

# TIME INTEGRATION ERRORS AND ENERGY CONSERVATION PROPERTIES OF THE STORMER VERLET METHOD APPLIED TO MPM

**Martin Berzins\***

\* Scientific Computing and Imaging Institute  
University of Utah  
Salt Lake City, UT 84112 USA  
e-mail: mb@sci.utah.edu, web page: <http://www.sci.utah.edu>

**Key words:** MPM, Time Integration, Stormer Verlet Method, Energy Conservation Accuracy

**Abstract.** The success of the Material Point Method (MPM) in solving many challenging problems nevertheless raises some open questions regarding the fundamental properties of the method such as the energy conservation since being addressed by Bardenhagen and by Love and Sulsky. Similarly while low order symplectic time integration techniques are used with MPM, higher order methods have not been used. For this reason the Stormer Verlet method, a popular and widely-used symplectic method is applied to MPM. Both the time integration error and the energy conservation properties of this method applied to MPM are considered. The method is shown to have locally third order accuracy of energy conservation in time. This is in contrast to the locally second order accuracy in energy conservation of the methods that are used in many MPM calculations. This third accuracy accuracy is demonstrated both locally and globally on a standard MPM test example.

## 1 INTRODUCTION

The Material Point Method (MPM) is often described as a solid mechanics method that is derived [10, 11] from the fluid implicit particle, FLIP and PIC methods. MPM has been very successful when applied to very many large deformation problems. However some of the properties of the method are still not as well-understood as they might be in areas such as time integration and conservation of energy. For example energy conservation is considered by Bardenhagen [1] and it is shown that the standard MPM method gives second order energy conservation over a timestep or first order overall. The analysis of Love and Sulsky [8] extends these results and shows that energy conservation is possible if a full mass matrix is used. The same authors also show that using a lumped mass matrix gives second order locally energy conservation. Other improved time integration methods based upon a central difference approach are considered by [12]. The relationship between MPM time integration and symplectic time integration methods is considered by [3]. Such symplectic methods have good conservation properties [6]. Furthermore the Stormer-Verlet [6] method has third order accuracy locally. This method is symplectic and very widely used in many applications [7] such as molecular dynamics and planetary orbits

---

and even dates back to Newton as was demonstrated by Feynman see [6]. The intention here is to apply the Stormer-Verlet method to MPM and to determine its accuracy and conservation properties. It is shown that the time continuity properties of the spatial methods used play an important role in time accuracy and in conservation. Furthermore it is shown that it is helpful for the basis functions to possess a commutative property so that a discrete version of integration by parts may be used. Although a model one dimensional problem is considered the results are more broadly applicable to higher dimensions. Section 2 describes the MPM method and the model problem used, while Section 3 explains how the Stormer Verlet method may be applied to MPM. Section 4 provides an analysis of the timestepping errors of the Stormer Verlet method and MPM while Sections 5 and 6 derives the energy conservation error of the method. Numerical experiments comparing the approaches on a model problem used by [5] are reported in Section 7, and show show that the Stormer Verlet method has better accuracy and conservation properties than the method considered in [1].

## 2 MPM MODEL PROBLEM AND METHOD

The description of MPM used here follows [5] in that the model problem used here is a pair of equations connecting velocity  $v$ , displacement  $u$  and density  $\rho$  (here assumed constant):

$$\frac{Du}{Dt} = v, \quad (1)$$

$$\rho \frac{Dv}{Dt} = \frac{\partial \sigma}{\partial x} + b(x, t), \quad (2)$$

with a linear stress model  $\sigma = E \frac{\partial u}{\partial x}$  for which Young's modulus,  $E$ , is constant, a body force  $b$ , which is initially assumed to be zero, and with appropriate boundary and initial conditions. For convenience a mesh of equally spaced  $N + 1$  fixed nodes  $X_i$  with intervals  $I_i = [X_i, X_{i+1}]$ , on on the interval  $[a, b]$  is used where

$$a = X_0 < X_1 < \dots < X_N = b, \quad (3)$$

$$h = X_i - X_{i-1}. \quad (4)$$

Theses fixed nodes are referred to as the  $i$  points. It will also be assumed that periodic boundary conditions exist in that

