Simulation of Reverse Osmosis Membrane Compaction using Material Point Method

SIAM Conference on Computational Science and Engineering (CSE2023), Amsterdam

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Date: March. 3rd , 2023

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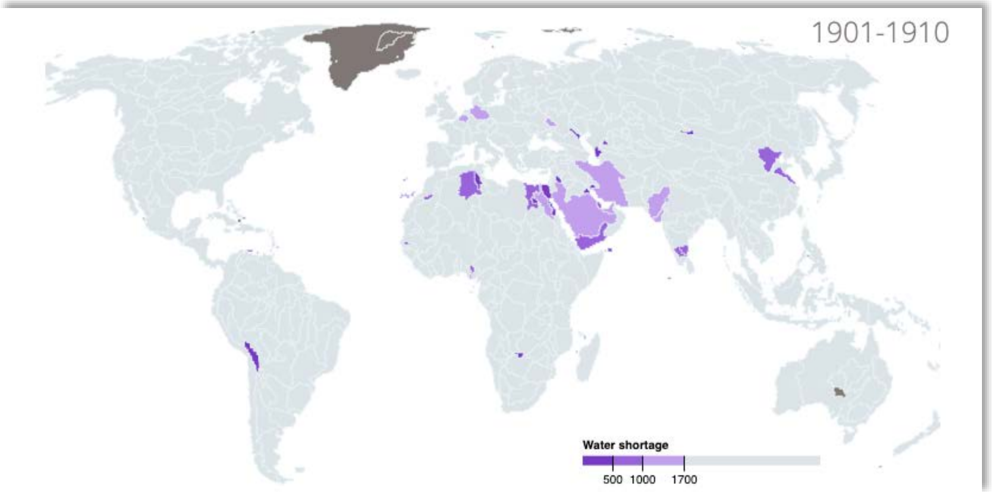
- Exagoop MPM Solver
- Application to RO membrane compaction problem

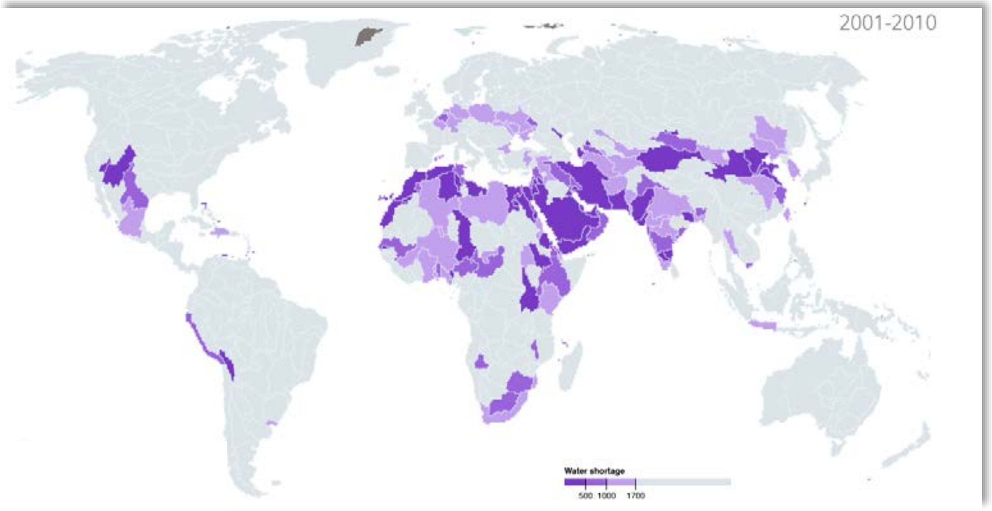
Background

Introduction



Global regions with water shortage in 1901-1910[1]

Regions with water contaminated by heavy metals[2]



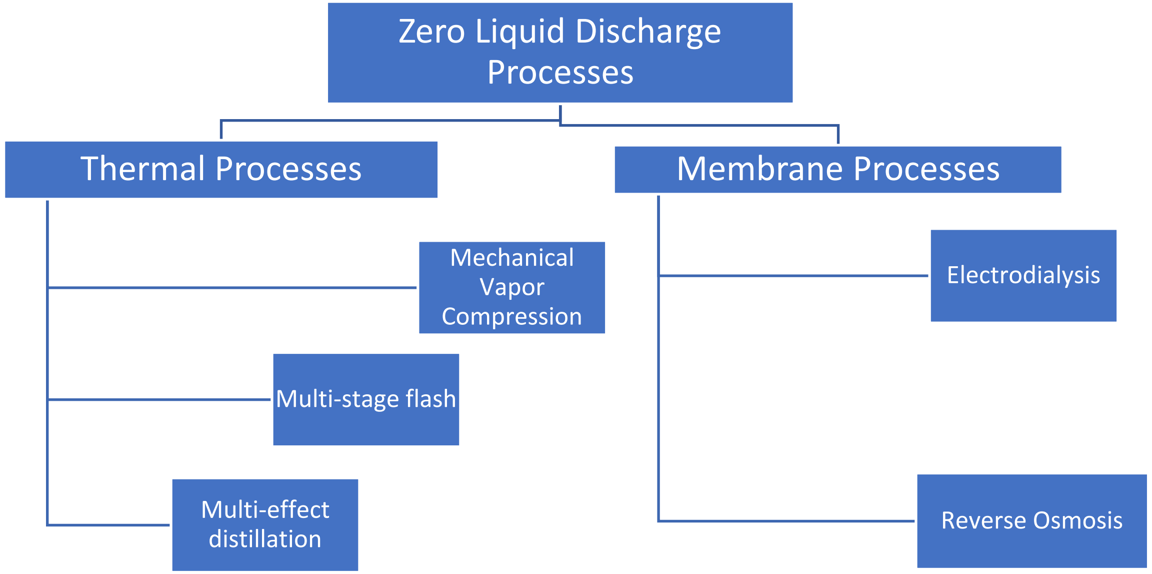
Global regions with water shortage in 2001-2010[1]

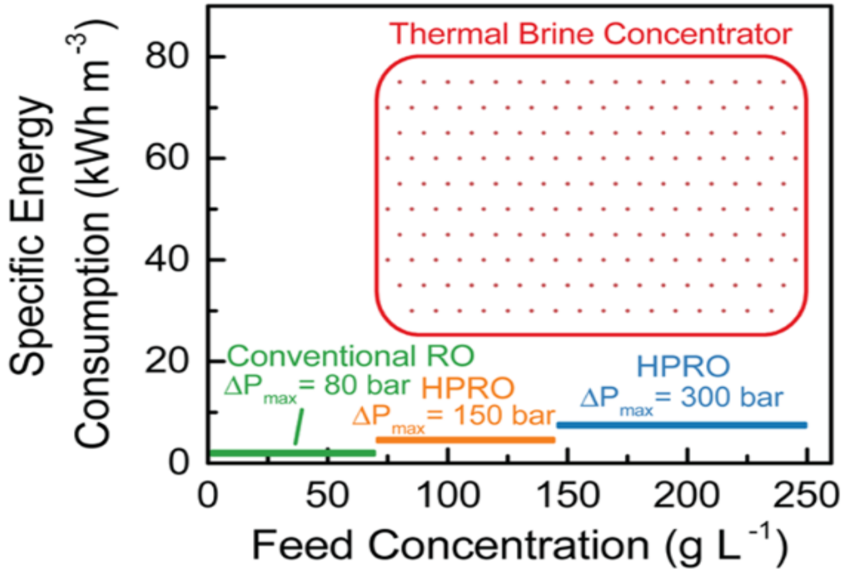
- 1.2 billion people across the world live in regions of water scarcity
- 2 million tons of industrial, sewage and agriculture waste discharged worldwide every day
- 14000 people die every day due to health reasons arising from drinking unhealthy water
- 140 million people regularly drink water with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

