Decoupling and Balancing of Space and Time Errors in the Material Point Method

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Outline

- Overview of Errors
- Observations and Motivation
- Moving Mesh MPM
- Balancing Space & Time Errors
- Sample Problem
  - Time Integration, Jump, and Quadrature Errors

Overview of Errors in MPM

- MPM simulations exhibit a variety of errors, e.g.:

Spatial	Temporal	Mixed
Approximation (h, ϕ)	Time-Integration (Δt)	Jump Error $(\Delta t, \Delta x, t)$
Mass Lumping (h, ϕ)		Quadrature $(\Delta x, t)$
		Geometric $(\Delta x, h, t)$

- MPM errors are not separable due to feedback
- Previously focused on spatial errors at one time-step
- Analysis of temporal errors is difficult due to feedback

Observations and Motivation

- Centered difference time-stepping scheme:

$$v^{k+1/2} = v^{k-1/2} + a^k \Delta t$$

$$u^{k+1} = u^k + v^{k+1/2} \Delta t$$

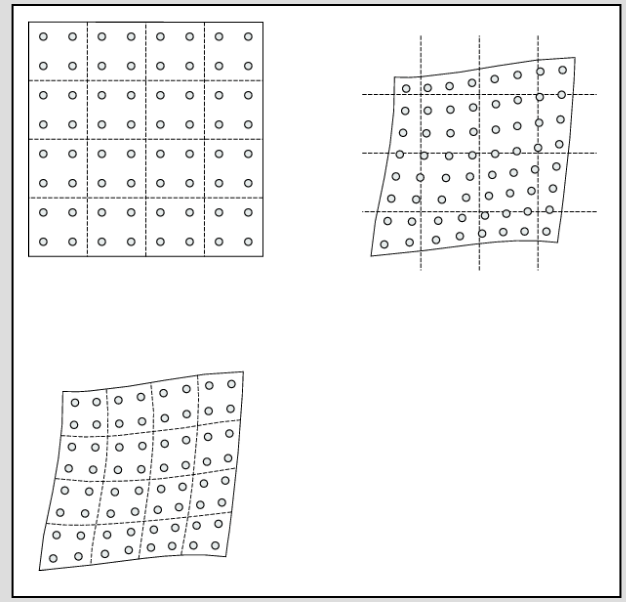
- "Formally second-order" in time for both velocity and displacement – assuming acceleration is well behaved

- MPM has spatial errors in acceleration:

$$v^{k+1/2} = v^{k-1/2} + \Delta t (a^k + c_1 \Delta x^2 + \cdots) + c_2 \Delta t^3 + \cdots$$

Moving Mesh MPM

- Moving mesh MPM
  - Mesh and material points move together
    - Can exhibit FEM mesh problems
    - Good for smooth test problems
  - Used in the MPM community
  - Particles stay in “nice” positions, quadrature jump errors no longer appear
  - Allows detailed analysis of temporal errors



Standard vs. Moving Mesh

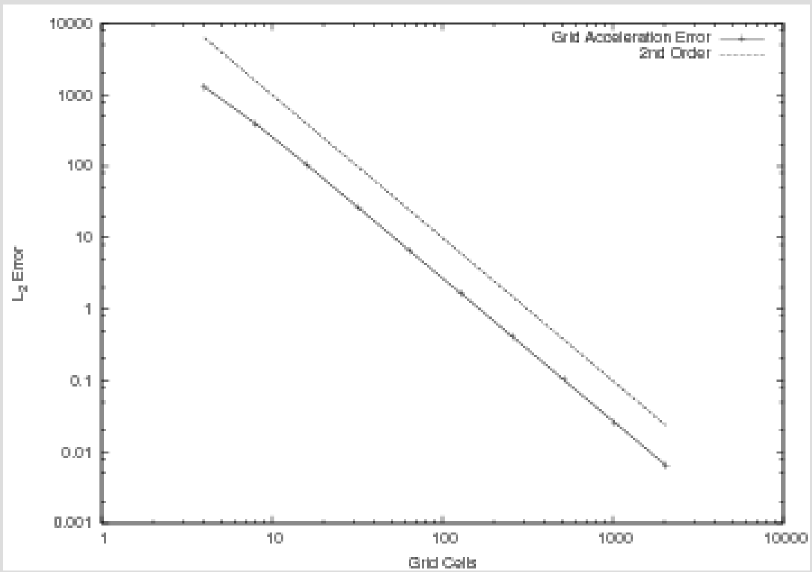
Observations

$$v^{k+1/2} = v^{k-1/2} + \Delta t(a^k + c_1 \Delta x^2 + \cdots) + c_2 \Delta t^3 + \cdots$$

- Second order temporal convergence has technically not been shown in MPM
- With moving mesh MPM, and measuring local truncation errors, we can demonstrate second order temporal convergence
- By finding constants c_1 and c_2, we can determine where spatial and temporal errors are balanced: $c_1 \Delta x^2 = c_2 \Delta t^2$