$$\sigma(a)v(a) = \sigma(b)v(b) \quad (5)$$

together with appropriate initial conditions. While the analysis of MPM for time integration error and energy conservation uses the model problem above it does apply more generally and in multiple space dimensions with a few obvious modifications. It will also be assumed that are  $n_p$  particles between each pair of nodes, situated at  $x_p^n$  points where at each time step,  $t^n = \delta t * n$ , where  $n$  is the  $n$ th time step, and the computed solution at the  $p$ th particles will be written as  $u_p^n = u(x_p^n, t^n)$ . Suppose that the particles in interval  $i$  lie between  $X_i$  and  $X_{i+1}$  and have positions  $x_{im+j}$ ,  $j = 1, \dots, m$ . The calculation of the internal forces in MPM at the nodes requires the calculation of the volume integral of the divergence of the stress [12] using

$$f_i^{int} = - \sum_p D_{pi}(x_p^n) \sigma_p V_p \quad (6)$$

---

In this case the subscript  $pi$  represents a mapping from particles  $p$  to node  $i$ . The subscript  $ip$  would represent a mapping from nodes  $i$  to particles  $p$ . The negative sign arises as a result of using integration by parts [5]. The mass at node  $i$  is defined by

$$m_i = \sum_p m_p S_{pi}(x_p^n) \quad (7)$$

It is important to note that the coefficients  $D_{pi}(x_p^n)$  and  $S_{pi}(x_p^n)$  depend explicitly on the background mesh and the particle positions and that they also be chosen to reproduce derivatives of constant and linear functions exactly [5]. It should also be noted that mappings from particles to derivatives on grids e.g.  $D_{pi}$  may possibly be very different from forming derivatives at particles using nodal values as denoted by  $D_{ip}$ . Similar comments apply to interpolating from particles to grids as denoted by the coefficients  $S_{pi}$  and from nodes to grids as denoted by  $S_{ip}$ . The initial volume of the particles is uniform for the  $n_p$  particles in an interval. The particle volumes are defined using the deformation gradient,  $F_p^n$ , and the initial particle volume,  $V_p^0$ ,

$$V_p^n = F_p^n V_p^0, \text{ where } V_p^0 = \frac{h}{n_p}, \text{ where } F_p^0 = 1 \quad (8)$$

From (7) the acceleration equation in the MPM method in this simple case is

$$a_i(t) = \frac{-1}{m_i} \sum_p D_{pi}(x_p(t)) \sigma_p(t) F_p(t) V_p^0 \quad (9)$$

The equation to update velocity at the nodes, as denoted by  $v_i^n$  is then given by

$$\dot{v}_i = a_i \quad (10)$$

The equation for the update of the particle velocity is then

$$\dot{v}_p = a_p \quad (11)$$

where the value of the acceleration at a point  $x_p^n$  is given by interpolation based upon nodal values of acceleration

$$a_p = \sum_i S_{ip}(x_p(t)) a_i \quad (12)$$

The equation for the particle position update is

$$\dot{x}_p = v_p \quad (13)$$

The update of the deformation gradients is given using,

$$\frac{\partial v}{\partial x}(x_p(t)) = \sum_i D_{ip}(x_p(t)) v_i \quad (14)$$

The deformation update equation is

$$\dot{F}_p = \frac{\partial v}{\partial x}(x_p(t), t) F_p \quad (15)$$

While the stress update equation is, using the appropriate constitutive model and Young's Modulus,  $E$ ,

$$\dot{\sigma}_p = E \frac{\partial v}{\partial x}(x_p(t)) \quad (16)$$

---

### 3 THE STORMER VERLET TIME INTEGRATION METHOD

In solving the system of equations defined above by equations (6) to (16) one standard approach used is to order the equations in a certain order and then to solve them in turn using explicit methods. Differences in how the equations are solved corresponds to whether or not the stress is updated first or last in a timestep, a choice that is discussed at length by [1] and [4]. These two different choices are related to the use of the semi-implicit Euler A or B method, [7], [3]. An alternative approach of Hairer et al.[6] defines a method with better time integration properties. Applying the method of p. 407 of [6] requires one extra step over the symplectic Euler Stress Last or Stress First methods [3, 1] to define both nodal and particle velocities, and spatial points at half timestep values. This approach applied to MPM will now be described. On the very first step the nodal accelerations and velocities have to be calculated.

$$v_i^n = \sum_p S_{pi}(x_p^n) \frac{m_p}{m_i} v_p^n \quad (17)$$

$$a_i^n = \frac{-1}{m_i} \sum_p D_{ip}(x_p^n) \sigma_p^n F_p^n V_p^0 \quad (18)$$

