PRACTICAL ERROR ESTIMATION FOR THE MATERIAL POINT METHOD.

Martin Berzins *

* SCI Institute and School of Computing University of Utah
72. S.Central Campus Drive, Salt lake City USA
e-mail: mb@sci.utah.edu, web page: http://sci.utah.edu/people/mb.html

Key words: Material Point Method Error Estimation

Summary. The Material Point Method (MPM) is widely used for challenging applications in engineering, and animation. The complexity of the method makes error estimation challenging. Error analysis of a simple MPM method is undertaken and the global error is shown to be first order in space and time for a widely-used variant of the method. Computational experiments illustrate the estimated accuracy.

1 INTRODUCTION

The Material Point Method (MPM) has proved to be capable of solving many challenging problems in computational mechanics [7, 11]. While for many methods in computational mechanics computational error estimates are available, they are very much lacking for the Material Point Method. In part this is due to the complex system of timedependent non-linear equations and the need to track the error as it evolves in time. This work is concerned with examining possible error estimation approaches for the Material Point Method. The first step is to make precise the sources and forms of the different MPM errors see [4]. estimating these errors may involve a finite element like method [1] or making use of a simpler linearity preservation formulation [6, 5] to define the accuracy in the different stages of the method. This was the approach in [4]. The first step is to use these estimates to understand the global order of accuracy. A preliminary step in this direction was taken by [10], to look at the form of the particle velocity and acceleration errors under reasonable but unproven assumptions about the assumed order of accuracy of the errors. Here the idea is to end this to use the error decomposition derived by [4] to develop expressions for the accuracy of all the computed components. This derivation shows first order accuracy for a widely-used MPM method. There are then two approaches that are possible. One is to explicitly model the error equations ,[4]. While the second is to use an extrapolation approach in which the main calculation is complemented by a subsidiary calculation on a coarse (or finer) mesh. This approach was initially explored by [9] but needs the order of accuracy derived here to be extended further. A number of computational experiments are used to illustrate the accuracy of MPM for a simple model problem.

2 MPM MODEL PROBLEM

A standard MPM model used here follows [5] in being a pair of equations connecting velocity v, displacement u, stress σ and density ρ (here assumed constant):

$$\frac{Du}{Dt} = v,\tag{1}$$

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

with a linear stress model $\sigma = \hat{E} \frac{\partial u}{\partial x}$ 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

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

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

It will also be assumed that periodic boundary conditions exist, together with appropriate initial conditions. The approach used corresponds to a stress-last [2] or a symplectic Euler A method [3]. Following Bardenhagen [2] it is preferable to increment stress last and to use the GIMP method for spatial discretization. It will also be assumed that are n_p particles initially 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 nth time step, and the computed displacement at the pth particles will be written as $u_p^n = u(x_p^n, t^n)$. 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 ,

$$V_p^n = F_p^n V_p^0$$
, where $V_p^0, = \frac{h}{n_p}$, where $F_p^0 = 1$ (5)

The nodal velocity is initially given by the mass-related mapping

$$v_i^n = \sum_p S_{pi}^n \frac{m_p}{m_i} v_p^n \tag{6}$$

At the beginning of each subsequent step it is assumed that particle positions and velocities x_p^n and v_p^n , stresses and deformation gradients σ_p^n and F_p^n exist. There are two key mappings in MPM. The first is an interpolation mapping from particles to grid (and back again) For example for the grid $(v_i^n a)$ and particle velocities. (v_p^n) at time t_n

$$v_i^n = \sum_p S_{pi}^n v_p^n \quad (andv_p^n = \sum_p S_{ip}^n v_i^n) \tag{7}$$

In this case the subscript pi represents a mapping from particles p to node i while the subscript ip represents a mapping from nodes i to particles p. Linearity preservation

means that $\sum_{p} S_{pi}^{n} = 1$ and that $\sum_{p} S_{pi}^{n} x_{p}^{n} = x_{i}$ The interpolation error in this mapping may be approximately written as [4] (where errors in v_{p}^{n} are ignored)

$$EIv_i^n = C_{EVi}h^2 \quad (or EIv_p^n = C_{EVp}h^2) \tag{8}$$

The second mapping uses particle values to compute a derivative at the nodes (or nodal values to compute a derivative at the particles).

$$\frac{\partial v}{\partial x}(x_i, t_n) = \sum_p D_{pi}^n v_p^n, \quad (or \frac{\partial v}{\partial x}(x_p, t_n) = \sum_p D_{ip}^n v_i^n)$$
(9)

