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On the issues associated with applying traditional Lagrangian mechanics to the material point method

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ABSTRACT

The material point method is marketed as *the* technique to solve problems involving large deformations, particularly in areas where conventional mesh-based methods struggle. However, there are issues with combining the method with traditional total and updated Lagrangian statements of equilibrium. This paper discusses the issues and then proposes a new Lagrangian statement of equilibrium which is ideal for material point methods. The method is applied to two large deformation elasto-plastic problems, with a specific focus on the convergence of the method towards analytical solutions with the standard and generalised interpolation material point methods. Although the focus of this work is on implicit material point formulations, the proposed framework can be applied to all existing material point methods and adopted for both implicit and explicit analysis.

KEY WORDS: Material point method; Lagrangian mechanics; elasto-plasticity; finite deformation mechanics; generalised interpolation.

INTRODUCTION

The material point method is ideally suited to modelling problems involving large deformations where conventional mesh-based methods would struggle. However, total and updated Lagrangian approaches are unsuitable and non-ideal, respectively, in terms formulating equilibrium for the method. This is due to the basis functions, and particularity their derivatives, of material point methods normally being defined based on an unformed, and sometimes regular (for example the generalised interpolation material point method of Bardenhagen and Kober (2004)), background mesh. It is possible to map the basis function spatial derivatives using the deformation at a material point (Charlton et al., 2017; Coombs et al., 2018a) but this introduces additional algorithm complexity and computational expense.

This paper starts by exploring the use of updated and total Lagrangian approaches with the material point method for large deformation elasto-plasticity, highlighting their deficiencies. The paper then formulates a new Lagrangian statement of equilibrium which is ideal for material point methods as it satisfies equilibrium on the undeformed background mesh at the start of a load step. The paper is organised as follows: Section 2 presents the large deformation framework adopted in this work and discusses issues with traditional statements of equilibrium, Section 3 presents the new Lagrangian formulation, numerical examples are presented in Section 4 and brief conclusions are drawn in Section 5. The majority of the paper uses index notation and is focused on two-dimensional quasi-static analysis for elasto-plastic materials.

FINITE DEFORMATION MECHANICS

In finite deformation mechanics, the deformation gradient, F_{ij}, provides the fundamental link between the original and deformed configurations

$$F_{ij} = \frac{\partial x_i}{\partial X_j}, \tag{1}$$

where X_i are the original (reference) coordinates and $x_i = \varphi(X_i, t)$ are the updated coordinates in the current (deformed) body, where φ is the motion of the body. In this paper, we assume that the deformation gradient can be multiplicatively decomposed into elastic and plastic components (Lee and Lu, 1967; Lee, 1969)

$$F_{ij} = F^e_{ik} F^p_{kj} \,, \tag{2}$$

where the superscripts e and p denote the elastic and plastic quantities. We also assume a linear relationship between elastic logarithmic strains and Kirchhoff stresses and combine these measures with an exponential map of the plastic flow rule to allow the use of conventional small-strain stress integration algorithms with a finite deformation framework. The elastic logarithmic strain is defined as

$$\varepsilon^e_{ij} = \frac{1}{2}\ln(b^e_{ij}), \qquad \text{where} \qquad b^e_{ij} = F^e_{ik} F^e_{jk} \tag{3}$$

is the left elastic Cauchy-Green strain and the Kirchhoff stress, τ_{ij}, can be obtained using

$$\tau_{ij} = D^e_{ijkl} \varepsilon^e_{kl} \,, \tag{4}$$

where D_{ijkl}^e is the linear elastic stiffness matrix. The Cauchy stress can be obtained from the Kirchhoff stress through

$$\sigma_{ij} = \frac{1}{J}\tau_{ij}, \qquad \text{where} \qquad J = \det(F_{ij}) \tag{5}$$

is the volume ratio between the deformed and reference configurations. In order to advance the non-linear solution, the finite deformation equations are discretised in pseudo-time by imposing the deformation over a number of load (or pseudo-time) steps. The stresses at each material point, for each load step, are updated using an elastic predictor-plastic corrector constitutive algorithm.

Total Lagrangian

An total Lagrangian formulation can be defined by the following weak statement of equilibrium

$$\int_\Omega \left(P_{ij}(\nabla_x \eta)_{ij} - b_i \eta_i\right) \mathrm{d}v - \int_{\partial\Omega} (t_i \eta_i)\, \mathrm{d}s = 0 \quad ,(6)$$

where the reference domain, **Ω**, is subjected to tractions, t_i, on the boundary of the domain (with surface, s), $\partial\Omega$, and body forces, b_i, acting over the volume, v of the domain, which lead to a first Piola Kirchhoff stress field, $P_{ij}= J\sigma_{ik}F_{jk}^{-1}$, through the body. The weak form is derived in the reference (or material) frame assuming a field of admissible virtual displacements, η_i, and the derivatives of these virtual displacements in the first term in (6) are taken with respect to the original material coordinates, X_i.

