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Error Analysis for Material Point Method and a case study from Gas Dynamics

Thanks to DOE for funding from 1997-2008

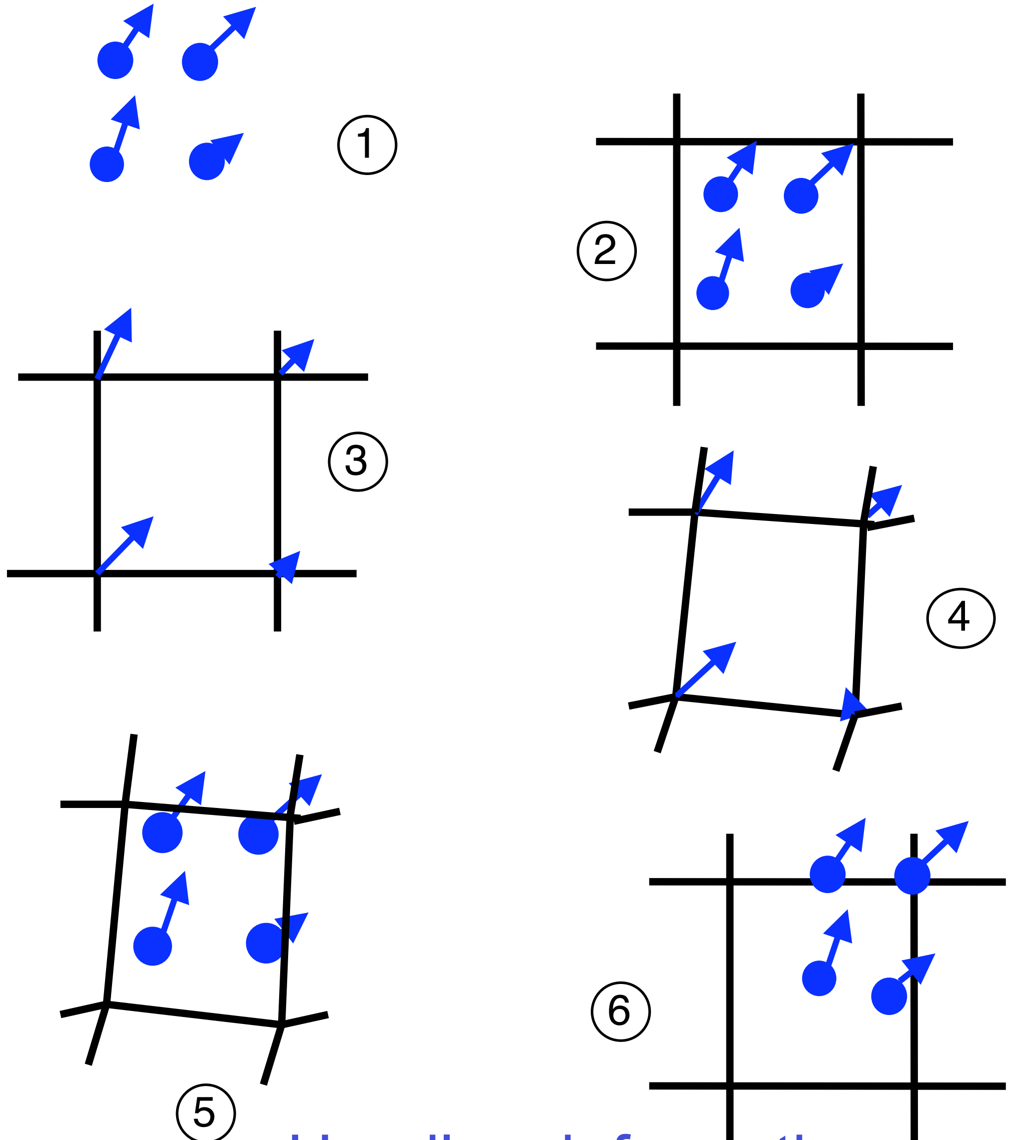
Material Point Method (MPM) Outline History
See Brackbill IJNMF 2005 47 693-705

- *1963 Harlow PIC methods then CiC ViC methods*
- *1980s -90s Flip methods Brackbill et al.*
- *1990s Sulsky Brackbill MPM-PIC*
- *2000+ Sulsky et al. + GIMP Bardenhagen et al*

Since then proved effective on difficult problems involving large deformations fracture e.g CSAFE [Guilkey et al.] + [Sulsky et al] + [Brydon] etc etc

A KEY ISSUE NOW IS THE THEORETICAL UNDERPINNING OF THE METHOD.

