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DIRICHLET BOUNDARY CONDITIONS IN ELEMENT FREE GALERKIN METHOD

L. Gavete[*], S. Falcón[†], and J.C.Bellido[††]

[*]Escuela Técnica Superior de Ingenieros de Minas
Universidad Politécnica
c/ Rios Rosas 21 ,28003 Madrid, Spain
[†] Union Fenosa Distribución
c/ Capitán Haya 53, 28020, Madrid, Spain
e-mail: sfalcon@uef.es
[††] CEU-Arquitectura
c/Camino de las Moreras s/n.,28040 Madrid, Spain
e-mail: jcbell@ceu.es

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Abstract. *Accurate imposition of essential boundary conditions is a main drawback in the use of the Element Free Galerkin (EFG) method. A way to solve the problem, is to use a constrained variational principle with a penalty function. This new treatment for essential boundary conditions is simple and logical and works very well in all numerical examples for 2-D potential problems that are presented here. It is shown that the present constrained variational formulation together with the EFG method and appropriated weighting function exhibit very high accuracy and stability.*

The method has been tested for the case of a complex domain with irregular grid of nodes. Also using penalty functions is important to use spline weighting functions with radius of influence as small as possible, but with small overlapping, in order to assure that the approximation function was closed to interpolation. A guide on the EFG penalisation method is given, considering the possibility of using variable radius of influence for each point.

1. INTRODUCTION

The diffuse element method developed by Nayroles et al.[1] is a new way for solving partial differential equations. In this method, only a mesh of nodes and a boundary description is needed to develop the Galerkin equations. The approximating functions are polynomials fitted to the nodal values of each local domain by a weighted least squares approximation.

Belytschko et al.[2,3] developed an alternative implementation using moving least squares (MLS) approximation as were defined by Lancaster and Salkauskas[4]. They called their approach the Element Free Galerkin (EFG) method. In their work, Belytschko and his co-workers have introduced a background cell structure in order to carry out integration by numerical quadrature and Lagrange multipliers to enforce essential boundary conditions. Liu et al.[5] have recently proposed a different kind of "gridless" multiple scale methods based on reproducing kernel and wavelet analysis (RPKM method).

Oñate et al.[6] focused on the application to fluid flow problems with a standard point collocation technique. All these methods can be considered as Finite Point or Meshless Methods.

On the one hand, Duarte and Oden[7] and on the other, Babuska and Melenk[8] have shown how meshless methods can be based on the partition of unity. In relation to, the first authors have developed a new method that they denominate h-p clouds.

This paper begins with a brief summary of EFG method. The rest of the paper is devoted to issues related to imposition of essential boundary conditions in the EFG method. The main contribution of the present paper is the proposal of a simple and effective strategy for the imposition of essential boundary conditions in the EFG method.

2. ELEMENT FREE GALERKIN METHOD

In the Element Free Galerkin Method, around a point x, the function $u^h(x)$ is locally approximated by:

$$u^h(\mathbf{x}) = \sum_{i=1}^{m} p_i(\mathbf{x}) a_i(\mathbf{x}) = \mathbf{p}^T(\mathbf{x})\mathbf{a}(\mathbf{x}) \tag{1}$$

where m is the number of terms in the basis, the monomial $p_i(x)$ are basis functions, and $a_i(x)$ are their coefficients, which as indicated, are functions of the spatial co-ordinates x.

The coefficients $a_i(x)$ are obtained by performing a weighted least square fit for the local approximation, which is obtained by minimising the difference between the local approximation and the function. This yields the quadratic form

$$J = \sum_{I=1}^{n} w(d_I)(\mathbf{p}^{\mathbf{T}}(\mathbf{x}_{\mathbf{I}})\mathbf{a}(\mathbf{x}) - u_I)^2 \tag{2}$$

where $w(d_I) = w(x-x_I)$ is a weighting function with compact support.

