Proceedings of the 24th UK Conference of the
Association for Computational Mechanics in Engineering
31 March - 01 April 2016, Cardiff University, Cardiff

GRADIENT ELASTICITY WITH THE MATERIAL POINT METHOD

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ABSTRACT

The Material Point Method (MPM) is a method that allows solid mechanics problems with large deformation and non-linearity to be modelled using particles at which state variables are stored and tracked. Calculations are then carried out on a regular background grid to which state variables are mapped from the particles. There have been a selection of extensions to the MPM, for example, a problem in the original method that arises when a material point crosses the boundary between one background grid cell and another is addressed by the Generalised Interpolation Material Point (GIMP) method [2]. An area yet to be studied in as much depth in MPM is that conventional analysis techniques constructed in terms of stress and strain are unable to resolve structural instabilities such as necking or shear banding. This is due to the fact that they do not contain any measure of the length of the microstructure of the material analysed such as molecule size of grain structure. Gradient elasticity theories provide extensions of the classical equations of elasticity with additional higher-order terms [3]. This use of length scales makes it possible to model finite thickness shear bands that is not possible with traditional methods. Much work has been done on including the effect of microstructure on a linear elastic solid and has previously been combined with the Finite Element Method and with the Particle In Cell Method. In this work the MPM will be developed to include gradient effects.

Key Words: *Material Point Method; Gradient Elasticity*

1. The Material Point Method

The Material Point Method (MPM) was first developed by Sulsky *et al.* [1] as an extension for solid mechanics of the Particle in Cell (PIC) method used in fluid dynamics. The MPM can be referred to as a meshfree method as although a background grid of connected nodes is required to perform calculations, material properties are carried by a series of particles which are free to move independently of each other. In the MPM, material points, known as particles, store state variables and move through a background grid or mesh which can be changed or reset following each time step or load increment. This can be seen in Figure 1 where a material has been deformed and the mesh has been reset with particles in updated positions.

Initially a material domain is split into a number of elements similar to the Finite Element Method (FEM). Each of these elements are then populated with a number of material points, with each material point being assigned a weight based on the volume of material that the particle represents. In addition to the mesh covering the material's initial position, the mesh must extend to where the material is expected to deform as the particles move through the mesh during deformation.

In each element containing particles, the state variables must be mapped from the particles to the grid nodes. This mapping process is carried out within each element using shape functions similar to those used in the FEM. For instance the external force at a grid node, $\{f_g^{ext}\}$, (shown in 2D) given by

$$\{f_g^{ext}\} = \sum_{i=1}^{n_p} \{N(\xi_i, \eta_i)\} f_{p_i}^{ext} \tag{1}$$

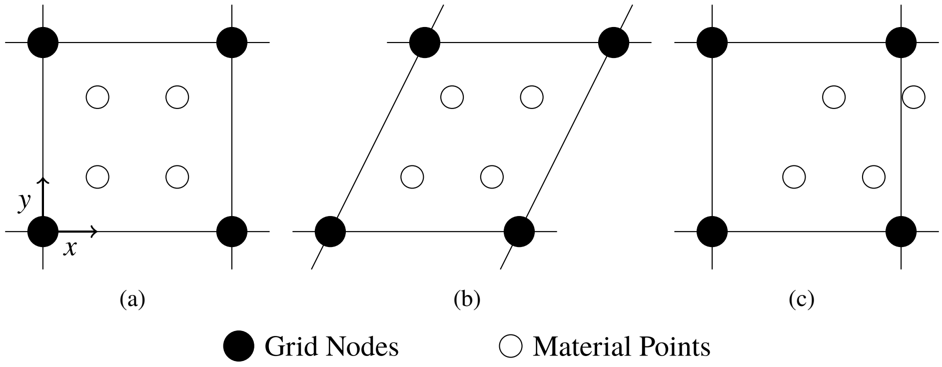

Figure 1: Material Point Method. Initial position of particles (a), deformed mesh and particles (b) and reset mesh with updated particles (c).

where f_p^{ext} is the particle external force, $\{N(\xi_i, \eta_i)\}$ are the nodal shape functions for the element containing the particle with local coordinates ξ and η and n_p refers to the number of material points in the grid element.

