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A Fully Implicit Particle-in-Cell Method for Granular Flows

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Abstract

An implicit-in-time method for granular materials is described. The method combines the Material Point Method (MPM), and a Newton-Krylov equation solver to give improved energy conservation and stabilization.

Introduction

A wide variety of numerical models have been used to capture the complexities of granular flow. Examples include Monte Carlo models, lattice gas models and numerical models to resolve the grains. The latter is the subject of this paper. In particular, an implicit formulation of the material point method (MPM) [1] is considered in the modeling of granular materials. MPM combines a Lagrangian treatment, using material points, with an Eulerian grid. These material points describe the grain dynamics, they resolve edges and allow history dependent effects to be recorded. The Eulerian grid allows for efficient computation of interactions between grains. Contacts between grains are computed with a model based on the immersed boundary method; interpenetration is prevented but grain separation, sliding and bonding are allowed [2].

Previous versions of the MPM algorithm advance the solution in time using a leapfrog algorithm. These work well for relatively high strain rates but implicit methods have the potential to be more robust, stable and efficient for low strain rate calculations. In this paper, a Newton-Krylov (NK) algorithm is applied to the solution of the implicit MPM equations [3]. The implementation is matrix-free, requiring only the evaluation of the residual error at each iterative step - ideal in the solution of the non-linear and non-analytic implicit MPM formulation.

In this paper, the granular flow model is presented and the implicit MPM formulation described. Next, the implementation of the Newton-Krylov technique is discussed and the results of numerical experiments for a single grain and an assembly of compressed grains presented.

A Model for Granular Material

Granular material is modeled as a collection of deformable grains[2]. The dynamics of each grain, g, is described by the continuum mechanics; the continuity equation,

$$\frac{d\rho_g}{dt} = -\rho_g \nabla \cdot \mathbf{v_g}, \tag{1}$$

and the stress evolution equation,

$$\frac{d\sigma_\mathbf{g}}{dt} = \mathbf{T_g} : \frac{d\mathbf{e_g}}{dt}, \tag{2}$$

where $\frac{d\mathbf{e_g}}{dt}$ is the strain rate,

$$\frac{d\mathbf{e_g}}{dt} = \frac{1}{2}\left(\nabla \mathbf{v_g} + \nabla \mathbf{v_g}^T\right). \tag{3}$$

The grains are modeled as elastic-plastic materials. The constitutive equation describes an elastic plastic material as described in detail in Sulsky *et al.* [4].

The momentum equation is written,

$$\rho \frac{d\mathbf{v_g}}{dt} = \nabla \cdot \sigma_\mathbf{g} + \mathbf{F_c}, \tag{4}$$

where $\mathbf{F_c}$ is the contact force between grains. In the absence of friction or bonding, the contact force prevents interpenetration of grains, but allows them to move apart freely. Interpenetration will not occur if the velocity for each grain at the point of contact, $\mathbf{x}_c$, satisfies the inequality,

$$\hat{\mathbf{n}}_\mathbf{g} \cdot (\mathbf{v_g} - \mathbf{v}) \leq 0, \tag{5}$$

where $\hat{\mathbf{n}}_\mathbf{g}$ is the outward directed surface normal for grain g, and $\mathbf{v}$ is the Fabre averaged velocity at the point of contact,

$$\mathbf{v} = \frac{\sum_g \rho_g \mathbf{v_g}}{\sum_g \rho_g}. \tag{6}$$

The summation includes all grains in contact at $\mathbf{x}_c$. The contact force is constructed to ensure the velocity satisfies the kinematic constraint and to allow for Coulomb friction between grains. See [2] for further details.

The Implicit MPM Formulation

In MPM, the material data is carried on Lagrangian mass points or particles. Each mass point p carries essential information such as the position $\mathbf{x}_p$, mass m_p, velocity $\mathbf{v}_p$, stress σ_p and volume V_p. History dependent variables are carried with the particles. The information carried by the particles is then projected onto a background grid where the equations of motion are solved. Shape functions, $\mathcal{S}$, typically formed from the tensor product of linear b-splines, are used to map information from the grid to the particles. The particle properties are then updated.