Equation (2) can be rewritten in the form

$$J = (P\,a - u)^T W(x)\,(P\,a - u) \tag{3}$$

where

$$u^T = (u_1,u_2,\ldots,u_n) \tag{4}$$

$$\mathbf{P} = \begin{bmatrix} \{\mathbf{P}(\mathbf{x}_1)\}^T \\ \ldots \\ \{\mathbf{P}(\mathbf{x}_n)\}^T \end{bmatrix} \tag{5}$$

$$\{\mathbf{P}(\mathbf{x}_i)\}^T = \{P_1(\mathbf{x}_i),\ldots,P_m(\mathbf{x}_i)\} \tag{6}$$

$$\mathbf{W} = diag\left[w_1(\mathbf{x}-\mathbf{x_1}),\ldots,w_n(\mathbf{x}-\mathbf{x_n})\right] \tag{7}$$

To find the coefficients a, we obtain the extremum of J by

$$\partial J/\partial a = A(x)\, a(x) - H(x)\, u = 0 \tag{8}$$

where

$$A = P^T\, W(x)\, P \tag{9}$$

$$H = P^T\, W(x) \tag{10}$$

and therefore

$$a(x) = A^{-1}(x)\, H(x)\, u \tag{11}$$

The dependent variable u^h can then be expressed as

$$u^h(\mathbf{x}) = \sum_{I=1}^{n(x)} \Phi_I(\mathbf{x})\, u_I \tag{12}$$

where

$$\Phi_I(x) = p^T(x)\, A^{-1}(x)\, H_I(x) \tag{13}$$

with H_I being the column I of H.

The partial derivatives of the MLS shape functions are obtained as

$$\Phi_{I,j}(\mathbf{x}) = \mathbf{p}_{,\mathbf{j}}^{\mathbf{T}}\, \mathbf{A}^{-1}\, \mathbf{H}_I + \mathbf{p}^{\mathbf{T}}\left[\mathbf{A}^{-1}\left(\mathbf{H}_{I,j} - \mathbf{A}_{,j}\mathbf{A}^{-1}\mathbf{H}_I\right)\right] \tag{14}$$

3. PENALTY FUNCTION

One of the biggest problems in the implementation of meshless methods resides in that the used approach is not an interpolation. In general, MLS approximation, lacks the delta function property of the usual FEM shape function, in that

$$\Phi_I(x_J) = d_{IJ} \tag{15}$$

where Φ_I is the Ith shape function evaluated at a nodal point x_J and δ_{IJ} is the Kronecker delta. This implies a difficulty when imposing the essential boundary conditions that it has led to the appearance of different solutions like they are, among other, Lagrange multipliers (Belytschko et al.[2]), or modified variational principles (Lu et al.[3]).

According to Krongauz and Belystchko[9], the most satisfactory solution is the use of a joining with finite elements. Other important method to treat essential boundary conditions is the one by Mukherjee and Mukherjee[10] taking into account that the method of moving least squares employed is an approximation instead of interpolation.

Another solution consists on to force that the weighting functions are singular in the boundary where the condition type Dirichlet is imposed (Duarte and Oden[11]). We can obtain interpolating shape functions using singular weights[4].

There are other techniques for meshless methods: in RPKM method, different procedures to generate admissible approximations for treatment of essential boundary conditions has been proposed by Günther and Liu[12] and Gosz and Liu[13]. Also in RPKM method, another interesting technique to treat essential boundary conditions has been introduced by Chen et al.[14] by the use of a method that transforms the generalised displacements to nodal displacements.

While these methods provide a means of overcoming the inherent difficulties of meshless methods, they also have some limitations and drawbacks. For example, Lagrange multipliers pose difficulties in that the resulting stiffness matrix is no longer positive definite or banded, and the size of the problem increases. While modified variational principles enable the stiffness matrix to remain positive definite and banded, they are reported to be less accurate and they are rather inconvenient. Coupling with finite elements wastes some of the advantages of meshless approximates and can result in discontinuities in the derivatives of the approximates.

In this paper we consider moving least squares method with appropriated weighting functions, and areas of influence for each one of them. Then, we obtain a local approximation that is close to the interpolation. As we employ a local approximation, we need to satisfy the essential boundary conditions only approximately. A way to do it, is to use a constrained variational principle with a penalty function.

Consider the problem of making a functional Π stationary, subject to the unknown u obeying some set of additional relationships or constraints, which can be introduced at some points or over boundaries of the domain Ω.