The equation to update velocity at the nodes is then given by

$$v_i^{n+1/2} = v_i^n + \frac{dt}{2} a_i^n \quad (19)$$

The value of the acceleration at a point  $x_p^n$  is given by interpolation based upon nodal accelerations is

$$a_p^n = \sum_i S_{ip}(x_p^n) a_i^n \quad (20)$$

The equation for the update of the particle velocity is then

$$v_p^{n+1/2} = v_p^n + \frac{dt}{2} a_p^n \quad (21)$$

Similarly the equation for the particle position update is

$$x_p^{n+1/2} = x_p^n + \frac{dt}{2} v_p^n \quad (22)$$

The velocity gradients at particles are calculated using

$$\frac{\partial v}{\partial x}(x_p^{n+1/2}, t_{n+1/2}) = \sum_i D_{ip}(x_p^{n+1/2}) v_i^{n+1/2} \quad (23)$$

These velocity gradients are used to update the stress and deformation gradients at particles

$$F_p^{n+1} = F_p^n + \frac{dt}{2} \frac{\partial v}{\partial x}(x_p^{n+1/2}, t_{n+1/2}) (F_p^n + F_p^{n+1}) \quad (24)$$

While stress is updated using the appropriate constitutive model and Young's Modulus,  $E$ ,

$$\sigma_p^{n+1} = \sigma_p^n + dt E \frac{\partial v}{\partial x}(x_p^{n+1/2}, t_{n+1/2}) \quad (25)$$

and the acceleration is updated with these two values which are the updated stresses and deformation gradients at the current grid points, but at the next time level  $t^{n+1}$ .

$$a_i^{n+1} = \frac{-1}{m_i} \sum_p D_{ip}(x_p^{n+1/2}) \sigma_p^{n+1} F_p^{n+1} V_p^0 \quad (26)$$

The equation to update velocity at the nodes is then given by

$$v_i^{n+1} = v_i^n + \frac{dt}{2} (a_i^{n+1} + a_i^n) \quad (27)$$

The value of the acceleration at a point  $x_p^n$  is given by interpolation based upon nodal accelerations:

$$a_p^{n+1} = \sum_i S_{ip}(x_p^{n+1/2}) a_i^{n+1} \quad (28)$$

The final equation for the update of the particle velocity is then

$$v_p^{n+1} = v_p^n + \frac{dt}{2} (a_p^{n+1} + a_p^n) \quad (29)$$

while the equation for the particle position update is

$$x_p^{n+1} = x_p^n + \frac{dt}{2} (v_p^{n+1} + v_p^n) \quad (30)$$

The conservation of energy analysis below will assume that the updated spatial position are substituted into equation (26) so that the nodal and particle accelerations and velocities at time  $t^{n+1}$  reflect the correct values of the spatial mesh points.

#### 4 Local Errors in Stormer-Verlet applied to MPM

In evaluating the local error in a step of the Stormer Verlet method it is important to note that the method consists of a half step using a forward Euler method. The values computed from this are substituted into what may be described as a Trapezoidal Rule or Midpoint Rule, before a final update that appears like part of a second-order Runge-Kutta Method. Considering the Forward Euler half step, the first error is that in the nodal velocity equation (19). In this case if this error is denoted as  $LEV_i$  its value is given by the standard Forward Euler local error as

$$LEV_i^{n+1/2} = \frac{dt^2}{8} \frac{da_i^n}{dt} + h.o.t \quad (31)$$

$$= \frac{dt^2}{8} \frac{d}{dt} \left( \frac{-1}{m_i} \sum_p D_{ip}(x(t)) \sigma_p(t) F_p(t) V_p^0 \right) + h.o.t. \quad (32)$$

This obviously require differentiability of the coefficients  $D_{ip}(x(t))$ , even when particles cross grid boundaries. Similarly at the particles

$$LEV_p^{n+1/2} = \frac{dt^2}{8} \sum_p \frac{d}{dt} (S_{ip}(x(t)) a_i(t)) + h.o.t. \quad (33)$$

For the particle update the local error as denoted by  $LEx_p^{n+1/2}$  is given by

$$LEx_p^{n+1/2} = \frac{dt^2}{8} \sum_p \frac{d}{dt} (S_{ip}(x(t))V_i(t)) + h.o.t. \quad (34)$$