To advance the solution forward by one time step Δt, grid velocities are first calculated using a lumped mass weighting of particle velocities [1] Lumping the mass matrix, as opposed to using a consistent mass matrix, results in a dissipation of kinetic energy in the transfer from particles to grid but allows for increased computational efficiency.

The momentum equation is next integrated forward in time. The momentum equation for explicit MPM is

$$m_i^n \frac{\left[\mathbf{v}_i^{n+1} - \mathbf{v}_i^n\right]}{\Delta t} = -\sum_p \nabla_{pi} \cdot {\sigma_p}^{n+1/2} {V_p}^{n+1/2} + \mathbf{F_c} \tag{7}$$

where $\nabla_{pi} = \nabla \mathcal{S}(\mathbf{x} - \mathbf{x}_i)|_{\mathbf{x}_p}$. The particle stress tensor $\sigma_p^{n+1/2}$ is calculated by solving the constitutive equations at the particles. The required particle strain increment is calculated by taking nodal velocity gradients,

$$\Delta \mathbf{e}_p^n = \frac{1}{2} \sum_i \left[\nabla_{pi} \mathbf{v}_i^n + \nabla_{pi} \mathbf{v}_i^{nT} \right] \Delta t \tag{8}$$

so that

$$\sigma_p^{n+1/2} = \sigma_p^{n-1/2} + \mathbf{T} : \Delta \mathbf{e}_p^n \tag{9}$$

The particle volume $V_p^{n+1/2}$ is calculated by integrating the particle's dilation,

$$V_p^{n+1/2} = V_p^{n-1/2} \left(1 + \Delta t \left(\nabla \cdot \mathbf{v}_p^n \right) \right). \tag{10}$$

The explicit leapfrog algorithm described above is extended here to incorporate the following fully implicit time centered discretisation,

$$\mathbf{v}_i^{n+\theta} = \mathbf{v}_i^n - \frac{\theta \Delta t}{m_i^n} \left(\sum_p \nabla_{pi} \cdot {\sigma_p}^{n+\theta} {V_p}^{n+\theta} + \mathbf{F_c} \right) \tag{11}$$

where θ is the time-centering variable and time centered particle stresses and volumes are

$$\sigma_p^{n+\theta} = \sigma_p^n + \mathbf{T} : \Delta \mathbf{e}_p^{n+\theta} \tag{12}$$

$$V_p^{n+\theta} = V_p^n \left(1 + \theta \Delta t \left(\nabla \cdot \mathbf{v} \right)_p^{n+\theta} \right). \tag{13}$$

Finally, the particle velocities are updated by mapping the nodal velocities to the particles. New particle positions are then calculated.

A Fully Implicit Algorithm using the Newton-Krylov Technique

The matrix-free Newton-Krylov (NK) method [3] is becoming an increasingly popular tool to solve the fully coupled transient and steady-state problems. It has been applied successfully to a wide range of applications such as combustion [5] and phase change [6] among others.

In this study, an inexact, matrix-free, Newton-Krylov technique is utilized to solve the fully implicit, non-linear equations of motion for granular flows with intergranular contact The nonlinear system of equations is represented by the vector $\mathbf{F}(\mathbf{v}) = [F_x(\mathbf{v}), F_y(\mathbf{v})]$. Typically, the NK method is utilized to find a single-valued vector field. In this study, a multi-valued velocity field is required since relative motion between the grains must be simulated in the contact algorithm. When grains come into close contact, a node i can be shared between more than one grain. Therefore, there will be more than one velocity field associated with i. Without a contact force, the grains would be decoupled and the NK technique could conceivably be applied to individual grains. However, the need for a contact force between grains couples the grains so that the full multi-valued velocity field must be solved for in the NK technique. The non-linear residual vector $\mathbf{F}$ must therefore contain the residuals for all nodes i belonging to each grain g, for all grains.