For instance, if we require that u obey

$$P(u) = 0 \qquad \text{on} \quad \partial\Omega \tag{16}$$

we would add to the original functional Π the term

$$a\int_{\partial\Omega} \mathbf{P}^{\mathbf{T}}(\mathbf{u})\mathbf{P}(\mathbf{u})d(\partial\Omega) \tag{17}$$

then we obtain

$$\Theta = \Pi + a\int_{\partial\Omega} \mathbf{P}^{\mathbf{T}}(\mathbf{u})\mathbf{P}(\mathbf{u})d(\partial\Omega) \tag{18}$$

in which α is a penalty number and then require the stationarity of the functional Θ will satisfy the constraints only approximately.

Alternatively, if the constraint P is applicable only at one or more points of the boundary, then the simple addition of $P^T(u)\ P(u)$ at these points to the general functional Π will introduce a discrete number of constraints.

In practical application with finite elements the method of penalty functions has proved quite efective[15]. Penalty method with Smooth Particle Hydrodynamics (SPH) techniques has been applied by Bonet and Kulasegaram[16].

In RPKM method[17], it is important the choice an optimal dilation parameter of a given windows function. Also in RPKM method[18], it has been demonstrated in 1D that when a given (arbitrary) window only covers three points and linear order polynomials are used as the basis functions, the RPKM shape function becomes a global linear finite element shape function.

In EFG method if our aim is to employ penalisation method with accuracy, it is necessary that the approximation involved is close to an interpolation. In order to do this, it is sufficient to consider areas of influence for each weighting function which are a little overlapped but with sufficient number of nodes for the involved approximation. Considering it, we take as functions P(u) directly the essential boundary condition.

4. TWO DIFFERENT APPROACHES: LAGRANGE MULTIPLIERS AND PENALTY FUNCTIONS

In order to compare the accuracy of the penalisation method, we consider two different approaches for approximation of essential boundary conditions in the EFG method: Lagrange multipliers and Penalty functions. We shall use Lagrange multipliers with physical meaning as originally proposed for EFG method by Lu, Belytschko and Gu[3] and the standard penalty function formulation together with the EFG method. In both cases a direct procedure (Gauss-Jordan) has been used to solve the system of linear equations. Ill conditioning of the resulting matrices has not been observed.

Different examples have been developed in other to check the capabilities of both numerical methods. Let us consider the Laplace equation in 2-D

$$\nabla^2 u = 0 \quad \text{in}\ \Omega \tag{19}$$

with boundary conditions $u = u_d$ on $\partial\Omega_u$, $\partial u/\partial n = v_d$ on $\partial\Omega_v$

where $\partial\Omega=\partial\Omega_u\cup\partial\Omega_v$ is the boundary of Ω and n is the usual unit outward normal to $\partial\Omega$ at any point of it being $\Omega =]0,1[\times]0,1[$.

Examples	Solution	Boundary conditions
E1	$u = x + y$	Dirichlet in all the boundary
E2	$u = -x^3 - y^3 + 3xy^2 + 3x^2y$	Dirichlet in all the boundary
E4	$u = -x^3 - y^3 + 3xy^2 + 3x^2y$	Neumann (v_d=0) in x= 0 or y =0 and Dirichlet in the rest of the boundary
T1	$u = x^2 - y^2$	Dirichlet in all the boundary
T2	$u = e^x \sin y$	Dirichlet in all the boundary
T3	$u = \mathrm{Log}(x^2+y^2)$	Dirichlet in all the boundary

A global error measure is defined as

$$Error_f = \frac{1}{|f|_{max}}\sqrt{\frac{1}{N_N}\sum_{i=1}^{N_N}(f_i^{(e)} - f_i^{(n)})^2} \qquad (20)$$

where f can be u, ∂u/∂x,∂u/∂y, the superscripts (e) and (n) refer to the exact and numerical solutions, respectively, and N_N is the total number of nodes. We take as numerical solution, the approximated values calculated using MLS shape functions.

The EFG method with linear shape functions was used including Penalty functions or flux Lagrange multipliers to enforce essential boundary conditions. Two regular meshes of nodes were considered: a mesh with 4x4 cells, 9×9 nodes and a mesh with 8×8 cells, 9x9 nodes(see fig.1). The integration space was defined in each case with cells formed by 9 or 4 nodes and in each cell Gauss quadrature was used.