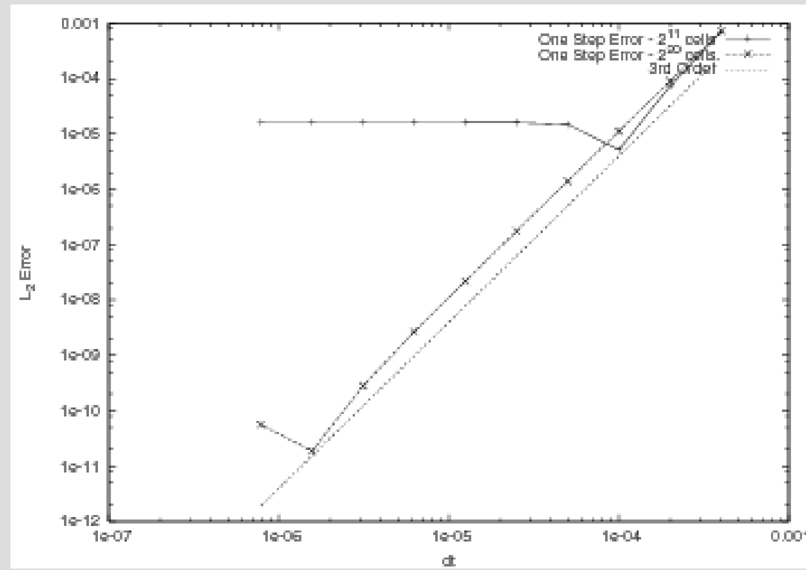
Balancing Space and Time Errors

$$v^{k+1/2} = v^{k-1/2} + \Delta t(a^k + c_1 \Delta x^2 + \cdots) + c_2 \Delta t^3 + \cdots$$



Spatial Acceleration Error

$$c_1 = \frac{E_a}{h^2} = 2.71 \times 10^4$$



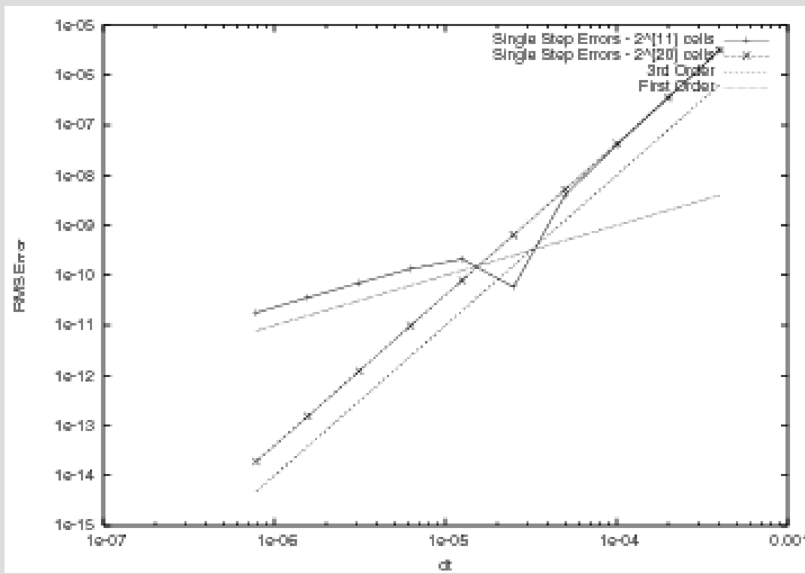
Temporal Velocity Error

$$c_2 = \frac{E_v}{\Delta t^2} = 1.13 \times 10^7$$

Balanced when: $\Delta t = h\sqrt{\frac{c_1}{c_2}} = 2.38 \times 10^{-5}$ for 2k grid cells

Balancing Space and Time Errors

$$v^{k+1/2} = v^{k-1/2} + \Delta t(a^k + c_1 \Delta x^2 + \cdots) + c_2 \Delta t^3 + \cdots$$



Estimate:

$$\Delta t = 2.38 \times 10^{-5}$$

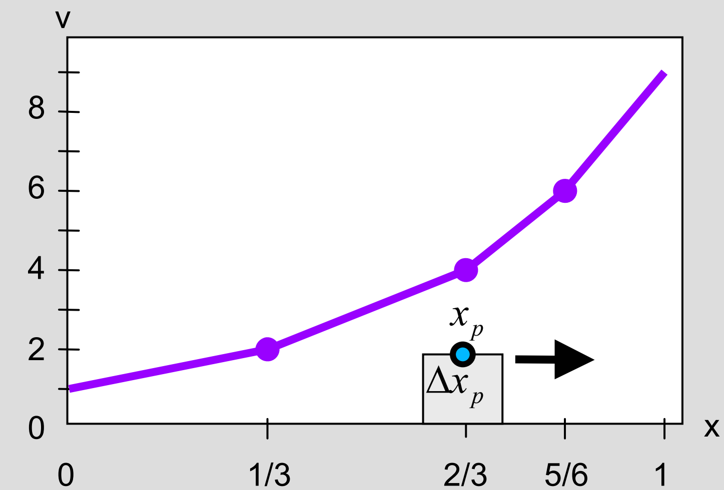
- Actual balance point (transition of convergence rate) occurs at estimate