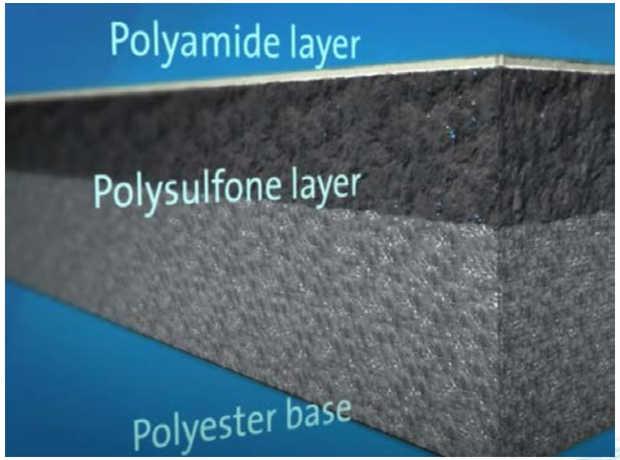
1. https://waterscarcityatlas.org/water-shortage/, Data: Kummu et.al., Nature SR, 2016
2. http://www.globalpollutionmap.org/sites.html, Data: Pure Earth TSIP

Introduction

Prominent ZLD Processes



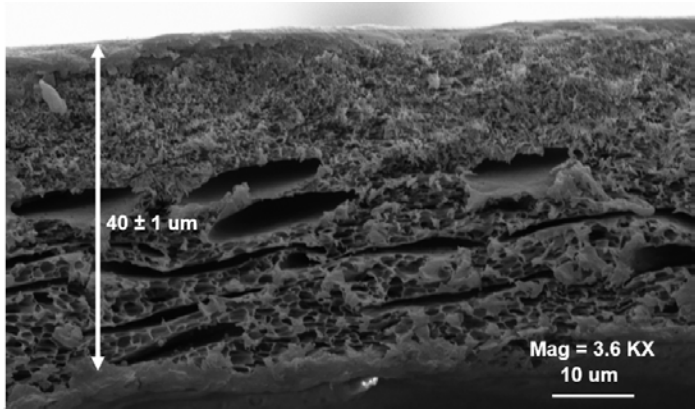




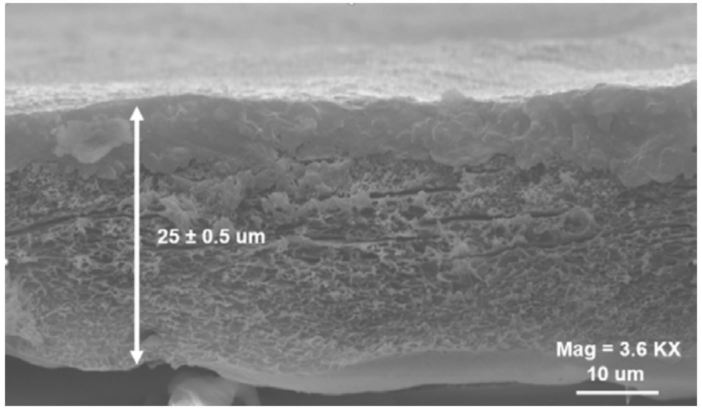
Typical HPRO Membrane structure*

Introduction

HPRO Membrane Compaction



Pristine Membrane (SEM image)



Compacted Membrane (SEM)

- Compaction arises from hydraulic pressure from feed water acting on membrane surface
- Alters the porous structure of the membrane
- Compacted membranes reduces permeate, increases pressure required for same flux and hence increases operating cost

Numerical Method?

MPM!

Material Point Method (MPM)

Governing equations

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

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

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

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

$\rho \rightarrow density$

$\boldsymbol{v} \rightarrow velocity$

$\boldsymbol{\sigma} \rightarrow stress$

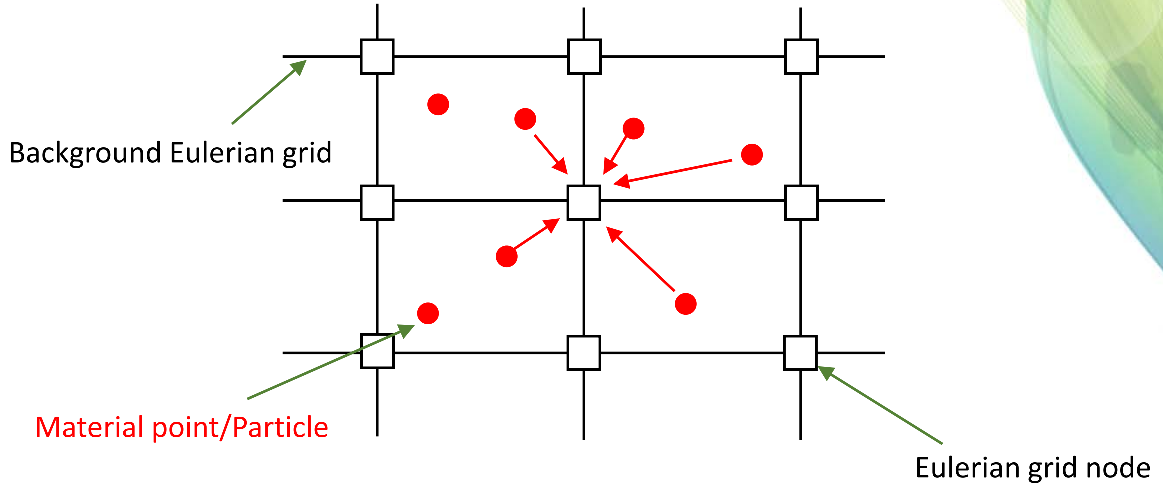
$\boldsymbol{b} \rightarrow body\ force$

E $\rightarrow youngs\ modulus$

$\nu \rightarrow poisson's\ ratio$

- For isothermal problems, energy equation is not solved
- Mass conservation equation implicitly satisfied

Basic components of MPM



- MPM is a variant of PIC method
    - Material represented as a collection of "particles"/"material points"
    - All material properties defined at "particles"
    - Density field $\rho = \sum m_i \delta(x - x_i)$
- 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

Exagoop MPM Solver

Material Point Method (MPM)

