Numerical analysis of regular material point method and its application to multiphase flows

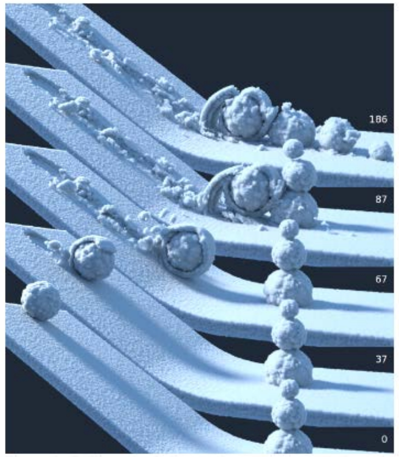
Presenter:
Dr. Sreejith N. A.
Researcher
National Renewable Energy Laboratory (NREL),
Golden, Colorado, USA
Date: Aug. 2nd , 2023

Other Contributors:

Dr. Nicholas Deak	NREL
Dr. Hariswaran Sitaraman	NREL
Dr. Marc Day	NREL

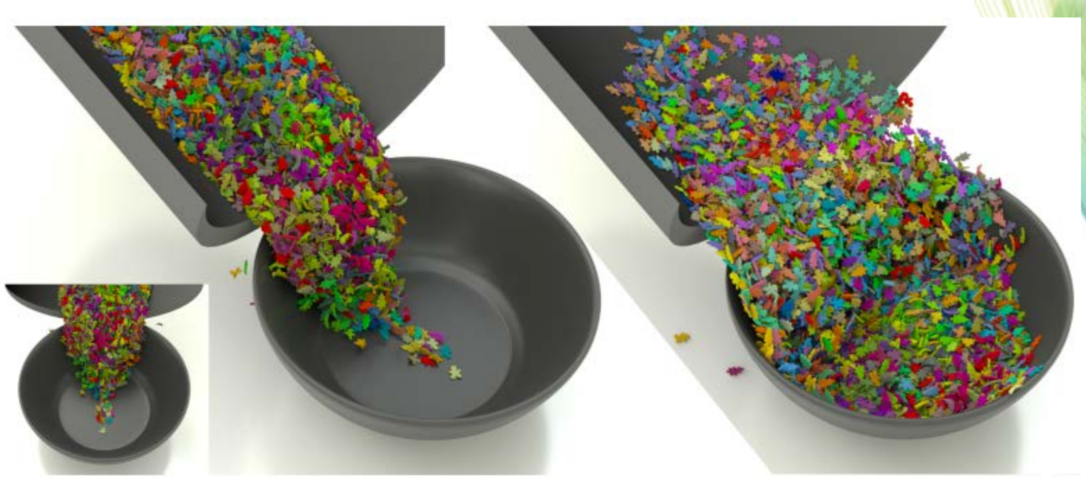
Background

Introduction

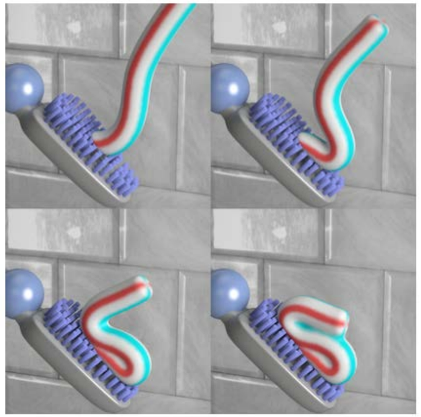


Rolling snowball simulation [1]

Concrete crushing simulation [2]



Pouring candies from a tube[2]



Simulation of toothpaste[3]

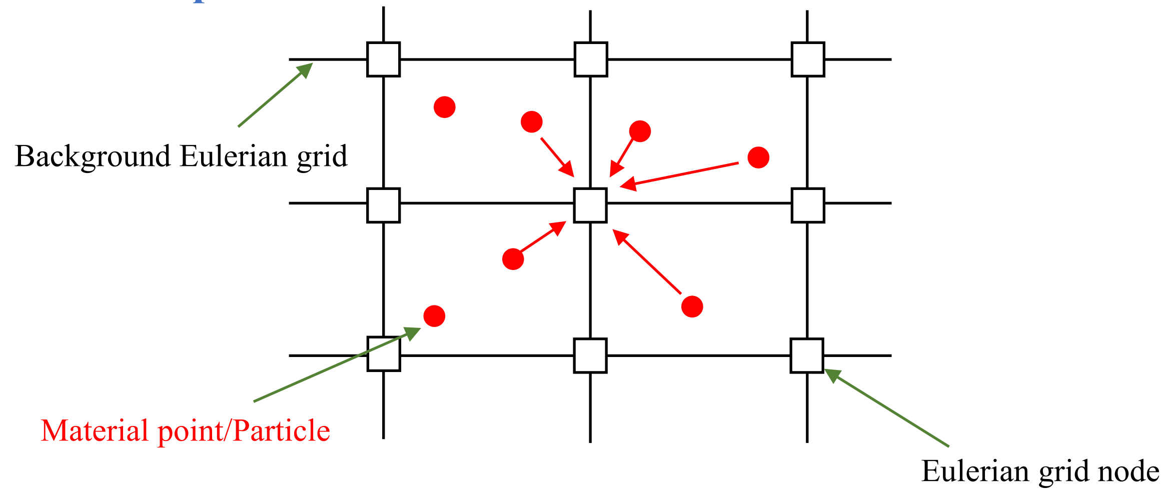
Ice cream poured on a conveyer belt[3]

1. A material point method for snow simulation, Stomakhin et. al. ACM Trans. Graph., Vol. 32, No.4, Article 30
2. A Massively Parallel and Scalable Multi-GPU Material Point Method, Wang et. al., ACM Trans. Graph., Vol. 39, No.4, Article 30
3. A Material Point Method for Viscoelastic Fluids, Foams and Sponges, Ram et. al., Proceedings of the 14th ACM SIGGRAPH, 2015

Material Point Method (MPM)
and
Exagoop Solver

Material Point Method (MPM)

Basic components of MPM



- MPM is a variant of particle-in-cell method
  - Material represented as a collection of “particles”/”material points”
  - All material properties defined at “particles”
- Advantages compared to regular FEM
  - No unstructured and deforming grids
  - Can handle large deformations
  - Flexibility with constitutive models
  - Complex geometries
  - Amenable to large-scale computing