To be able to map to the correct grid nodes it is necessary to know in which element each material point located at a point in time. Although trivial initially, after particles have moved this problem can become more complex, especially if the mesh is not uniform. To simplify this process it is common to reset the background mesh to a uniform grid after each load step.

The stiffness of each element is determined from the contributions from each of the particles currently inside. A global stiffness matrix is assembled and the grid node displacements determined in a similar manner to FEM. At the end of a load step the grid node displacements $\{d_g\}$ are then mapped back to particles to get particle displacements for that loadstep $\{d_p\}$ through

$$\{d_p\} = \sum_{i=1}^{n_g} N_i \{d_{g_i}\}, \tag{2}$$

where n_g is the number of element nodes. The particle positions are then updated. The grid node displacements are not used to update the position of nodes in the mesh; the original undeformed mesh is used. An important aspect that should be noted is that even for linear MPM the simulation is done over multiple load steps, that is the MPM is an incrementally linear method.

2. Overview of gradient elasticity

Gradient elasticity theories are an extension of classical elasticity equations to account for microstructure of a material with extra higher order derivatives, the term gradient elasticity comes from higher order terms being proportional to the laplacian of lower order terms. An overview introducing gradient elasticity can be found in [3] by Askes and Aifantis.

Theories relating to enriching elasticity equations by capturing effects of microstructure using higher order gradients can be seen as far back as the 19th century. Theories were based on modelling particular physical phenomenon rather than mathematical completeness. More interest in the area developed in the 1960s when many studies began to extend this into elaborate full gradient theories, a landmark paper being Mindlin [5]. In modern times there has been another shift of interest towards simplified theories. This simplification allows for easier implementation with the popular FEM an example of this is the Ru-Aifantis theorem [6].

The majority of the gradient elasticity publications in the literature show how it can be used to eliminate strains singularities from dislocation lines and crack tips. However one of the current problems is the perceived drawback of identifying coefficients needed for implementing the method. It is clear that these are somehow connected to the microstructure of a material however it is not clear what physically they represent. To be able to apply gradient elasticity to MPM it was necessary to choose a suitable method which should allow variables to be stored only at material points and not require any storage on the background grid. Due to the particles in the MPM being used as integration points the chosen method should not be too sensitive to slight errors in integration.

Mindilin's Theory of elasticity with microstructure [5] allows the deformation energy density U to be expressed as

$$U = \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} + \frac{1}{2}B_{ijkl}\gamma_{ij}\gamma_{kl} + \frac{1}{2}A_{ijklmn}\kappa_{ijk}\kappa_{lmn} + D_{ijklm}\gamma_{ij}\kappa_{klm} + F_{ijklm}\kappa_{ijk}\varepsilon_{lm} + G_{ijkl}\gamma_{ij}\varepsilon_{kl} \quad (3)$$

where the macroscopic strain ε_{ij} is defined from macroscopic displacements u_i, $\varepsilon_{ij} = \frac{1}{2}(u_{j,i} + u_{i,j})$. The microscopic deformation ψ_{ij} is used to calculate the micro-deformation gradient, $\kappa_{ijk} = \psi_{jk,i}$, and the relative deformation $\gamma_{ij} = u_{j,i} - \psi_{ij}$. However this is quite complicated, the constitutive tensors $C_{ijkl}, B_{ijkl}, A_{ijklmn}, D_{ijklm}, F_{ijklm}$ and G_{ijkl} contain 1764 coefficients of which 903 are independent. It can shown that this can be reduced to 18 for isotropic materials however this is still an unworkably large number. As such there have been numerous simplifications to the theory to allow practical use in Engineering applications.

A simpler version was formulated by Mindlin using different relationships between macroscopic displacement u_i and microscopic deformation gradient κ_{ijk}. One example being that $\kappa_{ijk} = \varepsilon_{jk,i} = \frac{1}{2}(u_{k,ij} + u_{j,ik})$, here the micro deformation coincides with the gradient of macro deformation.

Based on work from the 1980s on plasticity [4] an extension of linear elasticity which can be shown to be a simplification of Mindlin theory using the Laplacian of the strain in the constitutive relationship.

$$\sigma_{ij} = C_{ijkl}(\varepsilon_{kl} - \ell^2 \varepsilon_{kl,mm}) \quad (4)$$

where ℓ is a length scale parameter and C_{ijkl} is the classical constitutive tensor. Substituting this into the standard equilibrium equation gives

$$C_{ijkl}(u_{k,jl} - \ell^2 u_{k,jlmm}) + b_i = 0 \quad (5)$$

In [6] Ru and Aifantis show that this approach can be implemented in two steps with an uncoupled sequence of equations using an operator split.