The first-order interpolation and differentiation error in this mapping may be approximately written as [4] (again where errors in v_p^n (and v_i^n) are ignored)

$$EIv_{i,x}^{n} = C_{h}h \quad (orEIv_{p,x}^{n} = C_{h}h) \tag{10}$$

for obvious choices of constants C_h . Throughout in what follows such constants will be chosen and used to ease the complexity of the description. It should be note that, for example C_h will be any constant that multiplies h and that this is the lowest power of ,say, h in the error in this case. The errors in these mappings are fundamental in understanding the how the errors evolve in MPM. The calculation of the acceleration in MPM at the nodes requires the calculation of the volume integral of the divergence of the stress using the equations (and ignoring external forces)

$$a_i^n = \frac{-1}{m_i} \sum_p D_{pi}^n \sigma_p^n F_p^n V_p^0 \tag{11}$$

The negative sign arises as a result of using integration by parts [5]. The error in this approximation may be approximated by [4]

$$Ea_{i}^{n} = C_{h}h - \frac{1}{m_{i}}\sum_{p}D_{pi}^{n}(E\sigma_{p}^{n}F_{p}^{n} + \sigma_{p}^{n}EF_{p}^{n})V_{p}^{0}$$
(12)

Where $E\sigma_p^n$ and EF_p^n are the stress and deformation gradient errors at time t_n . The local error on just one time step assuming no error at the start of the step is

$$LEa_i^n = C_h h \tag{13}$$

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

$$v_i^{n+1} = v_i^n + dt a_i^n \tag{14}$$

The nodal velocity v_i error is Ev_i^n which is defined by existing particle errors and an interpolation error Ev_{ipi}^n by

$$Ev_i^n = \sum_p S_{pi}^n \frac{m_p}{m_i} Ev_p^n + EIv_{pi}^n \tag{15}$$

where EIv_{pi}^{n} is the mapping error associated with the coefficients S_{pi}^{n} and [4]

$$EIv_{ni}^n = C_{h2}h^2 \tag{16}$$

The global error in this forward Euler step at time t^{n+1} is given by Ev_i^{n+1} and its evolution may be approximated by

$$EV_i^{n+1} = Ev_i^n + \frac{dt^2}{2}\frac{d^2v_i^n}{dt^2} + dtEa_i^n + EIv_{pi}^n$$
(17)

The local part of this error assuming no error at the start of the step is

$$LEV_i^{n+1} = C_{dt2}dt^2 + C_{hdt}dth + C_{h2}h^2$$
(18)

and the second time derivative term is the local time error from the Euler approximation. The equation for the update of the particle velocity is then:

$$v_p^{n+1} = v_p^n + dt \sum_i S_{ip}^n a_i^n$$
(19)

The associated global error is Ev_p^{n+1} whose evolution may be approximated by

$$Ev_p^{n+1} = Ev_p^n + C_{dt2}dt^2 + dt\sum_i S_{ip}^n Ea_i^n + dtC_{h2}h^2$$
(20)

and where the rightmost term is the $O(h^2)$ mapping error associated with the coefficients S_{ip}^n . Again, the dt^2 term is the local time error. The local form of this, assuming no previous errors, is using (13)

$$LEv_p^{n+1} = C_{dt2}dt^2 + dt\sum_i S_{ip}^n C_h h + dt C_{h2} h^2$$
(21)

The velocity gradients at particles are calculated using the formula

$$\frac{\partial v^{n+1}}{\partial x}(x_p) = \sum_i D^n_{ip} v^{n+1}_i \tag{22}$$

with an associated derivative approximation error as denoted by Ev_{xp}^{i+1} , where

$$Ev_{xp}^{n+1} = C_h h + \sum_i D_{ip}^n Ev_i^{n+1}$$
(23)

The local error part of this is

$$LEv_{xp}^{n+1} = C_h h + \sum_i D_{ip}^n LEV_i^{n+1}$$
 (24)

Which may be written out in full as

$$LEv_{xp}^{n+1} = C_h h + \sum_i D_{ip}^n \left(C_{dt2} dt^2 + C_h h + C_{h2} h^2 \right)$$
(25)

or more straightforwardly rewritten by absorbing the D_{ip} terms into the constants as

$$LEv_{xp}^{n+1} = C_h h + C_{dt2} dt^2 + C_{h2} h^2$$
(26)

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

$$F_p^{n+1} = F_p^n + dt \frac{\partial v^{n+1}}{\partial x} (x_p^n, t_n) F_p^n dt$$
(27)