Governing equations

$$\rho \frac{Dv}{Dt} = \rho \boldsymbol{b} + \nabla . \boldsymbol{\sigma}$$

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\boldsymbol{D}, E, \nu)$$

$$\boldsymbol{D} = \frac{1}{2}(\boldsymbol{L} + \boldsymbol{L}^T)$$

$$\boldsymbol{L} = \nabla \boldsymbol{v}$$

$\rho \rightarrow density$

$\boldsymbol{v} \rightarrow velocity$

$\boldsymbol{\sigma} \rightarrow stress$

$\boldsymbol{b} \rightarrow body\ force$

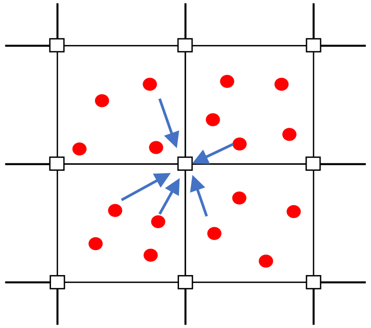
$\mathrm{E} \rightarrow youngs\ modulus$

$\nu \rightarrow poisson's\ ratio$

Mass conservation is implicitly satisfied

Material Point Method (MPM)-Different Steps

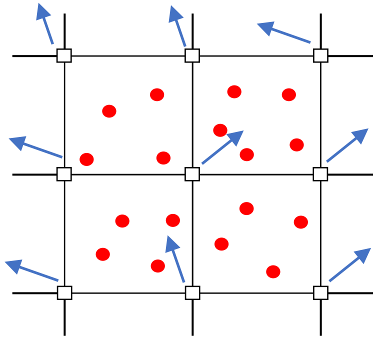
1. Particle to grid interpolation of mass, mom and forces



$$\theta_I^t = M^{-1}\sum m_p N_I(x_p)\theta_p^t,$$

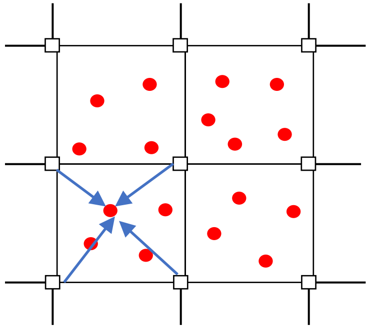
$$\theta \in \{m, mv, f_{int}, f_{ext}\}$$

2. Momentum equation solution & grid updation



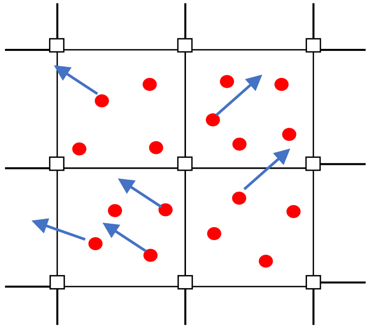
$$v_I^{t+\Delta t} = v_I^t + \Delta t\,\left(\frac{f_I}{m_I}\right)$$

3. Grid to particle interpolation



$$\mathbf{v}_p^{t+\Delta t} = \alpha \underbrace{\left(\mathbf{v}_p^t + \sum_I N_I\left(\mathbf{x}_p^t\right)\left[\mathbf{v}_I^{t+\Delta t} - \mathbf{v}_I^t\right]\right)}_{\text{FLIP update}} + (1-\alpha)\sum_I \overbrace{N_I\left(\mathbf{x}_p^t\right)\mathbf{v}_I^{t+\Delta t}}^{\text{PIC update}}$$

4. Position update and grid reset



$$x_p^{t+\Delta t} = x_p^t + \Delta t\, v_p^{t+\Delta t}$$

First order explicit time integration

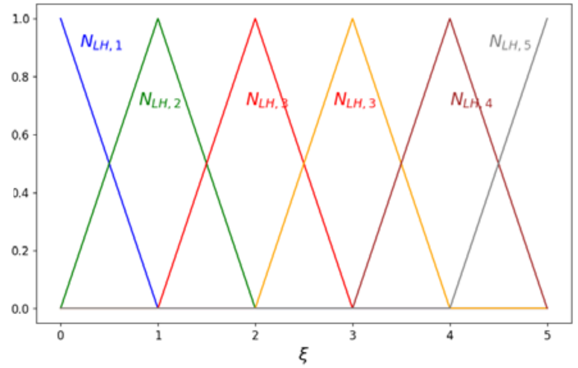
α determines the PIC-FLIP blending

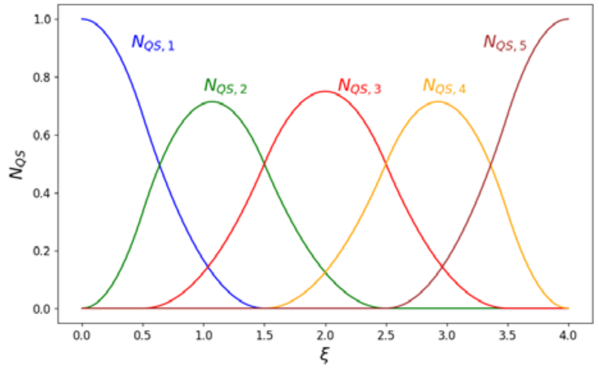
Material Point Method (MPM)-Shape Functions

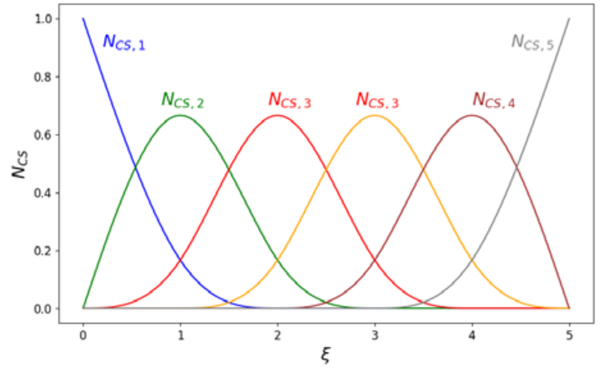
$$\xi = \frac{(x_p - x)}{\Delta x}$$

	Linear Hat (LH)	Quadratic B-Spline (QBS)	Cubic B-Spline (CBS)