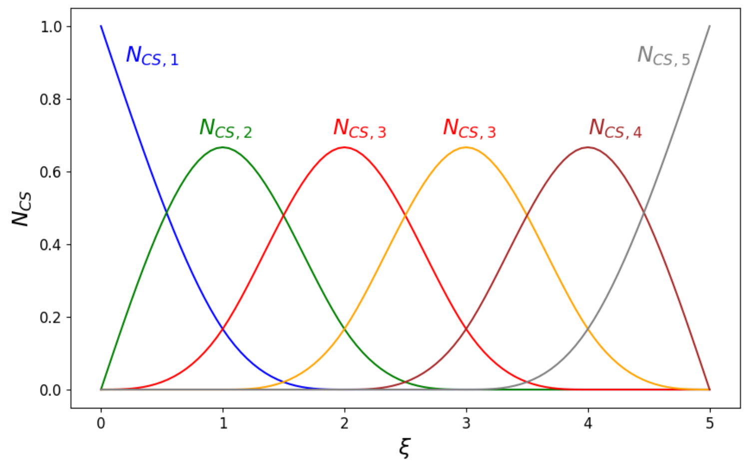
- MPM Solver Developed at NREL: *Exagoop*[1]
- Exagoop is developed based on AMReX[2] Framework
- Block-structured grid framework--> Used as background grid
- Embedded boundary method used to model complex geometry
- Particle class in AMReX used to model material point related operations
- Parallel capability→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

Shape Functions Used in Exagoop

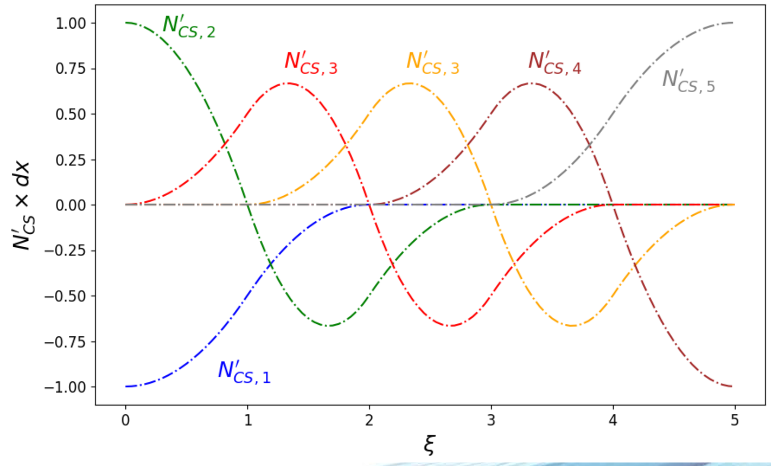
$$\xi = \frac{(x_p - x)}{dx}$$

Cubic B-Spline

Shape Function



Shape Function Derivative

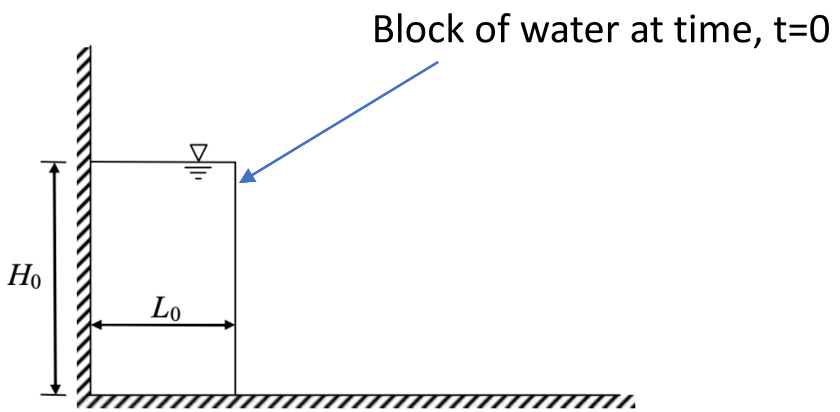


1. https://github.com/NREL/Exagoop
2. https://github.com/AMReX-Codes/amrex

Exagoop Solver: Validation

Test Case 1: Dam break

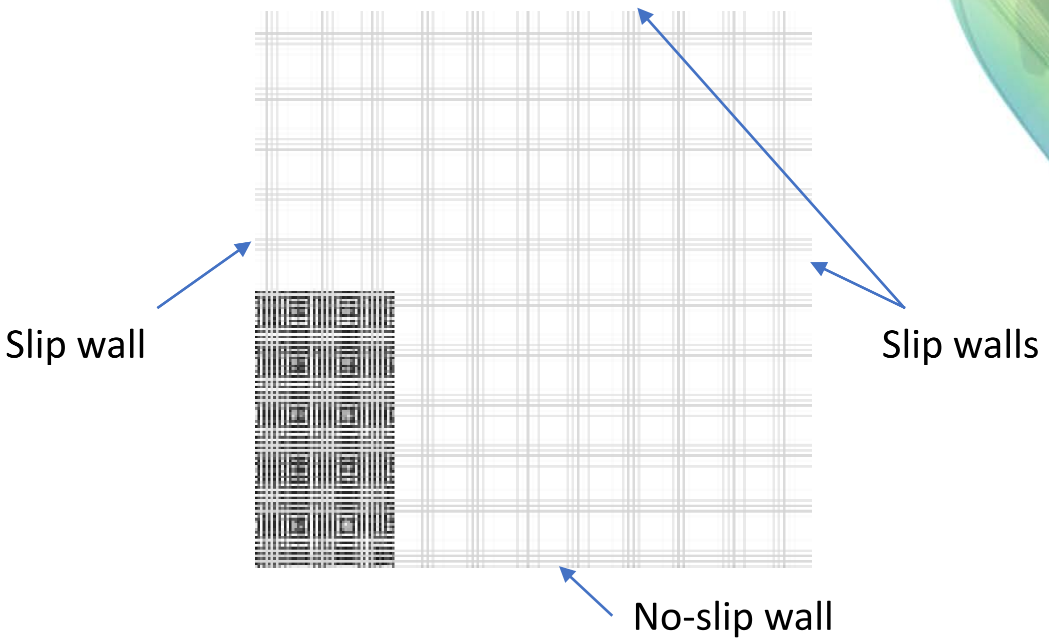
Experimental Configuration:



$L_0 = 0.1\ m$ $\rho = 997\ kg/m^3$

$H_0 = 0.2\ m$ $\mu = 0.001\ Nm/s$

MPM Model:

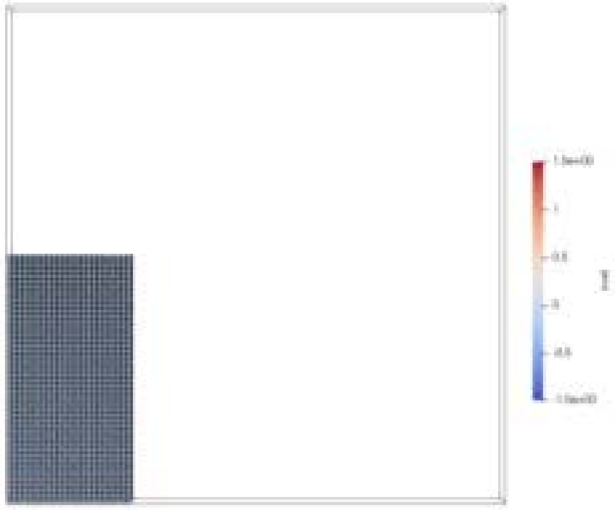


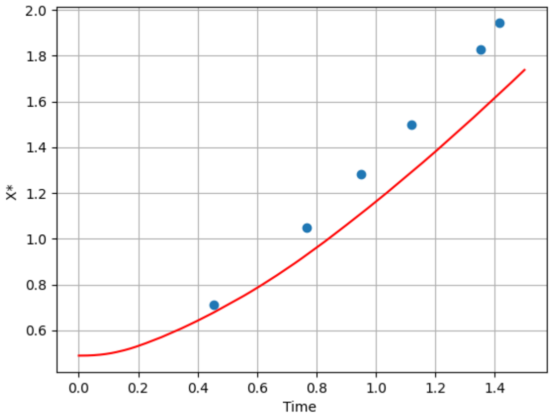
Domain Size: 0.5 x 0.4
Background grid size: 75x80
Shape Functions: Linear hat, Quadratic B-Spline, Cubic B-Spline
Constitutive Model: Barotropic fluid
Number of material points: 6250
CFL number =0.1
Number of particles per cell = 1

Exagoop Solver: Validation

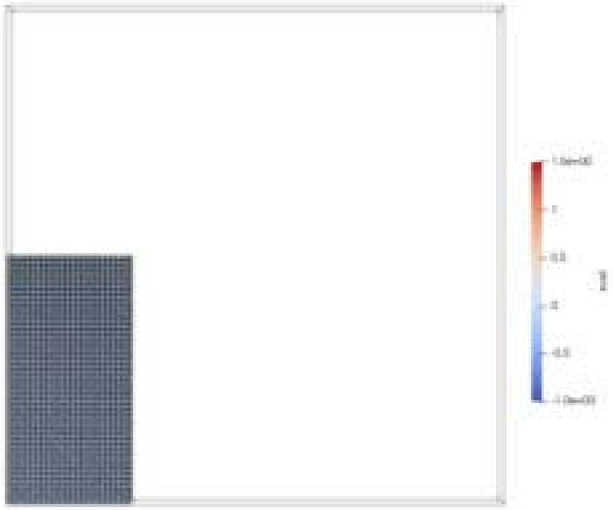
Test Case 1: Dam break

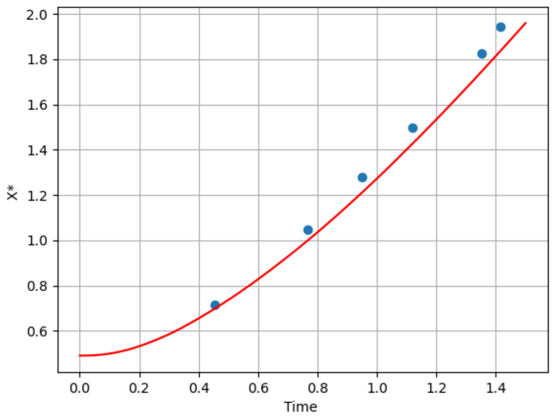
Linear Hat



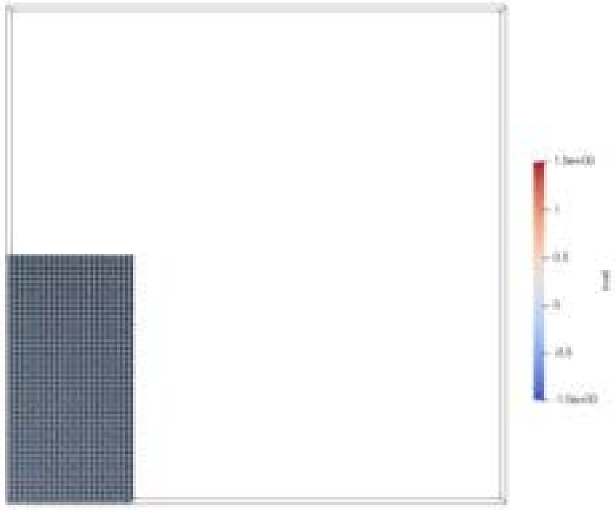


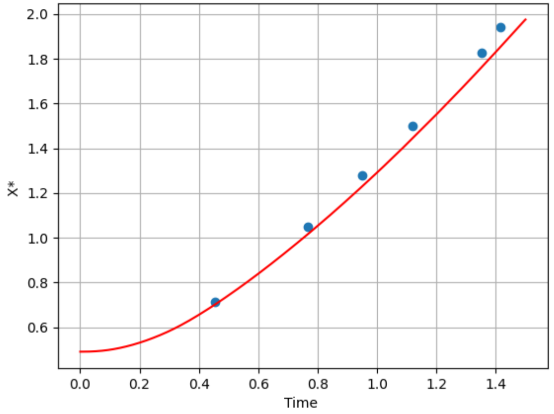
Quadratic B-Spline





Cubic B-Spline





Evolution of normalized position of water-front with time.

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

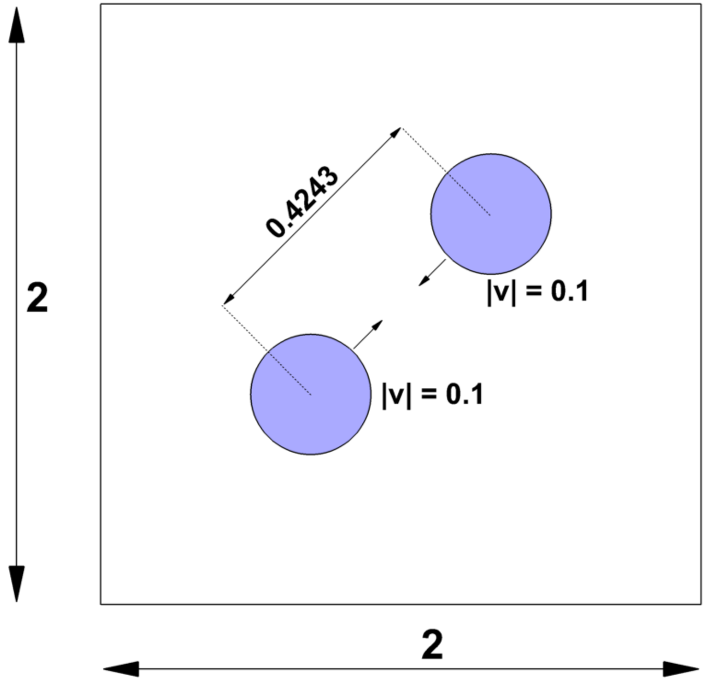
Excellent match with data with higher-order shape functions