Sample Problem

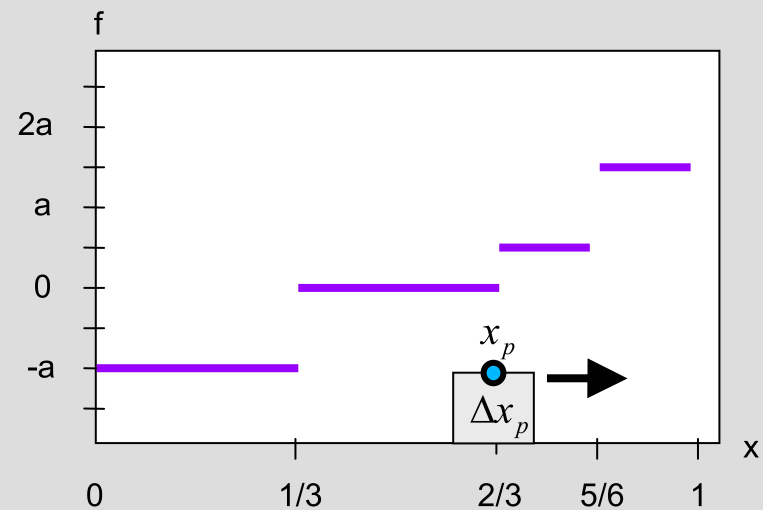
$$v_p^k = v(x_p^k) + v_{\text{ext}}^k \qquad a = \int_0^1 f(x)dx = 0$$

$$v_{\text{ext}}^{k+1} = v_{\text{ext}}^k + a_p^k \Delta t \qquad a_p^k = \int_{\Omega-\Omega_p^k} f(x)dx + f(x_p^k)\Delta x$$

$$x_p^{k+1} = x_p^k + v_p^k \Delta t$$



- Simpler Problem – exhibits similar errors as MPM
- Notice: dx/dt = v(x(t)). Analytic solution exists for piecewise-linear v(x).
- External acceleration should be 0
- Quadrature errors in acceleration calculation will affect time-stepping errors

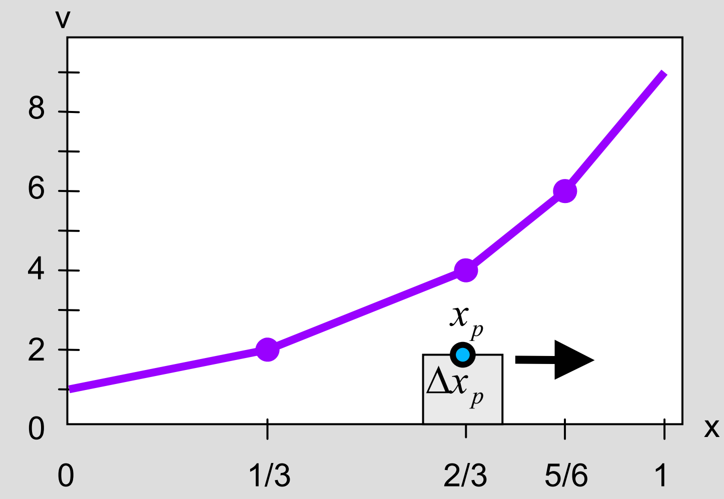


Analytic Solution

$$v_{\mathrm{ext}}^{k+1} = v_{\mathrm{ext}}^{k} + a_p^k \Delta t \qquad v_p^0 = 0$$

$$v_p^k = v(x_p^k) + v_{\mathrm{ext}}^k \qquad x_p^0 = 0$$

$$x_p^{k+1} = x_p^k + v_p^k \Delta t \qquad a_p^k = 0$$

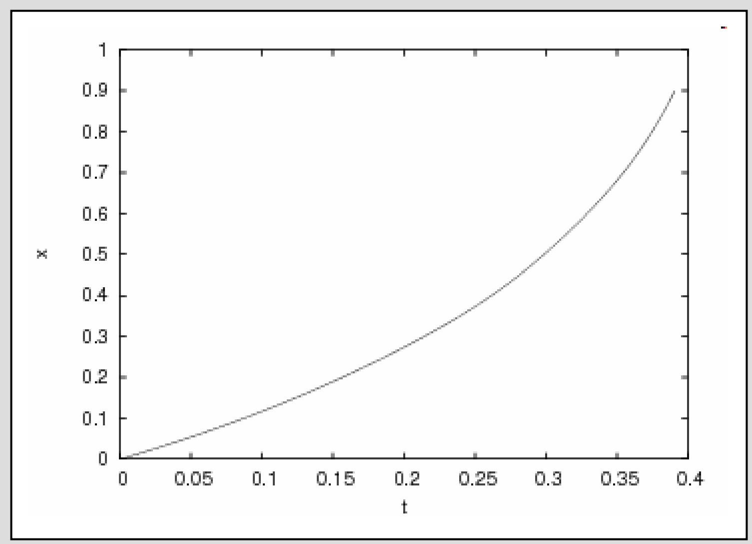


Analytic Solution (on 0 < x < 1/3):

$$x(t) = \frac{b + a x_0}{a e^{a t_0}} e^{at} - \frac{b}{a} \qquad 0 \le t < t_{\mathrm{cross}_1}$$

$$t_{\mathrm{cross}_1} = \frac{1}{a} \ln\left[\frac{x_{\mathrm{cross}} + b/a}{b + a x_0} a e^{a t_0} \right]$$

