Moving least squares method, revisited

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Abstract. The present paper is a first attempt towards implementing the Moving Least Squares (MLS) method within the frame of linear thermoelasticity. It presents the equations of the linear thermoelasticity, and the main features of the MLS method. The MLS method is used to solve a one-dimensional problem in the context of uncoupled linear thermoelasticity, 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.

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§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 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.

Recently, there have been developed a couple of methods concerning the idea of coupling between EFG (Element Free Galerkin)-FEM (Finite Element Method). These methods are also of great interest in applied mechanics, because they 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 D be a bounded domain in the three dimensional Euclidian space. Suppose that the domain D is filled by an isotropic and homogenous medium. As in [6], the basic equations of equilibrium of the linear thermoelasticity are:

the equilibrium equations:

$$t_{ji,j} + \rho_0 f_i = 0 \text{ on } \mathbf{D},$$
 (2.1)

the energy equation:

$$q_{i,i} = -\mathrm{s \ on \ D},\tag{2.2}$$

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the constitutive equations:

$$t_{ij} = 2\mu\varepsilon_{ij} + \lambda\varepsilon_{kk}\delta_{ij} - \beta\theta\delta_{ij} \tag{2.3}$$

$$q_i = k\theta_{,i} \tag{2.4}$$

the strain-displacement relations:

$$\varepsilon_{ij} = u_{i,j} + u_{j,i} \text{ on } \mathbf{D},$$
(2.5)

where u_i are the components of the displacement vector, t_{ij} are the components of the stress tensor, ε_{ij} are the components of the strain tensor, f_i are the components of the specific body force, s is the specific heat supplied, θ is the temperature measured from a constant reference temperature θ_0 , λ, μ, β, k are constants, characteristic of the material. We attach the following boundary conditions:

$$u_i = \overline{u}_i \text{ on } \Gamma_u, \ t_{ji} n_j = \overline{t}_i \text{ on } \Gamma_t \tag{2.6}$$

$$\theta = \theta \text{ on } \Gamma_{\theta}, \ q_i n_i = \overline{q} \text{ on } \Gamma_q,$$

$$(2.7)$$

where $\overline{u}_i, \overline{t}_i, \overline{\theta}, \overline{q}$ are continuous functions given on the specified boundary parts, and $\overline{\Gamma}_u \bigcup \Gamma_t = \overline{\Gamma}_\theta \bigcup \Gamma_q = \partial D$, $\Gamma_u \bigcap \Gamma_t = \Gamma_\theta \bigcap \Gamma_q = \Phi$. Thus the boundary value problem is to find u_i, θ which satisfy (2.1)-(2.5) and the boundary conditions (2.6) and (2.7). After some computations, we obtain the following equations:

$$\mu \ u_{i,jj} + (\lambda + \mu)u_{j,ji} + \rho_0 f_i = \beta \theta_{,i} \tag{2.8}$$

$$k\theta_{,ii} = -s. \tag{2.9}$$

We consider the transformed boundary conditions attached to these equations:

$$u_i = \overline{u}_i \text{ on } \Gamma_u, \ \lambda u_{r,r} n_i + \mu (u_{i,j} + u_{j,i}) n_j = \overline{t}_i + \beta \theta \ n_i \text{ on } \Gamma_t$$
(2.10)

$$\theta = \overline{\theta} \text{ on } \Gamma_{\theta}, \ k\theta_{i}n_{i} = \overline{q} \text{ on } \Gamma_{q}$$

$$(2.11)$$

In the remainder of this paper we will consider the corresponding one-dimensional problem on the domain $0 \le x \le 1$:

$$u_{,xx} + b = c\theta_{,x},\tag{2.12}$$

$$k\theta_{,xx} = -s \tag{2.13}$$

where $b = \frac{1}{\lambda + 2\mu} f_1$, $c = \frac{1}{\lambda + 2\mu} \beta$. In the following we will uncouple the problem; we will first solve the thermal problem: find θ which satisfies (2.13) and the boundary conditions:

$$\theta = \overline{\theta} \text{ on } \Gamma_{\theta}, \ \mathbf{k}\theta_{,x}n = \overline{q} \text{ on } \Gamma_{q} \tag{2.14}$$

Afterwards, we shall solve the mechanical problem: find u which satisfies (2.12) and the boundary conditions

$$u = \overline{u} \text{ on } \Gamma_u, \ u_{,x}n = \overline{t} \text{ n on } \Gamma_t, \tag{2.15}$$

where $\overline{t} = \frac{\overline{t} + \beta \theta}{\lambda + 2\mu}$. 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 ([1]):

I. The thermal problem: let the trial functions $\theta(x) \in H^1$ and the 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:

$$\int_{0}^{1} k \delta \varphi_{,x}^{T} \delta \theta_{,x} dx - \int_{0}^{1} \delta \varphi^{T} s dx - \delta \varphi^{T} \overline{q}|_{\Gamma_{q}} - \delta l^{T} (\theta - \overline{\theta})|_{\Gamma_{\theta}} - \delta \varphi^{T} l|_{\Gamma_{\theta}} = 0, \quad (2.16)$$

then (2.13) is satisfied together with the boundary conditions (2.14), where H^1 and H^2 denote Hilbert spaces of degree one and zero. A detailed discussion about these Hilbert spaces can be found in [3].