For the deformation gradient F_p^n the error evolution the associated global error as denoted by EF_p^{n+1} may be approximated by

$$EF_p^{n+1} = EF_p^n - \frac{dt^2}{2}\frac{d^2F_p}{dt^2} + dtF_p^n EV_{xp}^{n+1}$$
(28)

The second time derivative term corresponds to the local error from a semi-implicit Euler step with updated particle velocity derivatives at t^{n+1} . The local error accumulated on just one timestep is

$$LEF_{p}^{n+1} = dt^{2}C_{dt2} + dtF_{p}^{n}LEV_{xp}^{n+1}$$
(29)

Stress is updated using the appropriate constitutive model and Young's Modulus, \hat{E} ,

$$\sigma_p^{n+1} = \sigma_p^n + dt \hat{E} \frac{\partial v^{n+1}}{\partial x} (x_p^n)$$
(30)

The associated global error is $E\sigma_p^{n+1}$ In this case the stress global time and space error approximately evolves according to

$$E\sigma_p^{n+1} = E\sigma_p^n + dt^2 C_{dt2} + dt\hat{E} \ EV_{xp}^{n+1}$$
(31)

where, again, the dt^2 term is the local time integration error. The local stress error accumulated over one time step is

$$LE\sigma_{p}^{n+1} = dt^{2}C_{dt2} + dt\hat{E} \ LEv_{xp}^{i+1}$$
(32)

This may be written out in short form by using equation (26) as

$$LE\sigma_{p}^{n+1} = dt^{2}C_{dt2} + C_{dth}hdt + C_{h2dt}dth^{2}$$
(33)

The equation for the particle position update is

$$x_p^{n+1} = x_p^n + dt v_p^{n+1} (34)$$

The associated global error is denoted by Ex_p^{n+1} and for the particle update the global error evolves according to

$$Ex_p^{n+1} = Ex_p^n - \frac{dt^2}{2}\frac{d^2x_p^{n+1}}{dt^2} + dtEv_p^{n+1}$$
(35)

and the local form of this, assuming no prior errors, is

$$LEx_{p}^{n+1} = C_{dt2}dt^{2} + dtLEv_{p}^{n+1}$$
(36)

which again, after absorbing S_{ip} terms into the constants and keeping only the lowest powers of h and dt, is

$$LEx_{p}^{n+1} = dt^{2}C_{dt2} + dt^{2} \left[hC_{h} + h^{2}C_{h2}\right]$$
(37)

3 From Local to Global Errors

In general moving from the local error estimates to global error estimates is not straight forward. The main idea here is to show that adding the local errors on any step and estimating the new step results in the same lowest powers of dt and h. For example the acceleration error on the second step may be written as

$$Ea_i^{(2)} = C_h h + \frac{1}{m_i} \sum_p D_{pi}^1 (LE\sigma_p^1 F_p^1 + \sigma_p^1 LEF_p^1) V_p^0$$
(38)

Combining (26) (29) and (32) and rearranging gives

$$Ea_i^{(2)} = C_h h + C_{dt2} dt^2 + C_{hdt} h dt + h.o.t$$
(39)

3.1 Stress Error

In estimating the stress error, the acceleration error above is then transferred to the nodal velocity error via (18) yielding

$$EV_i^2 = C_{dt2}dt^2 + C_{hdt}hdt + C_{h2}h^2$$
(40)

and so onto the particle velocity derivative error via (24) giving

$$Ev_{xp}^{(2)} = C_h h + C_{dt2} dt^2 + C_{hdt} h dt + C_{dt2} h^2$$
(41)

And then to the stress error via (31) giving

$$E\sigma_p^{(2)} = C_{dt2}dt^2 + dt(C_hh + C_{h2}h^2) + dt(C_{dt2}dt^2 + C_hh + C_{h2}h^2)$$
(42)

Collecting together terms and ignoring higher powers of dt gives.

$$E\sigma_p^{(2)} = C_{dt2}dt^2 + C_{hdt}hdt + C_{h2dt}dt \ h^2$$
(43)

The stress error at the end of the second step thus has the same lowest powers of h and dt as at the first step.