Other intervals are calculated similarly



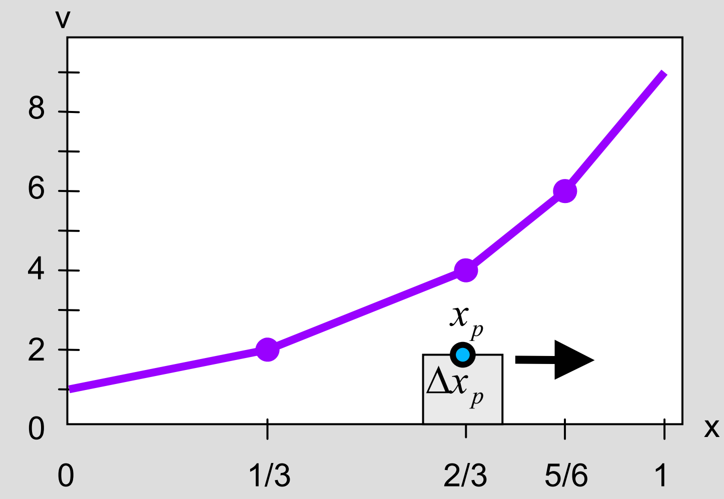
Analytic Solution

Euler Forward Error

$$v_{\text{ext}}^{k+1} = v_{\text{ext}}^{k} + a_p^k \Delta t \qquad v_p^0 = 0$$

$$v_p^k = v(x_p^k) + v_{\text{ext}}^k \qquad x_p^0 = 0$$

$$x_p^{k+1} = x_p^k + v_p^k \Delta t \qquad a_p^k = 0$$

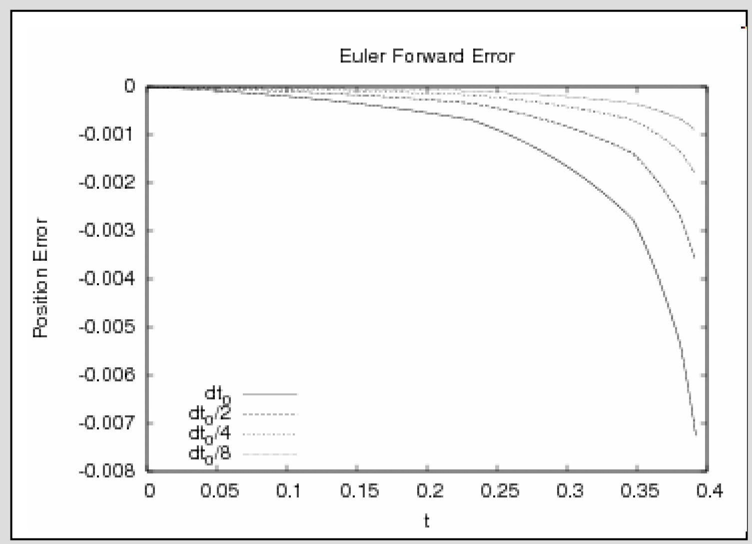


- Exact Spatial Integration
- Calculate Error:

$$\varepsilon_{EF} = x_p^k - x(t^k)$$

- Errors are $O(\Delta t)$

$$\varepsilon_{EF} \le \frac{T}{2} a_{\max} \Delta t$$

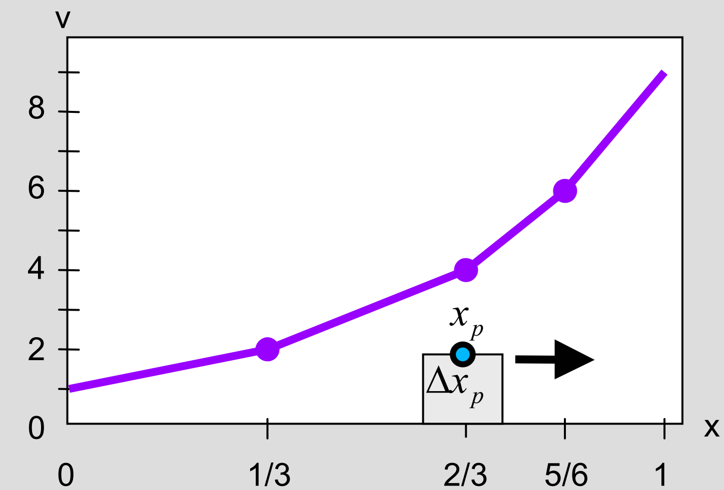


Centered Difference Error

$$v_{\text{ext}}^{k+1} = v_{\text{ext}}^{k} + a_p^k \Delta t \qquad v_p^0 = 0$$

$$v_p^k = v(x(t^{k+1/2})) + v_{\text{ext}}^k \qquad x_p^0 = 0$$

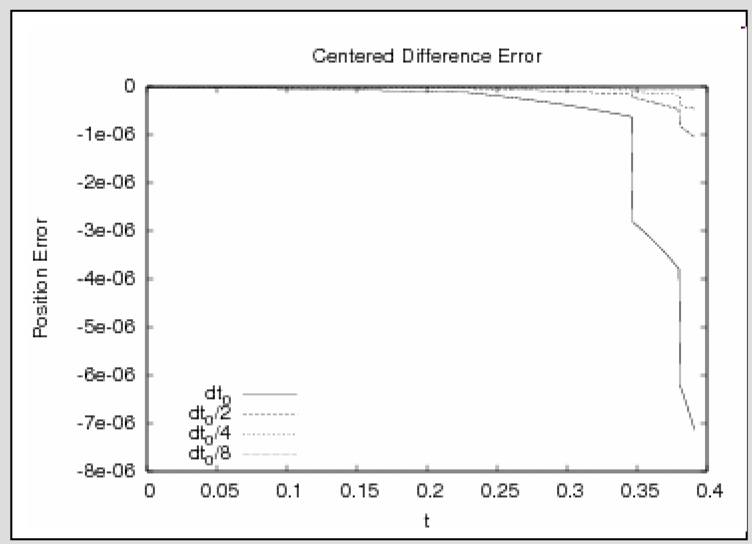
$$x_p^{k+1} = x_p^k + v_p^k \Delta t \qquad a_p^k = 0$$