Solution of the fully-coupled, non-linear problem is a concatenated velocity field $\mathbf{v}^{k+1}$ which satisfies $\frac{\mathbf{F}\left(\mathbf{v}^{k+1}\right)}{F_{scale}} <$ tol where tol is a chosen tolerance $= 10^{-6}$ and F_{scale} is a scaling factor that is problem dependent. Using Newton's method, the roots of this equation are calculated by solving the following linear system

$$\mathbf{J}^k \delta \mathbf{v}^k = -\mathbf{F}\left(\mathbf{v}^k\right); \mathbf{v}^{k+1} = \mathbf{v}^k + \delta \mathbf{v}^k \tag{14}$$

where $\mathbf{J}^k$ is the Jacobian matrix whose element (i,j) is $J_{i,j}^k = \frac{\partial F_i}{\partial v_j^k}$. In the non-linear granular flow equation set, the frictional component of the contact model and the plastic constitutive model are both governed by non-linear functions; in addition the plastic constitutive model is also non-analytic. The Jacobian matrix will therefore be difficult to invert. One of the primary advantages of employing the NK technique to granular flows is that the Jacobian does not need to be formed (hence the term 'matrix-free'). This occurs because a pertinent choice of the linear solver used in equation (14) requires the Jacobian only in the form of a matrix-vector product. One such solver is the Generalised Minimal RESidual (GMRES) algorithm [7], a variant of which is utilized in this report. GMRES constructs the solution of equation (14) from a basis of Krylov vectors $\left(\mathbf{r_0}, \mathbf{J r_0}, ..., \mathbf{J}^{l-1}\mathbf{r_0}\right)$ where the number of GMRES iterations is l and $\mathbf{r_0}$ is the initial linear residual, $\mathbf{r_0} = -\mathbf{F}\left(\mathbf{v}^k\right) - \mathbf{J}^k \delta \mathbf{v}^0$ constructed from an initial guess $\delta \mathbf{v}^0$. The matrix-vector product used is the following second-order approximation,

$$\mathbf{Jr} = \frac{\mathbf{F}\left(\mathbf{v} + \epsilon \mathbf{r}\right) - \mathbf{F}\left(\mathbf{v}\right)}{\epsilon}, \tag{15}$$

where ϵ is a heuristic perturbation parameter. At each Newton step, the linear problem is solved only to a tolerance that is proportional to the current non-linear residual, Hence the term 'inexact'. This tolerance is employed so that time is not spent needlessly solving the linear problem when the local gradient is far away from the root of the non-linear residual.

The Non-Linear Residual Function

For a given grain, the θ centered non-linear residual at node i is

$$\mathbf{F}_i^k = m_i^n \left(\frac{\mathbf{v}_i^{n+\theta,k} - \mathbf{v}_i^n}{\theta \Delta t} \right) - \left[\sum_p \nabla_{pi} \cdot \sigma_p^{n+\theta,k} + {\mathbf{F_c}_i}^{n+\theta,k} \right]. \tag{16}$$

at the kth Newton iteration. For notational convenience, the grain subscript g has been suppressed

Preconditioning

The overall efficiency of a Newton-Krylov solver is highly dependent on the choice of preconditioner used in the solution of the linear system. A preconditioner is indeed almost mandatory in a Newton-Krylov implementation. In most NK applications in the literature, an approximate matrix is constructed and either incomplete LU (ILU) factorizations [5] or smoothing techniques such as weighted Jacobi (WJ) or SSOR used in the preconditioner [6]. In these cases, the Newton-Krylov implementation is not strictly 'matrix-free' as a matrix that approximates the Jacobian is constructed and converted.

In this study, the linear system is right preconditioned so that the system to be solved is

$$\mathbf{J}^k \mathbf{M}^{-1} \left(\mathbf{M} \delta \mathbf{v}^k \right) = -\mathbf{F}\left(\mathbf{v}^k\right). \tag{17}$$

The solution is formed from the following basis of l Krylov vectors

$$\delta \mathbf{v}^k \approx \sum_{q=0}^{q=l} \beta_q \mathbf{M}_q^{-1} \mathbf{V}_q \tag{18}$$

where $\mathbf{V}_q$ = qth Krylov vector = $\left(\mathbf{J}^k\mathbf{M}_q^{-1}\right)\mathbf{V}_{q-1}$,

$$\mathbf{J}^k\mathbf{M}_q^{-1}\mathbf{V}_q = \frac{\mathbf{F}\left(\mathbf{v}^k + \epsilon\mathbf{M}_q^{-1}\mathbf{V}_q\right) - \mathbf{F}\left(\mathbf{v}^k\right)}{\epsilon}. \qquad (19)$$