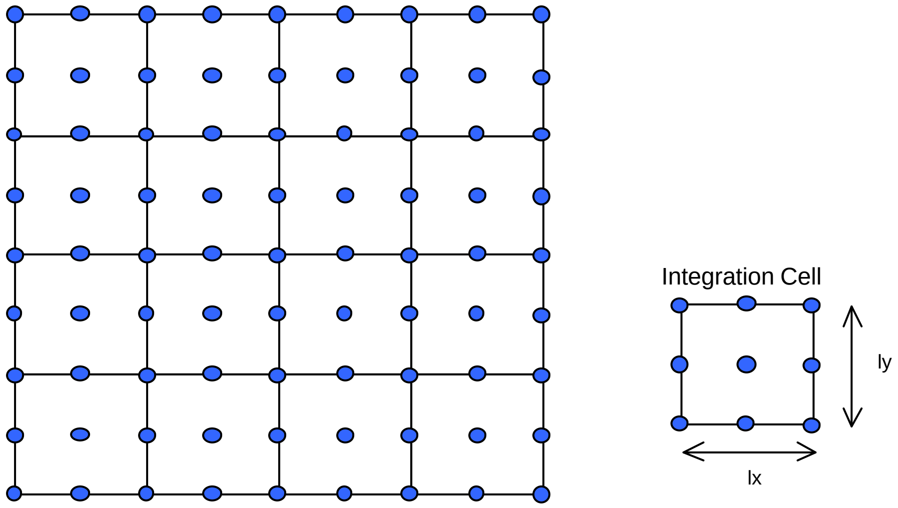


Figure 1: 9x9 mesh of nodes, 4x4 cells.

For both cases Penalty function and flux Lagrange multipliers, the following three weight functions were tested:

a) Polynomial weight function (Quartic Spline):

$$w_i(d) = 1 - 6\left(\frac{d}{dm}\right)^2 + 8\left(\frac{d}{dm}\right)^3 - 3\left(\frac{d}{dm}\right)^4 \qquad (21)$$

when $d \le dm$, and $w_i = 0$ when $d > dm$; and where

$d = \sqrt{(x - x_i)^2 + (y - y_i)^2}$ and dm = rinf

b) Polynomial weight function (Cubic Spline):

$$w_i(d) = \begin{cases} \frac{2}{3} - 4\left(\frac{d}{dm}\right)^2 - 4\left(\frac{d}{dm}\right)^3 & for\ d \le \frac{1}{2}dm \\ \frac{4}{3} - 4\left(\frac{d}{dm}\right) + 4\left(\frac{d}{dm}\right)^2 - \frac{4}{3}\left(\frac{d}{dm}\right)^3 & for\ \frac{1}{2}dm < d \le dm \\ 0 & for\ d > dm \end{cases} \tag{22}$$

$\mathrm{d} = \sqrt{(\mathrm{x}-\mathrm{x_i})^2 + (\mathrm{y}-\mathrm{y_i})^2}$ and dm = rinf

c) Exponential weight function (Gauss type):

$$w_i(d) = \frac{e^{-\left(\frac{d}{c}\right)^2} - e^{-\left(\frac{dm}{c}\right)^2}}{1 - e^{-\left(\frac{dm}{c}\right)^2}} \tag{23}$$

when d ≤ dm, and $w_i = 0$ when d > dm; and where

$d = \sqrt{(x-x_i)^2 + (y-y_i)^2}$

$c = \boldsymbol{b} \cdot c_i$

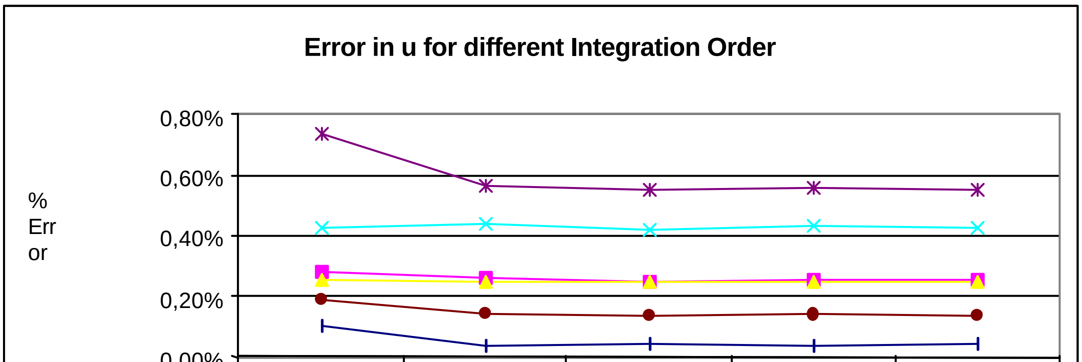
dm = rinf

with c_i is the side of the square cell

In the above, c is a parameter which controls the shape of the weight function and d_m is the size of the support for the weight function and determines the influence domain (rinf) of x_i.