- Exact Spatial Integration
- Calculate Error:

$$\varepsilon_{EF} = x_p^k - x(t^k)$$

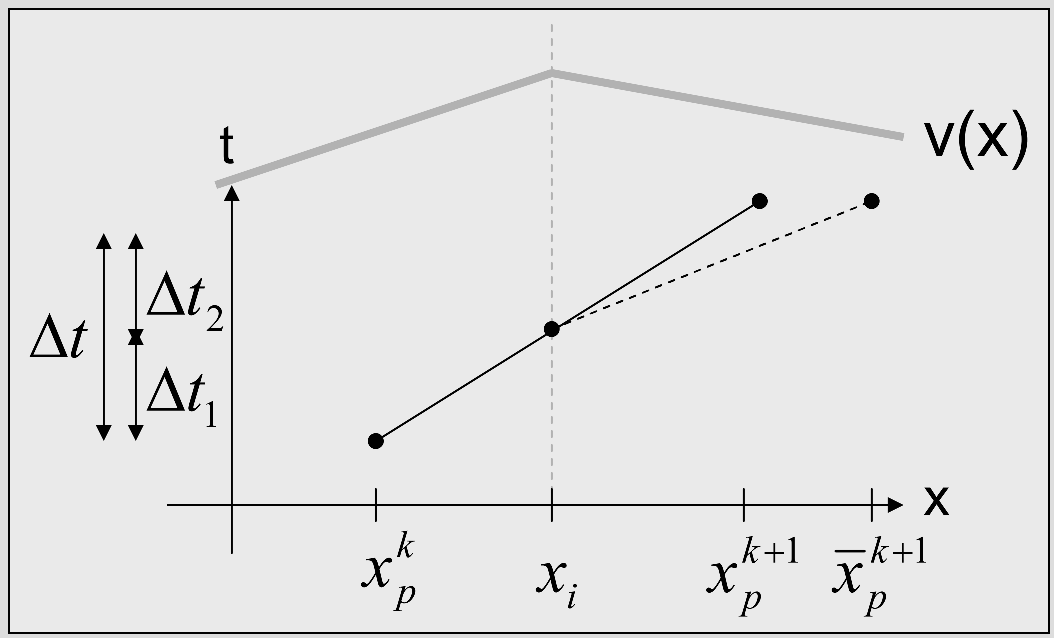
- Errors are $O(\Delta t^2)$



ODE Jump Error

- Different than the quadrature related grid crossing error treated in Steffen, et al.*
- Caused by integrating past spatial discontinuity in v’

One Step vs.
Two Step Method:



*M. Steffen, R. M. Kirby, M. Berzins. “Analysis and reduction of quadrature errors in the material point method (MPM).” *IJNME*, 2008

ODE Jump Error

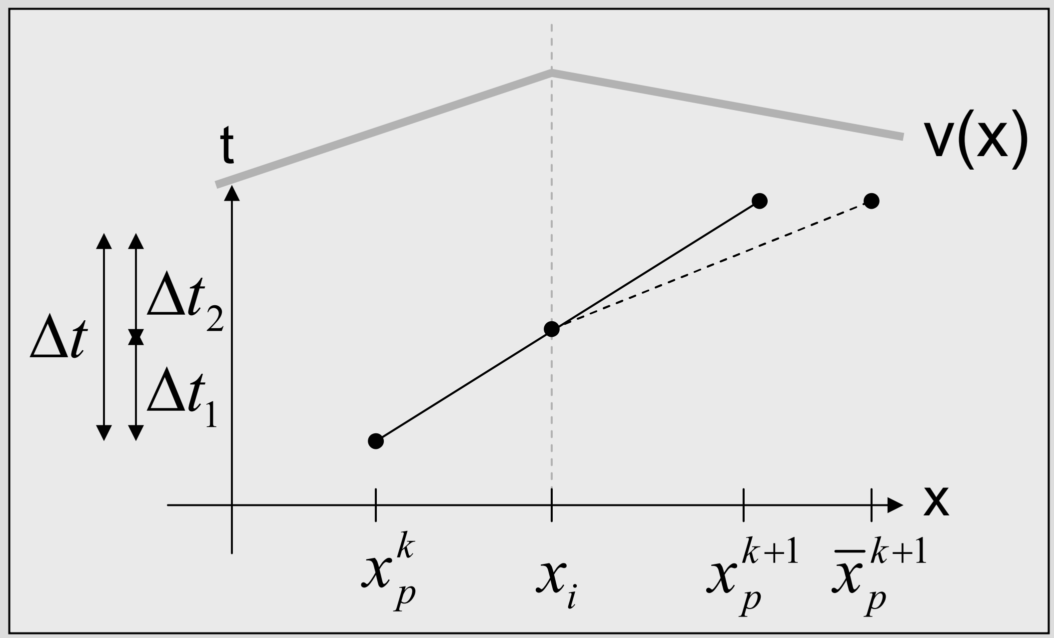
- Tran, et al., report this as a first-order temporal error in the MPM framework:*

$$\varepsilon_{\text{jump}} = \bar{x}_p^{k+1} - x_p^{k+1} = (v_i^{k+1} - v_{i-1}^{k+1})\left[\frac{x_i - x_p^k}{x_i - x_{i-1}}\right]\Delta t_2 + \left[a_{i-1}^k + \frac{x_p^k - x_{i-1}}{x_i - x_{i-1}}(a_i^k - a_{i-1}^k)\right]\Delta t_1 \Delta t_2$$

