are also observed, allowing to infer whether there is progress in the use of MECID in relation to MECDR.
Keywords: Boundary Element Method, Double Reciprocity, Direct Interpolation, Time Dependent Problems.

INTRODUCTION

Transient heat conduction problems are present in numerous industrial applications. In addition to producing changes in the geometry and materials of the equipment, temperature gradients are strongly related to the formation of thermal stresses, which are directly related to the problem of structural integrity. In physical terms, linear thermal problems, constituted solely by transient heat conduction, present a well-behaved response. This is because the phenomenon of transient diffusion is characterized by the slow transfer of energy from parts with higher potential toward regions of lower potential, Sagan (1963).

The flow of energy formed during the process tends to stabilize, reaching equilibrium, which characterizes the so-called stationary states or regimes. The period between the instant of application of external actions and the new stationary equilibrium position is called the transient stage. In mathematical terms, heat diffusion problems are expressed by parabolic partial differential equations, while acoustic wave propagation problems are given by hyperbolic partial differential equations. It is interesting to compare numerically the heat diffusion problems with the problems of scalar dynamics or propagation of acoustic waves.

In hyperbolic problems, energy from external actions propagates quickly, which causes severe gradients that may include discontinuities in the field of variables, as well as a vibratory response pattern, but not necessarily repetitive.

The formulations initially developed to analyze transient problems with the MEC employed fundamental time-dependent solutions, as reported by Mansur and Brebbia (1985). These formulations have high precision in their results, but demand considerable computational time in addition to elaborate programming.

In 1983, Nardini and Brebbia proposed a new formulation using a simpler fundamental solution, independent of time, which made it possible to obtain answers in a simpler way using the BEM: the formulation with Double Reciprocity (DEM), which uses an adequate sequence of functions radials to approximate the primal variable and thus transform the domain integral into a boundary integral.

MECDR uses a simplified but mathematically related fundamental solution to the stationary diffusion problem. When using this stationary fundamental solution, the best strategy to obtain a response over time is given by direct integration schemes, Bathe (1992). Such schemes require that the equilibrium of the system be obeyed only at discrete instants of the process, among which linear or constant variations are admitted for the variables of the problem and their temporal derivatives.

As exposed, the stability of the response with MECDR consists of its greater numerical difficulty. These difficulties are more accentuated in dynamic problems.

Aiming to improve the formulation of the Boundary Element Method using radial basis functions (Buhman, 2003), Loeffler et al. (2015) proposed a new model called MECID, which also transforms domain integrals into boundary integrals through the use of a sequence of radial basis functions, such as the MECDR. However, although it uses radial basis functions, it approximates the entire kernel to the domain integral, unlike MECDR, consisting of a numerical process very similar to a classical interpolation. In this model, the choice of primitive functions does not keep any compromise in reproducing the principles of reciprocity, that is, the differential operator of the primitive radial functions does not correspond to the particular solutions of the governing differential equation. This means that MECID can be used in more complex problems, with lower computational cost.

INTEGRAL GOVERNMENT EQUATION

Considering the mathematical procedures known from the MEC, the boundary integral equation referring to the transient heat transfer problem is given by Eq. (1).

$$c(\xi)u(\xi) + \int_\Gamma u(X)q^*(\xi;X)d\Gamma - \int_\Gamma q(X)u^*(\xi;X)d\Gamma =$$

$$-k\int_\Omega \dot{u}(X)\, u^*(\xi;X)d\Omega. \tag{1}$$

In Eq. (1), the scalar u(X) is the potential, q(X) is its normal derivative, u*(ξ;X) is the fundamental Laplace solution, and q*(ξ;X)) is its normal derivative. The diffusivity of the system is equal to k, ξ is a particular point called the source point, and X is the field point. The coefficient c(ξ) depends on the position of the source point relative to the domain: Ω(X); however, if this point is located on the contour $\Gamma(X)$, the value of (ξ) also depends on the smoothness of the same, Brebbia et al. (1984).