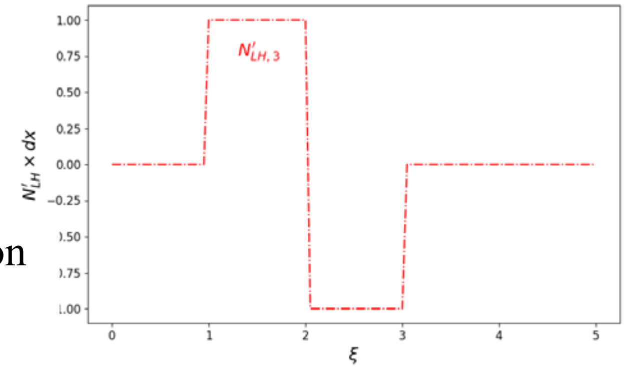
Shape Functions

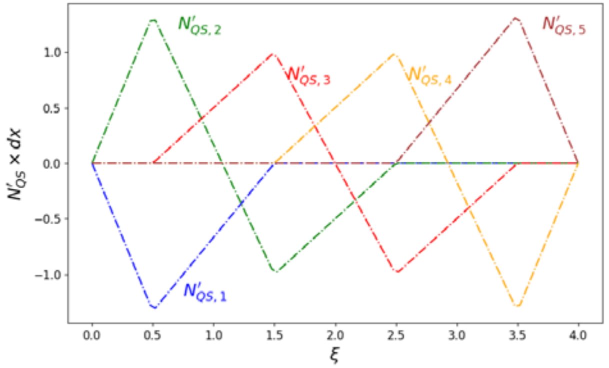


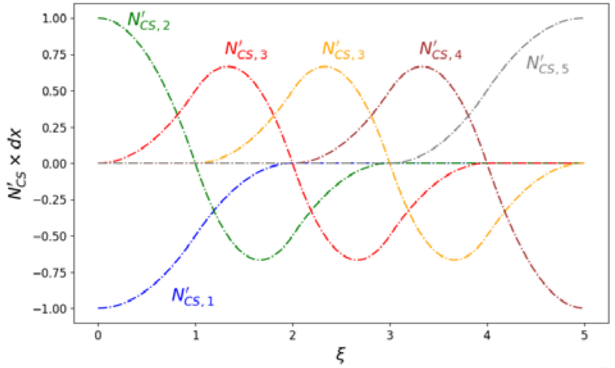




Shape Function Gradients







Discontinuous shape function gradients for LH causes grid crossing instability

Exagoop MPM Solver

- MPM Solver Developed at NREL: *Exagoop*[1]
- Exagoop is developed based on AMReX[2] Framework
- Particle class in AMReX used to model material point related operations
- Block-structured grid framework--> Used as background grid
- Level sets used to model complex geometry
- Parallel capability→ On CPUs and GPUs

1. https://github.com/NREL/Exagoop
2. https://github.com/AMReX-Codes/amrex

Spectral Stability Analysis of MPM

Spectral Stability Analysis-Methodology

Governing Equation:

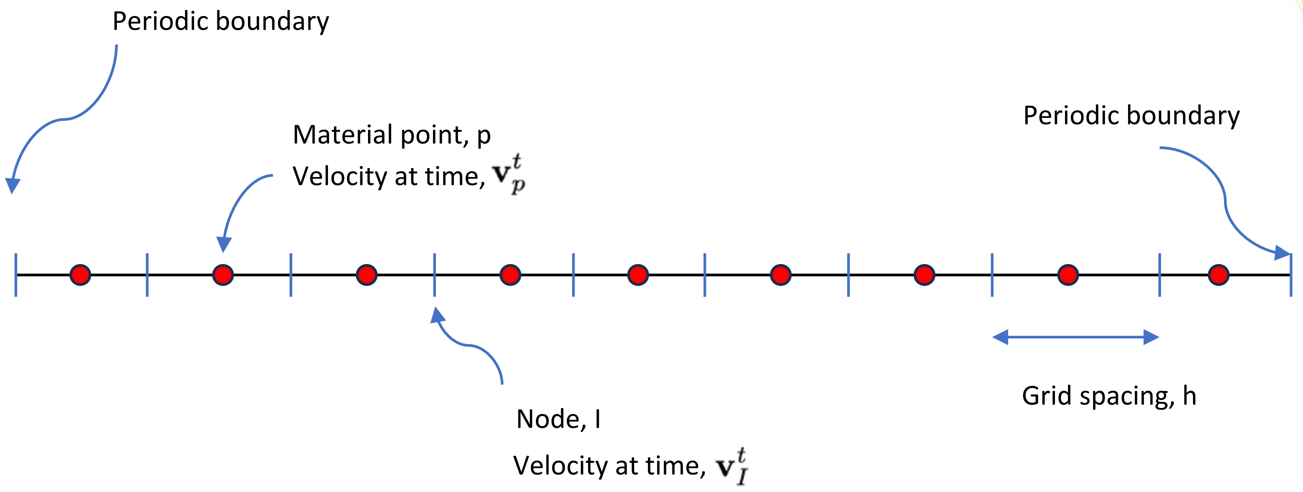
$$\rho \frac{D\mathbf{v}}{Dt} = \mathbf{F_i} + \cancel{\mathbf{F_e}}^{\,0} = \frac{\partial}{\partial x}\left[\nu \frac{\partial \mathbf{v}}{\partial x}\right]$$

MPM Governing Equation at nodes:

$$\sum_{p=1}^{n_p} m_p N_I(\mathbf{x}_p) N_J(\mathbf{x}_p)\,\mathbf{a_J} = -\sum_{p=1}^{n_p} m_p \sigma_p^s \nabla N_I(\mathbf{x}_p)$$

Assumptions:

- One-dimensional
- Periodic boundaries
- External forces assumed to zero
- All material point masses are equal and constant
- Stability studied assuming specific material points locations at a particular time instant