II. The mechanical problem: let the trial functions $u(x) \in H^1$ and the Lagrange multipliers $m \in H^0$ for all test functions $\delta v(x) \in H^1$ and $\delta m \in H^0$. If we have

$$\int_{0}^{1} \delta v_{,x}^{T} u_{,x} dx - \int_{0}^{1} \delta v^{T} (b - c\theta_{,x}) dx - \delta v^{T} \overline{t}|_{\Gamma_{t}} - \delta m^{T} (u - \overline{u})|_{\Gamma_{u}} - \delta v^{T} m|_{\Gamma_{u}} = 0 \quad (2.17)$$

then (2.12) is satisfied together with the boundary conditions (2.15). The next section presents the fundamentals of the MLS method for our particular one-dimensional case.

§3. MLS Aproximants

We further consider the domain $\Omega = [0, 1]$ discretized by a set of 11 evenly spaced nodes. In the theory proposed in [7], related to classical elasticity, each node has a corresponding 'nodal parameter': u_I associated with it. It was shown that in general $u_I \neq u(x_I)$. In the present theory, besides the parameter u_I that characterizes the mechanical behaviour at each node, we will consider the parameter θ_I that characterizes the thermal behaviour at each node. As we shell see, in general $\theta_I \neq -\theta(x_I)$.

Let's consider the approximations $u^{h}(\mathbf{x})$ and $\theta^{h}(x)$ as polynomials of order m with non-constant coefficients ([7]):

$$u^{h}(x) = \sum_{i=1}^{m} p_{i}(x)a_{i}(x) = \mathbf{p}^{T}(x)\mathbf{a}(x)$$
(3.1)

$$\theta^{h}(x) = \sum_{i=1}^{m} p_{i}(x)b_{i}(x) = \mathbf{p}^{T}(x)\mathbf{b}(x), \qquad (3.2)$$

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

$$\mathbf{p}^{T}(x) = (1, x).$$
 (3.3)

As a remark, it is possible to introduce singular functions in the basis as well. It was shown [3] 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 $a_i(x)$ and $b_i(x)$, at a given point, are to be determined by minimizing the differences between the local approximation at that point and the nodal parameters: u_i and, respectively θ_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 norms:

$$J_1 = \sum_{I=1}^n w(x - x_I) \left[p^T(x_I) a(x) - u_I \right]^2$$
(3.4)

$$J_2 = \sum_{I=1}^{n} w(x - x_I) \left[p^T(x_I) b(x) - \theta_I \right]^2,$$
(3.5)

where n is the number of nodes in the neighborhood of x for which the weight function $w(x-x_I) \neq 0$, u_I and θ_I are nodal values at $x = x_I$. In the calculus from the remainder of this paper we take w as a cubic spline weight function

$$w(x - x_I) = w(r) = \begin{cases} \frac{2}{3} - 4r^2 + 4r^3 \text{ for } r \leq \frac{1}{2} \\ \frac{4}{3} - 4r + 4r^2 - \frac{4}{3}r^3 \text{ for } \frac{1}{2} < r \leq 1 \\ 0 \text{ for } r > 1. \end{cases}$$
(3.6)

More details about the choice of the weight function can be found in [1]. For the sake of completeness, we will review the main steps in the determining the functional forms for θ . Minimizing the functional J_2 with respect to b(x), we obtain the following set of linear equations

$$\mathbf{A}(x)\mathbf{b}(x) = \mathbf{B}(x)\theta(x)orb(x) = \mathbf{A}^{-1}(x)\mathbf{B}(x)\theta(x), \qquad (3.7)$$

where

$$\mathbf{A}(x) = \sum_{I=1}^{n} w(x - x_I) \mathbf{p}(x_I) \mathbf{p}^T(x_I) \text{and}$$
(3.8)

$$\mathbf{B}(x) = [w(x - x_1)\mathbf{p}(x_1), w(x - x_2)\mathbf{p}(x_2), w(x - x_n)\mathbf{p}(x_n)]$$
(3.9)

$$\theta^T(x) = [\theta_1, \theta_2, \dots \theta_n]. \tag{3.10}$$

Substituting (3.7) into (3.2), we obtain the following form for the MLS approximants:

$$\theta^h(x) = \sum_{I=1}^n \Psi_I(x)\theta_I, \qquad (3.11)$$

where the shape functions $\Psi_I(x)$ are

$$\Psi_I(x) = \sum_{j=0}^m p_j(x) (A^{-1}(x)B(x))_{jI}.$$
(3.12)

In the same way, ([7]) we can obtain the following expressions for the displacement:

$$u^{h}(x) = \sum_{I=1}^{n} \Psi_{I}(x)u_{I}, \qquad (3.13)$$

where the shape functions $\Psi_I(x)$ are given by (3.12).