3.2 Displacement Error

On the second step the displacement error is, after combining dt^2 terms.

$$Ex_p^{(2)} = LEx_p^{(1)} + C_{dt2}dt^2 + dtLEv_p^{(2)}$$
(44)

which by using (21) and (37) may be written as

$$Ex_p^{n+1} = LEx_p^{(1)} + C_{dt2}dt^2 + dt\sum_i S_{ip}^2 Ea_i^{(2)} + dt^2 C_{h2}h^2$$
(45)

and may be summarized, after collecting together terms, and only including the lower order terms as

$$Ex_p^2 = C_{dt2}dt^2 + C_{dt2h}hdt^2 + dt^2C_{dt2h2}h^2$$
(46)

These are the same lowest powers of h and dt as in the local error in (37). This also shows that there is greater accuracy in the displacement than the stress or velocity, for example, as the results below will show. From the local error analysis above we can deduce that the global errors in stress acceleration velocity and displacement will be one power of dt less than the local error, following standard time integration theory for initial value problems. One complication arises with large Young's Modulus \hat{E} in that when E = 1000 say then this has a dramatic impact on the global error in stress.

4 Observed Order of Accuracy

The form of the error derived above now makes it possible to check the derived error accuracy against the observed error. The model problem used in that in [5, 4] except that the parameter A = 0.05 that multiplies the error does not depend on the mesh spacing h as in [4] and so the errors are one power of h lower than in that paper. The errors are measured by taking the L2 norm at each time step in each quantity and then finding its maximum value over all the time steps. These results show the higher accuracy of the

	E=1000				E=4			
h	Err x_p	Err v_p	Err σ_p	NGridX	Err x_p	Err v_p	Err σ_p	NGridX
1/10	2.5e-3	1.58	24	504	2.4e-3	3.4e-2	9.0e-2	32
1/20	6.7e-4	2.6e-1	9.3	1742	5.6e-4	7.6e-3	3.5e-2	112
1/40	3.4e-4	5.8e-2	6.3	6560	3.4e-4	3.0e-3	2.5e-2	416
1/80	3.4e-4	4.5e-2	6.2	25862	3.4e-4	2.8e-3	2.5e-2	1640

Table 1: Errors of MPM GIMP dt =2.5e-5, 4 particles per cell.

displacement errors and first order accuracy overall. The expected behavior as power of h is seen. For the finer meshes there may be little improvement in accuracy, because of the increased number of grid crossings (NGridX) and hence additional errors introduced, see [8]. It would be possible to modify the algorithm and/or the analysis to accommodate this. For large value of the Young's Modulus \hat{E} the Stress (and acceleration - not shown for brevity) errors are much larger than for smaller values of the modulus.

5 CONCLUSIONS

In this extended abstract an introductory discussion has been provided with regard to the errors in the material point method with a view to understanding better the error estimation approaches that may be used in the future to build on [4, 1]. Further work is needed on MPM convergence with grid crossing.

REFERENCES

- [1] A.S. Baumgarten and K Kamrin Analysis and mitigation of spatial integration errors for the material point method. *Int J Numer Methods Eng.* 2023;149
- [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. Energy Conservation and Accuracy of Some MPM Methods. *Computational Particle Mechanics*, February 04 2022.
- [4] Berzins M. Computational Error Estimation for the Material Point Method. *Computational Particle Mechanics* December 24 2022.
- [5] Gritton C. and Berzins M. Improving accuracy in the MPM method using a null space filter, *Computational Particle Mechanics*, 4, pp. 131142 2017.
- [6] Krongauz Y. and T. Belytschko T., Consistent pseudo-derivatives in meshless methods, Comput. Meths in Appl Mech and Engnrng, 146 (1997), pp. 371–386.
- [7] Solowski W.T., Berzins M., Coombs W.H, Guilkey J.E, Moller M., Tran Q.A., Adibaskoro T, Seyedan A., Tielen R., and Soga K. Material Point Method: overview and challenges ahead. Chapter 2 of Advances in Applied Mech. Vol. 54, 113-204, 2021.
- [8] Steffen M., Kirby R.M., Berzins M. Analysis and Reduction of Quadrature Errors in the Material Point Method (MPM), Int. J. for Numer. Meths in Engnrng, 76, 6, 922–948, 2008.
- [9] Steffen M. Analysis-Guided Improvements of the Material Point Method, Ph.D. Thesis, School of Computing, University of Utah, 2009. http://www.sci.utah.edu/ publications/Ste2009a/Steffen_PhDThesis2009.pdf
- [10] Steffen M., Kirby R.M., Berzins M. Decoupling and Balancing of Space and Time Errors in the Material Point Method (MPM), Int. J. for Numer. Meths. in Engnng, 82, No. 10, pp. 1207–1243. 2010.
- [11] de Vaucorbeil A., Nguyen V.P., Sinaie S., Wu J.Y, Chapter Two Material point method after 25 years: Theory, implementation, and applications, Editor(s): Stphane P.A. Bordas, Daniel S. Balint, Adv. in Appl. Mech., Elsevier, 2020 53, 2020, 185-398.