The fundamental solution used in Eq. (1) corresponds to the analytical expression for the potential produced in an infinite medium governed by the Poisson equation in which a concentrated source acts at the source point ξ, that is:

$$u^*_{,ii}(\xi;X) = -\Delta(\xi;X). \tag{2}$$

In Eq. (2), the function: Δ(ξ;X) is called the Dirac Delta function. Solving Equation 2), we have:

$$u^*(\xi;X) = -\frac{\ln[r(\xi;X)]}{2\pi} \tag{3}$$

$$q^*(\xi;X) = -\frac{1}{2\pi r(\xi;X)} r_i(\xi;X)n_i(X). \tag{4}$$

In the Equation 3) and Equation 4) r(ξ,X) is the Euclidean distance between the source point and the field point, and ni(X) is the external normal to the contour (X). The difference between MECDR and MECID concerns the approach of the domain integral referring to the thermal inertia of the system, that is, the right side of Equation 1).

The basic idea of MECID is to interpolate the complete kernel of the domain integral on the right-hand side of Equation (1), including the fundamental solution, as shown in

Equation 5).

$$\dot{u}(X)u^*(\xi;X) \cong {}^{\xi}\dot{\alpha}^i F^i(X^i;X). \quad (5)$$

The same radial functions are used here and the same type of procedure performed for MECDR is also applied, but now the difference is that the coefficients ξαi depend on the source point. Such coefficients can be obtained by solving the system after the discretization, in Eq. (6):

$$[{}^{\xi}\dot{\alpha}] = [F]^{-1}[{}^{\xi}\Lambda][F]\dot{\alpha} = [F]^{-1}[{}^{\xi}\Lambda](\dot{u}). \quad (6)$$

The domain integral term is transformed into a boundary integral using a primitive function:

$$\int_{\Omega} {}^{\xi}\alpha^i F^i(X^i;X)d\Omega = \int_{\Omega} {}^{\xi}\alpha^i \Psi^{\,i}_{,jj}(X^i;X)d\Omega = \int_{\Gamma}$$

$${}^{\xi}\alpha^i \Psi^{\,i}_{,j}(X^i;X)n_j(X)d\Gamma = {}^{\xi}\alpha^i \int_{\Gamma} \eta^i(X^i;X)d\Gamma. \quad (7)$$

For convex domains, the procedure shown in Equation 7) can be done avoiding the adoption of a primitive function, using a special integration technique, Campos (2020). In MECID, as the fundamental solution also composes the core to be interpolated, so that the source point ξ has the same position as the field points X, it is necessary to carry out a regularization procedure, as proposed by Hadamard (1932) and detailed by Loeffler, Zamprogno, Bulcão and Mansur (2017).

In this sense, the following procedure is performed on the integral term on the right side of Eq. (1):

$$c(\xi)u(\xi) + \int_{\Gamma} [u(X)q^*(\xi;X) - q(X)u^*(\xi;X)]d\Gamma = -k\int_{\Omega} u^*$$

$$(\xi;X)[\dot{u}(X) - \dot{u}(\xi)]d\Gamma - k\dot{u}(\xi)\int_{\Omega} u^*(\xi;X)d\Omega \quad (8)$$

Due to the regularization procedure, the basic sentence given by Eq. (5) includes the first two integrals on the right-hand side of Eq. (8):

$$\int_{\Omega} u^*(\xi;X)[\dot{u}(X) - \dot{u}(\xi)]d\Gamma \approx \int_{\Omega} {}^{\xi}\dot{\alpha}^i F^i(X^i;X)d\Omega. \quad (9)$$

The matrix treatment of this equation, considering typical MEC procedures, is detailed in a previous work, Loeffler, Cruz and Bulcão (2015), resulting in the following matrix system, according to Eq. (10):

$$[H]\{u\} - [G]\{q\} = -k[C]\{\dot{u}\} \quad (10)$$

Note that the thermal inertia matrix [C] is built from the interpolation of the entire core of the transient term of the governing equation (Eq. 10), accompanied by numerical procedures that include the regularization of the integrals. This means that the MECID procedure is eminently an interpolation procedure, and therefore requires a significant number of internal points to obtain a good representation of the potential within the domain.

