Spectral Analysis of Regular Material Point Method and its Application to Study High Pressure Reverse Osmosis Membrane Compaction and Embossing

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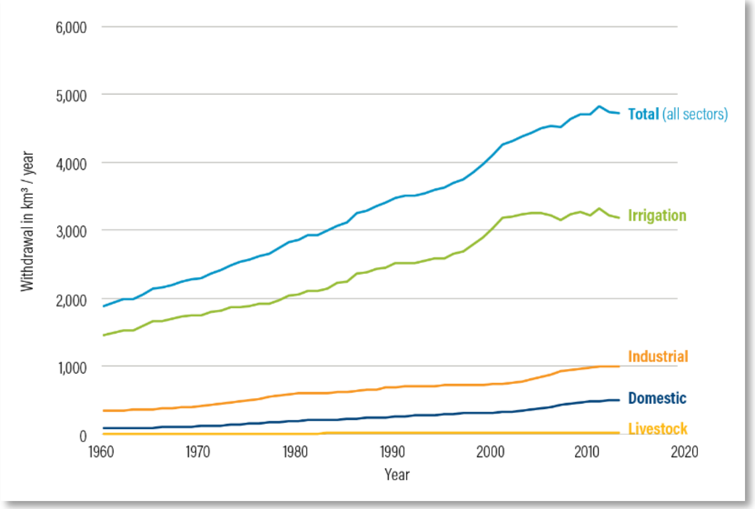
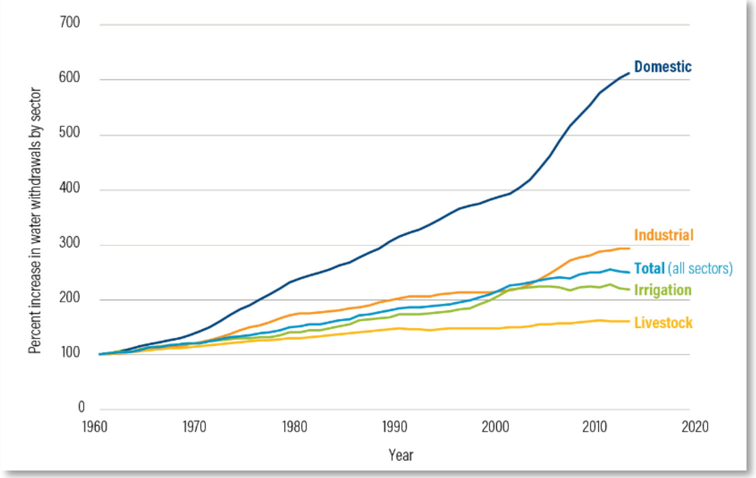
- Introduction and background on NAWI UHPRO project
- Analysis of regular material point method
- Application of MPM to UHPRO membrane compaction problem
- Conclusions & Perspectives

Introduction

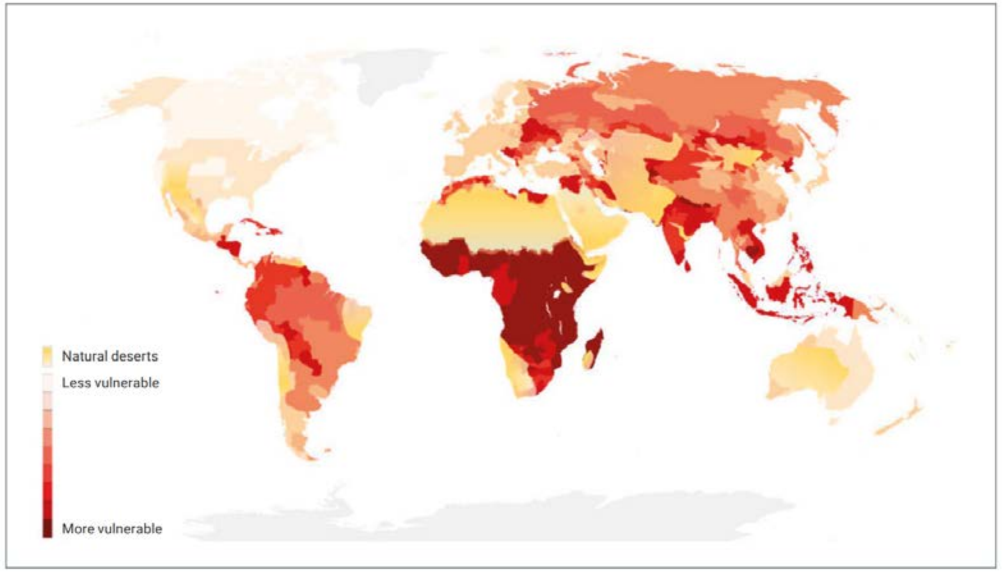
Introduction – World Water Shortage



Water withdrawals in km^3/year[1]



Percentage water withdrawals increase over time[1]

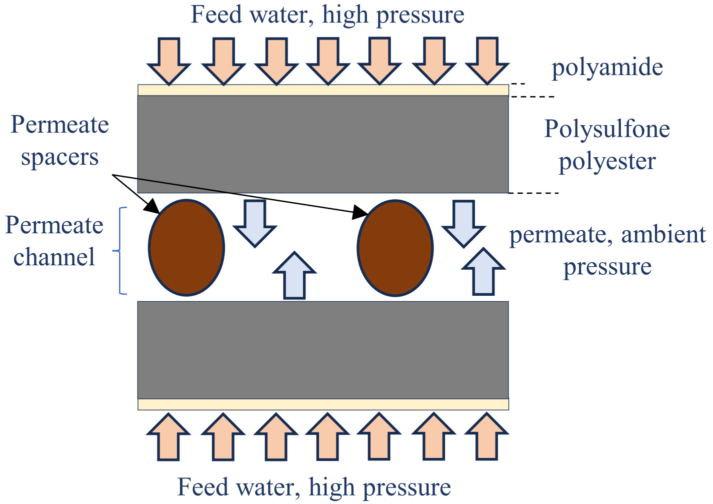


Drought vulnerability index, 2022[2]

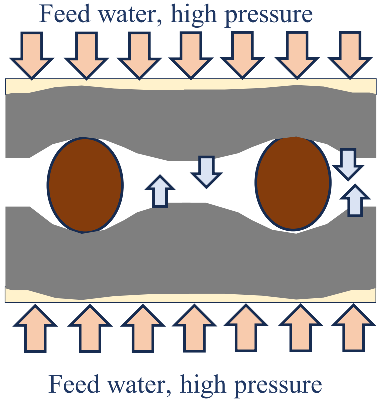
- 2.2 billion people across the world live in regions of water scarcity
- 2 million tons of industrial, sewage and agriculture waste discharged worldwide every day
- 14000 people die every day due to health reasons arising from drinking unhealthy water
- 140 million people regularly drink water with contaminants more than WHO provided guidelines

1. *https://www.wri.org/insights/domestic-water-use-grew-600-over-past-50-years*, Otto and Schleifer (2020)
2. *Carrao et. al., Climate Dynamics (2018) (50) 2137-2155*
3. *Caretta et.al., Climatic Change (2023) 176:100*