In material point methods, at the end of each load (or time) step the background mesh is normally reset or, in some cases, replaced with a new mesh. This causes issues when trying to adopt a total Lagrangian formulation as information is lost regarding the deformation of the background mesh between load steps. For example, the statement of equilibrium (6) requires derivatives of the basis functions with respect to the original coordinates, but a there is no guarantee that a material point is in the same element as at the start of the analysis. There are also issues associated with determining the external force vector in the reference frame due to the material points moving between elements. These two issues make total Lagrangian formulations unsuitable for material point analysis.

Updated Lagrangian

An updated Lagrangian formulation can be defined by the following weak statement of equilibrium expressed in the deformed (or current) frame

$$\int_{\varphi_t(\Omega)}\big(\sigma_{ij}(\nabla_x\eta)_{ij} - b_i\eta_i\big)\,\mathrm{d}v - \int_{\varphi_t(\partial\Omega)}(t_i\eta_i)\,\mathrm{d}s = 0 \tag{7}$$

φ_t is the motion of the material body with domain, Ω, which is subjected to tractions, t_i, on the boundary of the domain (with surface, s), $\partial\Omega$, and body forces, b_i, acting over the volume, v of the domain, which lead to a Cauchy stress field, σ_{ij}, through the body. The weak form is derived in the current frame assuming a field of admissible virtual displacements, η_i, and the spatial gradient of these displacements are taken with respect to the deformed coordinates, x.

As discussed previously, in material point methods there is no concept of the current (deformed) nodal coordinates as information is lost between incremental steps. Spatial derivatives therefore should be calculated using the method proposed by Charlton et al. (2017), that is

$$\frac{\partial(\cdot)}{\partial_{x_j}} = \frac{\partial(\cdot)}{\partial\tilde{X}_i}\frac{\partial\tilde{X}_i}{\partial_{x_j}} = \frac{\partial(\cdot)}{\partial\tilde{X}_i}(\Delta F_{ij})^{-1} \tag{8}$$

where $\tilde{X}_i$ are the coordinates at the start of the load step. It is essential that the spatial derivatives are used in the statement of equilibrium to converge towards the correct solution based on the internal force contribution of each material point Charlton et al. (2017); Coombs et al. (2018a). However, this mapping adds complexity to the numerical implementation of the method and computational expense as the mapping must be applied to each material point for each iteration within every load step.

PREVIOUSLY CONVERGED LAGRANGIAN MECHANICS

This section provides a new approach for satisfying equilibrium in material point analysis. The updated Lagrangian weak statement of equilibrium (7) can be recast within a previously converged formulation where equilibrium is satisfied at the starting point of a load step (or the previously converged state). The statement of equilibrium becomes

$$\int_{\varphi_{t_n}(\Omega)}\big(\tilde{P}_{ij}(\nabla_{\tilde{X}}\eta)_{ij} - b_i\eta_i\big)\,\mathrm{d}v - \int_{\varphi_{t_n}(\partial\Omega)}(t_i\eta_i)\,\mathrm{d}s = 0 \tag{9}$$

where φ_{t_n} is the motion of the material body evaluated at the previously converged (or for the first load step, the initial) state and $\tilde{P}_{ij}$ is the Cauchy stress pulled back to the previously converged state, $\tilde{X}_i$, that is

$$\tilde{P}_{ij} = \Delta J\ \sigma_{im}(\Delta F^{-1})_{jm}, \tag{10}$$

The advantage of the proposed formulation is that it does not require mapping of spatial derivatives. Therefore all equilibrium calculations truly take place on the background mesh at the start of the load step. The material points are convected through the mesh once equilibrium has been obtained.

The proposed formulation was implemented within an implicit quasi-static material point code with a full Newton solution algorithm to achieved asymptotic quadratic convergence of the global equilibrium equation, (9). The overall program structure is very similar to conventional updated Lagrangian implementation (see Charlton et al. (2017); Coombs et al. (2018a), for example) and details of the implementation can be found in Coombs et al. (2018b). The formulation has been implemented for the standard and the generalised interpolation material point methods using regular Cartesian background meshes. The basis functions for these methods can be found in Bardenhagen and Kober (2004) and Coombs et al. (2018a), amongst others. Although an implicit implementation has been used in this paper, (9) is equally applicable to explicit analysis.