Total number of nodes: N_I

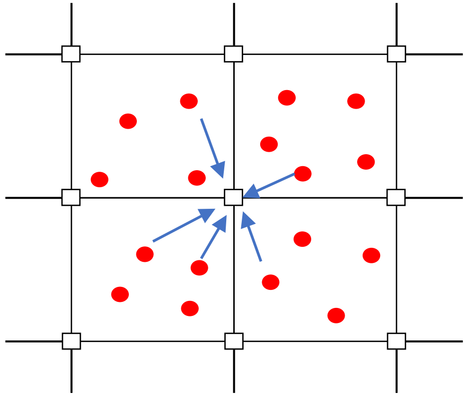
Total number of material points: N_p

Material points

Grid Nodes

Spectral Stability Analysis-Methodology

1. Particle to grid interpolation



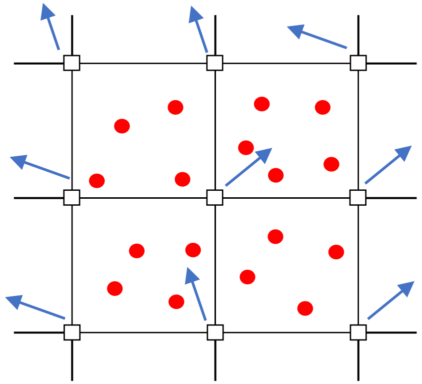
$$\mathbf{v}_I^t = \bar{\bar{\mathbf{T}}}_{p\to I}\mathbf{v}_p^t$$

$$\bar{\bar{\mathbf{T}}}_{p\to I} = \bar{\bar{\mathbf{M}}}^{-1}\bar{\bar{\mathbf{C}}}$$

Mass matrix (N_I X N_I)

Coefficient matrix, (N_I X N_p)

2. Nodal time integration



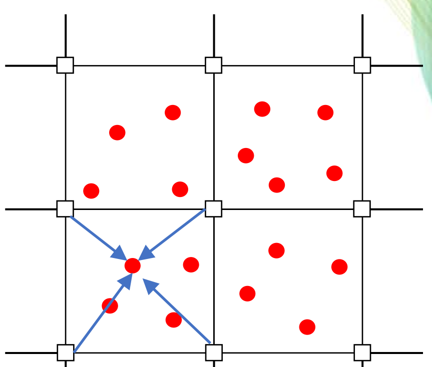
$$\bar{\mathbf{v}}_I^{t+\Delta t} = \left[\bar{\bar{\mathbf{I}}} - Fo\,\bar{\bar{\mathbf{G}}}_{P\to I}\bar{\bar{\mathbf{G}}}_{I\to P}\right]\bar{\mathbf{v}}_I^t$$

$$Fo = \frac{\nu\Delta t}{h^2}$$

P2G Gradient matrix

G2P Gradient matrix

3. Grid to particle interpolation



$$\mathbf{v}_p^{t+\Delta t} = \alpha\left(\mathbf{v}_p^t + \sum_I N_I\left(\mathbf{x}_p^t\right)\left[\mathbf{v}_I^{t+\Delta t} - \mathbf{v}_I^t\right]\right) + (1-\alpha)\sum_I N_I\left(\mathbf{x}_p^t\right)\mathbf{v}_I^{t+\Delta t}$$

$$\bar{\mathbf{v}}_p^{t+\Delta t} = \left[\bar{\bar{\alpha}} + \bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Theta}}\bar{\bar{\mathbf{T}}}_{P\to I} + (\bar{\bar{I}} - \bar{\bar{\alpha}})\bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Phi}}\bar{\bar{\mathbf{T}}}_{P\to I}\right]\bar{\mathbf{v}}_p^t$$

$$\bar{\bar{\Theta}} = -Fo\,\bar{\bar{\mathbf{G}}}_{P\to I}\bar{\bar{\mathbf{G}}}_{I\to P}$$

$$\bar{\bar{\Phi}} = \bar{\bar{\mathbf{I}}} - \bar{\bar{\Theta}}$$

Spectral Stability Analysis-Methodology

Exact amplification factor

$$\mathbf{v}(x,t) = \int \hat{\mathbf{V}}(k,t)e^{ikx}dk$$

$$\mathbf{v}(x,t+\Delta t) = \int \mathbf{G}\hat{\mathbf{V}}(k,t)e^{ikx}dk$$

Theoretical amplification factor

MPM amplification factor

$$\bar{\mathbf{v}}_p^{t+\Delta t} = \left[\bar{\bar{\alpha}} + \bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Theta}}\bar{\bar{\mathbf{T}}}_{P\to I} + (\bar{\bar{I}} - \bar{\bar{\alpha}})\bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Phi}}\bar{\bar{\mathbf{T}}}_{P\to I}\right]\bar{\mathbf{v}}_p^t$$

$$\mathbf{v}_{p,l}^{t+\Delta t} = \underbrace{\left[\bar{\bar{\alpha}} + \bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Theta}}\bar{\bar{\mathbf{T}}}_{P\to I} + (\bar{\bar{I}} - \bar{\bar{\alpha}})\bar{\bar{\mathbf{T}}}_{I\to P}\bar{\bar{\Phi}}\bar{\bar{\mathbf{T}}}_{P\to I}\right]}_{\bar{\bar{\mathbf{A}}}}\bar{\mathbf{v}}_p^t$$

$$\begin{aligned}\mathbf{v}_{p,l}^{t+\Delta t} &= \int \bar{\bar{\mathbf{A}}}_{l,m}\hat{\mathbf{V}}(k,t)e^{ikx_m}dk \\ &= \int \bar{\bar{\mathbf{A}}}_{l,m}\hat{\mathbf{V}}(k,t)e^{ikx_l}e^{ik(x_m-x_l)}dk \\ &= \int \underbrace{\bar{\bar{\mathbf{A}}}_{l,m}\bar{\bar{\mathbf{P}}}_{m,l}}_{G_{MPM}}\hat{\mathbf{V}}(k,t)e^{ikx_l}dk\end{aligned}$$

Function of kh and Fo

Knowing shape functions evaluated at specified material points location, one can calculate amplification factor