1. "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*

Exagoop Solver: Validation

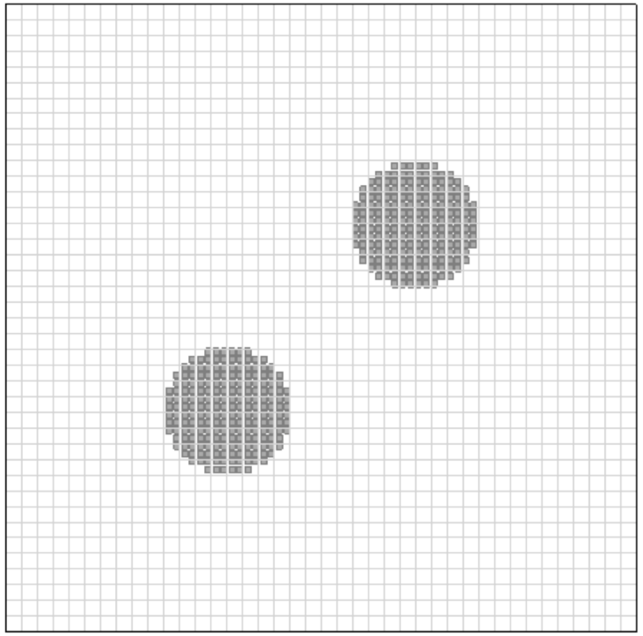
Test Case 2: Elastic Collision of Disks

Problem Definition:



Young's modulus = 1000
Poisson's ratio = 0.3

MPM Model:

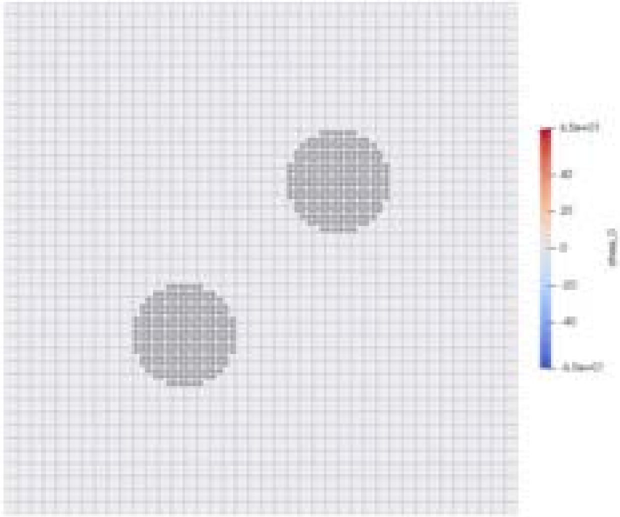


Domain size: 2m x 2m
Background grid: 40 x 40
Constitutive Model: Linear Elastic
Number of material points: 416
Shape Functions: Linear hat, Quadratic B-Spline, Cubic B-Spline
CFL number =0.1
Number of particles per cell = 4