In the following results firstly, we study the use of the penalisation function, and secondly we compare with flux Lagrange multipliers. As it is shown in figure 2, in the penalisation method the error is stable with the integration order for the different cases considered.

The penalisation parameter α can take any value between 10^3 and 10^{31}, obtaining similar results. For $\alpha < 10^3$ the method can not give correct results because the parameter is very small. The results obtained for $\alpha > 10^{31}$ are due to the limited sizes of the variables.



	2x2	3x3	4x4	5x5	6x6
E1 4x4 cells	0,1035%	0,0360%	0,0449%	0,0369%	0,0387%
E2 4x4 cells	0,2819%	0,2624%	0,2476%	0,2525%	0,2510%
E2 8x8 cells	0,2517%	0,2506%	0,2503%	0,2502%	0,2503%
E4 4x4 cells	0,4256%	0,4392%	0,4229%	0,4321%	0,4286%
T1 4x4 cells	0,7331%	0,5670%	0,5517%	0,5597%	0,5528%
T2 4x4 cells	0,1874%	0,1420%	0,1365%	0,1371%	0,1363%

Figure 2: Error in u for different integration orders. (rinf = 0.292, Penalisation Parameter 10^{15}, Quartic Spline weight function).

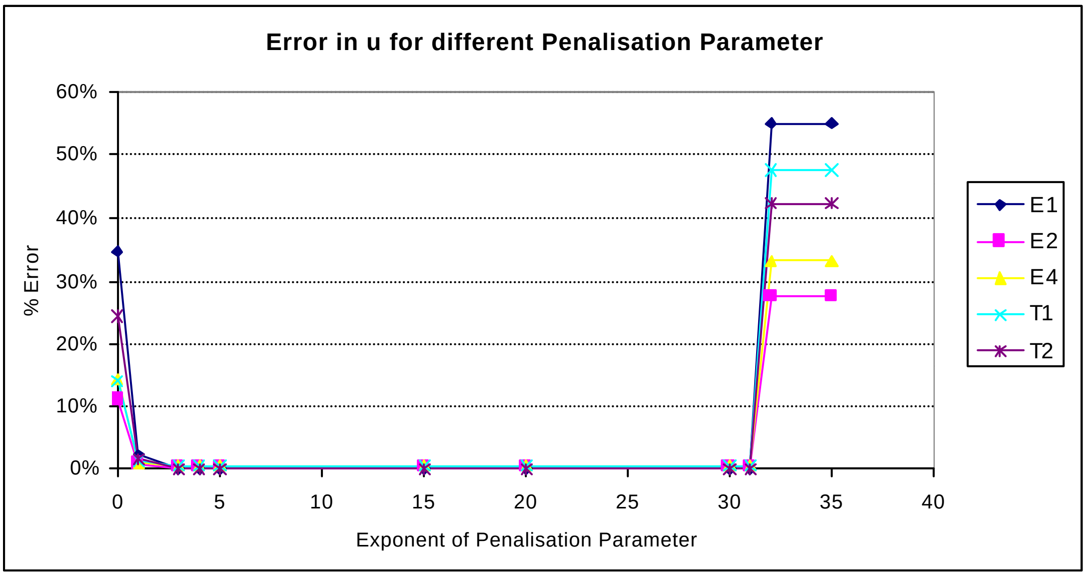


Figure 3: Error in u for different penalisation parameters.

As it is shown in figure 4, the area of influence of the weighting function is an important parameter in the accuracy of the results obtained. To obtain a better local approximation is necessary to take the areas of influence which are a little overlapped, assuring at the same time that the number of the points covered is sufficient for the approximation chosen.