The Material Point Method (MPM)



Errors at each stage of this process

Particles with properties (velocity, mass etc) defined on a mesh

Particle properties mapped onto mesh points

Forces, accelerations, velocities calculated on mesh points

Mesh point motion calculated but only the particles moved by mapping velocities back to particles

Handles deformation, contact, high strain

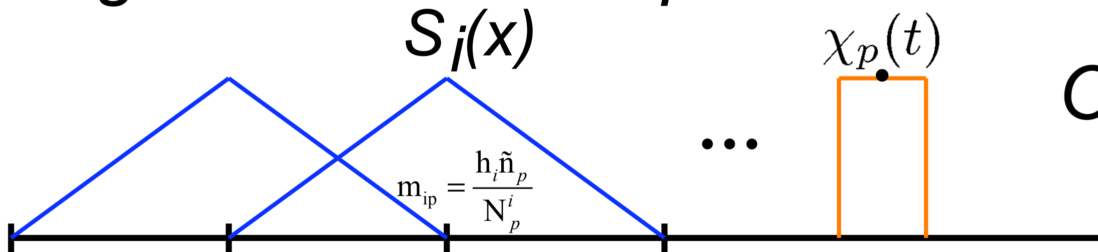
Explicit MPM Algorithm Errors

- Particle to grid projection — Projection Error
- Interpolation from grid back to particles — Interpolation Error
- Time integration of particles — Time Error
- Finite element + mass matrix lumping — FE +Mass Error
- Analysis of mesh/particle interplay from [Grigorev,Vshivkov and Fedoruk PIC 2002] - more particles may not be better on a given mesh. Both cell size and particles per cell matter.

1D : 4-8 particles per cell is optimal

MPM Basis Overview

grid basis fns *particle basis fns*



Or delta fn ..

point Velocity

point mass $m_{ip} = \frac{h_i \tilde{n}_p}{N_p^i}$

$$v_i = \sum_{p=1}^{np} \lambda_p v_p, \qquad \lambda_p = \frac{m_{ip} S_{ip}}{\sum_{ip=1}^{np} m_{ip} S_{ip}}, \qquad S_{ip} = \frac{1}{V_p} \int_{\Omega_i} S_i(x) \chi_p(x) dx$$

$$a_i = \sum_{p=1}^{np} \mu_p V_p, \qquad \mu_p = \frac{p_{ip} G_{ip}}{\sum_{ip=1}^{np} m_{ip} S_{ip}}, \qquad G_{ip} = \frac{1}{V_p} \int_{\Omega_i} \frac{dS_i}{dx} \chi_p(x) dx$$

Forward Euler time integration

$$\mathrm{v}_i^{n+1} = \mathrm{v}_i^{n} + \delta t\, \mathrm{a}_{\mathrm{i}}, \quad \mathrm{v}_p^{n+1} = \mathrm{v}_p^{n} + \delta t \sum_{i=1}^{nv} S_{ip}\, \mathrm{a}_{\mathrm{i}},$$

$$x_p^{n+1} = x_p^{n} + \delta t \sum_{i=1}^{nv} S_{ip}\, \mathrm{v}_{\mathrm{i}}^{\mathrm{n+1}}$$

V^{n+1} *n.b. semi-implicit*

Local errors are second order in time

Global error is first order in time

Second derivatives of x and v are involved in error estimates

These terms may be discontinuous

If $x_p \in [x_{i-1}, x_i]$ then (a) $\ddot{x}_p = \alpha_i a_{i-1} + (1-\alpha_i) a_i, \quad \alpha_i = \dfrac{x_p - x_i}{x_{i-1} - x_i}$

If $x_p \in [x_i, x_{i+1}]$ then (b) $\ddot{x}_p = \alpha_{i+1} a_i + (1-\alpha_{i+1}) a_{i+1}, \quad \alpha_{i+1} = \dfrac{x_p - x_{i+1}}{x_i - x_{i+1}}$

Hence differentiating gives

(a) $$\dddot{x}_p = \alpha_i \dddot{x}_{i-1} + (1-\alpha_i)\dddot{x}_i + v_p \frac{a_{i-1} - a_i}{x_{i-1} - x_i}$$

(b) $$\dddot{x}_p = \alpha_{i+1} \dddot{x}_i + (1-\alpha_{i+1})\dddot{x}_{i+1} + v_p \frac{a_i - a_{i+1}}{x_i - x_{i+1}}$$

Limits global accuracy
To first order

Hence jump in $\dddot{x}$ is $[\dddot{x}^+ - \dddot{x}^-]_{x_i} = v_p \left[\dfrac{a_i - a_{i+1}}{x_i - x_{i+1}} - \dfrac{a_{i-1} - a_i}{x_{i-1} - x_i} \right]$