To achieve this, first displacements u_i^c are are used obeying classical elasticity,

$$C_{ijkl}u^c_{k,jl} + b_i = 0, \quad (6)$$

this is then followed

$$u_k^g - \ell^2 u^g_{k,mm} = u_k^c, \quad (7)$$

where u_i^g are the gradient enriched displacements. This separation makes numerical solutions possible where they were not before with Mindlin's general theory. This split approach has the potential to be a good method to use with the MPM. Although this method doesn't remove all singularities at tips of sharp cracks this is not a major goal of the current MPM code as we are more interested in being able to model a shear band with a finite thickness.

In [7] this displacement based approach is compared with approaches where the displacements are replaced with strains and stresses. It is shown that all singularities are removed when the gradient enrichment is evaluated in terms of strains where this is not the case for the displacement approach. Both of these approaches will be considered when developing the MPM.

The Ru and Aifantis approach has been implemented in FEM in 1D to test the method before applying it to MPM. A bar with a young's modulus in one half 5 times greater than the other half (as shown in [7]), with original length of $10mm$, is extended by $0.1mm$. The axial strain is calculated using a classic FEM approach and a displacement based Ru and Aifantis gradient approach (u-RA) with $\ell = 2mm$. The results of this can be seen in figure 2 with the gradient approach eliminating the jump in strain.

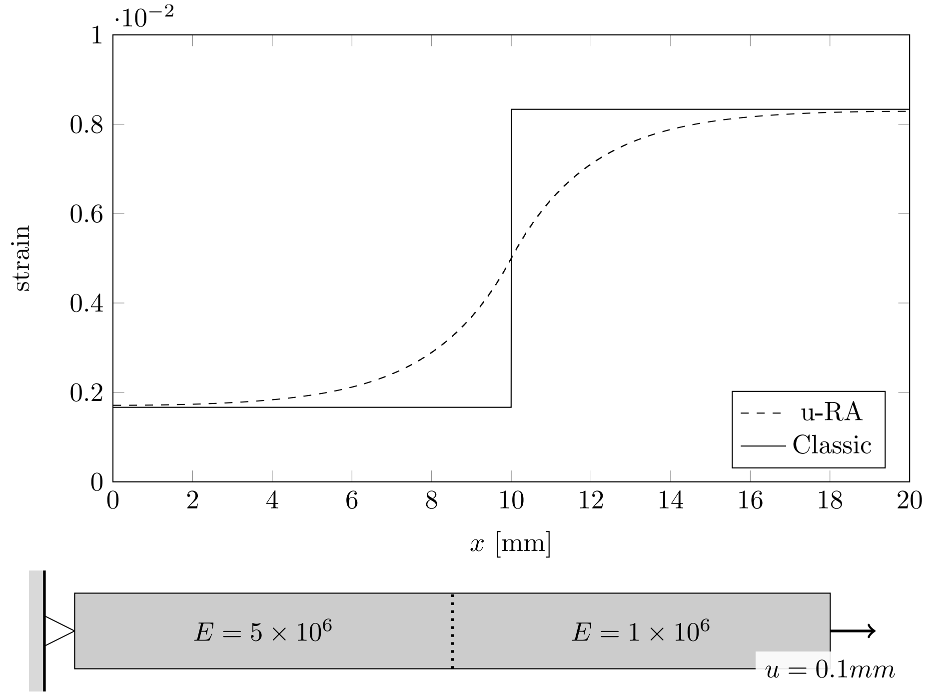

Figure 2: Strain along an extended bar using the FEM with and without gradient elasticity.

3. Current development and intended progress

As the operator split technique outlined above can be added as a post processing step it is possible to directly apply this to the MPM however due to the multiple steps in MPM it needs to be thought about whether gradient effects should be applied at the end of each loadstep or just at the end of the whole simulation. A further related question is will gradient dependent deformations map between grid and material points or are they only related to the grid? This work so far outlines the very basics of applying gradient effects to the MPM, for more interesting geomechanics problems it is likely that it will be necessary to implement plasticity and look at gradient plasticity methods.

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