Second order accuracy requires that the coefficients  $S_{ip}(x(t))$  are differentiable in time. The local errors in the updates of the deformation gradient as defined in (24) is similar to that of the Trapezoidal Rule and is given by

$$LEF_p^{n+1} = \frac{dt^3}{12} \frac{d^2}{dt^2} \left( F \frac{\partial v}{\partial x}(x_p(t), t) \right) + h.o.t. \quad (35)$$

Stress is updated using the appropriate constitutive model and Young's Modulus,  $E$ , at the mid point and so  $LE\sigma_p^{n+1}$  is the stress local time error obtained from the Mid-point Rule

$$LE\sigma_p^{n+1} = \frac{Edt^3}{24} \frac{d^2}{dt^2} \left( \frac{\partial v}{\partial x}(x_p(t), t) \right) + h.o.t. \quad (36)$$

Again the differentiability of the coefficients  $D$  is required. The full local errors including those carried from the velocity calculation at the half step are given by

$$leF_p^{n+1} = LEF_p^{n+1} + dtF \sum_q \frac{\partial}{\partial x_q} \left( \frac{\partial v}{\partial x}(x_q(t), t) \right) LEx_q^{n+1/2} + h.o.t. \quad (37)$$

and

$$le\sigma_p^{n+1} = LE\sigma_p^{n+1} + dtE \sum_q \frac{\partial}{\partial x_q} \left( \frac{\partial v}{\partial x}(x_q(t), t) \right) LEx_q^{n+1/2} + h.o.t. \quad (38)$$

When updating the velocity and position at the particles the nodal errors are carried by interpolation. For the final velocity update at nodes the local error as denoted by  $LEV_i^{n+1}$  is given by

$$LEV_i^{n+1} = \frac{dt^3}{12} \frac{d^2}{dt^2} (a_i(t)) + h.o.t. \quad (39)$$

The full local error in the equation to update velocity at the nodes (29) is then given by

$$lev_i^{n+1} = dtlea_i^{n+1} + LEV_i^{n+1} \quad (40)$$

where the propagated error from the stress and deformation gradients in the acceleration is (ignoring products of these errors) given by

$$lea_i^{n+1} = \frac{-1}{m_i} \left[ \sum_p D_{ip}(x_p^{n+1/2} + LEx_p^{n+1/2})(\sigma_p^{n+1} + LE\sigma_p^{n+1})(F_p^{n+1} + LEF_p^{n+1})V_p^0 - \sum_p D_{ip}^{n+1/2} \sigma_p^{n+1} F_p^{n+1} V_p^0 \right] \quad (41)$$

$$lea_i^{n+1} \approx \frac{-1}{m_i} \left[ \sum_p D_{ip}(x_p^{n+1/2})(LE\sigma_p^{n+1} F_p^{n+1} + LEF_p^{n+1} \sigma_p^{n+1}) + \sum_p \frac{\partial D_{ip}(x_p(t))}{\partial x_p(t)} LEx_p^{n+1/2} F_p^{n+1} \sigma_p^{n+1} \right] V_p^0 \quad (42)$$

---

The time local error in the value of the acceleration at a point  $x_p^n$  as defined by (28) is given by interpolating nodal acceleration errors

$$lea_p^{n+1} = \sum_i S_{ip}(x_p^n) lea_i^{n+1} \quad (43)$$

The equation for the full local time error in the update of the particle velocity as defined by (29) is then

$$lev_p^{n+1} = dt lea_p^{n+1} + LEV_p^{n+1} \quad (44)$$

where the Trapezoidal Rule-like error is given by

$$LEV_p^{n+1} = \frac{dt^3}{12} \sum_p \frac{d^2}{dt^2} (S_{ip}(x_p(t)) a_i(t)) + h.o.t. \quad (45)$$

For the particle update the local error, as denoted by  $LEx_p^{n+1}$ , is given by

$$LEx_p^{n+1} = \frac{dt^3}{12} \sum_p \frac{d^2}{dt^2} (S_{ip}(x_p(t)) V_i^n) \quad (46)$$

The equation for the full local time error in the particle position update as given by (30) is

$$lex_p^{n+1} = dt lev_p^{n+1} + LEx_p^{n+1} \quad (47)$$

In summary, even after taking into account the propagated errors from the different MPM stages, the local error appears to be third order, providing that the coefficients of the MPM method  $S_{ip}(x(t))$  and  $D_{ip}(x(t))$  are sufficiently differentiable.

## 5 ENERGY CONSERVATION OF MPM

The focus here is on the energy of the particles as this corresponds to the points moved in computation and solution values that used and displayed. The starting point is, for the moment, to ignore the body forces and then to use the approach of [1].