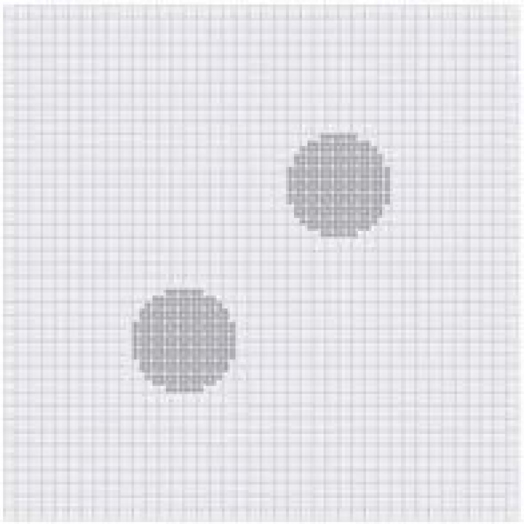
Exagoop Solver: Validation

Test Case 2: Elastic Collision of Disks

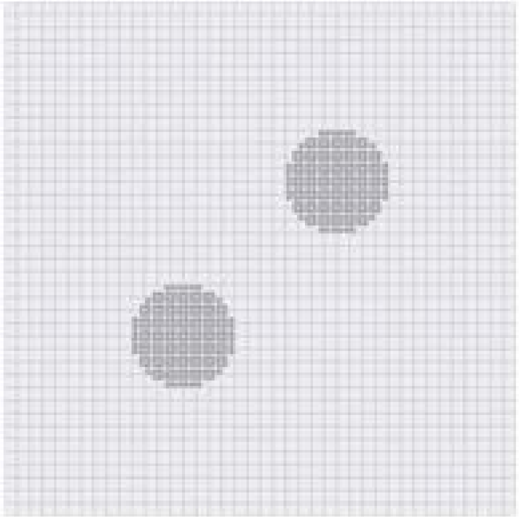
Linear Hat



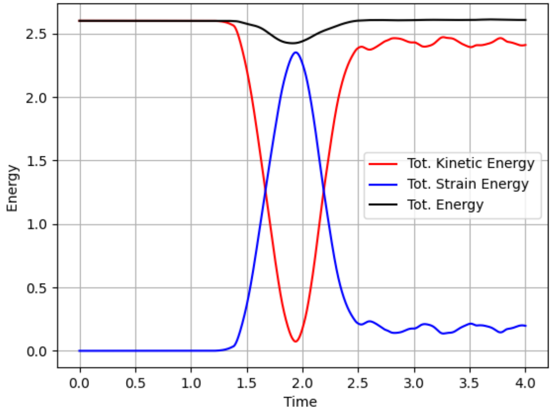
Quadratic B-Spline

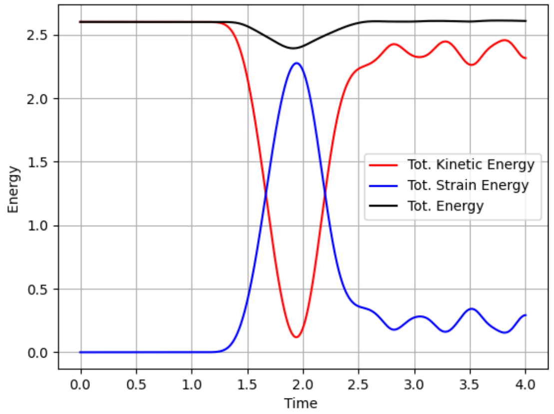


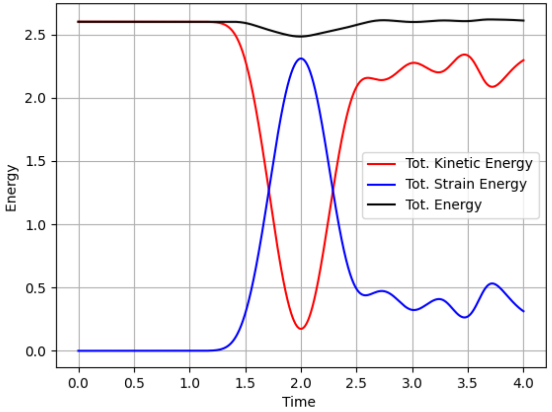
Cubic B-Spline



Disks collision colored by contours of stress, σ_{xx}





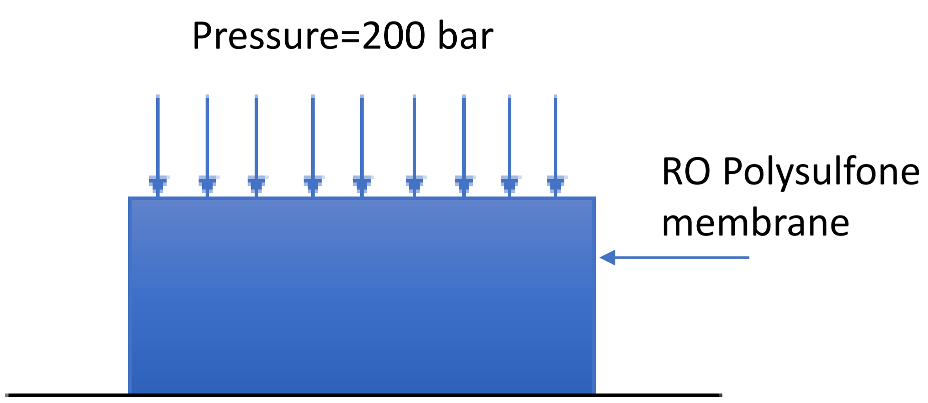


Evolution of energy with time

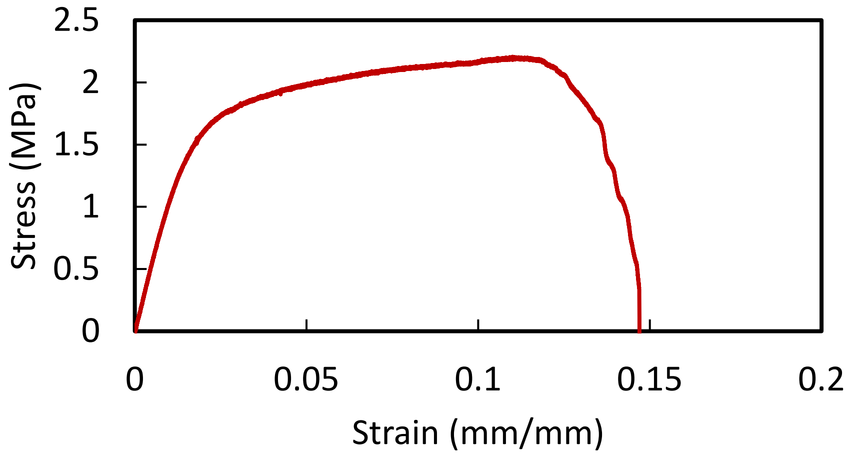
Full recovery of total energy observed for all shape functions

Application to RO membranes

Application to simulation of RO 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

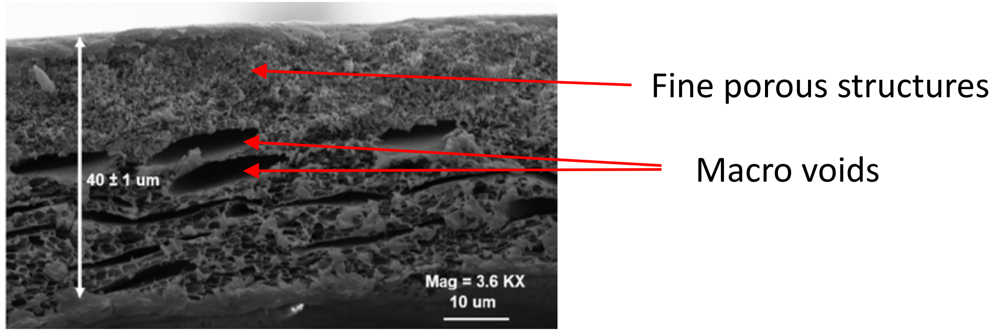
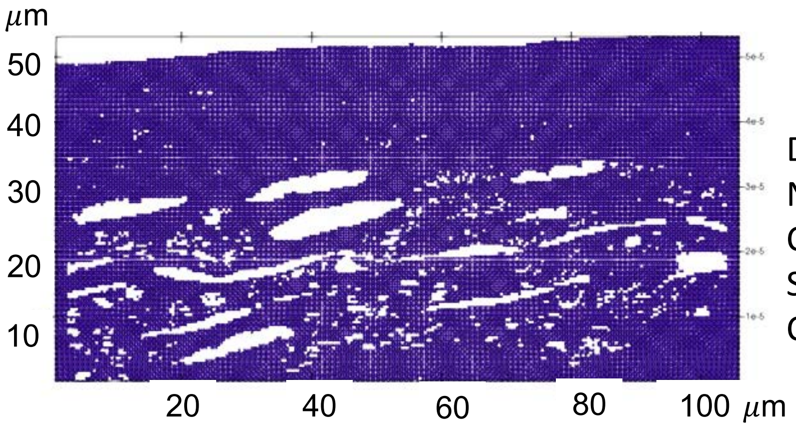
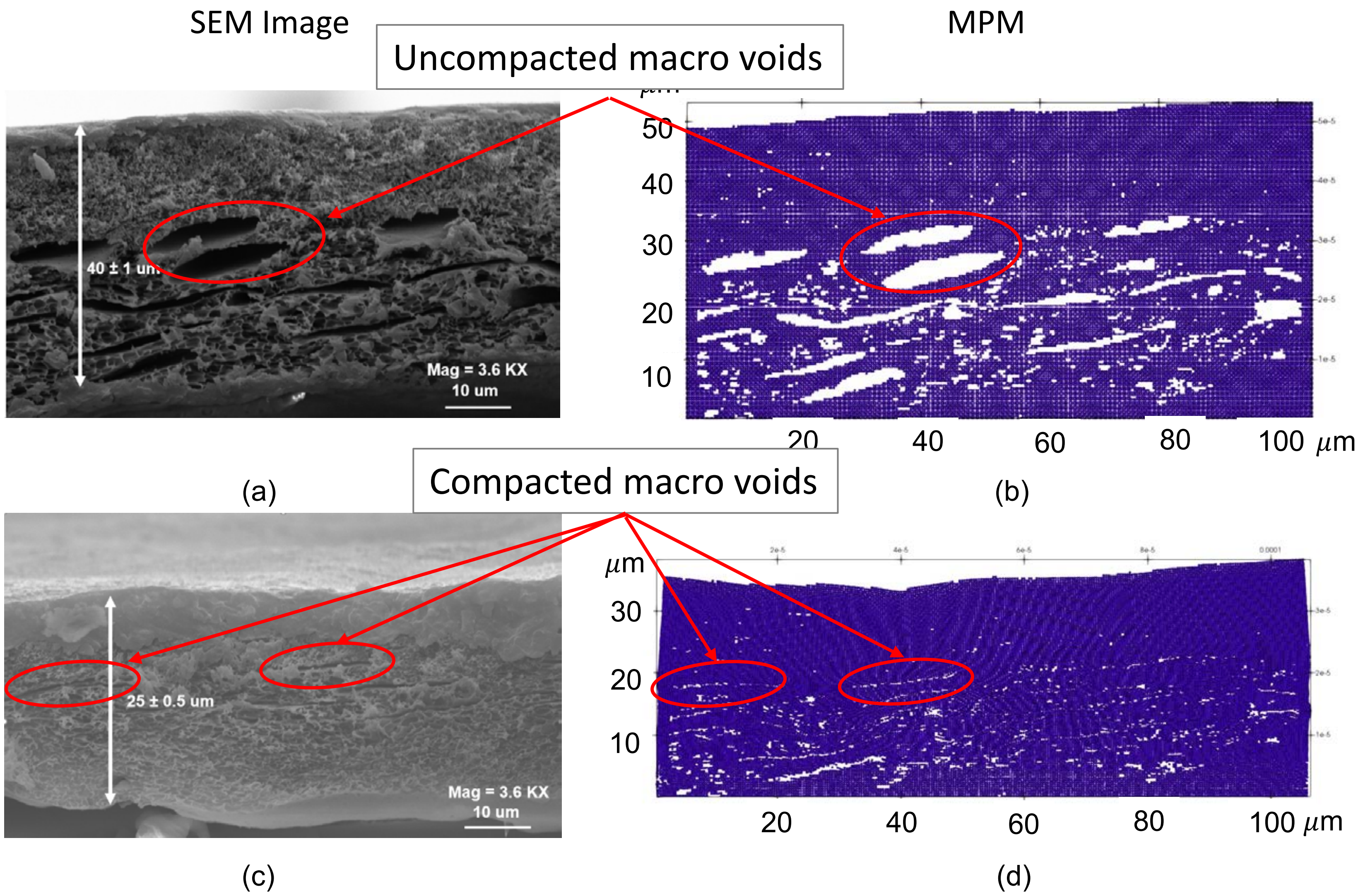