Acceleration continuous but its derivative is not
Because of linear basis functions and moving points

Particle Acceleration Derivative Potentially Discontinuous as Particle Crosses Boundary

If $x_p \in [x_{i-1}, x_i]$ then (a) $\ddot{x}_p = \alpha_i a_{i-1} + (1-\alpha_i)a_i, \quad \alpha_i = \dfrac{x_p - x_i}{x_{i-1} - x_i}$

If $x_p \in [x_i, x_{i+1}]$ then (b) $\ddot{x}_p = \alpha_{i+1} a_i + (1-\alpha_{i+1})a_{i+1}, \quad \alpha_{i+1} = \dfrac{x_p - x_{i+1}}{x_i - x_{i+1}}$

Hence differentiating gives

(a) $\dddot{x}_p = \alpha_i \dddot{x}_{i-1} + (1-\alpha_i)\dddot{x}_i + v_p \dfrac{a_{i-1} - a_i}{x_{i-1} - x_i}$

(b) $\dddot{x}_p = \alpha_{i+1} \dddot{x}_i + (1-\alpha_{i+1})\dddot{x}_{i+1} + v_p \dfrac{a_i - a_{i+1}}{x_i - x_{i+1}}$

Limits global accuracy To first order

Hence jump in $\dddot{x}$ is $[\dddot{x}^+ - \dddot{x}^-]_{x_i} = v_p \left[\dfrac{a_i - a_{i+1}}{x_i - x_{i+1}} - \dfrac{a_{i-1} - a_i}{x_{i-1} - x_i}\right]$

Particle Methods applied to Euler Equations

Energy

$$\varepsilon_p^{n+1} = \varepsilon_p^{n+1} - \frac{p_p^n}{\rho_p^n}\frac{\partial v_p}{\partial x}\delta t$$

Density

$$\rho_p^{n+1} = \rho_p^n(1 - \frac{\partial v_p}{\partial x}\delta t)$$

Pressure

$$p_p^{n+1} = \varepsilon_p^{n+1}\rho_p^{n+1}(\gamma - 1) + ArtVis$$

Acceleration $a = \frac{1}{\rho}\frac{dp}{dx}$

Positive density requires $0 < (1 - \frac{\partial v_p}{\partial x}\delta t)$

Note differing particle velocity gradients in different cells may lead to new extrema when particles cross over cells

Arbitrary point Quadrature Error [Hickernell]

$$\left| \frac{1}{\mathrm{h}} \int_{x_i}^{x_{i+1}} f(x)dx - \frac{1}{\mathrm{N}_p^i} \sum_{i=1}^{\mathrm{N}_p^i} f(z_i) \right| \leq \mathrm{D}_2(\mathrm{P}, \mathrm{N}_p^i)\mathrm{h}^{1/2} \left\| \frac{df}{dx} \right\|_{2,h}$$

$$\left| \int_{x_i}^{x_{i+1}} f(x)dx - \frac{h}{N_p^i} \sum_{i=1}^{N_p^i} f(z_i) \right| \leq \mathrm{D}_2(\mathrm{P}, \mathrm{N}_p^i)\mathrm{h}^2 \left| \frac{df}{dx}(\varsigma) \right|$$

Where

$$\mathrm{D}_2(\mathrm{P}, \mathrm{N}_p^i) = \left[\frac{1}{12(\mathrm{N}_p^i)^2} + \frac{1}{\mathrm{N}_p^i} \sum_{i=1}^{\mathrm{N}_p^i} \left(z_i - \left(x_i + \frac{(2i-1)h}{2\mathrm{N}_p^i} \right) \right)^2 \right]^{1/2} \approx \left[\frac{1}{12(\mathrm{N}_p^i)^2} + Ch^2 \right]^{1/2}$$