### 5.1 Grid Point Kinetic Energy of MPM

The change in kinetic energy as denoted by  $\Delta K^{\mathcal{E}_{grid}}$  on the points is given by [1]

$$\Delta K^{\mathcal{E}_{pts}} = \frac{1}{2} \sum_p m_p (v_p^{n+1})^2 - \frac{1}{2} \sum_p m_p (v_p^n)^2 \quad (48)$$

where  $m_p$  is the mass at particle point  $x_p$ . Hence the grid Kinetic energy is also given by

$$\Delta K^{\mathcal{E}_{pts}} = \frac{1}{2} \sum_p m_p (v_p^{n+1} - v_p^n)(v_p^{n+1} + v_p^n) \quad (49)$$

This may be written in terms of the acceleration as

$$\Delta K^{\mathcal{E}_{grid}} = \frac{dt}{4} \sum_p m_p (a_p^{n+1} + a_p^n)(v_p^{n+1} + v_p^n) \quad (50)$$

Substituting for the acceleration at a point using (12) gives

$$\Delta K_{\mathcal{E}_{grid}} = \frac{dt}{4} \left[ \sum_p m_p (v_p^{n+1} + v_p^n) \left( \sum_i S_{ip}(x_p^{n+1/2}) a_i^{n+1} + \sum_i S_{ip}(x_p^n) a_i^n \right) \right] \quad (51)$$

and again for the nodal acceleration using (9) gives

$$\begin{aligned} \Delta K_{\mathcal{E}_{grid}} = \frac{-dt}{4} \sum_p (v_p^{n+1} + v_p^n) & \left[ \sum_i S_{ip}(x_p^{n+1/2}) \frac{m_p}{m_i} \sum_q D_{qi}(x_q^{n+1/2}) \sigma_q^{n+1} F_q^{n+1} V_q^0 \right. \\ & \left. + \sum_i S_{ip}(x_p^n) \frac{m_p}{m_i} \sum_q D_{qi}(x_q^n) \sigma_q^n F_q^n V_q^0 \right] \end{aligned} \quad (52)$$

Using the extension to define velocities and accelerations at the final particle positions  $x_p^{n+1}$  gives

$$\begin{aligned} \Delta K_{\mathcal{E}_{grid}} = \frac{-dt}{4} \sum_p (v_p^{n+1} + v_p^n) & \left[ \sum_i S_{ip}(x_p^{n+1}) \frac{m_p}{m_i} \sum_q D_{qi}(x_q^{n+1}) \sigma_q^{n+1} F_q^{n+1} V_q^0 \right. \\ & \left. + \sum_i S_{ip}(x_p^n) \frac{m_p}{m_i} \sum_q D_{qi}(x_q^n) \sigma_q^n F_q^n V_q^0 \right] \end{aligned} \quad (53)$$

## 5.2 Strain Energy of MPM

The rate of change of strain energy is given by (28) in [1]. Hence integrating this equation from  $t^n$  to  $t^{n+1}$  and using the Trapezoidal Rule gives

$$\Delta S_{\mathcal{E}} = \frac{dt}{2} \sum_p \left( \sigma_p^{n+1} F_p^{n+1} \frac{\partial v_p^{n+1}}{\partial x} + \sigma_p^n F_p^n \frac{\partial v_p^n}{\partial x} \right) V_p^0 + O(dt^3) \quad (54)$$

This expression is different from that derived by Bardenhagen [1] using piecewise linear approximations for  $\sigma$  and for  $F$ . The error in equation (54) is  $\frac{dt^3}{12} \frac{\partial^2}{\partial t^2} (\sigma F \frac{\partial V_p}{\partial x})$ , while the error in Bardenhagen's expression is about a factor of three larger. Substituting for the spatial derivatives in equation (54) gives

$$\begin{aligned} \Delta S_{\mathcal{E}} = \frac{dt}{2} & \sum_p \left( \sigma_p^{n+1} F_p^{n+1} \sum_i D_{ip}(x_p^{n+1}) \sum_q S_{qi}(x_q^{n+1}) v_q^{n+1} \frac{m_q}{m_i} + \sigma_p^n F_p^n \sum_i D_{ip}(x_p^n) \sum_q S_{qi}(x_q^n) v_q^n \frac{m_q}{m_i} \right) V_p^0 \end{aligned} \quad (55)$$