NUMERICAL EXAMPLES

This section presents two numerical analyses to demonstrate the performance of the proposed framework. In both cases the material's behaviour was governed by an isotropic linear elastic perfectly plastic constitutive model with a von Mises yield surface of the form

$$f = \rho - \rho_y = 0 \tag{11}$$

where ρ_y is the yield strength of the material, $\rho = \sqrt{2J_2}$, $J_2 = s_{ij}s_{ji}/2$, $s_{ij} = \tau_{ij} - \tau_{kk}\delta_{ij}/3$ and δ_{ij} is the Kronecker delta tensor. The analyses were conducted in two-dimensions with a plane strain assumption in the out of plane direction. The background mesh was comprised of bi-linear quadrilateral elements and all of the examples used the proposed previously converged Lagrangian formulation.

Compaction Under Self Weight

The first example is an elasto-plastic column compressed under its own weight. Initially the column had a height of $l_0 = 50$m and a width linked to the size of the background grid used to analyse the problem such that there was always one element in the horizontal direction. The base of the column was restrained vertically and both sides of the column were restrained in the horizontal direction. The column had a Young's modulus of 1MPa and Poisson's ratio of 0, the yield strength of the material was set to 20kPa and an initial density of %$_0$ = 80kg/m^3. A body force of -800N/m^3 was applied in the vertical (Z, z) direction over 50 equal loadsteps. The analytical solution for the vertical Cauchy stress is

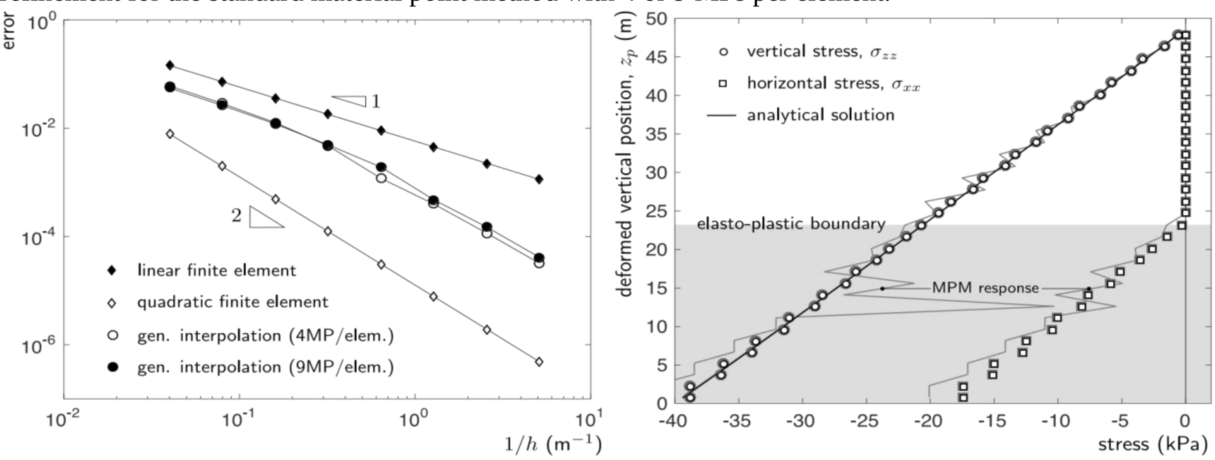
$$\sigma_{zz} = \rho_0 g(l_0 - Z) \tag{12}$$

where g is gravity (10m/s^2) and Z is a material point's initial vertical position. The normal stress in the other directions are given by Charlton et al. (2017) and the shear stresses are zero.

Figure 1 (a) shows the convergence of the generalised interpolation material point method with 4 and 9 material points (MPs) per element under uniform h refinement, where the dimensionless error is defined as

$$\text{error} = \sum_{p=1}^{n_p} \frac{\| (\sigma_p)_{zz} - \sigma_{zz}^a(Z_p) \| \, V_p^0}{(\rho_0 g l_0) V_0} \, . \tag{13}$$

n_p is the total number of material points, $(\sigma_p)_{zz}$ is the Cauchy stress in the vertical direction at a material point, Z_p is the material point's original position, V_p^0 is the original volume associated with the material point, σ_{zz}^a is the analytical Cauchy stress solution in the vertical direction and $V_0 = \sum V_p^0$ is the initial volume of the column. The convergence rate is between that of linear and quadratic finite elements. The stress response of both the generalised interpolation and standard material point elements are shown in Figure 1 (b) with h = 3.125m and 4MPs/element. As expected, and widely reported in the literature, the standard material point method suffers from stress oscillations cased by cell crossing instabilities. A consequence of this is that (13) does not reduce with mesh refinement for the standard material point method with 4 or 9 MPs per element.