As it can be easily found in the literature, see Wrobel and Brebbia (1984), the final matrix equation for the MECDR formulation is given according to Equation (11).

$$[H]\{u\} - [G]\{q\} = -k\{[G][\eta] - [H][\psi]\}\{\dot{u}\} \quad (11)$$

The matrices [η] e [ψ] are interpolation matrices, formed by primitives of radial functions. However, the procedure is not a simple interpolation as in the case of MECID.

DISCRETIZATION OF TIME

For linear problems, incremental time advance schemes have been widely used in the main methods based on the idea of domain discretization, such as the Finite Element Method, the Finite Volume Method and the Boundary Element Method. It can be observed that the behavior of these algorithms is quite simple and satisfactory. However, many of the demonstrations and postulations of stability criteria were based on matrix systems of equations generated by the Finite Difference Method.

In transient heat problems, the energy flux formed during the process tends to stabilize, reaching a state of equilibrium typical of parabolic problems. It can be observed that linear thermal problems constituted only by heat conduction present, in general, a well-behaved response.

The finite difference scheme approximates the rate of temperature change in the form of Eq. (12):

$$\dot{u}_n = \frac{u_n - u_{n-1}}{\Delta t} \tag{12}$$

In the Equation (12), Δt is the interval of integration and n are the equilibrium instants. For the heat problems solved here, the equilibrium matrix equation, expressed in terms of a present instant: t_n, is given by Equation (13):

$$[H]\{u_n\} - [G]\{q_n\} = -k[C]\{\dot{u}_n\} \tag{13}$$

Substituting Eq. (12) in Eq. (13), we obtain Eq. (14):

$$\{k[C] + \Delta t[H]\}\{u_n\} = \Delta t[G]\{q_n\} - k[C]\{u_{n-1}\} \tag{14}$$

It is observed by the structure of Equation (14) that it describes a transitory balance between two consecutive instants of time, involving the present instant and the immediately previous instant. Choosing the time step is a crucial step. An estimate used in earlier work, Wrobel and Brebbia (1984), is given by Eq. (15):

$$\Delta t = \frac{\Delta L^2}{k} \tag{15}$$

In this last equation, ΔL is the length of the largest contour element used. However, this criterion was proposed for a boundary element formulation that uses a time-dependent fundamental solution, thus being a different formulation from the one used here. Therefore, a new criterion for the integration step must be investigated.

APPLICATION EXAMPLE

Fig. 1 shows a square plate with unit sides subjected to a temperature gradient. The left vertical edge is subjected to zero temperature and the right vertical edge to a unit flow. Horizontal edges have zero flow condition. The thermal diffusivity is unity. The analytical solution to the problem is given by Eq. (16).

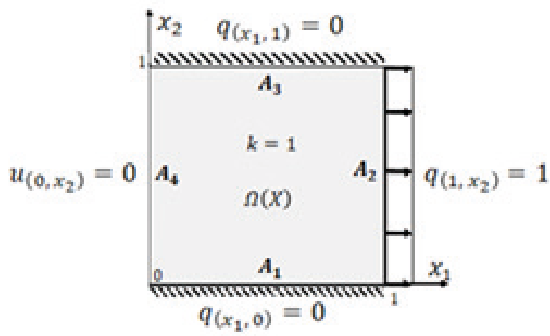

Figure 1 - Temperature gradient on the square plate

$$u(x,t) = 1.0 - \sum_{n=1,3,5,7}^{\infty} \frac{8}{n^2\pi^2} e^{-\frac{n\pi t}{2}}. \tag{16}$$

Two meshes with double nodes at the vertices and different amounts of linear contour elements and internal interpolation points (poles) were considered: the simplest mesh has 84 nodal points on the contour and 25 poles, while the most refined mesh has 164 nodal points and 25 poles. 144 poles. In addition, two different radial functions were used: the simple radial function (r) and the logarithmic or thin-plate function (r2ln(r)). Based on the results of several previous works, these functions were the most successful, Loeffler, Cruz and Bulcão (2015).