Introduction- UHPRO membrane compaction

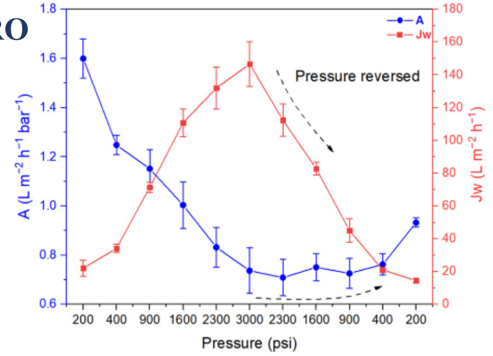


Uncompacted

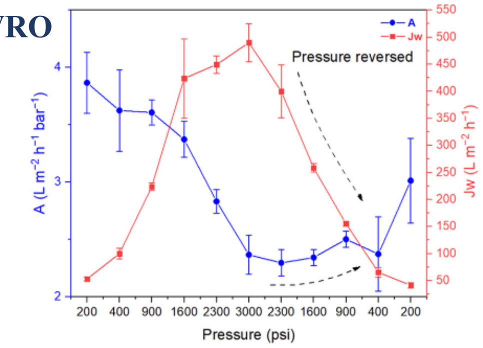


Compacted

HPRO



BWRO

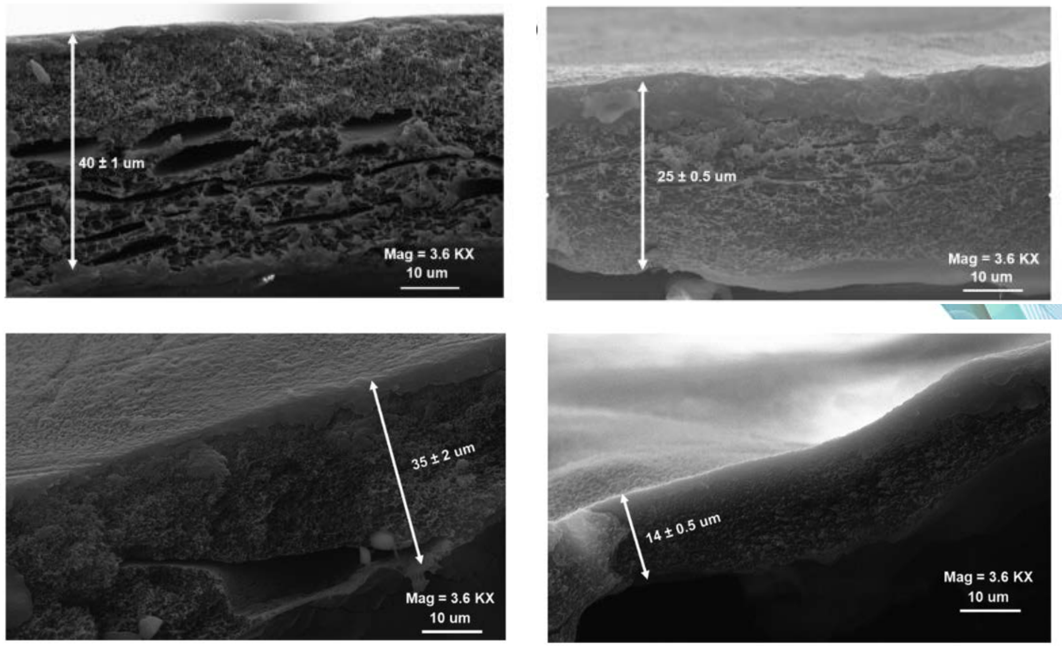


Reduction of membrane permeance and water flux at higher pressures due to compaction

Uncompacted **Compacted**

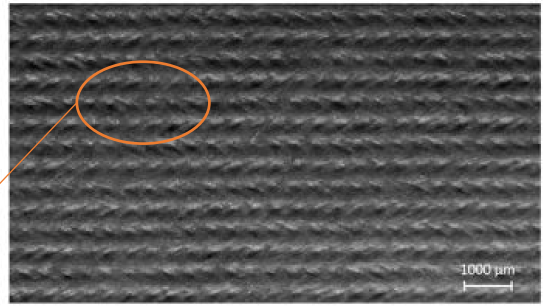
HPRO

BWRO



X-sectional SEM images of pristine and compacted membranes[1]