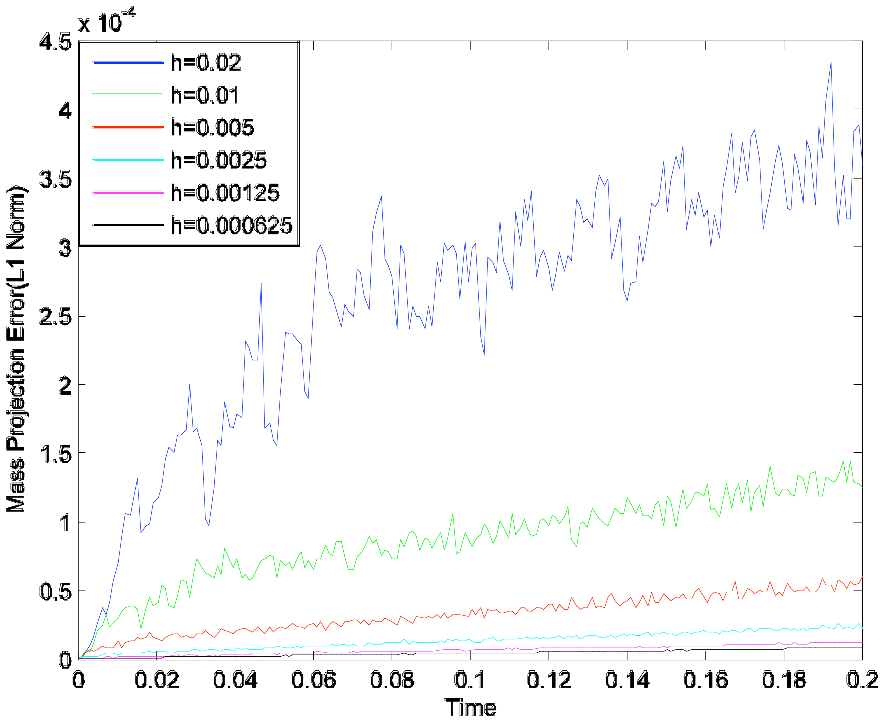
$$\frac{1}{4} \leq C \leq \frac{1}{3}$$

Mass Projection Error

$$E_m^i = \left| \int_{x_{i-1}}^{x_{i+1}} S_i(x)\rho(x)dx - \frac{h}{N_p^i}\sum_{i=1}^{N_p^i} \rho_p S_i(x_{ip}) \right|$$

$$\le D_2(P, N_p^i)h^2 \left| \frac{d(S_i\rho)}{dx}(\varsigma_1) \right| + D_2(P, N_p^{i+1})h^2 \left| \frac{d(S_i\rho)}{dx}(\varsigma_2) \right|$$

$$\le D_2(P, N_p^i)h \ \left|\rho(\varsigma_1)\right| + D_2(P, N_p^{i+1})h \ \left|\rho(\varsigma_2)\right| \qquad n.b. \frac{dS_i(x)}{dx} = \frac{\pm 1}{h}$$



$$D_2(P, N_p^i) \le \left[\frac{1}{12(N_p^i)^2} + Ch^2 \right]^{1/2}$$

$$\frac{1}{4} \le C \le \frac{1}{3}$$

First order in space for small mesh sizes, and may achieve a second order of convergence for large mesh.

Momentum projection error

$$E_P^i = \left| \int_{x_{i-1}}^{x_{i+1}} S_i(x)\rho(x)v(x)dx - \frac{h}{\mathrm{N}_p^i}\sum_{i=1}^{\mathrm{N}_p^i} \rho_p \mathrm{v}_p \mathrm{S}_i(x_{ip}) \right|$$

$$\leq \mathrm{D}_2(\mathrm{P},\mathrm{N}_p^i)\mathrm{h}^2 \left| \frac{d(S_i\rho v)}{dx}(\varsigma_1) \right| + \mathrm{D}_2(\mathrm{P},\mathrm{N}_p^{i+1})\mathrm{h}^2 \left| \frac{d(S_i\rho v)}{dx}(\varsigma_2) \right|$$

$$\leq \mathrm{D}_2(\mathrm{P},\mathrm{N}_p^i)\mathrm{h} \ \left| (\rho v)(\varsigma_1) \right| + \mathrm{D}_2(\mathrm{P},\mathrm{N}_p^{i+1})\mathrm{h} \ \left| (\rho v)(\varsigma_2) \right|$$

$$\mathrm{D}_2(\mathrm{P},\mathrm{N}_p^i) \leq \left[\frac{1}{12(\mathrm{N}_p^i)^2} + Ch^2 \right]^{1/2}$$

Momentum projection error is also first order in space for small mesh sizes, and second order of convergence for large mesh.

Force Projection Error

$$F_i^{proj} = \int_{x_{i-1}}^{x_{i+1}} p(x) G_{ip}(x) dx = \frac{1}{h_i} \int_{x_{i-1}}^{x_i} p(x) dx - \frac{1}{h_{i+1}} \int_{x_i}^{x_{i+1}} p(x) dx$$