As it was very well pointed out in [7], [1], the shape functions are not real interpolants, because the Kronecker's delta criterion is not satisfied: $\Psi_I(x_J) \neq \delta_I J$.

§4. Numerical implementation

Let us first solve the thermal problem (2.16). Thus, let's consider the approximate solution θ and the test function $\delta\varphi$ of the form given in (3.11). After some elementary computations, we obtain the following system of linear algebraic equations

$$\begin{pmatrix} M & N \\ N^T & 0 \end{pmatrix} \begin{pmatrix} \theta \\ l \end{pmatrix} = \begin{pmatrix} b \\ r \end{pmatrix}$$
(4.1)

where,

$$M_{IJ} = \int_{0}^{1} k \Psi_{I,x}^{T} \Psi_{J,x} dx$$
 (4.2)

$$N_{IJ} = -\Psi_K |\Gamma_{\theta I} \tag{4.3}$$

$$g_I = \Psi_I q_x |\Gamma_q + \int_0^1 \Psi_I s dx, r_K = -\overline{\theta}_K.$$
(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 ([7]). Then, the shape functions are computed and the equations (4.1) are assembled.

In order to solve the mechanical problem (2.17), we will consider the approximate solution u and the test function δv of the form given in (3.13). As before, after some elementary computations, we obtain the following system of linear algebraic equations

$$\begin{pmatrix} P & Q \\ Q^T & 0 \end{pmatrix} \begin{pmatrix} u \\ m \end{pmatrix} = \begin{pmatrix} d \\ e \end{pmatrix}$$
(4.5)

where,

$$P_{IJ} = \int_{0}^{1} \Psi_{I,x}^{T} \Psi_{J,x} dx$$
 (4.6)

$$Q_{IJ} = -\Psi_K |\Gamma_{uI} \tag{4.7}$$

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$$d_I = \Psi_I t_x |\Gamma_t + \int_0^1 \Psi_I (b - c\theta_{,x}) dx, \ e_K = -\overline{u}_K.$$

$$(4.8)$$

The equations (4.5) are to be assembled like (4.1), using Gaussian quadrature.

§5. Numerical example

In this section we implement the MLS method: consider a one-dimensional bar of unit length subjected to a body force of magnitude x and to a specific heat of magnitude x. Assume that the displacement of the bar is fixed at the left end, and the right end is traction free. Moreover, suppose that the temperature is constant on the left end and the heat flux is null at the right end. The bar has constant cross sectional area of unit value. This problem was also studied for a pure mechanical case in [7]. Thus, the thermal problem can be written:

$$k\theta_{,xx} + x = 0 \ x \in (0,1) \tag{5.1}$$

$$\theta(0) = 0 \tag{5.2}$$

$$\theta_{,x}(1) = 0.$$
 (5.3)

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

$$\theta(x) = \frac{1}{k} \left(\frac{1}{2}x - \frac{1}{6}x^3 \right).$$
 (5.4)

In order to compute the MLS solution of the thermal problem, one would have to follow the steps described in the previously, taking s = x, $\overline{\theta} = 0$, $\overline{q} = 0$. We will take k = 1 and c = 1 in the calculus. The mechanical problem can be written

$$u_{,xx} + x - c\theta_{,x} = 0 \ \mathbf{x} \in (0,1) \tag{5.5}$$

$$u(0) = 0 \tag{5.6}$$

$$u_{,x}(1) = 0. (5.7)$$

As previously, substituting (5.4) in (5.5), we obtain the following exact solution of the problem (5.5)-(5.7):

$$u(x) = -\frac{c}{36k}x^4 - \frac{1}{6}x^3 + \frac{c}{4k}x^2 - \left(\frac{7}{18}c - \frac{1}{2}\right)x$$
(5.8)

The MLS solution is obtained, like for the thermal problem; we have to assembly the equation (4.5), computing the equations (4.6)-(4.8). In Fig.1 we can compare the exact solution with the MLS solution for the thermal problem. In Fig. 2 we can compare the exact solution with the MLS solution for the mechanical problem. We can see that the errors in the approximation for the thermal problem are negligible;

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Fig. 1 Temperature vs. position



Fig. 2 Displacement vs. position

for the mechanical problem there are some grater errors, and so we can conclude that the method provides a better solution for the thermal problem.

§6. Conclusions

This paper proposes the implementation of MLS method in linear thermoelasticity. This numerical method has been implemented in elasticity [5], since 1977. 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 thermoelasticity. It is presented the case of linear uncoupled thermoelasticity, 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.

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