Clear imprinting of spacer shape on membrane surface

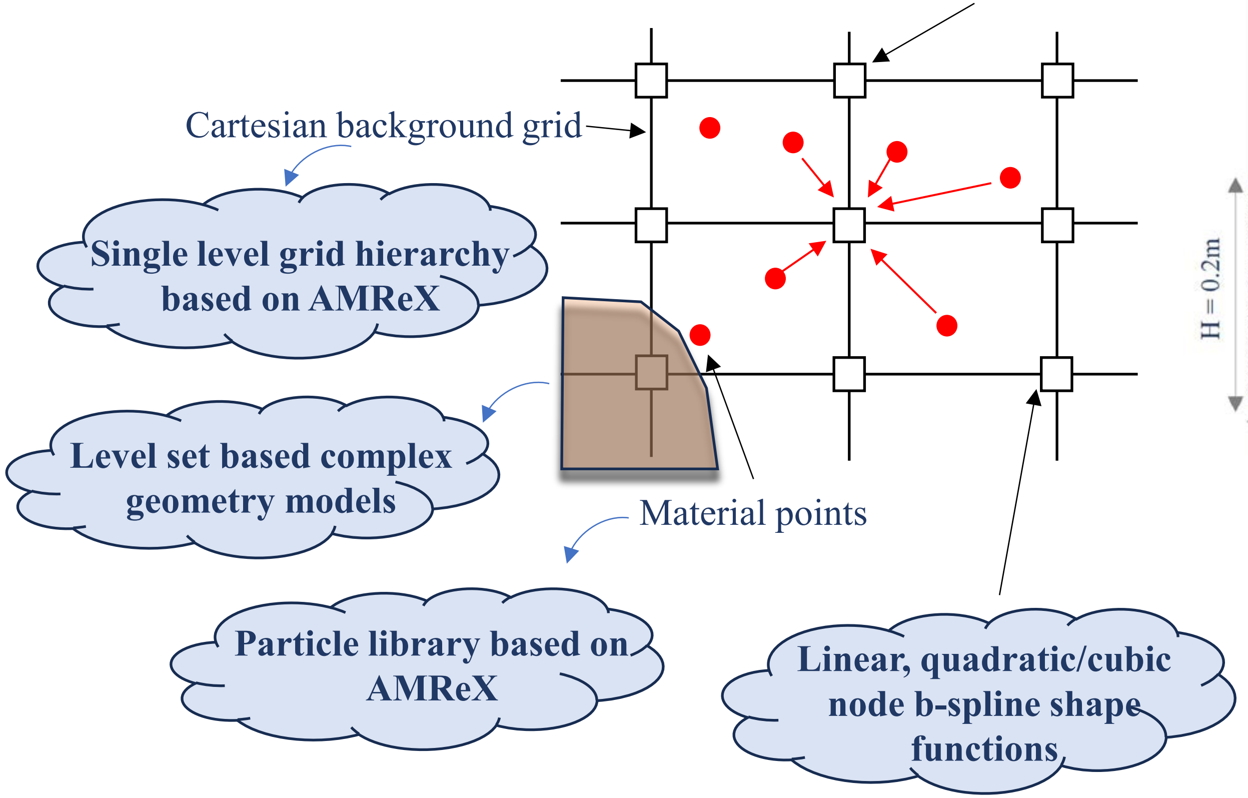


SEM images of compacted HPRO membrane fabric layer

1. Wu et.al., Reverse osmosis membrane compaction and embossing at ultra-high pressures, Desalination, 2022

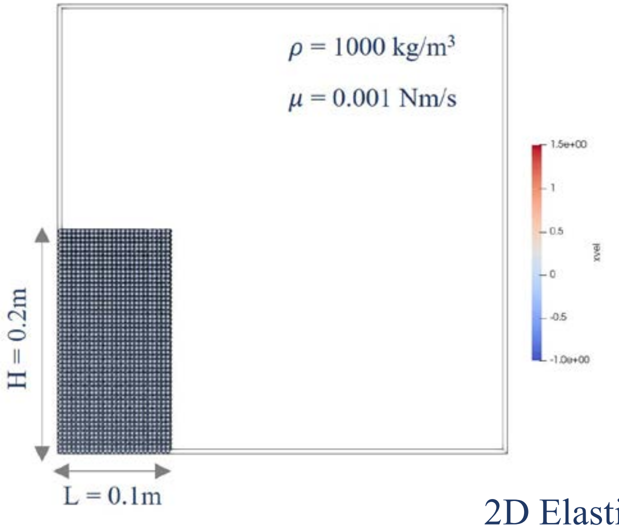
ExaGOOP MPM Solver

ExaGOOP Material Point Method Solver[1]



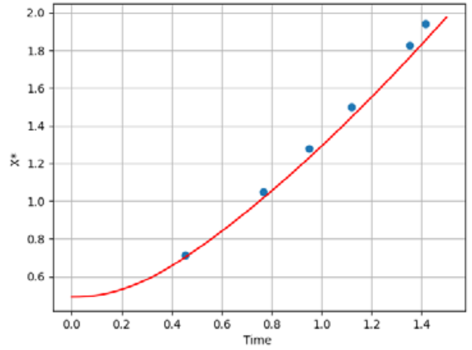
AMReX library provides parallelism for heterogenous (CPU+GPU) computing platforms

2D- dam break simulation

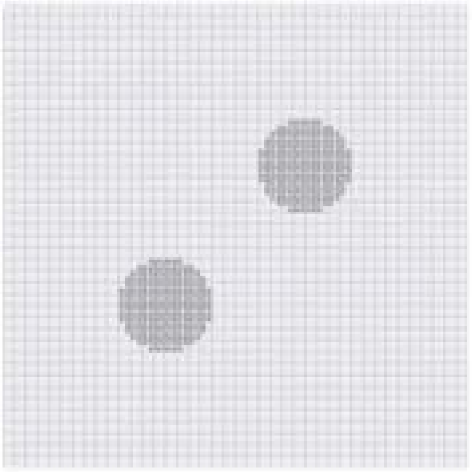


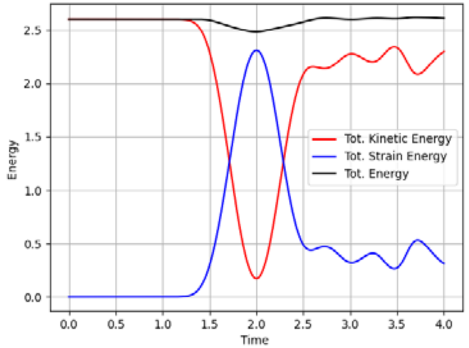
Evolution of normalized position of water-front with time.

(Curve: MPM, Dots: Experimental data[1])



2D Elastic Disk Collision





Validation and verification of ExaGOOP solver

1. https://github.com/NREL/Exagoop
2. "An experimental study of the collapse of liquid columns on a rigid horizontal plane", Martin & Moyce, 1952, *Philosophical Transactions of the Royal Society of London*

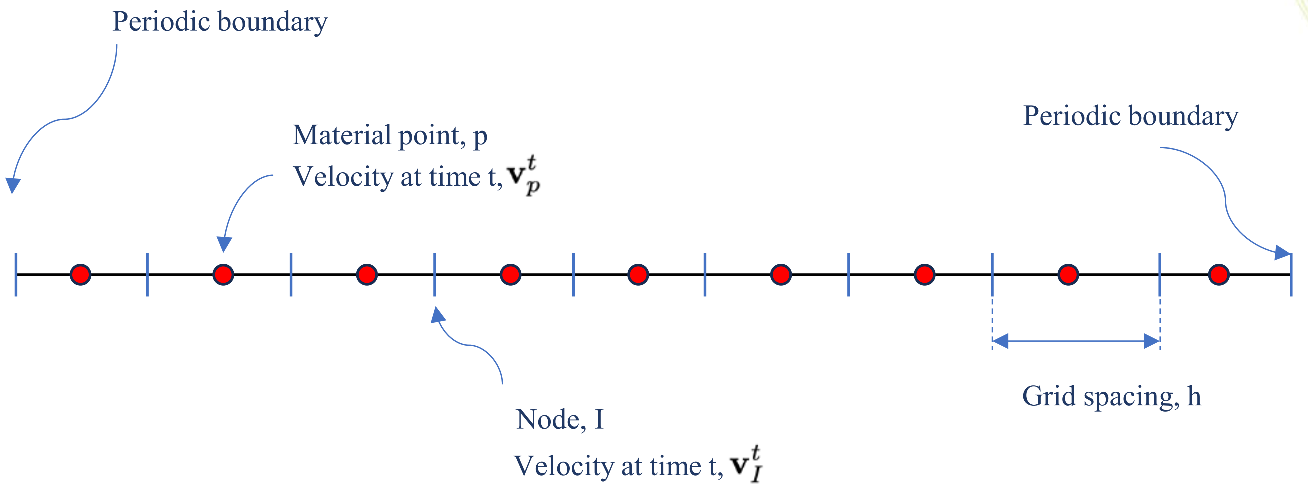
Analysis of MPM

Spectral Stability Analysis-Methodology

Governing Equation:

$$\rho \frac{D\mathbf{v}}{Dt} = \mathbf{F_i} + \mathbf{F_e} \quad (\mathbf{F_e} \rightarrow 0)$$

$$= \frac{\partial}{\partial x}\left[\nu \frac{\partial \mathbf{v}}{\partial x}\right]$$



MPM Governing Equation at nodes:

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

Total number of nodes: N_{nodes}

Total number of material points: N_{part}

● Material points

+ Grid Nodes

$m_p = mass\ of\ material\ point$

$N_I(x_p) = shapefunction\ defined\ at\ node\ I\ and\ evaluated\ at\ material\ point\ position\ x_p$

$\sigma_p^s = stress\ tensor\ defined\ at\ material\ point$

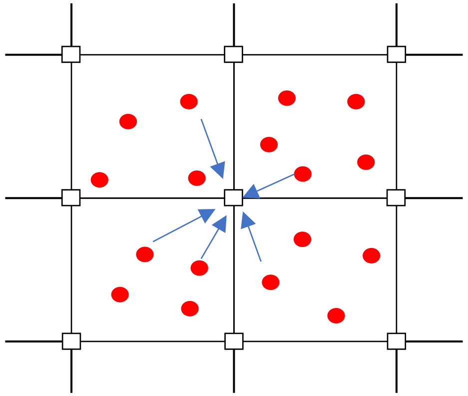
$a_J = acceleration\ at\ node\ J$

Assumptions:

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

Spectral Stability Analysis-Methodology

1. Particle to grid interpolation



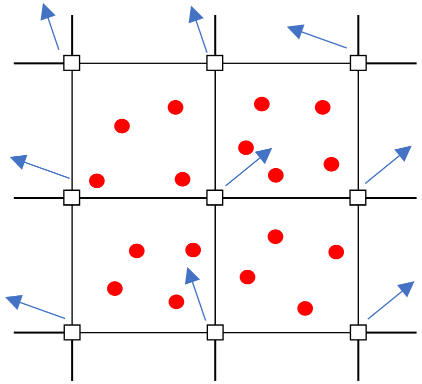
$$\mathbf{v}_I^t = \bar{\bar{\mathbf{T}}}_{p\to I}\mathbf{v}_p^t$$

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

Mass matrix (N_{nodes} X N_{nodes})

Coefficient matrix, (N_{nodes} X N_{part})

2. Nodal time integration



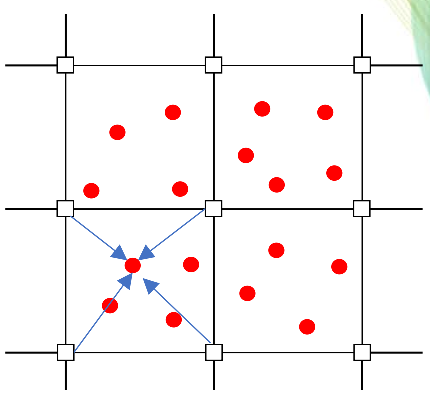
$$\bar{\mathbf{v}}_I^{t+\Delta t} = \left[\bar{\bar{\mathbf{I}}} - Fo\,\bar{\bar{\mathbf{G}}}_{P\to I}\bar{\bar{\mathbf{G}}}_{I\to P}\right]\bar{\mathbf{v}}_I^t$$

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

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

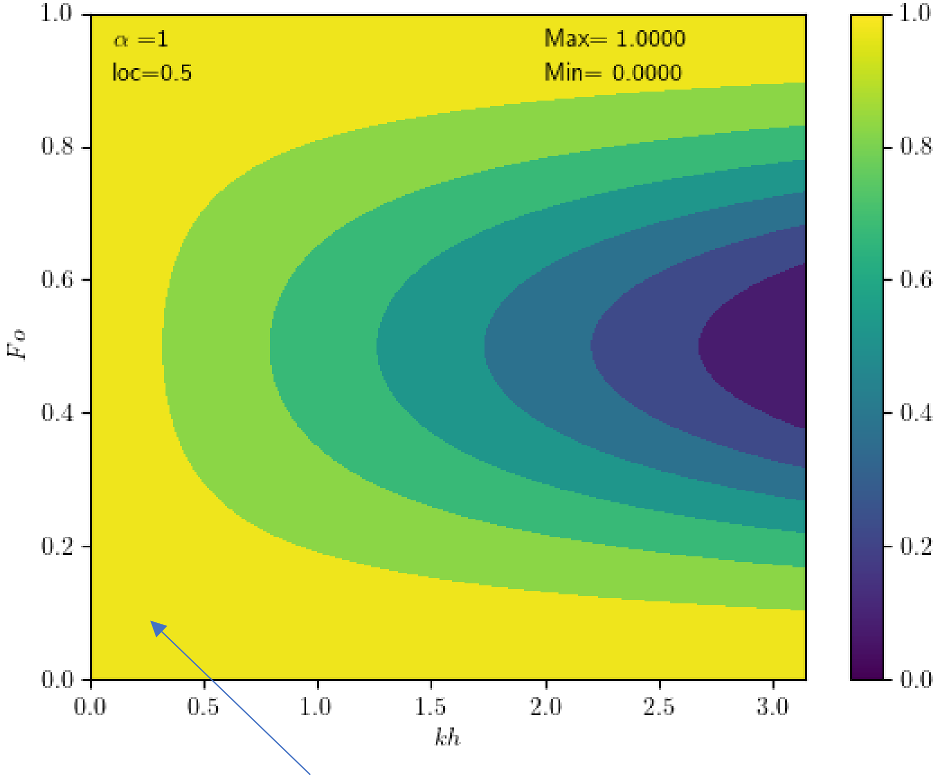
Spectral Stability Analysis- Results (|G|)

Effect of α (PIC and FLIP update)

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

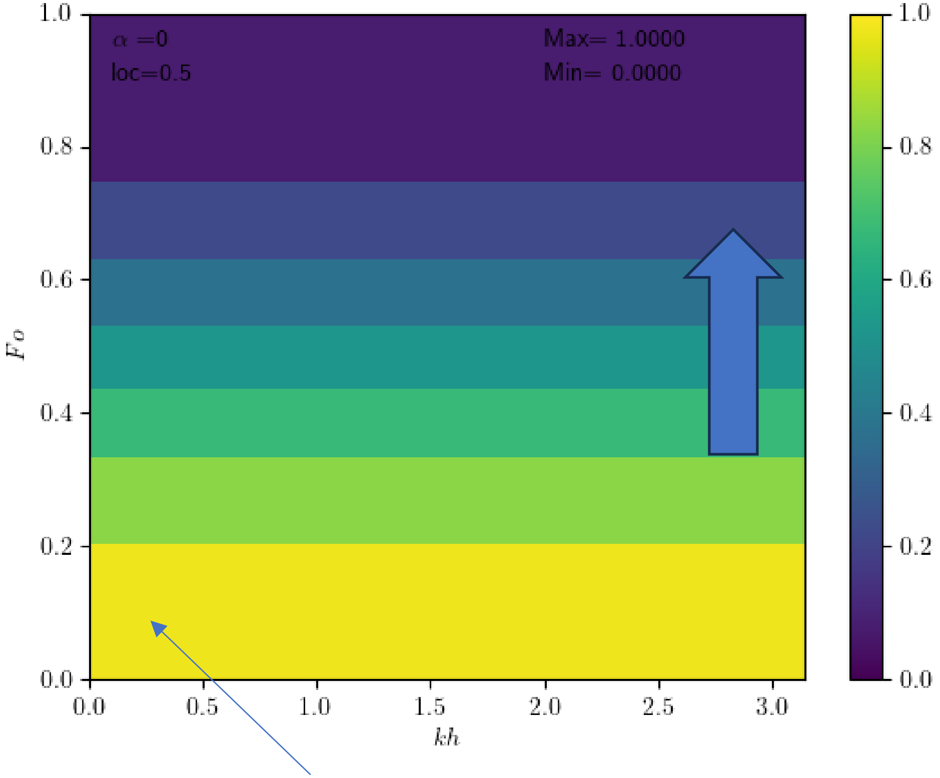
$$\mathbf{v}_p^{t+\Delta t} = \alpha \left(\mathbf{v}_p^t + \sum_I N_I \left(\mathbf{x}_p^t\right) \left[\mathbf{v}_I^{t+\Delta t} - \mathbf{v}_I^t\right] \right) + (1-\alpha) \sum_I N_I \left(\mathbf{x}_p^t\right) \mathbf{v}_I^{t+\Delta t}$$

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|)