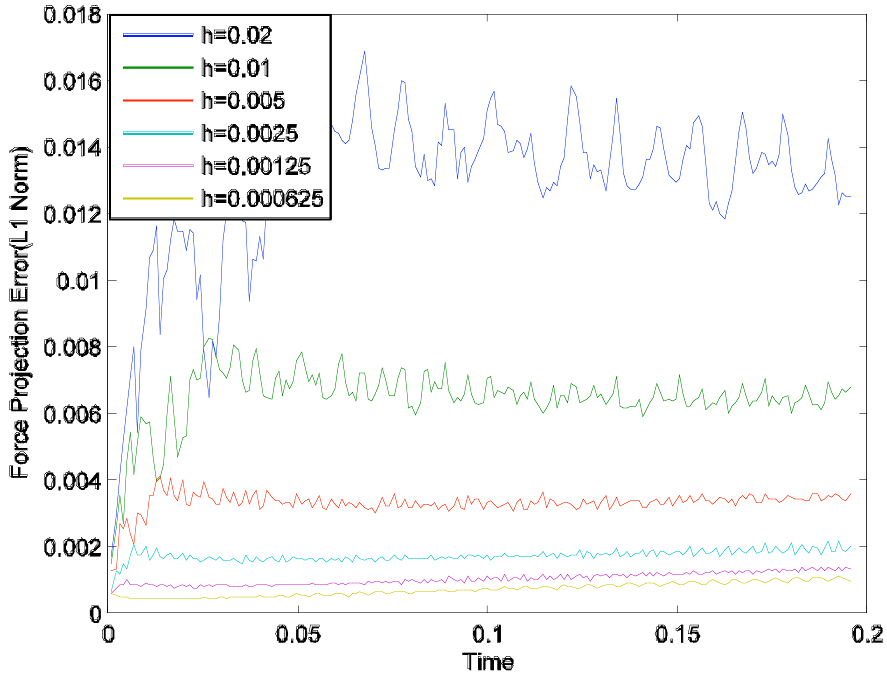
$$\left|E_F^i\right| \le \left| \frac{1}{h} \int_{x_{i-1}}^{x_i} p(x) dx - \frac{1}{N_p^i} \sum_{p:x_p \in I_i} p_p \right| + \left| \frac{1}{h} \int_{x_i}^{x_{i+1}} p(x) dx - \frac{1}{N_p^{i+1}} \sum_{p:x_p \in I_{i+1}} p_p \right|$$

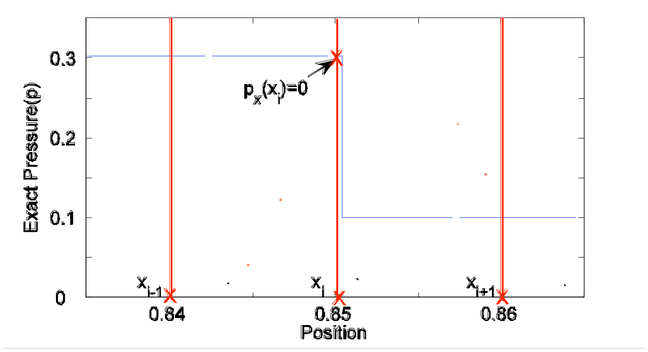
Using Hickernel:

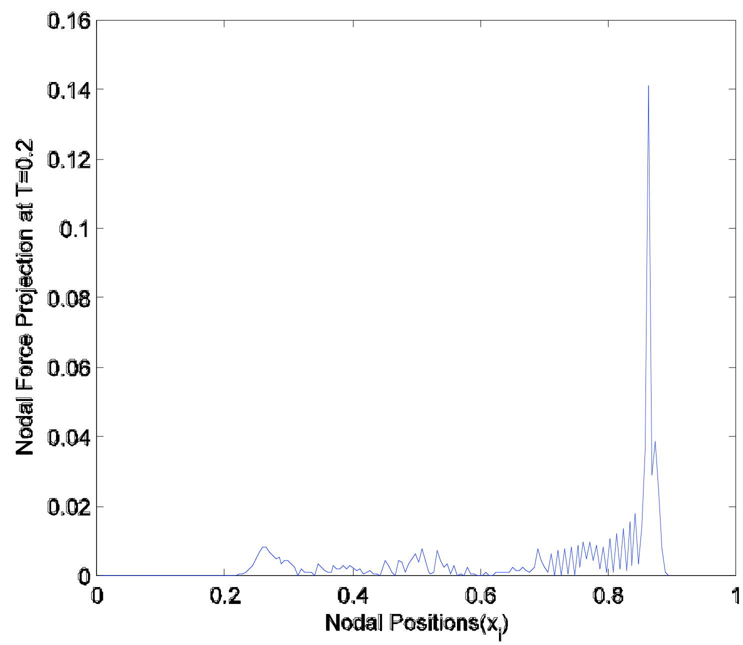
$$\left|E_F^i\right| \le \mathrm{D}_2(\mathrm{P}, \mathrm{N}_p^i)\mathrm{h} \left| \frac{dP}{dx}(\varsigma_1) \right| + \mathrm{D}_2(\mathrm{P}, \mathrm{N}_p^{i+1})\mathrm{h} \left| \frac{dP}{dx}(\varsigma_2) \right|$$

Force Projection Error is first order in space for small mesh sizes, and may achieve up to second order of convergence for large meshes.