Image converted to material point collection using python script



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

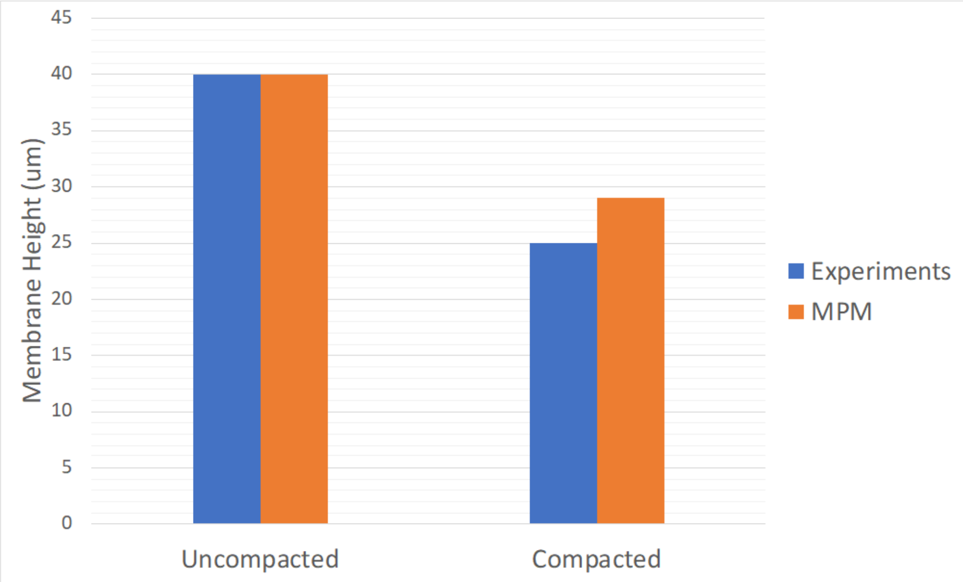
Application to simulation of RO membrane compaction



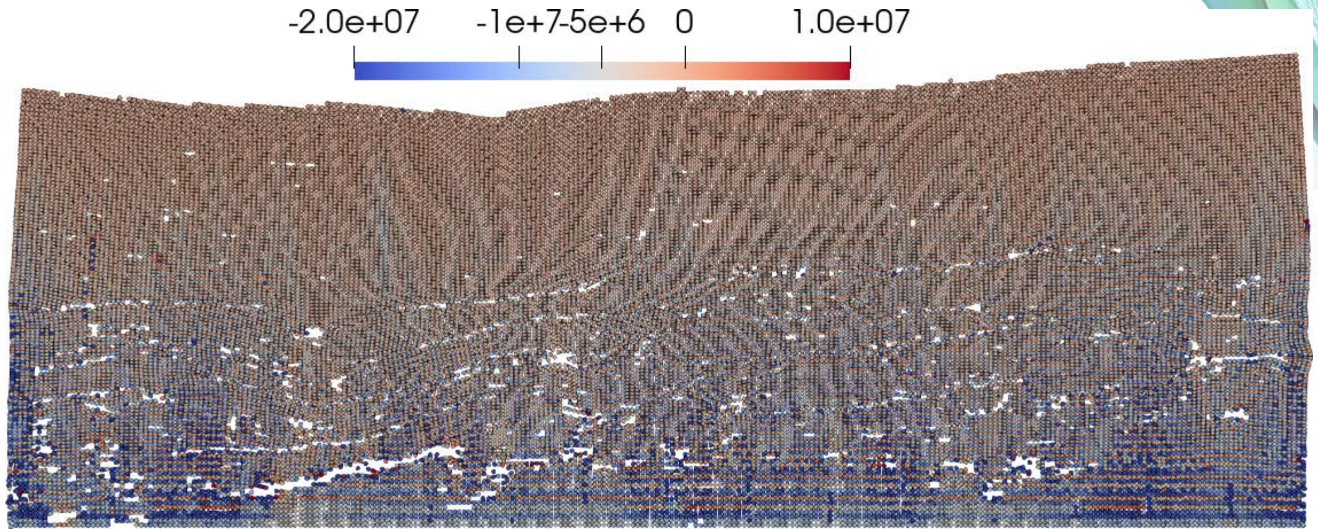
Uncompacted membrane

Compacted membrane

Application to simulation of RO membrane compaction



Comparison of membrane heights observed in experiments and MPM



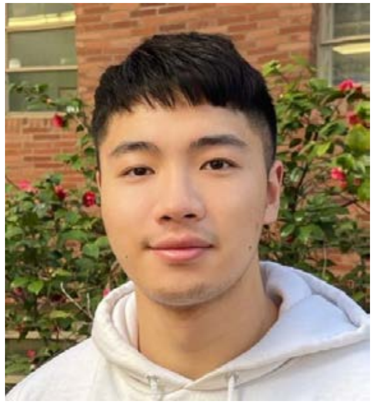
Normal stress contours at material points

Conclusions

- Material point method-based solver used to simulate RO membrane compaction
- MPM solver- Exagoop developed based on the AMReX framework
- Exagoop solver validated and verified with canonical test cases and shows excellent match with available solutions
- Higher order shape functions are costlier when compared to linear hat shape functions. However, cubic B-spline function exhibits maximum accuracy
- Application of MPM to membrane compaction problem shows good qualitative and visual match with macro void structure observed from SEM images
- MPM predicts membrane deformation within an accuracy of 16% when compared to experiments

Other researchers who contributed to this project

Dr. Hariswaran Sitaraman



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THANK YOU

NREL/PR-2C00-85437

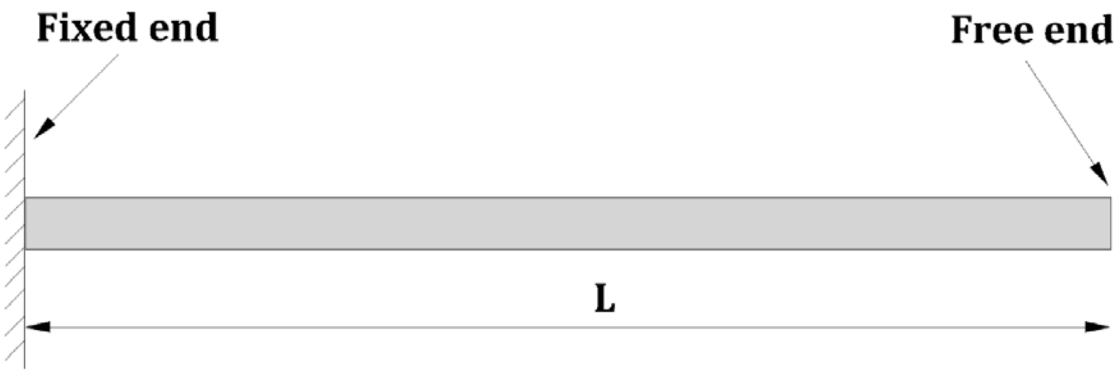
This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by U.S. Department of Energy Office of Science and National Nuclear Security Administration. 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.