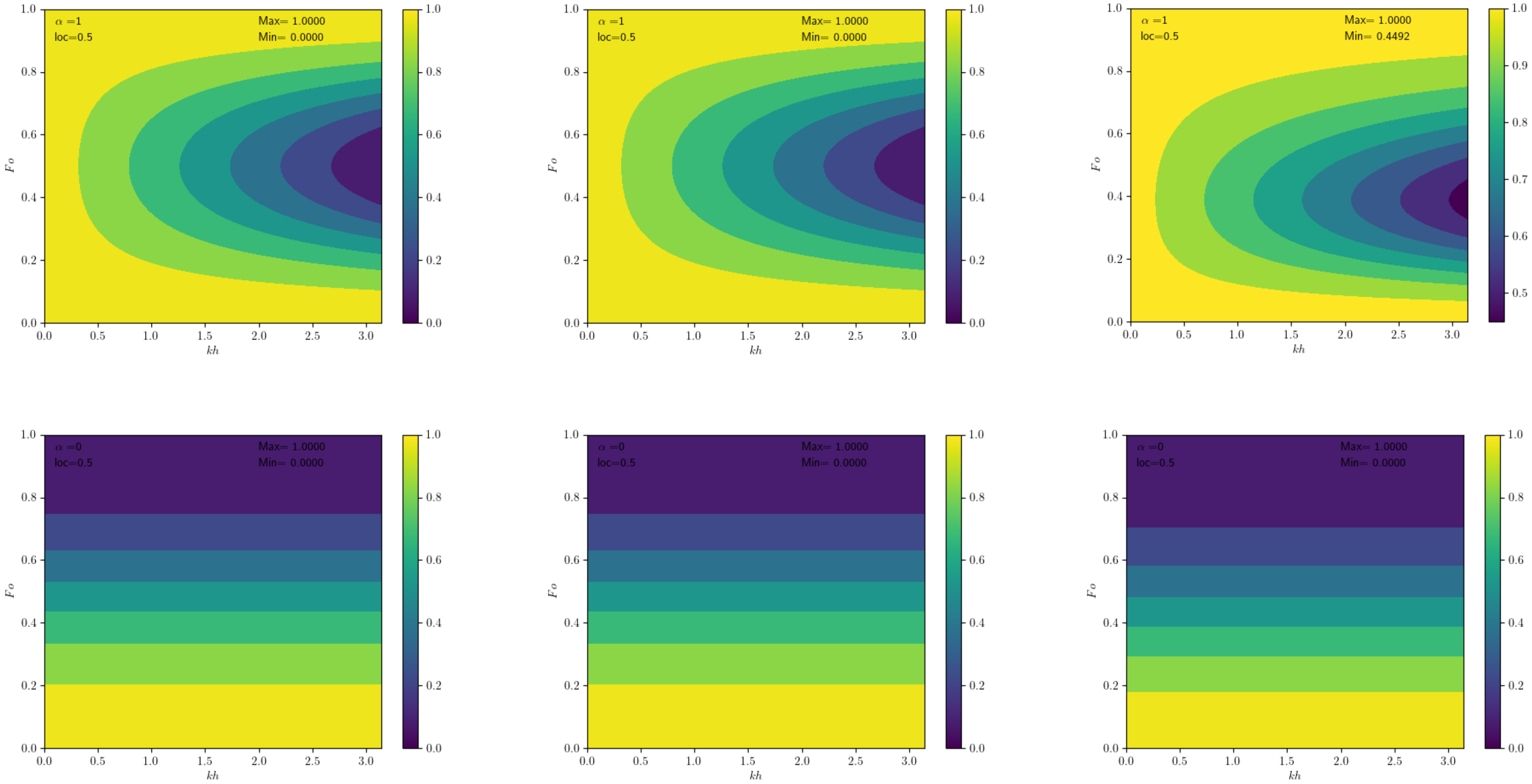
Effect of shape functions

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 $\alpha = 0.0$

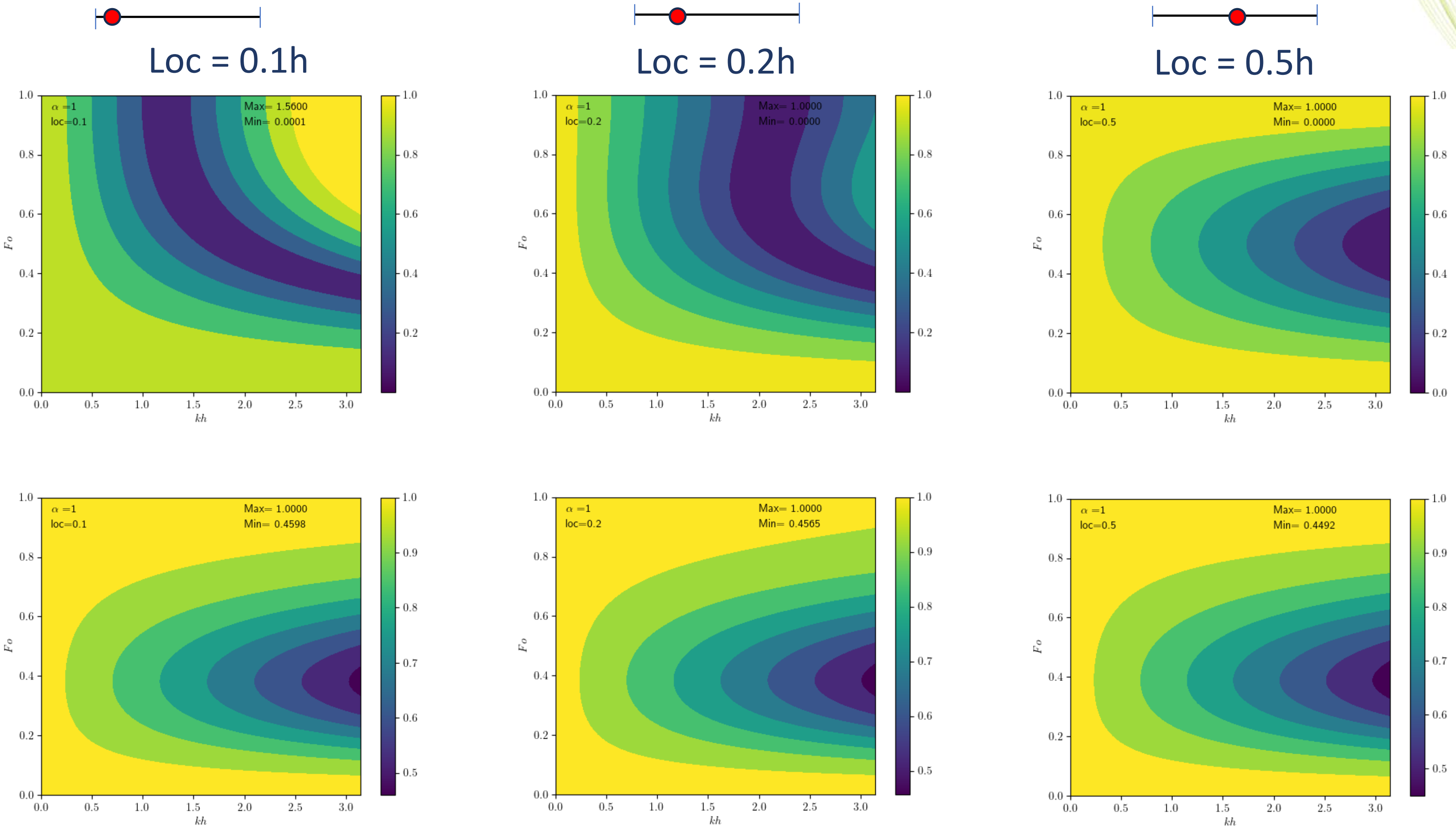
Spectral Stability Analysis- Results (|G|)