To evaluate the preconditioned Krylov vector, $\mathbf{y} \approx \mathbf{M}^{-1}\mathbf{V}$ a WJ smoother is employed where the matrix-free approximation is retained,

$$\mathbf{M}\mathbf{y} = \frac{\tilde{\mathbf{F}}\left(\mathbf{v}^k + \epsilon\left(\mathbf{y}\right)\right) - \tilde{\mathbf{F}}\left(\mathbf{v}^k\right)}{\epsilon}. \qquad (20)$$

As the preconditioning matrix M need only approximate the Jacobian, a simplified form of the Newton residual $\tilde{\mathbf{F}}$ is employed for efficiency. The Fabre-averaged velocity is assumed constant allowing the contact force can be calculated in one pass of the grid rather than two.

In order to retain the matrix-free approximation, each element in the diagonal is effectively calculated by passing in a unit vector into equation (20). Thus element a in diagonal $\mathbf{D}$ is $\mathbf{D}_a = \mathbf{M}\mathbf{e}_a$ where $\mathbf{e}_a$ is the zero vector with a unit entry at element a. For a two-dimensional system with n nodes, this operation requires $2n$ and quickly becomes prohibitive for large systems. The work required in the diagonal calculation is reduced from $2n$ to 18 calls to the matrix free approximation by recognizing the sparsity of the matrix M due to the compact nature of the MPM stencil.

Results

Single Elastic Grain

The problem of an elastic grain rebounding of a solid wall is examined using the implicit and explicit MPM formulations. Figure 1 shows the initial physical configuration and reveal the grain positions for the implicit and explicit MPM formulations respectively at time $t = 2.00$ (after five wall rebounds). The explicit results are run with a CFL stability limit of 0.25. Despite this, they reveal grain spallation as the edges of the grain separate from the main body. Plots of total energy, elastic energy and momentum transfer for both implicit and explicit cases are presented in Figure 2. For the explicit leapfrog, the total energy grows by an order of magnitude, due primarily to the spurious growth in elastic energy. An inelastic deformation is occurring after each wall contact and residual stresses remain. The explicit momentum plot in Figure 2 also shows a spurious increase in momentum after each interaction.

Elastic energy accumulates after each wall contact for the implicit scheme. The accumulation is, however, approximately two orders of magnitude less that that seen in the explicit case. The implicit momentum plot reveals an overall dissipation in kinetic energy which is due to the use of a lumped mass matrix.

In [8], the energy conservation and stability properties of the implicit and explicit schemes were discussed. Both schemes conserve total energy to $0\left(\Delta t^2\right)$ (due to use of the lumped mass matrix). If one considers the grid solution only, the implicit scheme conserves total energy for $\theta = \frac{1}{2}$, while the explicit leapfrog scheme conserves total energy to at best $O\left(\Delta t^3\right)$. In addition, the explicit scheme is non-linearly unstable to an aliasing error that exists for all particle-in-cell calculations [9]. Elastic and kinetic energies are not positive definite and therefore are not bounded by the total energy. The implicit scheme is stable to this aliasing error as elastic and kinetic energies are positive definite and bounded by the total energy.

Compressed Grains

The second problem examined is the dynamic loading of an assembly of 5 grains. The motivation behind the simulation of this problem comes from the experimental work of Rossmanith [10]. Here, investigations of dynamic wave propagation in granular media were undertaken in order to study impact wave propogation and load transfer in granular materials.

Figure 3 displays the contours of the fringe patterns of the in-plane principal stress differences at time $t = 50$ (nearly twice the time taken for a stress wave to propagate through the entire assembly). In the explicit results, the fringe patterns are dominated by high frequency noise; this is a further example of the finite grid instability discussed in Section . The total energy grows as seen in Figure 3. In contrast, the implicit formulation does not exhibit this high frequency noise and total energy is conserved to within 1%.