Force Projection Error(cont.)







Nodal Acceleration Projection Error

$$a_i = \frac{F_i}{m_i} = \frac{\int_{x_{i-1}}^{x_{i+1}} p(x) G_{ip}(x)\,dx}{\int_{x_{i-1}}^{x_i} \rho(x) S_i(x)\,dx}$$

$$E_a^i = \frac{E_F^i}{m_i} - \frac{F_i}{m_i}\frac{E_m^i}{m_i} = \frac{E_F^i}{m_i} - a_i \frac{E_m^i}{m_i}$$

Acceleration projection error is one order less in space than the order of convergence for Force projection error and mass projection error, since mass is first order in space.

Nodal Velocity projection (particle to grid) error

$$v_i = \frac{P_i}{m_i} = \frac{\int_{x_{i-1}}^{x_{i+1}} \rho(x) v(x) S_{ip}(x) dx}{\int_{x_{i-1}}^{x_i} \rho(x) S_{ip}(x) dx}$$

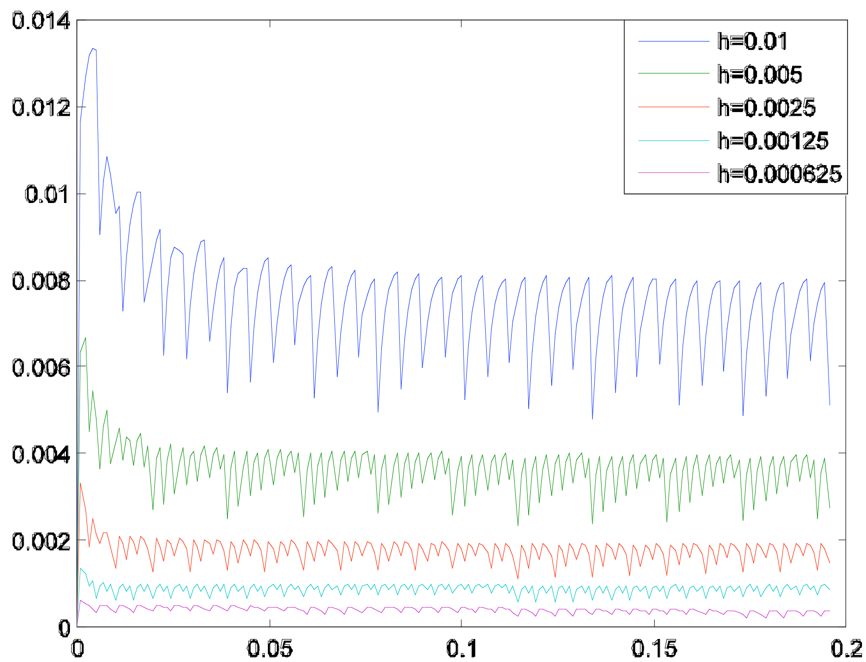
$$E_v^i = \frac{E_P^i}{m_i} - v_i \frac{E_m^i}{m_i}$$

Let: $E_{v1}^i = v_i^{exact} - v_i$

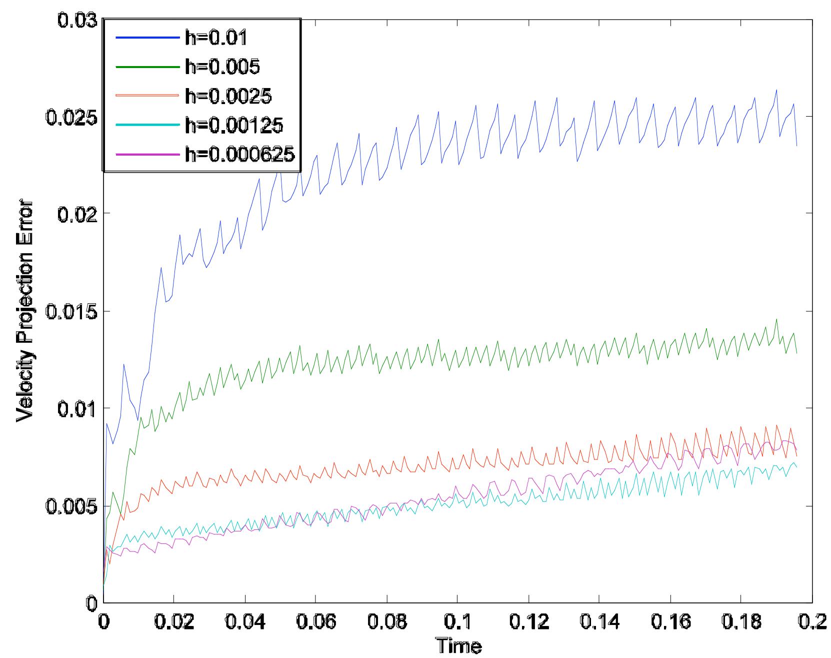
$$E_v^i = \frac{E_P^i}{m_i} - v_i^{exact} \frac{E_m^i}{m_i} + E_{v1}^i \frac{E_m^i}{m_i}$$