Effect of material point location

$\alpha = 1.0$

Linear Hat (LH)

Cubic B-Spline (CBS)

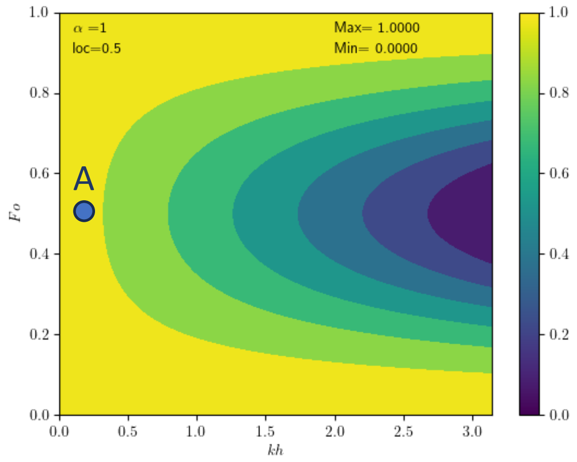


Cubic spline properties least sensitive to material point location
Linear hat susceptible to grid crossing instability

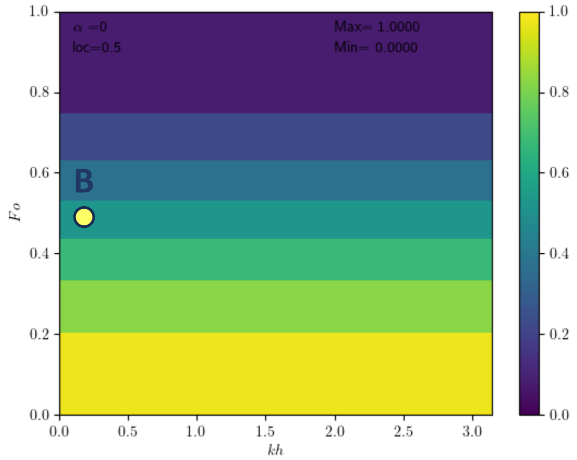
Spectral Stability Analysis- Validation

Test Case Description: Effect of α

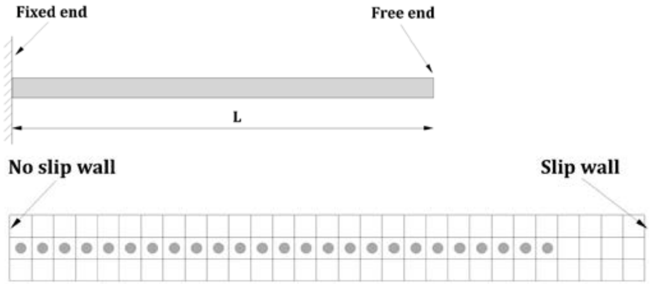
$\alpha = 1.0$
Shape Function: LH
kh = 0.13
Fo = 0.5



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



Validation test case



Initial solution

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

Exact solution

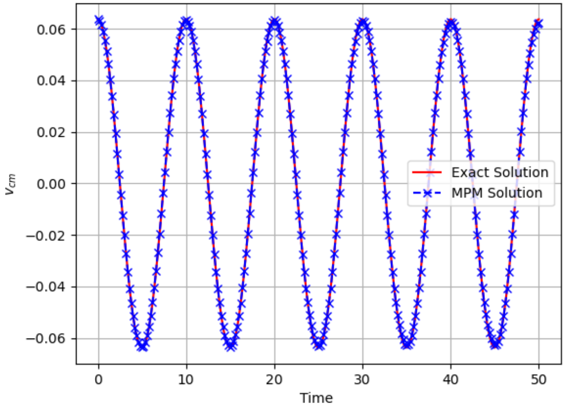
$$u(x,t) = V_0/\omega_1 \sin\left(\frac{\pi x}{2L}\right) \sin(\omega_1 t)$$

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

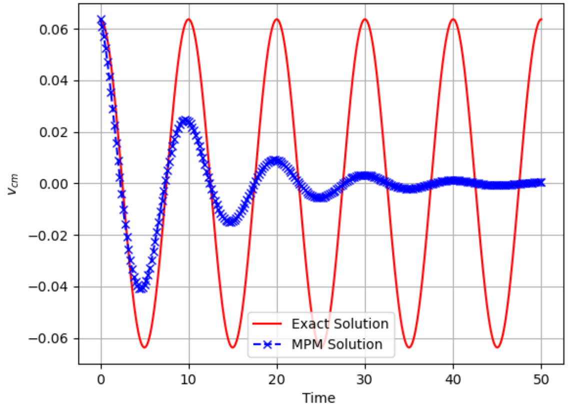
|G| computed from analysis

	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



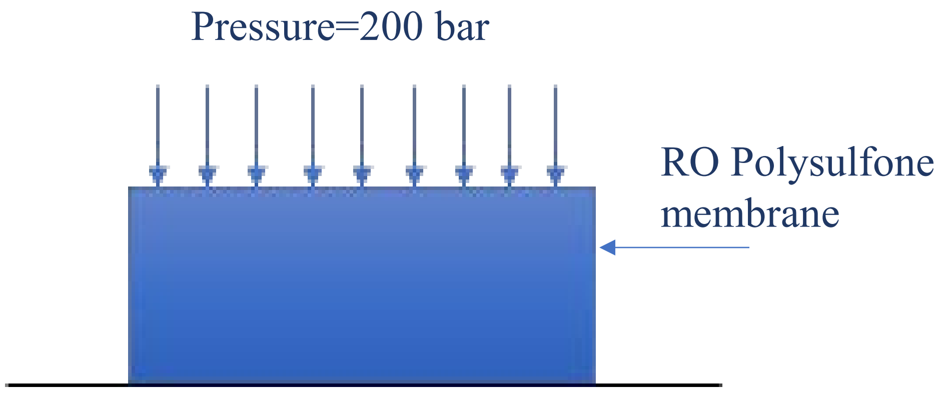
Test B



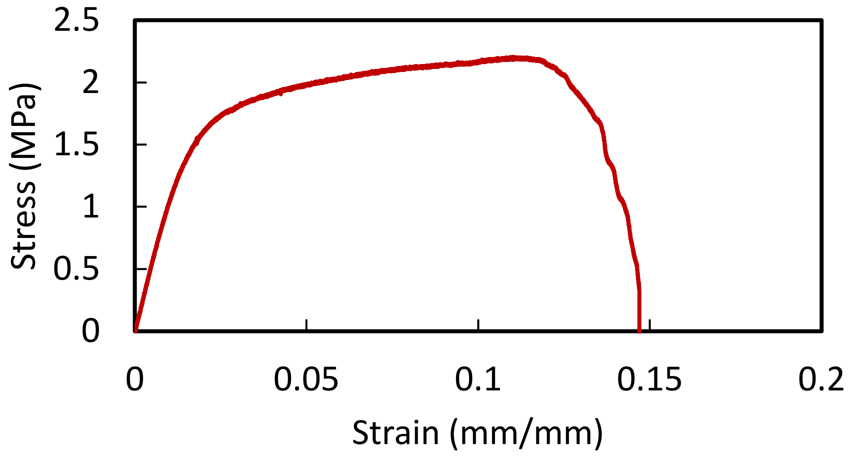
$\alpha = 0.0$ induces solution damping

Application to UHPRO Membrane Compaction

Simulation of HPRO membrane compaction



PS membrane modeled as linear elastic body



Young's modulus, E = 100MPa obtained from tensile test

MPM Model:

SEM image of uncompacted membrane cross-section

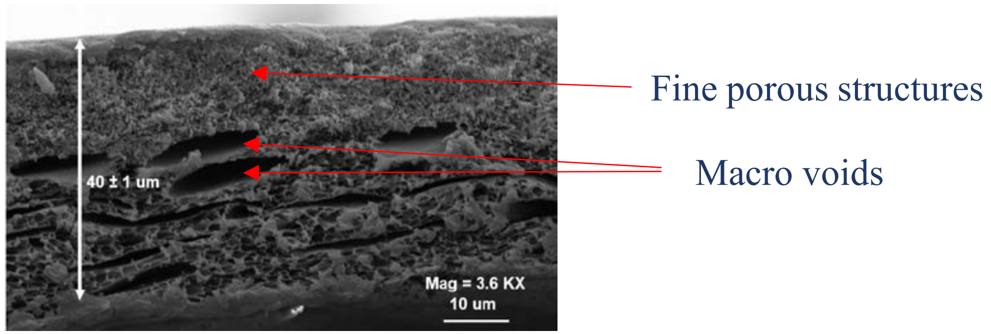
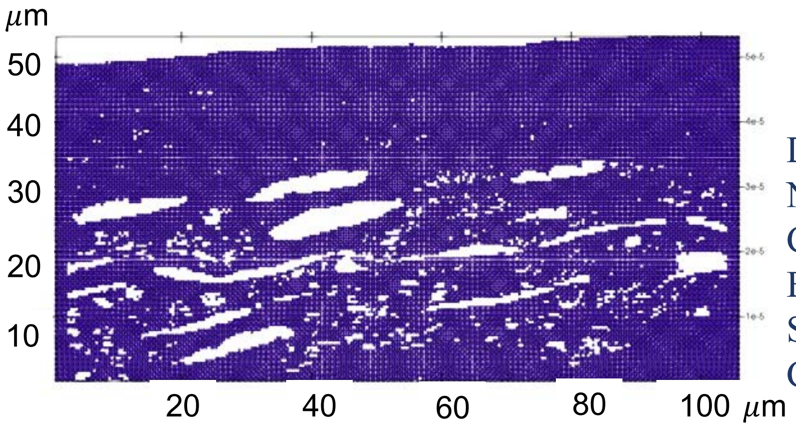


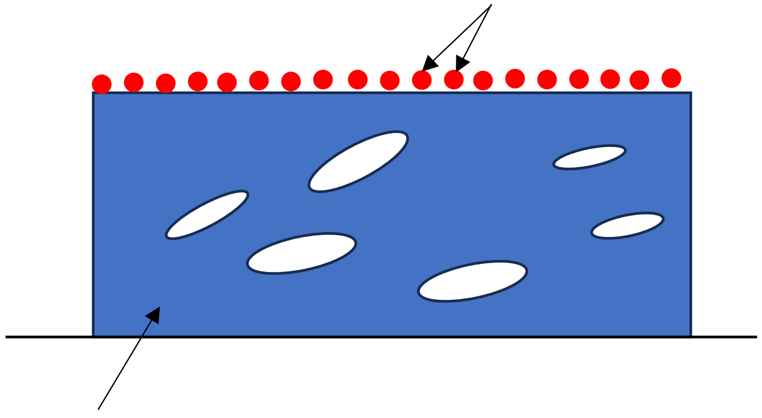
Image converted to material point collection using python script



Domain size: 100um x 60um
Number of material points: 180K
Constitutive Model: Linear Elastic
Shape Function: Linear Hat
CFL = 0.1

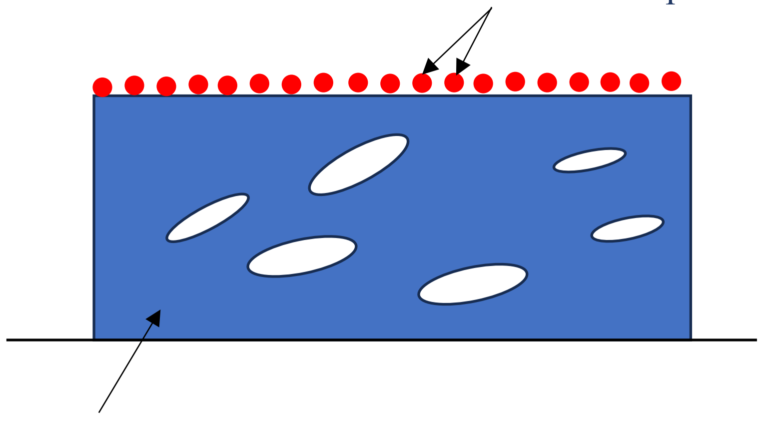
Load Application Strategy

Strategy-1



- Weight of fictitious material points enforces the desired pressure
- Scaling Youngs' modulus and density→ dt remains unaltered
- Numerical damping induced by reducing $\boldsymbol{\alpha}$