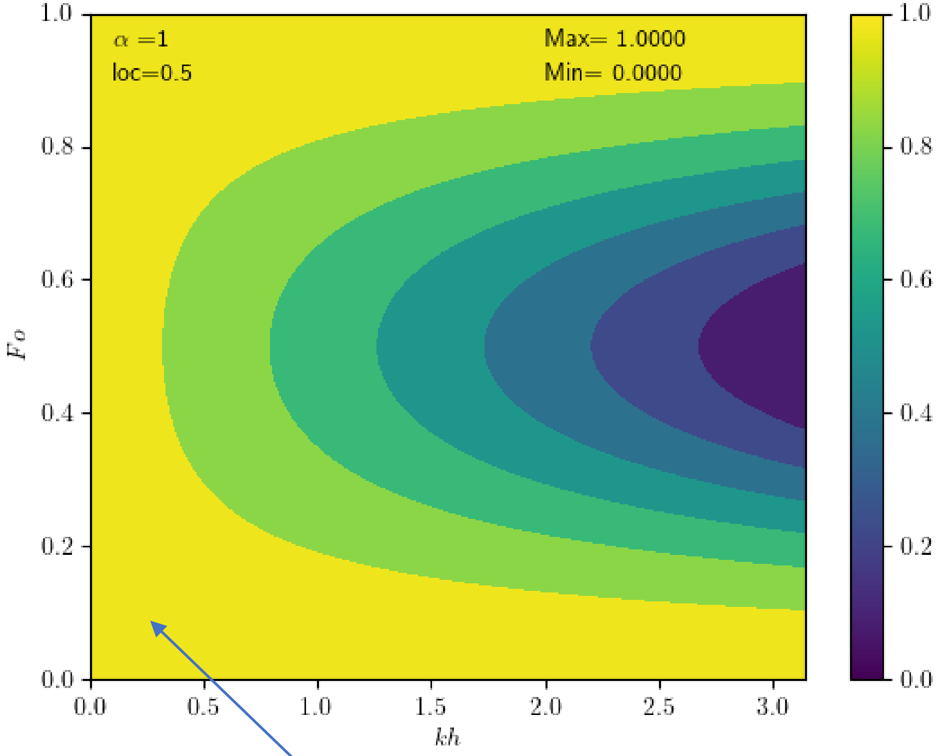
Spectral Stability Analysis- Results (|G|)

Effect of α (PIC and FLIP update)

Shape Function: Linear Hat
Material point location: Mid-cell

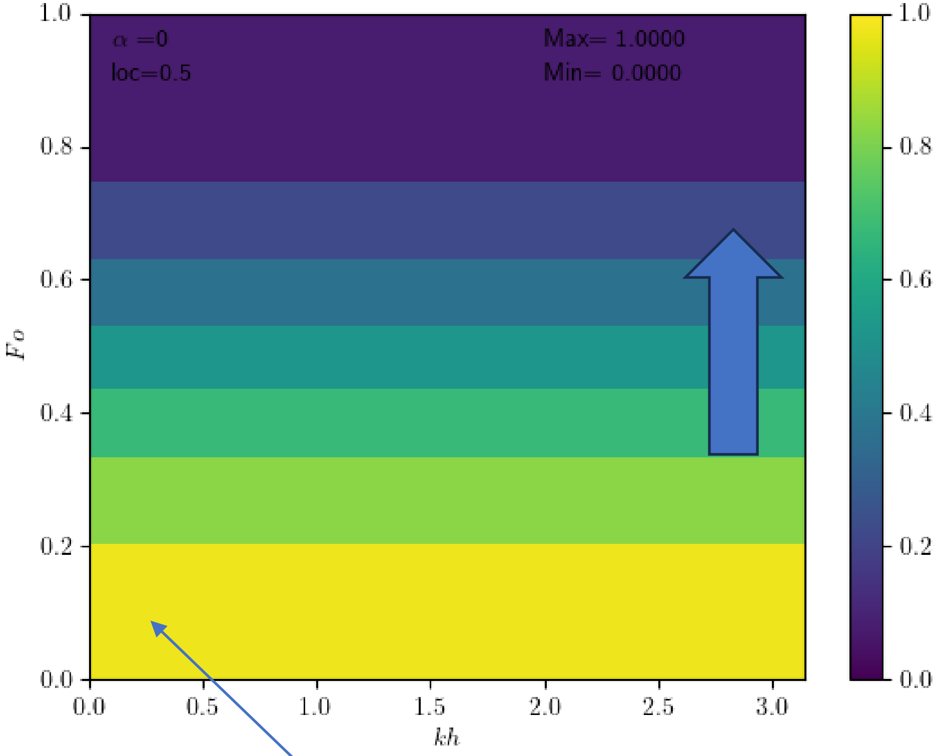
$$\mathbf{v}_p^{t+\Delta t} = \alpha \left(\mathbf{v}_p^t + \sum_I N_I\left(\mathbf{x}_p^t\right)\left[\mathbf{v}_I^{t+\Delta t} - \mathbf{v}_I^t\right] \right) + (1-\alpha) \sum_I N_I\left(\mathbf{x}_p^t\right) \mathbf{v}_I^{t+\Delta t}$$

α = 1.0



Good region to compute

α = 0.0



Good region to compute

Progressive damping with higher Δt for all wavenumbers

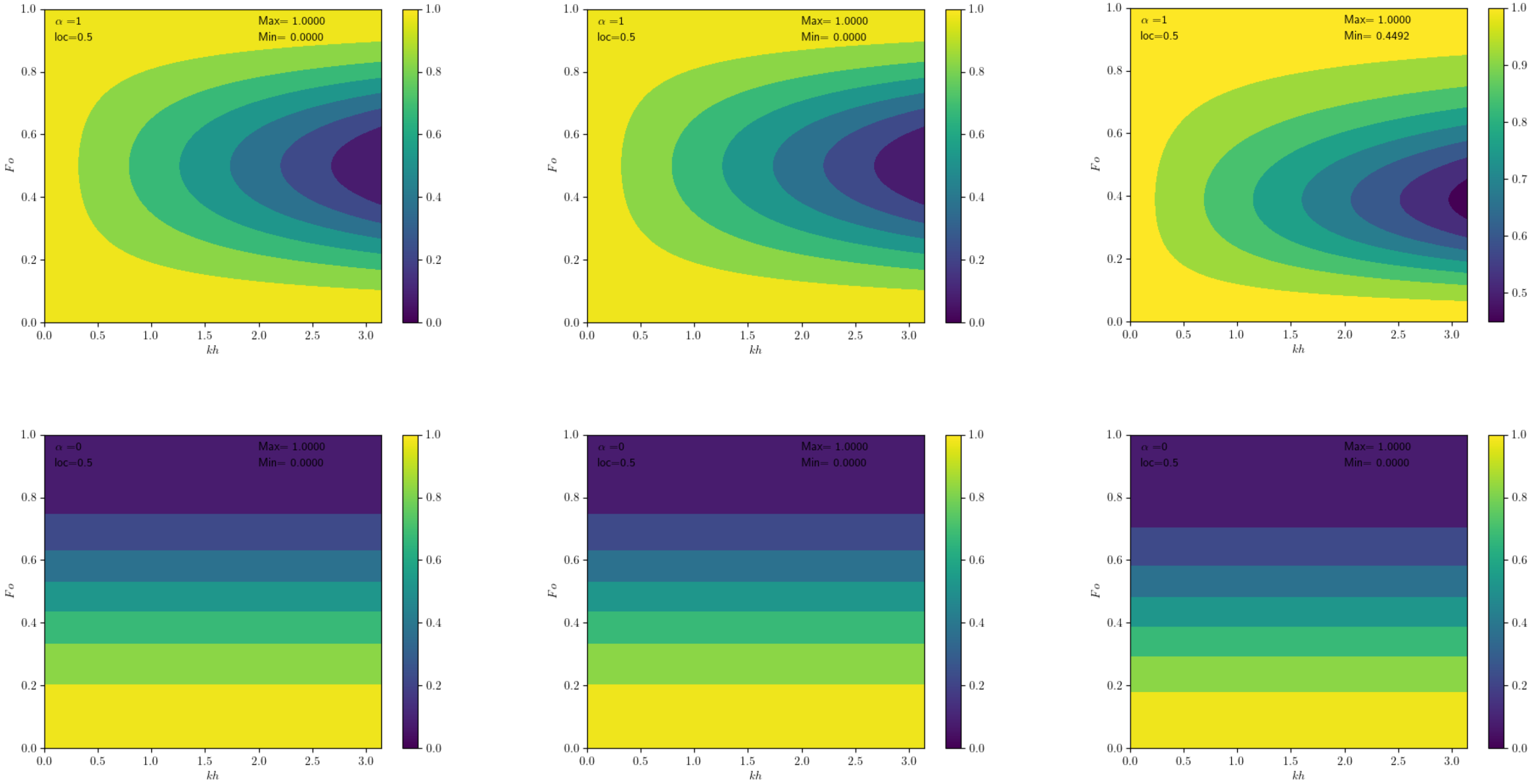
Damping at all spatial frequencies for α = 0.0