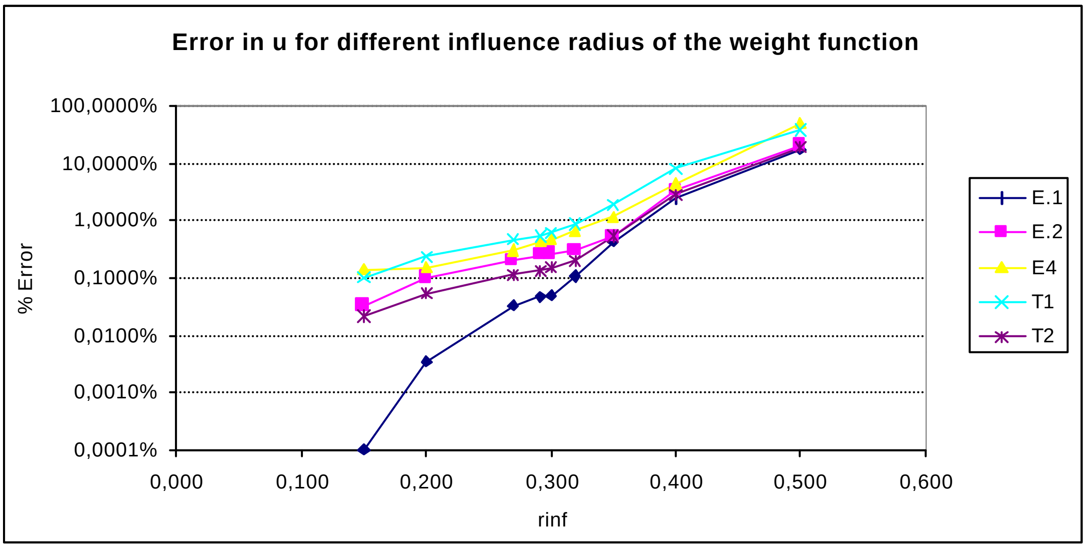


Figure 4: Error in u for different areas of influence.

In table 1, we can see the results obtained for the function u as compared with those of Mukherjee and Mukherjee[10], using their new strategy (including fluxes as Lagrange multipliers with new definition of J) and old strategy (also considering flux Lagrange multipliers as defined in Lu et al.[3]), for the case of 4x4 cells and 9x9 nodes.

Strategy of treatment of Essential Boundary Conditions	Penalty Function (10^{15})		Muk. & Muk.[10] New Strategy	Muk. & Muk.[10] Old Strategy
Weighting Function Data	Quartic Spline rinf = d= 0.15	Gauss rinf=d= 0.15 c = 0.48	Gauss, d = 0.32 ; c = 0.48	
Integration Order	4x4	4x4	6x6	6x6
E1	0.0001 %	0.0732 %	0.51 %	---
E2	0.0318 %	0.2073 %	1.85 %	17.97 %
E4	0.1432 %	2.9071 %	0.5 %	3.06 %

Table 1 : Comparison of results

In Table 2 we have the results obtained with flux Lagrange multipliers and Penalisation for the cases E2 and T3 with different number of cells of integration for the three weighting functions considered and rinf = 0.32. Best results for penalisation method are obtained with quartic and cubic spline weighting functions. Decreasing rinf can ameliorate the penalisation results.

Strategy of treatment of Essential Boundary Conditions		Flux Lagrange Multipliers			Penalisation Penalty Function (10^{15})		
Weighting Function Data		Quartic Spline rinf = d= 0.32	Cubic Spline rinf = d= 0.32	Gauss rinf=d= 0.32 c=0.48	Quartic Spline rinf = d= 0.32	Cubic Spline rinf = d= 0.32	Gauss rinf=d= 0.32 c = 0.48
Integration Order		6x6	6x6	6x6	6x6	6x6	6x6
E2 8x8 cel. 9x9 nod.	u	10.609	10.619	11.974	0.293	0.316	4.964
	∂u/∂x	19.819	20.284	29.275	1.944	2.241	36.133
	∂u/∂y	19.819	18.164	29.281	1.944	4.435	36.133
E2 4x4 cel. 9x9 nod.	u	10.610	10.619	11.889	0.293	0.317	5.014
	∂u/∂x	19.817	20.289	29.619	1.951	2.239	36.813
	∂u/∂y	19.817	18.169	29.565	1.951	4.437	36.813
T3 8x8 cel. 9x9 nod.	u	8.945	7.937	15.735	2.176	1.916	4.114
	∂u/∂x	10.619	11.970	21.303	8.138	7.856	6.448
	∂u/∂y	7.019	7.878	12.945	8.138	8.472	6.448
T3 4x4 cel. 9x9 nod.	u	8.948	7.941	15.575	2.177	1.916	4.261
	∂u/∂x	10.613	11.971	21.266	8.138	7.856	6.365
	∂u/∂y	7.017	7.878	12.877	8.138	8.472	6.365