Changing the order of summation gives

$$\begin{aligned} \Delta S_{\mathcal{E}} = \frac{dt}{2} & \left( \sum_q v_q^{n+1} \sum_i S_{qi}(x_q^{n+1}) \frac{m_q}{m_i} \sum_p D_{ip}(x_p^{n+1}) \sigma_p^{n+1} F_p^{n+1} V_p^0 + \right. \\ & \left. \sum_q v_q^n \sum_i S_{qi}(x_q^n) \frac{m_q}{m_i} \sum_p D_{ip}(x_p^n) \sigma_p^n F_p^n V_p^0 \right) \end{aligned} \quad (56)$$

The two symmetry relations mentioned in the introduction are now needed

$$S_{qi}(x_q(t)) = S_{iq}(x_q(t)) \quad (57)$$



and

$$D_{qi}(x_q(t)) = D_{iq}(x_q(t)) \quad (58)$$

to be able to write equation (56) as

$$\Delta S_{\mathcal{E}} = \frac{dt}{2} \left( \sum_q v_q^{n+1} \sum_i S_{iq}(x_q^{n+1}) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^{n+1}) \sigma_p^{n+1} F_p^{n+1} V_p^0 + \sum_q v_q^n \sum_i S_{iq}(x_q^n) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^n) \sigma_p^n F_p^n V_p^0 \right)$$

## 6 Energy Conservation Error of the Stormer Verlet Scheme

Combining the kinetic and strain energy expressions gives the energy conservation error

$$\begin{aligned} \Delta \mathcal{E}_{err} = & \frac{-dt}{2} \left( \sum_p \frac{(v_p^{n+1} + v_p^n)}{2} \left[ \sum_i S_{ip}(x_p^{n+1}) \frac{m_p}{m_i} \sum_q D_q(x_q^{n+1}) \sigma_q^{n+1} F_q^{n+1} V_q^0 \right. \right. \\ & \left. \left. + \sum_i S_{ip}(x_p^n) \frac{m_p}{m_i} \sum_q D_{qi}(x_q^n) \sigma_q^n F_q^n V_q^0 \right] - \right. \\ & \left. \left( \sum_q v_q^{n+1} \sum_i S_{iq}(x_q^{n+1}) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^{n+1}) \sigma_p^{n+1} F_p^{n+1} V_p^0 + \sum_q v_q^n \sum_i S_{iq}(x_q^n) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^n) \sigma_p^n F_p^n V_p^0 \right) \right) \end{aligned}$$

Assuming for the moment that the  $D$  and  $S$  values are updated to have the final velocities this may now be simplified to be

$$\begin{aligned} \Delta \mathcal{E}_{err} = & \frac{dt}{2} \left( \left( \sum_q (v_q^{n+1} - \frac{(v_q^{n+1} + v_q^n)}{2}) \sum_i S_{iq}(x_q^{n+1}) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^{n+1}) \sigma_p^{n+1} F_p^{n+1} V_p^0 \right. \right. \\ & \left. \left. + \sum_q (v_q^n - \frac{(v_q^{n+1} + v_q^n)}{2}) \sum_i S_{iq}(x_q^n) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^n) \sigma_p^n F_p^n V_p^0 \right) \right) \quad (59) \end{aligned}$$

and again to

$$\begin{aligned} \Delta \mathcal{E}_{err} = & \frac{dt}{2} \sum_q \left( \frac{(v_q^{n+1} - v_q^n)}{2} \right) \\ & \left( \sum_i S_{iq}(x_q^{n+1}) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^{n+1}) \sigma_p^{n+1} F_p^{n+1} V_p^0 - \sum_i S_{iq}(x_q^n) \frac{m_q}{m_i} \sum_p D_{pi}(x_p^n) \sigma_p^n F_p^n V_p^0 \right) \quad (60) \end{aligned}$$

Using (18,20,25) and (28) this may now be written as

$$\Delta \mathcal{E}_{err} = \frac{dt}{2} \sum_q \left( \frac{(v_q^{n+1} - v_q^n)}{2} \right) m_q (a_q^{n+1} - a_q^n) \quad (61)$$