Spectral Stability Analysis- Results (|G|)

Effect of shape functions

Material point location: Mid-cell

	Linear Hat (LH)	Quadratic B-Spline (QBS)	Cubic B-Spline (CBS)
$\alpha = 1.0$			
$\alpha = 0.0$			



All schemes behave alike at $\alpha = 0.0$

Spectral Stability Analysis- Results (|G|)

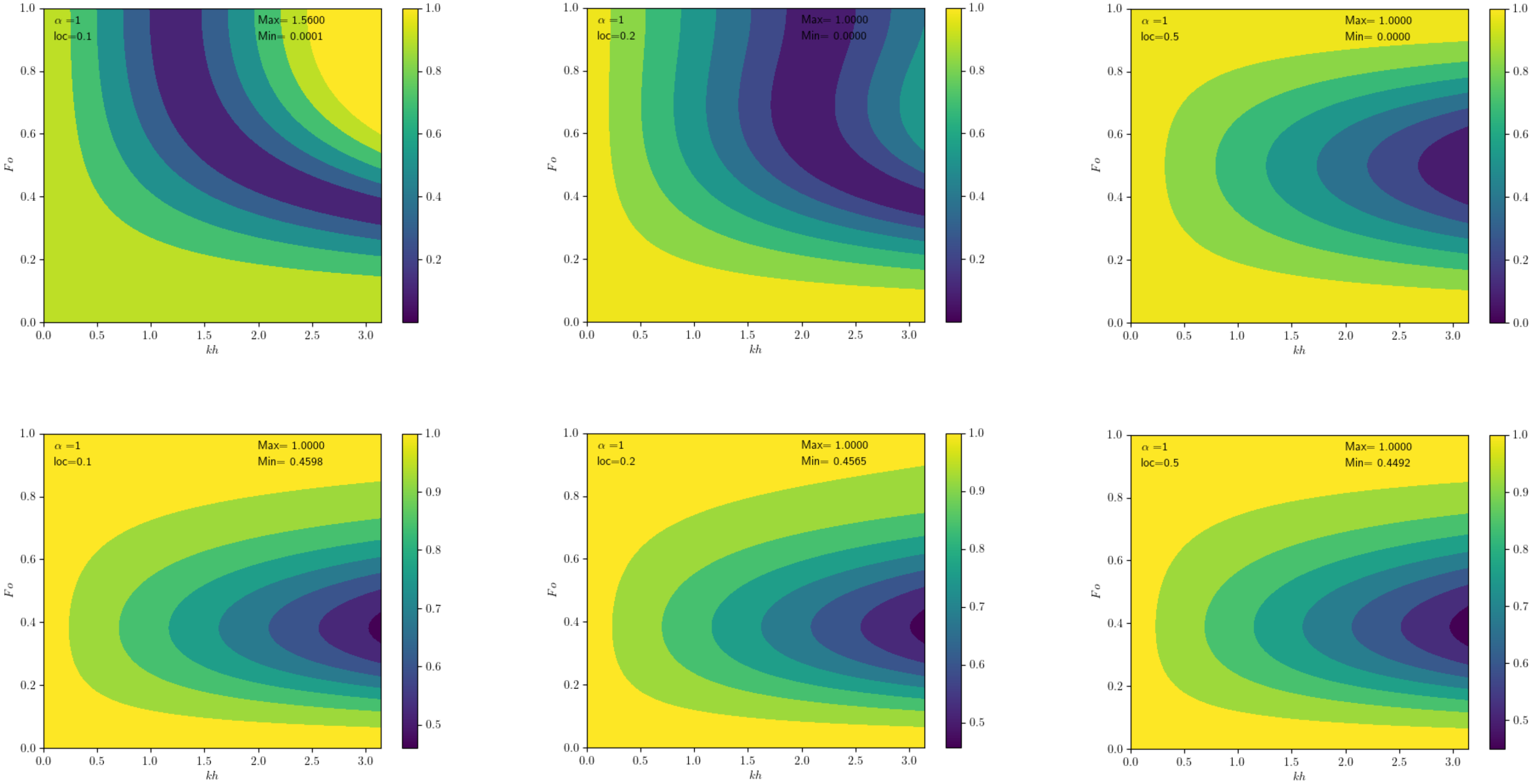
Effect of material point location

$\alpha = 1.0$

Loc = 0.1h | Loc = 0.2h | Loc = 0.5h

Linear Hat (LH)

Cubic B-Spline (CBS)