The term: $(v_i^{k+1} - v_{i-1}^{k+1})\left[\frac{x_i - x_p^k}{x_i - x_{i-1}}\right]\Delta t_2$

looks to be clearly first-order in time. It *is* when x_p^k is not dependent on Δt

*L.T. Tran, J. Kim, M. Berzins, "Solving Time-Dependent PDEs using the Material Point Method, A Case Study from Gas Dynamics", IJNMF, 2009



ODE Jump Error

$$\varepsilon_{\text{jump}} = \bar{x}_p^{k+1} - x_p^{k+1} = (v_i^{k+1} - v_{i-1}^{k+1})\left[\frac{x_i - x_p^k}{x_i - x_{i-1}}\right]\Delta t_2 + \left[a_{i-1}^k + \frac{x_p^k - x_{i-1}}{x_i - x_{i-1}}(a_i^k - a_{i-1}^k)\right]\Delta t_1 \Delta t_2$$

Rewriting: $(v_i^{k+1} - v_{i-1}^{k+1})\left[\frac{x_i - x_p^k}{x_i - x_{i-1}}\right]\Delta t_2$ assuming: $x_i = x_p^k + v_p \Delta t_1 \qquad \Delta t_1 \le \Delta t$

gives: $\frac{v_i^{k+1} - v_{i-1}^{k+1}}{x_i - x_{i-1}}(x_i - x_p^k)\Delta t_2 \approx \frac{\partial v}{\partial x_-} v_p \Delta t_1 \Delta t_2$

Therefore: $\varepsilon_{\text{jump}} = \left[\frac{\partial v}{\partial x_-} v_p + a_p\right]\Delta t_1 \Delta t_2$

The ODE jump error is then bounded by:

$$\varepsilon_{\text{jump}} \le \left[\frac{\partial v}{\partial x_-} v_p + a_p\right]\frac{\Delta t^2}{4}$$

If: $\Delta t_1 = \alpha \Delta t$, $\Delta t_2 = (1-\alpha)\Delta t$ $\qquad 0 < \alpha < 1$

Then: $\Delta t_1 \Delta t_2 = \alpha(1-\alpha)\Delta t^2$

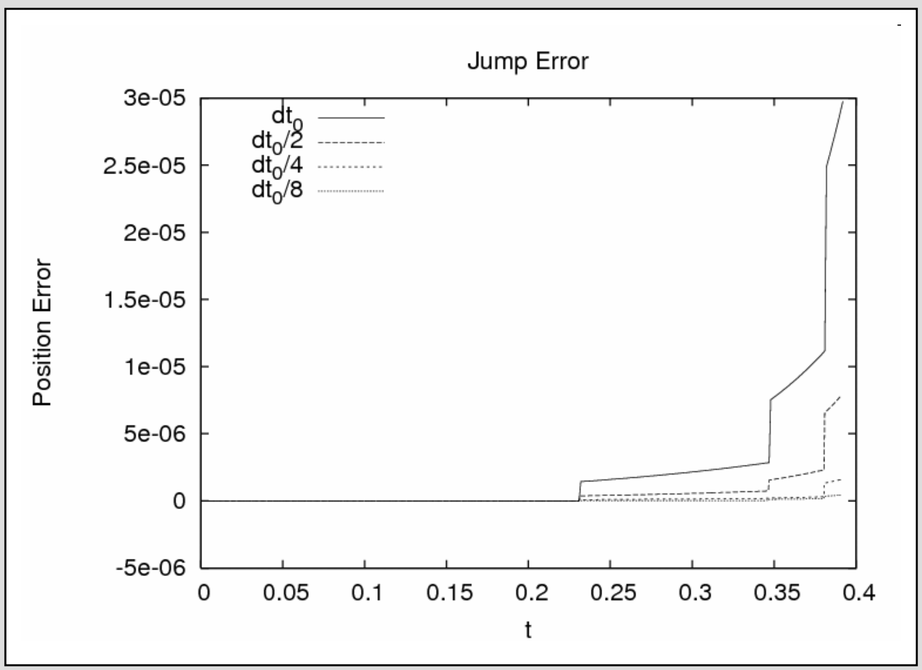
Therefore: $\Delta t_1 \Delta t_2 \le \frac{1}{4}\Delta t^2$