E_{v1}^i is first order in space so the order of velocity projection error is determined by $\frac{E_P^i}{m_i} - v_i^{exact} \frac{E_m^i}{m_i}$

Nodal velocity projection error(cont)



The velocity error E_{v1}^{i} for different mesh sizes



So velocity projection error has constant order as the mesh size get smaller.

Velocity gradient projection error

$$\frac{\delta v}{\delta x}(x_p) = \frac{v_{i+1} - v_i}{x_{i+1} - x_i} - \left(\frac{x_i + x_{i+1}}{2} - x_p \right) \frac{\delta^2 v}{dx^2}(x_p) + H.O.T$$

$$E_{VG}^p = \frac{E_{v*}^{i+1} - E_{v*}^i}{h} - \left(\frac{x_i + x_{i+1}}{2} - x_p \right) \frac{\delta^2 v}{\delta x^2}(x_p)$$

$$E_{VG}^i = \frac{E_{v*}^{i+1} - E_{v*}^i}{h} \qquad E_{v*}^i = E_v^i + \Delta t E_a^i$$

$$E_{VG}^i = \frac{E_v^{i+1} - E_v^i}{h} + \frac{\Delta t}{h}\left[E_a^{i+1} - E_a^i \right]$$

$$E_{VG}^i \approx \frac{E_v^{i+1} - E_v^i}{h}$$

Velocity gradient projection error(cont)

Velocity projection error at nodes for h:

$$\left(E_v^{i-2}\right)_h \qquad \left(E_v^{i-1}\right)_h \qquad \left(E_v^{i}\right)_h$$

Velocity projection error at nodes for 2h:

$$\left(E_v^{i-1}\right)_{2h} \qquad \left(E_v^{i}\right)_{2h}$$

With: $E_v^i = Ch^p$,We have:

$$\left(E_v^{i}\right)_{2h} = 2^p \left(E_v^{i}\right)_h$$

$$\left(E_v^{i-1}\right)_{2h} = 2^p \left(E_v^{i-2}\right)_h$$

Velocity gradient projection error

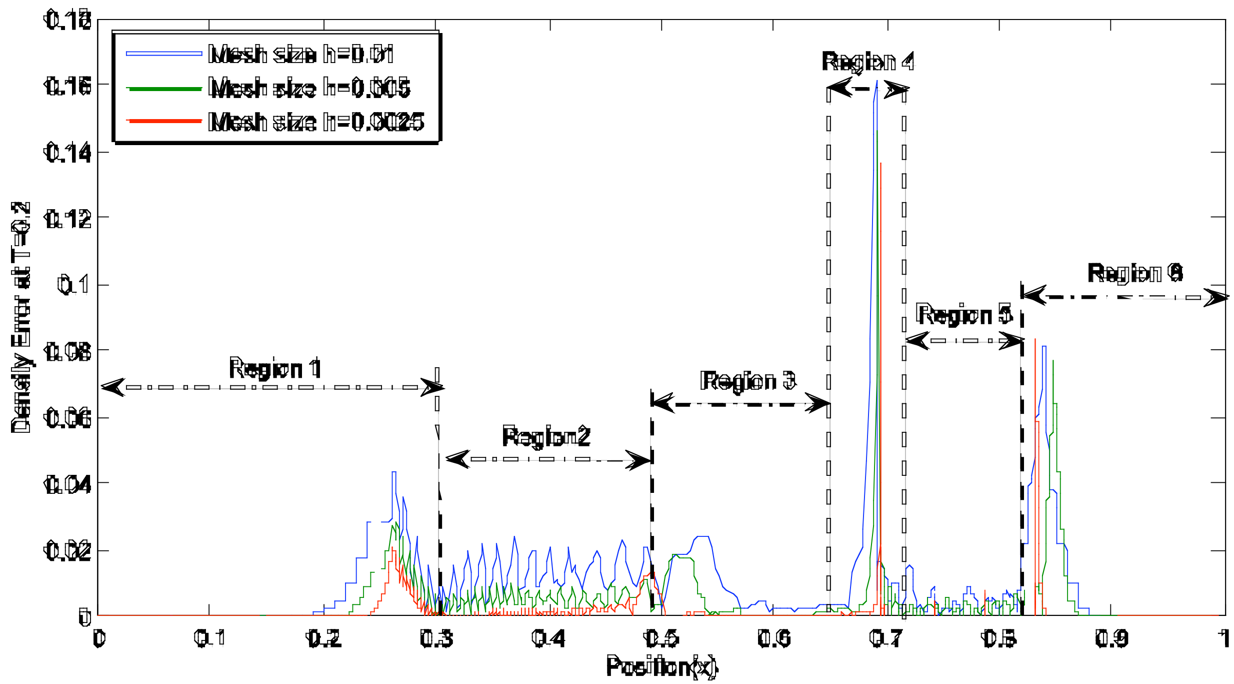
$$2^p \frac{\left(E_v^i\right)_h - \left(E_v^{i-1}\right)_h}{h} \approx 2^p \frac{\left(E_v^i\right)_h - \frac{\left(E_v^i\right)_h + \left(E_v^{i-2}\right)_h}{2}}{h} \approx 2^p \frac{\left(E_v^i\right)_h - \left(E_v^{i-2}\right)_h}{2h}$$