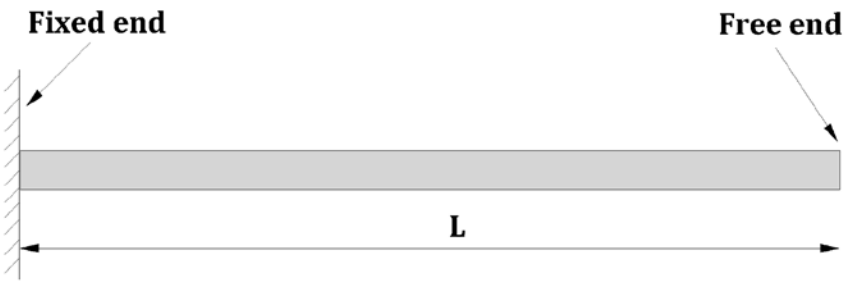
Cubic spline properties least sensitive to material point location

Linear hat susceptible to grid crossing instability

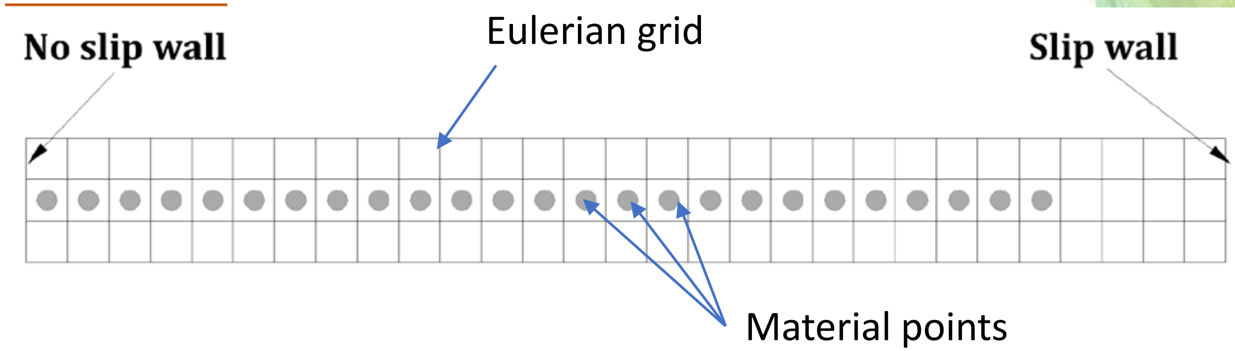
Spectral Stability Analysis- Validation

Test Case Description:

Problem Definition



MPM Model



Boundary Conditions

$$u(0,t) = 0 \quad \frac{\partial u}{\partial x}(L,t) = 0$$

Initial Conditions

$$u(x,0) = 0 \quad \frac{\partial u}{\partial t}(x,0) = V_0 \sin(\frac{\pi x}{2L})$$

Exact Solution

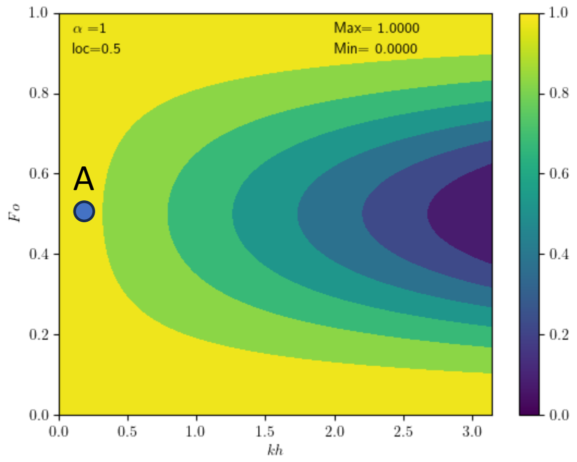
$$u(x,t) = V_0/\omega_1 \sin\left(\frac{\pi x}{2L}\right) \sin(\omega_1 t)$$

$$v(x,t) = V_0 \sin\left(\frac{\pi x}{2L}\right) cos(\omega_1 t)$$

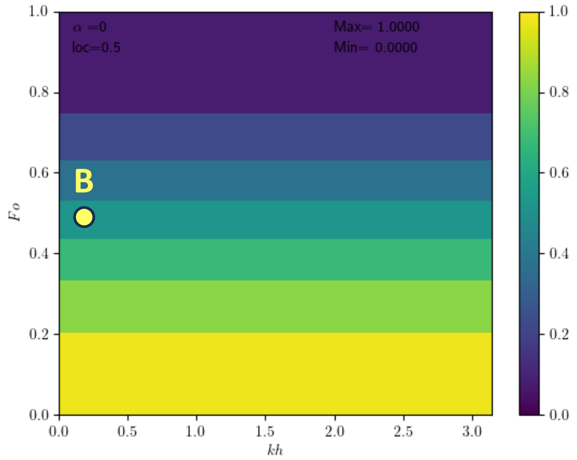
Spectral Stability Analysis- Validation

Test Case Description: Effect of alpha

$\alpha = 1.0$
Shape Function: LH
kh = 0.13
Fo = 0.5



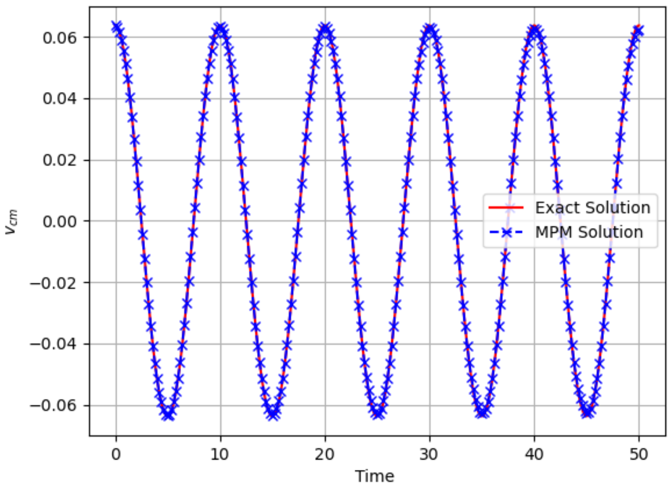
$\alpha = 0.0$
Shape Function: LH
kh = 0.13
Fo = 0.5