The direct comparison with the analytical solution was made in two instants: at t = 1 s and t = 3 s. The analytical values at these instants are respectively 0.83148 and 0.9927 temperature units.

It must be noted that the proposed optimal time increment, given by Eq. (15), did not present positive results in the simulations presented here. This proposal was used in previous works with double reciprocity, Loeffler, Cruz and Bulcão (2015), using constant elements and problems with other geometry. Furthermore, in the present work linear contour elements are used.

RESULTS FOR THE FORMULATION WITH DOUBLE RECIPROCITY

Table 1 presents the results obtained using the simple radial function for two different meshes, considering the temperature values on the right vertical edge, where the unitary flux is applied. It can be observed that the refinement of the mesh improves the threshold value and the accuracy of the response curve, also increasing the minimum values of the step capable of producing stable results. However, it was possible to obtain stable results only for step values greater than 0.05 s.

In dynamics, the biggest restriction of double reciprocity consists of limiting a minimum integration step, a practically non-existent requirement in other discrete methods. In general, large steps produce instability if certain conditions are not met; however, reduced steps can be used. Unnecessarily small integration steps add computational time.

Table 2 shows the results with the logarithmic function. The results for small steps are also unstable, and the sensitivity of this function was even greater in this respect, producing stable results only for delta $\Delta t > 0.1$s.

Comparing the behavior of the two radial functions with regard to stability, it can be seen that using the less refined mesh, the simple radial basis function works better than the logarithmic function, as it is possible to find stable results from a step Δt equal to 0.05, although the accuracy obtained is low. However, with the finer mesh the results are better for this same step. The results can be considered good for both functions from a time increment equal to 0.1.

Finally, it is observed that the results of the simple radial function tend to exceed the analytical value, while the results of the logarithmic function are always below the limit value, tending to take a long time for the unit. Fig. 2 illustrates this behavior for the mesh with 84 contour points and 25 internal interpolation points.

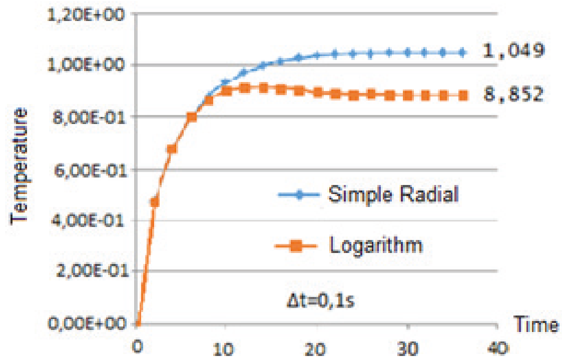

Figure 2 - Comparison of MECDR response curves over time for temperature on the right edge

RESULTS WITH THE FORMULATION WITH DIRECT INTERPOLATION

Table 3 shows the results obtained with MECID using the same grids used previously. It is observed that it is possible to obtain results with much smaller integration steps than the MECDR. This indicates greater precision in the construction of the matrix referring to the thermal inertia or the transient term of the governing equation. Mesh refinement also reduces the value of the integration step without producing instability and improves the accuracy of the results. Interestingly, when using the logarithmic function with MECID, the results were even slightly better than those obtained with the simple radial function, as shown in Table 4.

Numerical values of temperature with the logarithmic function were higher than those of the simple radial function at time t = 1s, that

Time increment Δt	Mesh with 84PN/25PI		Mesh with 164PN/144PI	
	Temp. t =1s. Analytics =0,83148	Temp. t =3s Analytics =0,9927	Temp. t =1s Analytics =0,83148	Temp. t =3s Analytics =0,9927
Δt=0.02	30.814	1189.05	1.4958	3.5180
Δt=0.03	1.4763	4.0395	1.2032	1.6957
Δt=0.05	1.0579	1.2932	1.0086	1.1712
Δt=0.1	0,9391	1,0496	0,9482	1,0695
Δt=0.2	0,9004	1.0092	0,8961	1.0060