Therefore:

$$2^p \frac{\left(E_v^i\right)_h - \left(E_v^{i-1}\right)_h}{h} \approx \frac{\left(E_v^i\right)_{2h} - \left(E_v^{i-1}\right)_{2h}}{2h}$$

So velocity gradient projection error is the same order as velocity projection error.

Final Error Combination



Region 1 and Region 3 capture the error at left and right rarefaction

Region 4 captures the error at contact discontinuity

Region 6 captures the error at shock-front

Region 2 is the region of smooth solution of density and velocity

Region 5 contains the error propagation from the shock-front

Final Error Combination(cont.)

h	L1-Norm	L2-Norm
0.01	0.00830833	0.0158701
0.005	0.00433578	0.0104553
0.0025	0.00230507	0.0075895
0.00125	0.00126351	0.0057596
0.000625	0.00109963	0.0061870
0.0003125	0.00101256	0.0062115

Burgers' Problem

$$\frac{\partial v}{\partial t} + v(x,t)\frac{\partial v}{\partial x} = \varepsilon \frac{\partial^2 v}{\partial x^2} \qquad (x,t) \in [0,2] \times [0.0, T)$$

Solving with MPM:

$$v_i = \sum_p \lambda_{ip} v_p \qquad \lambda_{ip} = \frac{S_{ip} N_p^j}{\sum_p S_{ip} N_p^j}$$

$$a_i = -\varepsilon \frac{v_i - v_{i-1}}{h^2 N_p^i} \sum_{p:x_p \in I_i} 1 + \varepsilon \frac{v_{i+1} - v_i}{h^2 N_p^{i+1}} \sum_{p:x_p \in I_{i+1}} 1$$

Follow the consequence steps of standard MPM method.

Burgers' Problem(cont.)

Error at T=0.5 for different mesh sizes:

		h=0.01	**h=0.005**	**h=0.0025**	**h=0.00125**	**h=0.000625**
Update Velocity Using Exact Acceleration	ε=0.045	2.67e-4	1.24e-4	6.07e-5	3.03e-5	1.52e-5
	ε=0.04	2.67e-4	1.25e-4	6.09e-4	3.06e-5	1.53e-5
	ε=0.03	2.78e-4	1.27e-4	6.19e-4	3.09e-5	1.55e-5
	ε=0.02	2.97e-4	1.24e-4	6.16e-4	3.10e-5	1.55e-5
	ε=0.01	5.34e-4	1.58e-4	6.18e-4	3.10e-5	1.55e-5
Update Velocity Using Calculated Acceleration	ε=0.045	9.82e-4	5.39e-4	2.84e-4	1.42e-4	7.09e-5
	ε=0.04	8.54e-4	4.61e-4	2.35e-4	1.17e-4	5.86e-5
	ε=0.03	5.97e-4	3.20e-4	1.61e-4	8.05e-4	4.03e-4
	ε=0.02	3.73e-4	1.93e-4	9.91e-5	4.95e-4	2.47e-4
	ε=0.01	4.12e-4	1.51e-4	6.52e-5	3.20e-4	1.60e-5

Conclusions

Nodal mass, momentum and force projection error converges with order $h^p (1 \le p \le 2)$

Nodal acceleration projection error is order $h^p (0 \le p \le 1)$

Nodal velocity projection error is order $h^p (0 \le p \le 1)$

Nodal velocity gradient projection error is the same order with velocity projection error

The overall error at particles as density, energy… will stop converging as the mesh size get smaller.