(a) convergence (b) stress response

Figure 1 Elasto-plastic compaction under self weight

Elasto-Plastic Collapse

The second example is the collapse of a 16m by 8m elasto-plastic body under self weight. The domain was discretised by 3^2 and 6^2 generalised interpolation material points points per initial background grid element. Due to symmetry only half of the body was modelled and roller boundary conditions were imposed directly on the background mesh on the base and the line of symmetry (see Figure 2). The body had a Young's modulus of 1MPa, Poisson's ratio of 0.3 and a yield stress of ρ_y= 20kPa and was subjected to a body force of −10,000N/m^3 over 40 equal loadsteps.

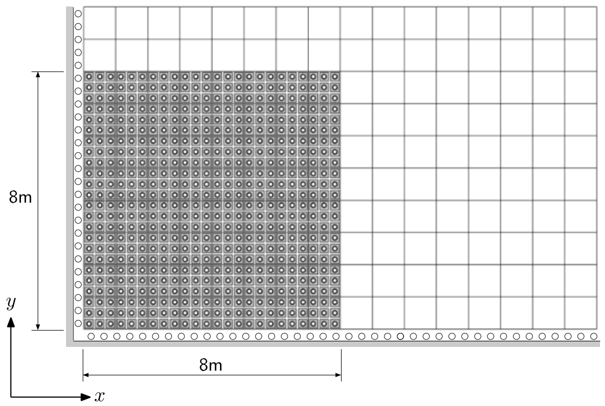


Figure 2 Elasto-plastic collapse: problem definition and initial discretisation

Figure 3 shows the deformed material point positions coloured according to the vertical stress, σ_{yy}, for different background grid sizes (h = 1, 0.5 and 0.25m) and numbers of material points per initially populated grid cell (3^2 and 6^2 MPs/element). With coarse meshes, especially with low numbers of material points per initially populated element, there are severe stress oscillations through the body. These reduce with background and the material point refinement, however oscillations between adjacent elements still exist due to discontinuous spatial derivatives of the basis functions between elements.

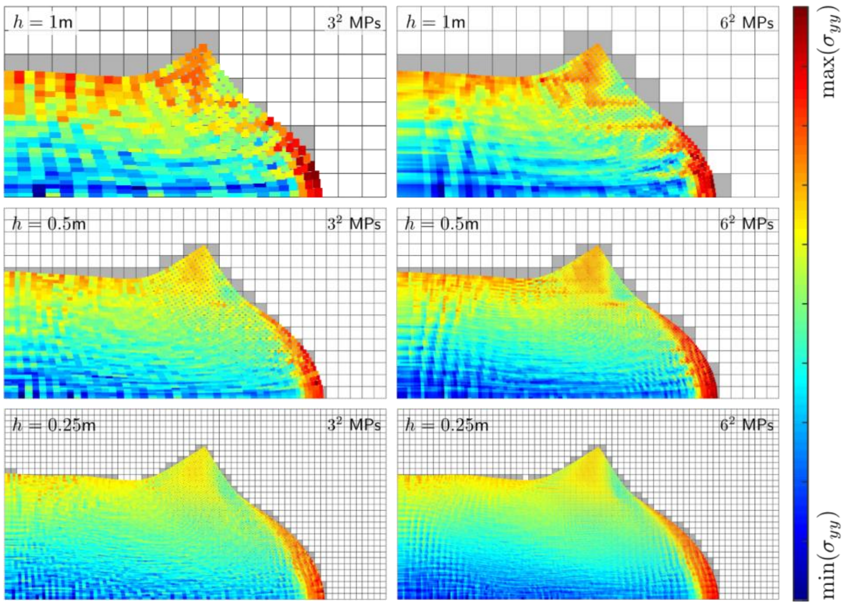


Figure 3 Elasto-plastic collapse: deformed material point positions coloured according to vertical normal Cauchy stress, σ_{yy}, where the mesh size, h, is given in each subfigure. The analysis was run with 3^2 and 6^2 material points per initially populated background grid cell

CONCLUSION

This paper has discussed issues associated with applying traditional Lagrangian equilibrium equations to material point methods and proposed a new statement of equilibrium which, in the authors' opinion, is ideally suited to material point analysis. Although it is possible to use an updated Lagrangian formulation with the material point method it requires the derivatives of the basis functions to be mapped into the current (deformed) configuration. This step is avoided in the proposed formulation, which simplifies the implementation of the method and increases its computational efficiency (by approximately 5% based on the numerical analyses conducted to date). The proposed Lagrangian formulation is still susceptible cell-crossing instabilities; in this paper we mitigate this by adopting generalised interpolation basis functions.

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