Table 1 - Summary of results for double reciprocity with simple radial function

Time increment Δt	Mesh with 84PN/25PI		Mesh with 164PN/144PI	
	Temp. t=1s Analytics =0,83148	Temp. t=3s Analytics = 0,9927	Temp. t=1s Analytics =0,83148	Temp. t=3s Analytics = 0,9927
Δt=0.05	49,772	instabilidade	6.05734	122.3080
Δt=0.1	0,9020	0.8855	0,8708	0,8980
Δt=0.2	0,8928	0,9835	0,8878	0,9793
Δt=0.3	0,8815	0,9950	0,7941	0,9922

Table 2 - Summary of results for double reciprocity with thin plate function

Time increment Δt	Mesh with 84PN/25PI		Mesh with 164PN/144PI	
	Temp. t=1s Analytics =0,83148	Temp. t=3s Analytics =0,9927	Temp. t=1s Analytics =0,83148	Temp. t=3s Analytics =0,9927
Δt=0.005	increasing instability	increasing instability	0,9946	1.0938
Δt=0.01	13,4232	increasing instability	0,9315	1.0026
Δt=0.02	0,9353	1,0914	0,9274	0,9949
Δt=0.1	0,9101	0,9972	0,9106	0,9988
Δt=0.2	0,8902	0,9977	0,8908	0,9978

Table 3- Summary of results for MECID with simple radial function

Time incremente Δt	Mesh with 84PN/25PI		Mesh with 164PN/144PI	
	Temp. t=1s Analytics = 0,83148	Temp. t=3s Analytics = 0,9927	Temp. t=1s Analytics =0,83148	Temp. t=3s Analytics =0,9927
Δt=0.005	increasing instability	increasing instability	0,9724	1,0911
Δt=0.01	0,9338	increasing instability	0,9743	0,9994
Δt=0.02	0,8420	0.9983	0,9366	0,9982
Δt=0.1	0,9107	0,9973	0,9107	0,9997
Δt=0.2	0,9209	1,0003	0,9998	0,9998

Table 4- Summary of results for MECID with logarithmic function

is, at moments still in the initial phase of the transient process, mainly with smaller time increments, as for Δt = 0,02s. Mesh refinement allowed the adoption of smaller integration steps. Fig. 3 shows the MECID response curve for the two radial functions employed, which now has a similar performance for an integration step Δt = 0.1s. The mesh used was the least refined.

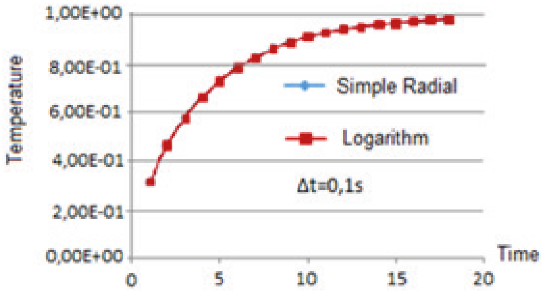

Figure 3 - Comparison of MECID response curves over time for temperature on the right edge

CONCLUSIONS

As noted, due to the inadequacy of the time increment criterion presented in the literature, it would be possible to choose a more adequate estimate of the integration step, both for MECDR and MECID, which must be similar. However, a greater number of simulations must be performed in this sense, varying the size and order of the boundary elements used, as well as the type of boundary conditions involved.

The presented results confirm the conclusions obtained in the solution of other scalar field problems: the matrix resulting from the application of the typical MECID interpolation procedure is more precise than the corresponding matrix obtained by MECDR. Not only the transient response curves prove this greater robustness of the MECID, but also the greater stability of the smallest time increment values was clearly observed.

The relatively efficient numerical behavior of parabolic problems in relation to hyperbolic or dynamic problems has induced many works to disregard questions related to the stability of the first order algorithm in the discretization of temperature rates. The simulations presented here show that some care is needed when choosing the integration step. Certainly, the use of MECID in dynamic problems will face much greater challenges in this regard, since the stable representation of the response over time, in these cases, is much more complex. However, the indication that the matrix related to the transient term in heat conduction problems was much better built by MECID, compared to MECDR, encourages its immediate application in cases of dynamic response.

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