It follows that if all the components of the above equation are differentiable then

$$\Delta \mathcal{E}_{err} = O(dt^3) \quad (62)$$

## 6.1 Contribution from the Body Forces

The body forces may be divided by nodal mass to get body accelerations at the nodes, denoted here by  $\hat{b}_i$ . The body accelerations at the particles are denoted by  $\hat{b}_p$ . It is then routine to show that the energy error due to the body forces,  $\Delta \mathcal{E}_{err}^B$  is given by

$$\Delta \mathcal{E}_{err}^B = \frac{-dt}{2} \left( \sum_p \frac{(v_p^{n+1} + v_p^n)}{2} \left[ \sum_i S_{ip}(x_p^{n+1/2}) \hat{b}_i^{n+1} + \sum_i S_{ip}(x_p^n) \hat{b}_i \right] - \sum_q v_q^{n+1} \hat{b}_q^{n+1} - \sum_q v_q^n \hat{b}_q^n \right)$$

Using the expression

$$\hat{b}_p^n = \sum_i S_{ip}(x_p^n) \hat{b}_i^n + (\hat{b}_p^n - \sum_i S_{ip}(x_p^n) \hat{b}_i^n) \quad (63)$$

allows the above equation to be written as

$$\Delta \mathcal{E}_{err}^B = \frac{dt}{2} \left( \sum_q (v_q^{n+1} - \frac{(v_q^{n+1} + v_q^n)}{2}) \hat{b}_q^{n+1} + \sum_q (v_q^n - \frac{(v_q^{n+1} + v_q^n)}{2}) \hat{b}_q^n + ERR_b \right) \quad (64)$$

and as

$$\Delta \mathcal{E}_{err}^B = \frac{dt}{2} \left( \sum_q \left( \frac{(v_q^{n+1} - v_q^n)}{2} \right) (\hat{b}_q^{n+1} - \hat{b}_q^n) + ERR_b \right) \quad (65)$$

where the term  $ERR_B$  is given by

$$ERR_B = \frac{dt}{2} \left( \sum_p \frac{(v_p^{n+1} - v_p^n)}{2} (b_p^n - b_p^{n+1} + \sum_i S_{ip}^{n+1} b_i^{n+1} - \sum_i S_{ip}^n b_i^n) \right) \quad (66)$$

Again all these terms are  $O(dt^3)$  if there is sufficient smoothness in time.

## 6.2 Energy Conservation Errors of The Stress First/Last Schemes

The above analysis may easily be extended to the stress first and stress last schemes discussed by [1]. In the case of Stress First this gives, in terms of the particular Stress First accelerations and velocities the energy conservation error

$$\Delta \mathcal{E}_{err}^{first} = \frac{-dt}{2} \sum_q v_q^n m_q (a_q^{n+1} - a_q^n) \quad (67)$$

While in the case of Stress Last the sign is reversed. It follows that both these errors are  $O(dt^2)$ .

## 7 COMPUTATIONAL EXPERIMENTS

In order to illustrate the above results the model 1D bar problem used by [5] and [3] is used. The cell width is  $h = 10^{-2}$ , the material density is  $\rho_0 = 1$  and the time interval is  $[0,1]$ . The initial spatial discretization uses two evenly spaced particles per cell with the spatial domain being  $[0, 1]$ . The Young's modulus values are  $E = 256$  and  $E = 64$ . The maximum displacement is  $A = 0.015$ , and  $A = 0.05$  and the time step values used are  $dt = 10^{-6}, 10^{-5}, 10^{-4}, 10^{-3}$ . In

---

both these cases for the values given of  $A$  it should be noted that with the use of the above parameters particles will cross from one cell to another.

Experiments were undertaken with the MPM GIMP method [9] These experiments were run with fixed time steps as shown in Table 1 in which the time step,  $dt$  is varied appropriately. The number of grid crossings varies greatly, see [3]. Roughly speaking the case with  $A = 1.5e - 2$  has about half the grid crossings of the case when  $A = 5.0e - 2$ . The results in Table 1 show for the maximum over th timesteps of the sum of squares of energy and displacement errors that the Stormer Verlet method is much better at conserving energy that a standard MPM approach, as indeed the theoretical results suggest. Moreover the theoretical local second and third order accuracies also in this case give rise to global second and third order accuracy.

## 8 CONCLUSIONS

This approach addresses the conservation properties of the MPM method by deriving the conservation properties of the Stormer Verlet Method and by contrasting it in experiments with the Stress First and Stress Last methods discussed by [1]. The Stormer Verlet method appears to have superior energy conserving properties.

### Acknowledgements

Chris Gritton is thanked for the use of his code for the model problem used to obtain the results shown in Section 6. This research was partially sponsored by the Army Research Laboratory under Cooperative Agreement Number W911NF-12-2-0023. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies of the Army Research Laboratory or the U.S. Government.