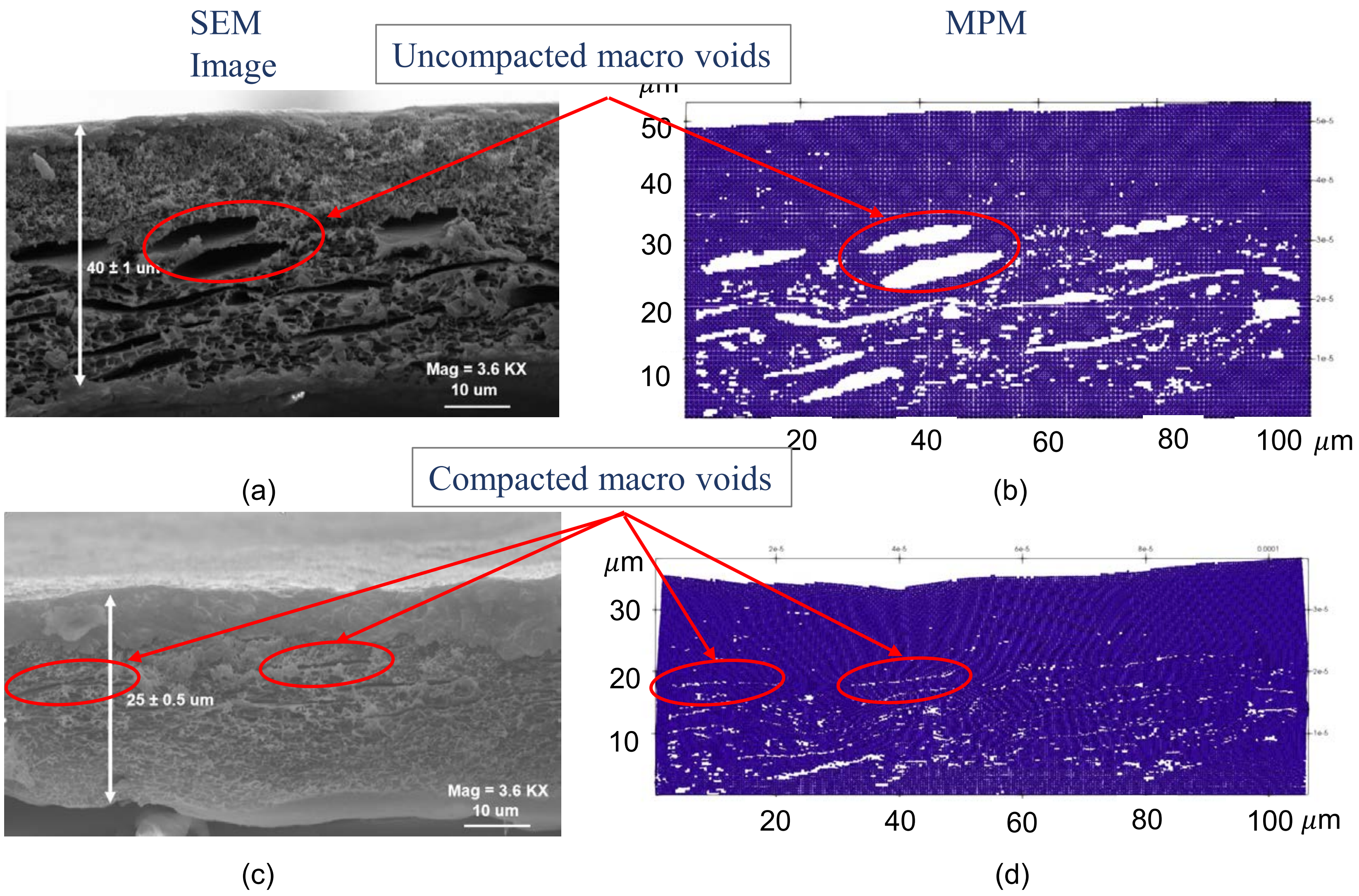
Strategy-2



- Reactive force from membrane calculated by interpolating stress on rigid material points
- External damping can be varied to reduce oscillations and reach steady state

Fictitious body forces added to match applied pressures due to numerical instabilities

Application to simulation of RO membrane compaction

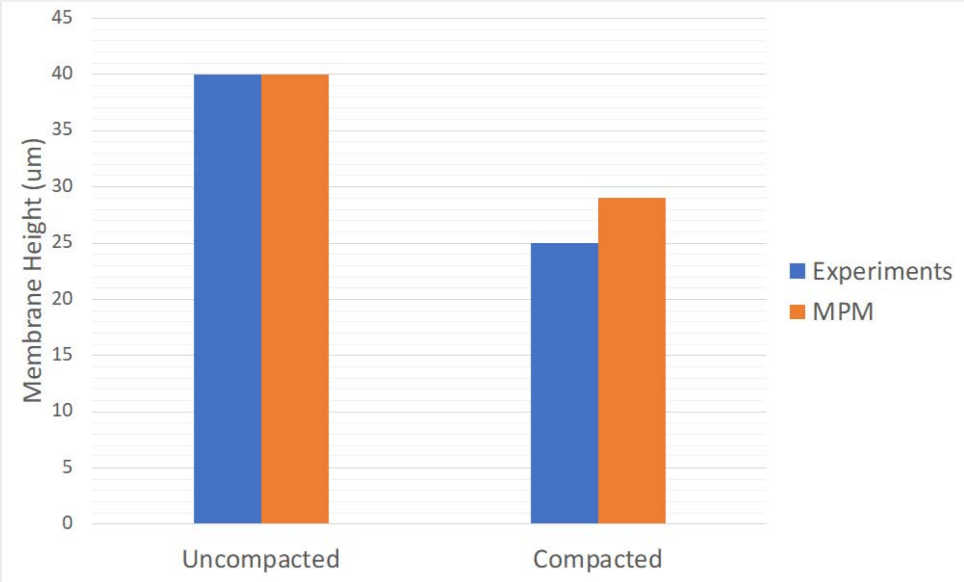


Uncompacted membrane

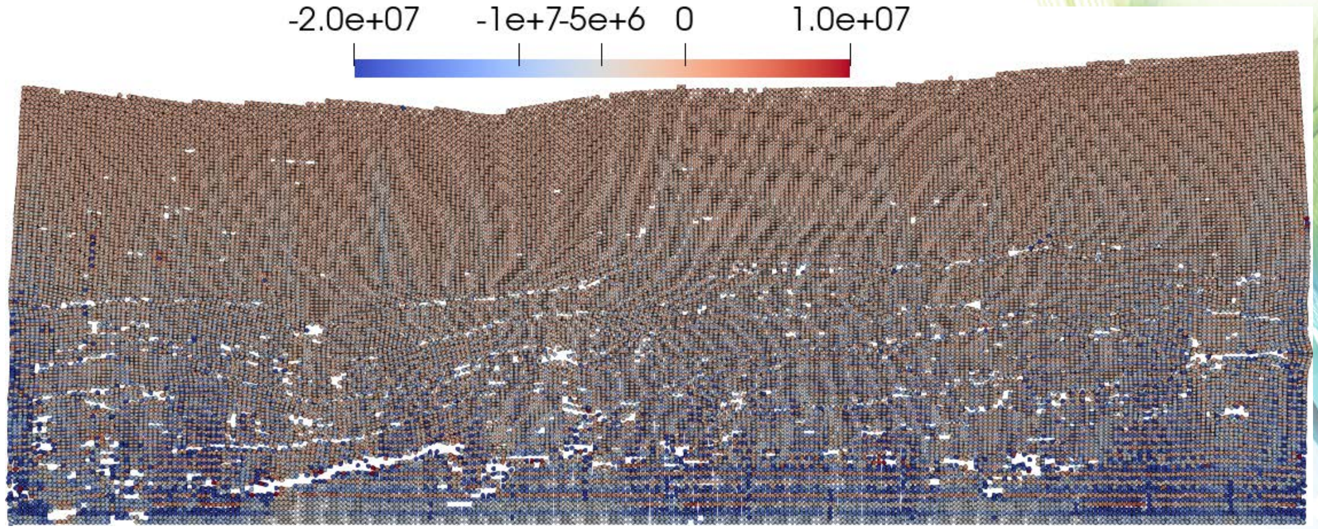
Compacted membrane

Good qualitative match between MPM results and SEM images

Application to simulation of RO membrane compaction



Comparison of membrane heights observed in experiments and MPM



Normal stress contours at material points

Simulated membrane deflection under compaction matches well with experimental data

Conclusions & Perspectives

- MPM solver ExaGOOP developed based on AMReX library. Works on heterogenous platforms. Validated against experimental and analytical solutions

- Spectral analysis of regular MPM method reveals numerical properties of regular MPM methods using linear hat, B- spline shape functions with explicit time integration schemes

- MPM applied to study HPRO membrane compaction. Numerical instabilities observed with load application strategies- a simplified approach adopted for now. 3-D, full-membrane simulations in progress.

THANK YOU

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NREL Transforming ENERGY

NAWI National Alliance for Water Innovation