ODE Jump Error

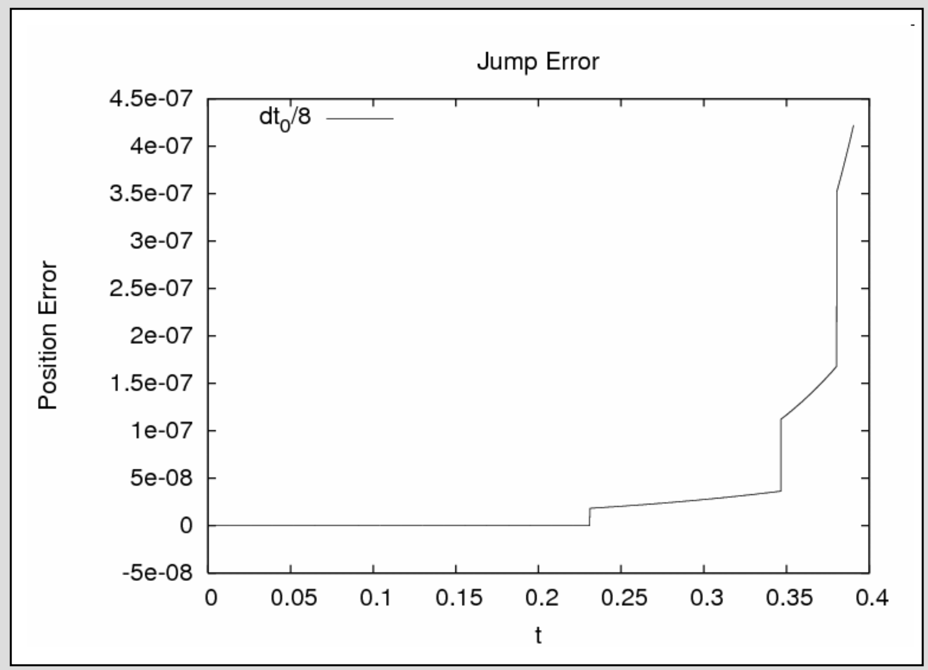
- Calculated: $\varepsilon^k_{jump} = x^k_p - \bar{x}^k_p$

- Error Bound: $\varepsilon_{\text{jump}} \le \left[\frac{\partial v}{\partial x_-} v_p + a_p \right] \frac{\Delta t^2}{4}$

Jump	Jump Bound	Calculated Jump
1	2.34×10^{-8}	1.81×10^{-8}
2	9.36×10^{-8}	7.60×10^{-8}
3	2.81×10^{-7}	1.84×10^{-7}



Multiple Time Step Sizes



Single Time Step Size

Quadrature Error

- Integrating Piecewise-Constant Functions with the Midpoint Rule:*

Bounds for each time-step: $E_{\text{MAX}} = \frac{1}{2}[[f(x)]]\Delta x$

One Time-Step:

$$v^{k+1} = v^k + (a^k + C\Delta x)\Delta t$$

$$x^{k+1} = x^k + v^{k+1}\Delta t$$

$$= x^k + v^k\Delta t + a^k\Delta t^2 + C\Delta x\Delta t^2$$

N Time-Steps:

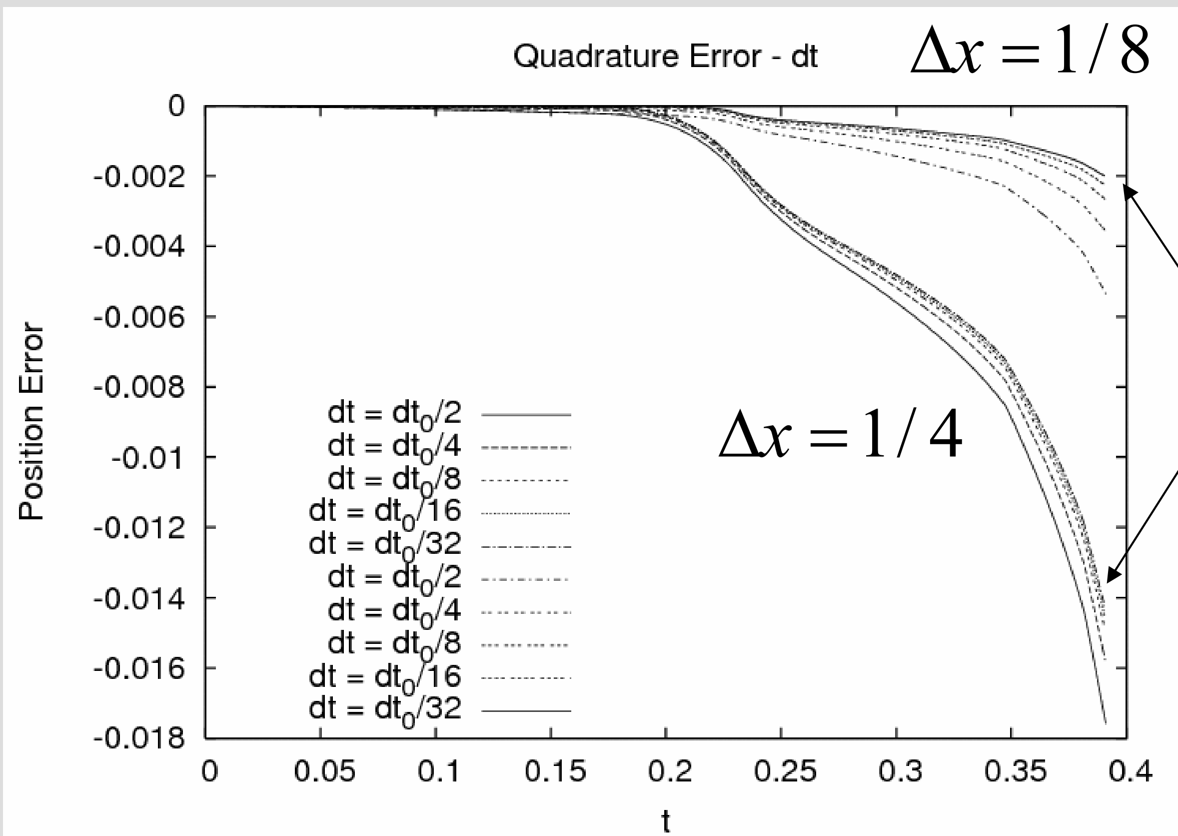
$$x^N = x^0 + Nv^0\Delta t + \sum_{j=1}^{N}\sum_{i=1}^{j} a^i\Delta t^2 + \frac{1}{2}TC\Delta x\Delta t + \frac{1}{2}T^2C\Delta x$$