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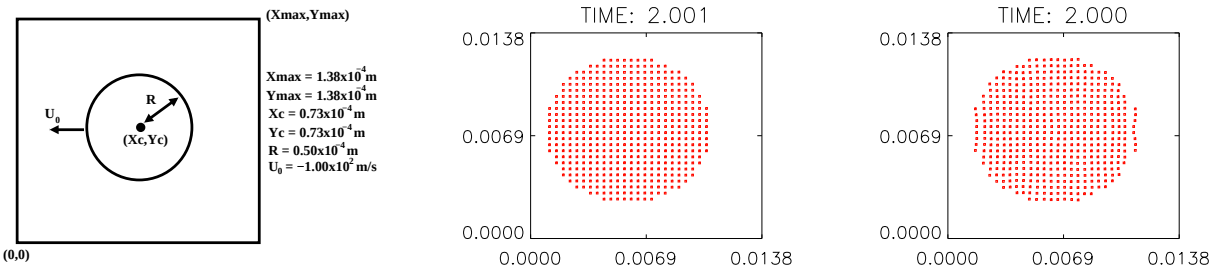

Figure 1: Elastic grain initial configuration, implicit and explicit positions at time $t = 2.00$

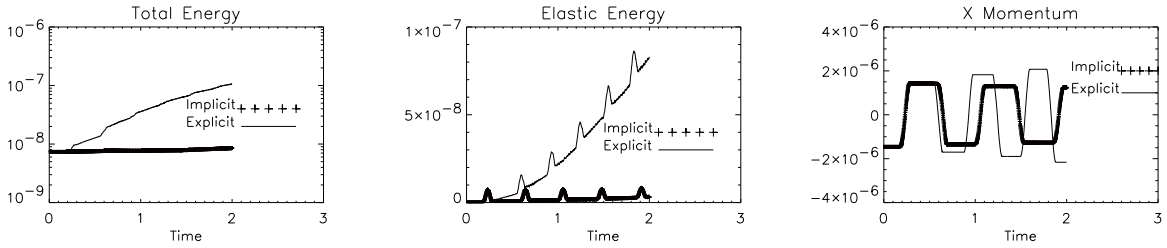

Figure 2: Elastic grain initial configuration, implicit and explicit positions at time $t = 2.00$

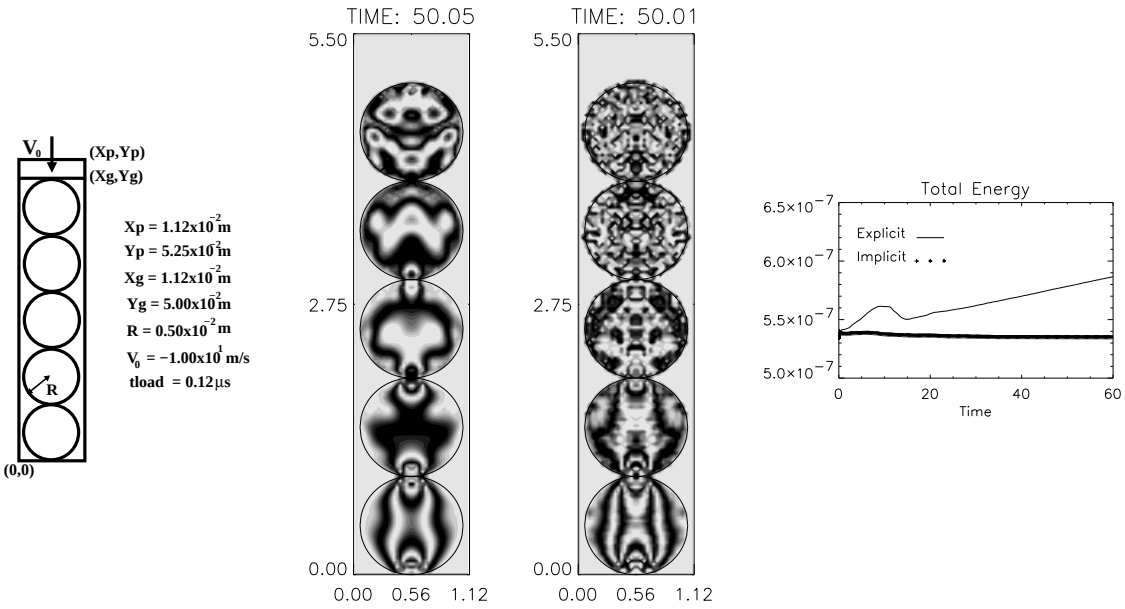

Figure 3: Compressed grains initial configuration, implicit and explicit principal stress differences at time $t = 50.00$ and total energy comparisons.