### REFERENCES

- [1] Bardenhagen S., Energy conservation error in the material point method for solid mechanics, *Journal of Computational Physics*, 180, 2002, 383-403.
- [2] Bardenhagen s. and Kober E., The generalized interpolation material point method, *Computer Modeling in Engineering and Science*, 5 (2004), 477-495.
- [3] Berzins M. Nonlinear stability and time step selection for the MPM method, *Computational Particle Mechanics*, Jan, 2018.
- [4] Buzi O., Pedroso D.M. and Giacomini A. Caveats on the Implementation of the Generalized Material Point Method. *CMES*. vol 31, 2, 85-106, 2008
- [5] Gritton C.E. and Berzins M., Improving Accuracy In the MPM Methods by Using a Null Space Filter, *Computational Particle Mechanics* 2017, 4 131-142.
- [6] Hairer E., Lubich C., and Wanner G., Geometric numerical integration illustrated by the Stormer-Verlet Method. *Acta Numerica* 2003, pp.399-450, Cambridge University Press.
- [7] Leimkuhler B. and Reich S., *Simulating Hamiltonian dynamics*. Cambridge Monographs on Applied and Computational Science. Cambridge University Press 2004.

**Table 1:** Maximum Energy and Maximum Displacement Errors over Timesteps

A=1.5e-2 E = 256				A=5e-2 E =256			
dt	Method	Energy Error	Displacement Error	dt	Method	Energy Error	Displacement Error
1e-3	GIMP	3.2e-2	5.2e-5	1e-3	GIMP	4.5e-4	2.4e-3
	SVGP	7.5e-6	7.8e-5		SVGP	2.4e-4	3.0e-3
1e-4	GIMP	2.3e-4	2.2e-5	1e-4	GIMP	7.0e-3	2.9e-3
	SVGP	7.7e-9	2.1e-5		SVGP	1.0e-6	3.0e-3
1e-5	GIMP	2.5e-6	2.3e-5	1e-5	GIMP	1.0e-4	2.8e-3
	SVGP	8.5e-12	2.3e-5		SVGP	1.5e-9	2.8e-3
1e-6	GIMP	2.5e-8	2.3e-5	1e-6	GIMP	1.0e-6	2.7e-3
	SVGP	9.0e-15	2.3e-5		SVGP	1.6e-12	2.7e-3
A=1.5e-2 E = 64				A=5e-2 E =64			
dt	Method	Energy Error	Displacement Error	dt	Method	Energy Error	Displacement Error
1e-3	GIMP	1.2e-3	1.8e-5	1e-3	GIMP	1.9e-2	9.3e-4
	SVGP	2.0e-7	2.5e-5		SVGP	7.9e-6	6.3e-4
1e-4	GIMP	1.2e-5	6.2e-6	1e-4	GIMP	2.5e-4	7.0e-4
	SVGP	1.7e-10	6.5e-6		SVGP	1.3e-8	6.9e-4
1e-5	GIMP	1.4e-7	7.4e-6	1e-5	GIMP	2.8e-6	7.3e-4
	SVGP	2.0e-13	7.4e-6		SVGP	1.8e-11	7.3e-4
1e-6	GIMP	1.5e-9	7.5e-6	1e-6	GIMP	2.9e-8	7.3e-4
	SVGP	2.0e-16	7.5e-5		SVGP	2.0e-14	7.0e-4

- [8] Love, E and Sulsky, D. An energy consistent material point method for dynamic finite deformation plasticity. *International Journal for Numerical Methods in Engineering*. 65. 1608 - 1638, 2006.
- [9] Steffen M., Wallstedt P.C., Guilkey J.E. , Kirby R.M. and Berzins M., Examination and analysis of implementation choices within the Material Point Method (MPM), *Computer Modeling in Engineering & Sciences*, 2008, 31, 2, 107-127.
- [10] Sulsky D., Chen Z. and Schreyer H.L. A particle method for history-dependent materials. *Computer Methods in Applied Mechanics and Engineering* 118 (1994):179-196.
- [11] Sulsky D., Zhou S.-J. and Schreyer H.L. Application of a particle-in-cell method to solid mechanics. *Computer Physics Communications* 87 (1995):236-252 .
- [12] Wallstedt P.C. and Guilkey J.E., An evaluation of explicit time integration schemes for use with the generalized interpolation material point method. *Journal of Computational Physics* 2008, 227, 22, 9628-9642.