Table 2 : % Error in u, ∂u/∂x, ∂u/∂y

However, the primary interest of the meshless methods is that they should work on arbitrary geometries and on irregular grids. We will consider as a second example the case of Laplace equation on a more complex domain with an irregular grid of nodes. (See fig. 5).

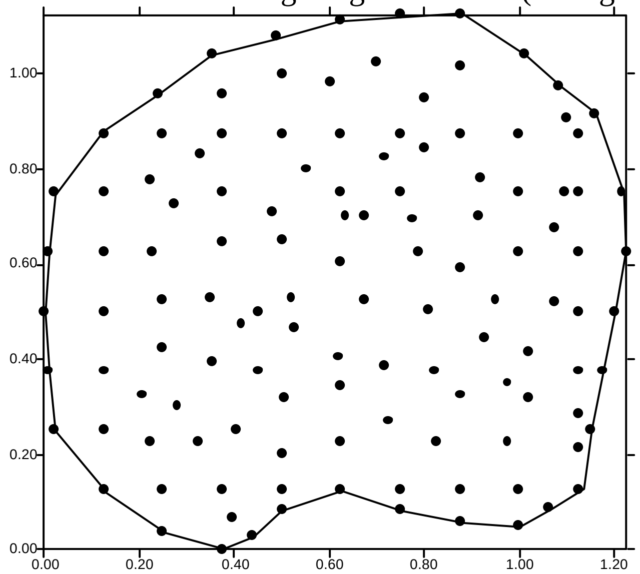


Figure 5: A more complex domain with an irregular grid of nodes.

The numerical integration over this more complex domain is made using triangular and square cells as it is shown in figure 6.

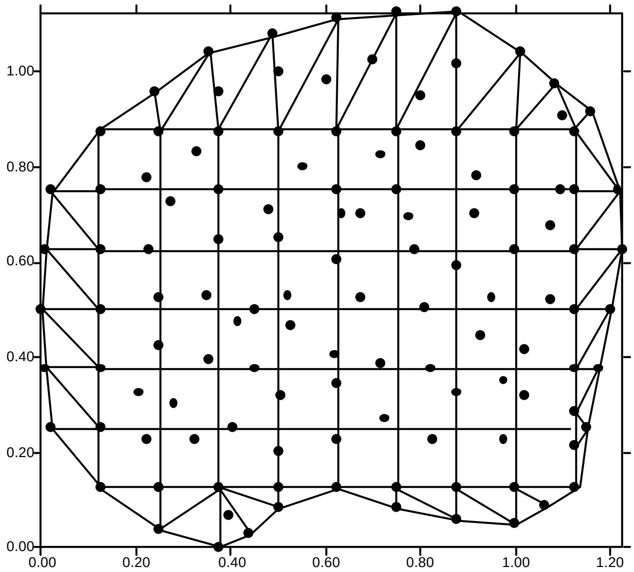


Figure 6: Triangular and square cells used for numerical integration.

In Table 3 we can see the results obtained for Lagrange Multipliers and Penalisation for the T3 case considered before (essential boundary conditions with a singularity in the gradients at x=0 y =0), for two different values of radius of influence rinf.

We use, as it is shown in figure 6, 52 triangles (13 integration points) and 64 cells (4x4) for numerical integration.