*M. Steffen, R.M. Kirby, M. Berzins, “Analysis and Reduction of Quadrature Errors in the Material Point Method (MPM)”, *IJNME*, 2008

Quadrature Error – Final T

Effect of Time-Step

- Integration error in acceleration – effect on particle position errors:



Bounded by Quadrature Error

Conclusions

- Spatial and temporal errors in MPM are interconnected, making analysis difficult.
- Moving-Mesh MPM has allows these errors to remain independent – no feedback errors
- Analysis of local truncation errors allows us to operate in unstable regimes – demonstrating expected temporal error behaviors
- Simplified problem demonstrates errors similar to MPM – easier to analyze. Hope to extend to the full MPM framework.

Acknowledgments

- Center for the Simulation of Accidental Fires and Explosions (CSAFE) DOE Grant W-7405-ENG-48

Future Work

- Extended Error analysis of simplified problem to full MPM framework.
- Through extrapolation techniques, we hope to achieve > $O(h^2)$
  - Should be easy for Moving Mesh MPM

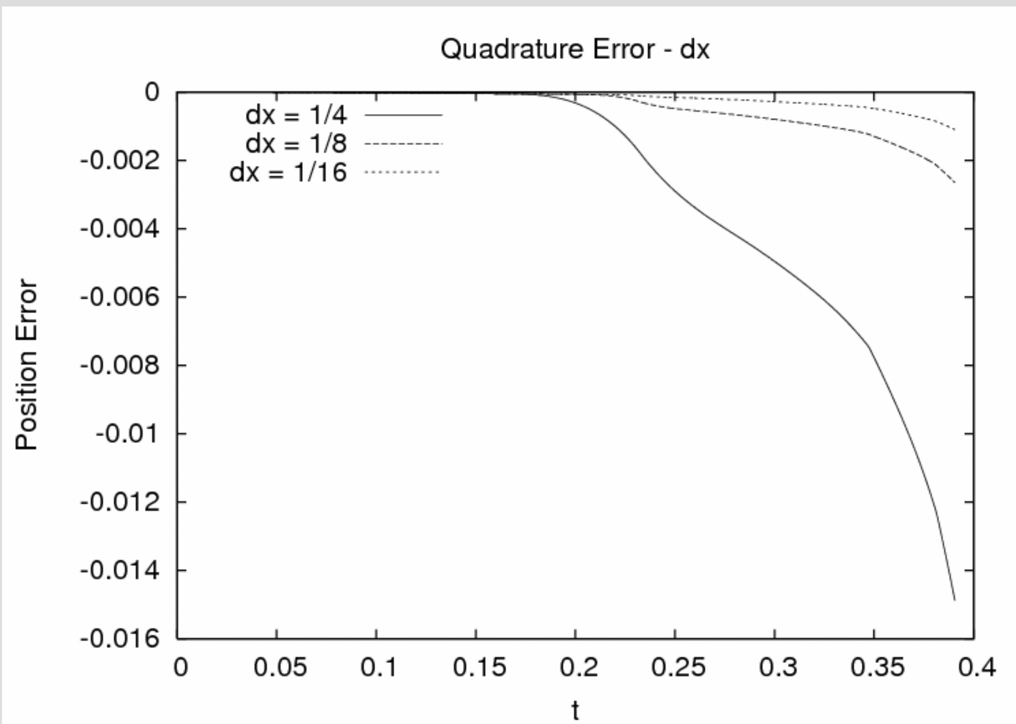
Conclusions

- Approximation Error, Mass Lumping Error, Quadrature Error, Time integration Error, Jump Error, Feedback
- Moving Mesh MPM
  - Approximation: $O(h^2)$
  - Mass Lumping Error: $O(h^2)$
  - Quadrature Error: $O(dx^2)$
  - Time integration: $O(dt^2)$
  - No Jump Error, No Feedback.
  - Should give $O(h^2, dt^2)$ errors
- Standard MPM
  - Quadrature, Time-Stepping, Jump Error interplay
  - Interplay forces things to $O(dt)$

Quadrature Error – Final T

Effect of Particle Width

- Integration error in acceleration – effect on particle position errors:



Reminder, for $\Delta t = \Delta t_0 / 8$:

$$\varepsilon_{\mathrm{ODE}} \approx 1 \cdot 10^{-3}$$

$$\varepsilon_{\mathrm{jump}} \approx 4 \cdot 10^{-7}$$