COMPUTATIONAL ASPECTS OF THE MLS METHOD

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Abstract The present paper introduces the Moving Least Squares (MLS) method in electrostatics. It presents the equations of the linear electrostatics, and the main features of the MLS method. The MLS method is used to solve a one-dimensional problem in the context of linear electrostatics, and an algorithm for implementing numerically this method is proposed. Finally, a numerical example is proposed and the exact solution is compared with the approximate one.

Keywords: Meshless methods, electrostatics, numeric analysis

1. INTRODUCTION

Presently, there are some numerical methods such as: smooth particle hydrodynamics, reproducing kernel particle methods, hp-clouds, and element free Galerkin that are of great importance in numerical modelling of mechanical and electrical phenomena. Their main advantage consists in the fact that these methods are mesh free, i.e. they don’t use a mesh in order to assemble the system of equations. Mesh free methods are of great interests in the study of problems that involves discontinuous fields, such as crack problems or phase changes, and adaptive refinement. The MLS method was implemented for the first time in thermoelasticity by R. Raducanu in [5].

Coupling methods EFG (Element Free Galerkin)-FEM (Finite Element Method) are also of great interest in applied electro-mechanics, because these methods can reduce considerably the computational cost. Pure FEM methods are primarily used by the engineers, because are more common, but the advantages of meshless methods are not to be negligible.
2. BASIC EQUATIONS

Let Ω be a bounded domain in the three dimensional Euclidian space. Suppose that the domain Ω is occupied by an isotropic and homogenous medium. As in [3], the basic equations of linear electrostatics are:

- Gauss Law:
  \[ \text{div} \mathbf{D} = \rho \quad (2.1) \]

- Electrostatic form of the Faraday law:
  \[ \text{rot} \mathbf{E} = 0 \quad (2.2) \]

- Constitutive relation:
  \[ \mathbf{D} = \varepsilon \mathbf{E} \quad (2.3) \]

where \( \mathbf{E} \) is the electric field intensity and \( \mathbf{D} \) is the electric flux density or, alternatively the electric displacement, \( \varepsilon \) is the electrical permittivity and \( \rho \) represents charge density.

We can see from (2.2) that \( \mathbf{E} \) is a potential field, i.e. there exists an electric potential \( V \) (voltage) defined by:

\[ \mathbf{E} = -\nabla V \quad (2.4) \]

In this way, supposing that \( \varepsilon \) is constant, from the relations (2.1)-(2.4) we can write:

\[ -\varepsilon \Delta V = \rho \quad (2.5) \]

To this equation we’ll attach the following mixt boundary conditions:

\[ V = V_1 \text{ on } \Gamma_1 \text{ and } V_n = V_2 \text{ on } \Gamma_2 \quad (2.6) \]

where \( V_1, V_2 \) are continuous functions given on the specified boundary parts, and \( \bar{\Gamma}_1 \cup \bar{\Gamma}_2 = \partial \Omega, \ \Gamma_1 \cap \Gamma_2 = \emptyset \). Thus the boundary value problem is to find \( V \) which satisfy (2.5) and the boundary conditions (2.6).
In order to impose essential boundary conditions, a couple of methods have been developed [1], [4]. In the following we will use the Lagrange multipliers method. We consider the following weak forms for our problem: let trial functions \( V(x) \in H^1 \) and Lagrange multipliers \( l \in H^0 \) for all test functions \( \delta \varphi(x) \in H^1 \) and \( \delta l \in H^0 \). If we have:

\[
\int_0^1 \varepsilon \delta \varphi^T \cdot x \, \delta V, x \, dx - \int_0^1 \delta \varphi^T \rho dx - \delta \varphi^T V_2 |_{\Gamma_2} \\
- \delta l^T (V - V_1) |_{\Gamma_1} - \delta \varphi^T l |_{\Gamma_2} = 0 \quad (2.7)
\]

then (2.5) is satisfied together with the boundary conditions (2.6), where \( H^0 \) and \( H^1 \) denote Hilbert spaces. A detailed discussion about these Hilbert spaces can be found in [2] and [6]. The next section presents the fundamentals of the MLS method for our particular one-dimensional case.

3. MLS APPROXIMANTS

Let us consider the domain \( = [0, 1] \) discretized by a set of 11 evenly spaced nodes. Let’s suppose that each node has a corresponding 'nodal parameter': \( V_I \) associated with it. It was shown that in general \( V_I \neq V(x_I) \). Let’s we will consider the approximations \( V^h(x) \) as polynomials of order \( m \) with non-constant coefficients:

\[
V^h(x) = \sum_{i=1}^{m} p_i(x) a_i(x) = p^T(x) a(x) \quad (3.1)
\]

where \( m \) represents the number of terms in the base, \( p_i(x) \) are the basis functions (usually monomials) and \( a_i(x) \) are their coefficients. For example, in an one dimensional space:

\[
p^T(x) = (1, x) \quad (3.2)
\]

As a remark, it is possible to introduce singular functions in the basis as well. It was shown [2] that any function included in the basis could be reproduced exactly by an MLS approximation. This fact is very useful in the study of domains with cracks.