Strategy of treatment of Essential Boundary Conditions		Flux Lagrange Multipliers			Penalisation Penalty Function (10^{15})		
Weighting Function Data		Quartic Spline	Cubic Spline	Gauss rinf/c=2/3	Quartic Spline	Cubic Spline	Gauss rinf/c=2/3
Integration Order		4x4/13	4x4/13	4x4/13	4x4/13	4x4/13	4x4/13
T3 8x8 cel. 52 triangles. rinf.=0.32	u	22.370	20.617	23.821	22.217	19.740	23.707
	∂u/∂x	35.332	42.195	29.279	32.683	38.563	29.875
	∂u/∂y	31.786	32.003	27.407	45.742	35.134	28.305
T3 8x8 cel. 52 triangles. rinf.=0.15	u	34.657	19.989	15.482	2.431	2.069	2.573
	∂u/∂x	>100	83.390	40.071	7.169	7.143	10.819
	∂u/∂y	>100	>100	72.179	11.348	10.211	13.731

Table 3 : % Error in u, ∂u/∂x, ∂u/∂y for T3

Best results are obtained for penalisation method with spline weighting functions using small radius of influence (rinf=0.15), because in this case, we obtain an approximation that is close to an interpolation.

5. THE USE OF PENALISATION METHOD IN EFG

Using the penalisation method we can obtain very accurate results in EFG method, but it is necessary to take into account some recommendations:

The use of spline weighting functions (21) or (22) is recommended.

It is necessary that with the MLS functions employed, we obtain an approximation close to an interpolation. It can be easily verified, by obtaining the differences between the value of u (equations system solution), and the approximated value u^h calculated by (12). For example, interpolation at a point I will give 0% interpolation error at this point, that is the case when $u_I = u_I^h$. We shall use formula (20) to calculate the global interpolation error, taking $u = u^{(e)}$ and $u^h = u^{(n)}$. This formula (20) has been applied in the following table 4 to calculate "% error in interpolation".

Item 2 can also be considered, using variable rinf. In this case, rinf is adjusted for each point taking into account just the neighbourhood area covering the nearest points. We can multiply the distance to n^{th} point by a parameter (as in table 4), in order to assure a small overlapping of the areas of influence of each point.

Strategy of treatment of Essential Boundary Conditions		Penalisation Penalty Function (10^{15})	
Weighting Function Data		Quartic Spline	Cubic Spline
Integration Order		4x4/13	4x4/13
rinf=1.05×distance to the nearest third node.	% error in interpolation	0.013	0.006
	% error in u	11.211	10.394
	% error in ∂u/∂x	34.063	33.566
	% error in ∂u/∂y	27.751	27.383
rinf=1.1×distance to the nearest fourth node.	% error in interpolation	0.136	0.1867
	% error in u	1.835	1.718
	% error in ∂u/∂x	6.919	9.171
	% error in ∂u/∂y	8.079	10.117
rinf=1.1×distance to the nearest fifth node.	% error in interpolation	1.034	0.687
	% error in u	2.519	2.068
	% error in ∂u/∂x	7.851	7.669
	% error in ∂u/∂y	11.311	10.497
rinf=1.1×distance to the nearest sixth node.	% error in interpolation	2.143	1.351
	% error in u	2.6091	2.154
	% error in ∂u/∂x	8.1615	7.947
	% error in ∂u/∂y	11.675	10.350

Table 4 : % Error in u, ∂u/∂x, ∂u/∂y for T3

In table 4, we find the results obtained considering a variable rinf adjusted to the nearest third, fourth, fifth, and sixth node of the neighbourhood area.

In table 4, the interpolation global error of the function calculated according formula (20), decreases with the number of nodes used to calculate the radius of influence of the weighting function. However the error in u, $\partial u/\partial x$, $\partial u/\partial y$ increases when we are very close to interpolation, as it is the case when we use three points of support. Bests results are obtained considering four points.

6. CONCLUSIONS

Some aspects of the treatment of essential boundary conditions in EFG method have been studied. In this paper, a new strategy is proposed in this paper using penalty functions for the purpose of alleviating problems encountered in imposing essential boundary conditions in the EFG method. A high accuracy has been obtained. The method seems also very effective and stable for a wide range of penalisation coefficients.

The method has been tested for the case of a complex domain with irregular grid of nodes. Also using penalty functions is important to use spline weighting functions with radius of influence as small as possible, but with a small overlapping, in order to assure that the approximation function is close to interpolation. A guide about the EFG penalisation method is given, considering the possibility of using variable radius of influence for each point.

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