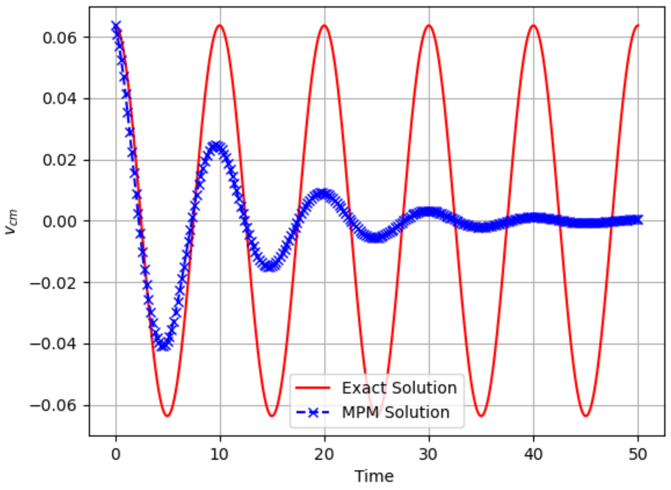
|G| computed from analysis

	Kh	Fo	Scheme	α	|G|
Test A	0.126	0.5	LH	1.0	0.96
Test B	0.126	0.5	LH	0.0	0.5

Test A



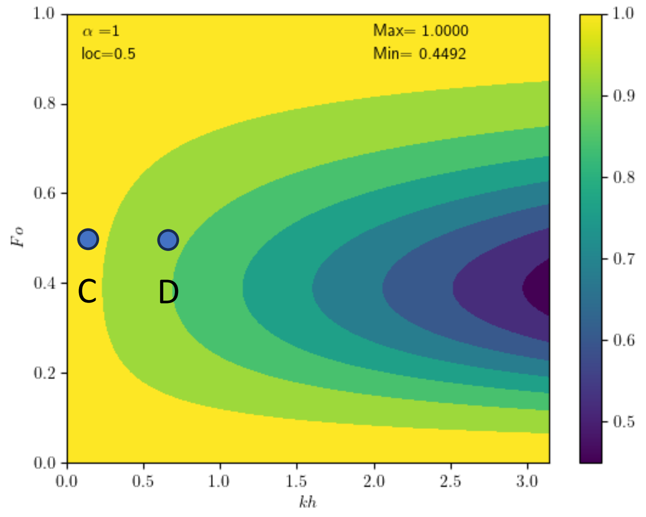
Test B



$\boldsymbol{\alpha} = 0.0$ induces solution damping

Spectral Stability Analysis- Validation

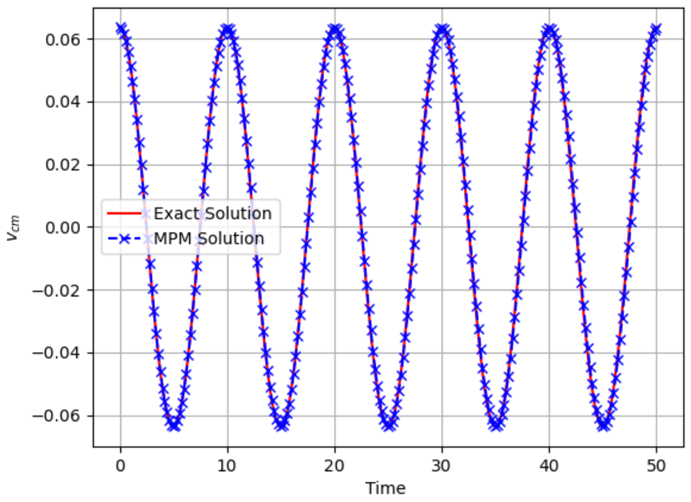
Test Case Description: Effect of grid resolution



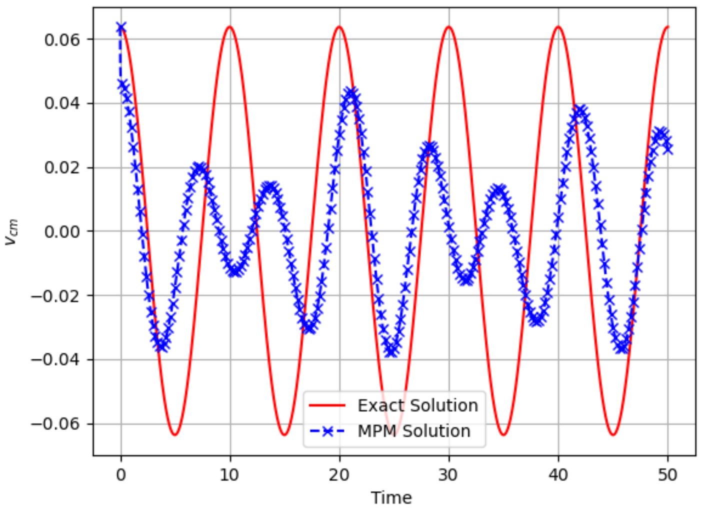
|G| computed from analysis

	Kh	Fo	Scheme	α	|G|
Test C	0.126	0.5	CBS	1.0	0.98
Test D	0.628	0.5	CBS	1.0	0.90

Test C



Test D



$\alpha = 1.0$ does not guarantee undamped solution even for CBS scheme!!

Conclusions

- Material point method solver developed based on AMReX framework

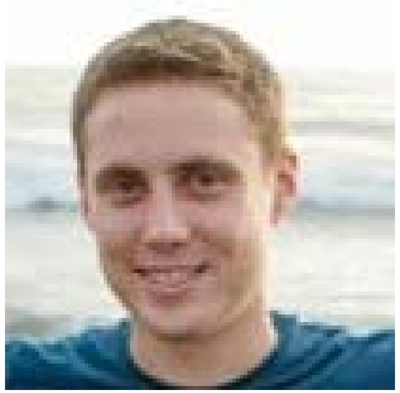
- Spectral stability analysis framework developed that studies amplification factor in the velocity update step

- Verification with a 1-dimensional axial vibration of bar test case shows excellent match with stability analysis prediction

- PIC update is observed to dampen all wavenumbers for progressively increasing time steps, where as FLIP update is observed to be undampened at low wavenumbers

- Cubic B-spline is observed to show minimal variances between different material point locations

Other researchers who contributed to this project



Dr. Nicholas Deak (NREL)

Dr. Hariswaran Sitaraman (NREL)

Dr. Marc Day (NREL)

THANK YOU

NREL/PR-2C00-87103

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Science and National Nuclear Security Administration. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes. This research was supported by the NAWI UHPRO project, a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration. A portion of the research was performed using computational resources sponsored by the Department of Energy's Office of Energy Efficiency and Renewable Energy and located at the National Renewable Energy Laboratory.