The unknown parameters \( a_i(x) \) at a given point, are to be determined by minimizing the differences between the local approximation at that point and the nodal parameters: \( V_I \). Let the nodes whose support include \( x \), be numbered locally from 1 to \( n \). The functional to be minimized are the following weighted, discrete \( L_2 \) norm:
\[ J = \sum_{I=1}^{n} w(x - x_I) \left[ p^T(x_I) a(x) - V_I \right]^2 \] (3.3)

where \( n \) is the number of nodes in the neighborhood of \( x \) for which the weight function and are nodal values at. In the calculus from the remainder of this paper we'll take as a cubic spline weight function:

\[
w(x - x_I) = w(r) = \begin{cases} 
\frac{2}{3} - 4r^2 + 4r^3 & \text{for } r \leq \frac{1}{2} \\
\frac{4}{3} - 4r + 4r^2 - 4r^3 & \text{for } \frac{1}{2} < r \leq 1 \\
0 & \text{for } r > 0
\end{cases}
\] (3.4)

More details about the choice of the weight function can be found in [8].

Next, we will review the main steps in the determining the functional forms for \( V \). Minimizing the functional \( J \) with respect to \( a(x) \), we obtain the following set of linear equations:

\[
A(x)a(x) = B(x)V(x) \text{ or } a(x) = A^{-1}(x)B(x)V(x),
\] (3.5)

where

\[
A(x) = \sum_{i=1}^{n} w(x - x_I)p(x_I)p^T(x_I)
\] (3.6)

\[
B(x) = [w(x - x_1)p(x_1), w(x - x_2)p(x_2), ..., w(x - x_n)p(x_n)]
\] (3.7)

\[
V^T(x) = [V_1, V_2, ..., V_n]
\] (3.8)

Substituting (3.5) into (3.1), we obtain the following form for the MLS approximants:

\[
V^h(x) = \sum_{I=1}^{n} \Phi_I(x)V_I
\] (3.9)

where the shape functions \( \Phi_I(x) \) are:

\[
\Phi_I(x) = \sum_{j=0}^{m} p_j(x) \left( A^{-1}(x)B(x) \right)_{jI}
\] (3.10)

As it was very well pointed out in [1], [6], the shape functions are not real interpolants, because the Kronecker’s delta criterion is not satisfied: \( \Phi_I(x,J) \neq \delta_{IJ} \).
4. NUMERICAL IMPLEMENTATION

Let's consider the approximate solution $V$ and the test function $\delta \phi$ of the form given in (3.9). After some elementary computations, we obtain the following system of linear algebraic equations:

$$
\begin{pmatrix}
M & N \\
N^T & 0
\end{pmatrix}
\begin{pmatrix}
V \\
1
\end{pmatrix} =
\begin{pmatrix}
b \\
r
\end{pmatrix}
$$

(4.1)

where,

$$M_{IJ} = \int_0^1 \varepsilon \Phi_I^T \Phi_J dx$$

(4.2)

$$N_{IJ} = -\Phi_K |\Gamma_I|$$

(4.3)

$$b_I = \Phi_I V_{2x} |\Gamma_2| + \int_0^1 \Phi_I \rho dx, \ r_K = -V_{1K}$$

(4.4)

To assemble these equations, we should integrate over the domain using Gauss quadrature. First we will determine the quadrature points, and second, the domain of influence of the nodes is determined. Then, the shape functions are computed and the equation (4.1) is assembled.

5. NUMERICAL EXAMPLE

In this section we'll implement the MLS method: consider a one-dimensional bar of unit length subjected to a charge density of magnitude $x$. Let's suppose that the electric potential of the bar is null at the left end, and its normal derivative is null at the right end. The bar has constant cross sectional area of unit value. Thus, our problem can be written:

$$k V_{xx} + x = 0, \ x \in (0, 1)$$

(5.1)

$$V(0) = 0$$

(5.2)

$$V_x(1) = 0.$$  

(5.3)

The exact solution to (5.1)-(5.3) is given by:

$$V(x) = \frac{1}{k} \left( \frac{1}{2} x - \frac{1}{6} x^3 \right)$$

(5.4)

In order to obtain the MLS solution, we have to assemble the equation (4.1), computing the equations (4.2)-(4.4). In the fig.1 we can compare the exact solution with the MLS solution. One can see that the errors in the approximation are negligible.
6. CONCLUSIONS

This paper proposes the implementation of MLS method in linear electrostatics. This numerical method has been implemented in elasticity [6] since 1977 and in thermoelasticity [5] since 2002. In 1995, the method was further developed by a great number of scientists, who proposed new meanings and interpretations. Meshless methods have to be developed in the future, especially regarding the computational cost which presently is too high. At this stage, the optimum way of implementing these methods is coupling with FEM. This paper represents the first step in implementing MLS in electrostatics. It is presented the case of linear electrostatics, and an algorithm for numerical implementation was proposed as well. Finally the exact solution was compared to the approximate one and the errors were discussed.

References