APPENDIX

Exagoop Solver: Validation

Test Case 1: Axial vibration of bar

Problem Definition



Governing Equations, Boundary conditions, Initial Conditions

Governing Equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad 0 \le x \le L$$

Boundary Conditions

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

Initial Conditions

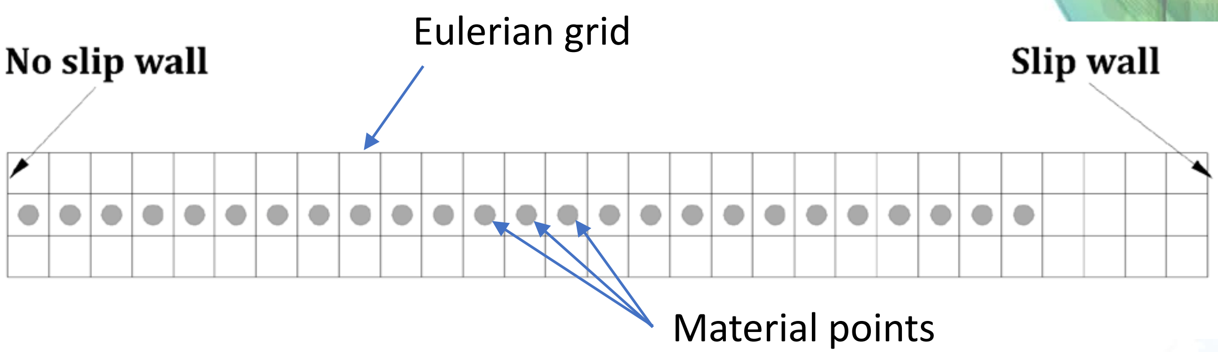
$$u(x,0) = 0 \quad \frac{\partial u}{\partial t}(x,0) = V_0 \sin(\frac{\pi x}{2L})$$

Exact Solution

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

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

MPM Model:

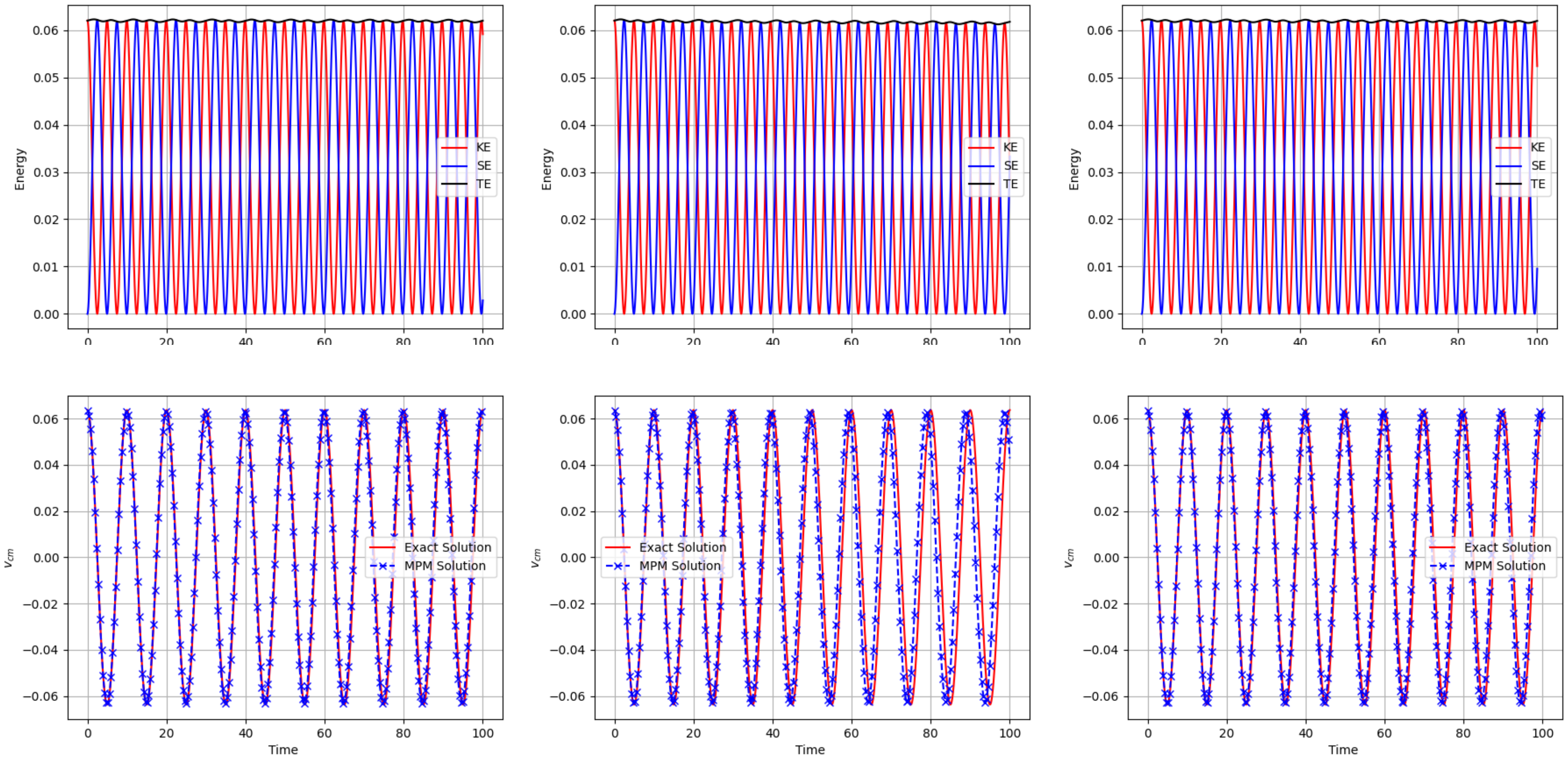


Number of cells in background grid = 29 x 3
L = 25
Number of particles per cell = 1
Shape Functions: Linear hat, Quadratic B-Spline, Cubic B-Spline
Constitutive Model: Linear Elastic
Courant-Friedrichs-Lewy (CFL) number = 0.1

Exagoop Solver: Validation

Test Case 1: Axial vibration of bar

Linear Hat | Quadratic B-Spline | Cubic B-Spline

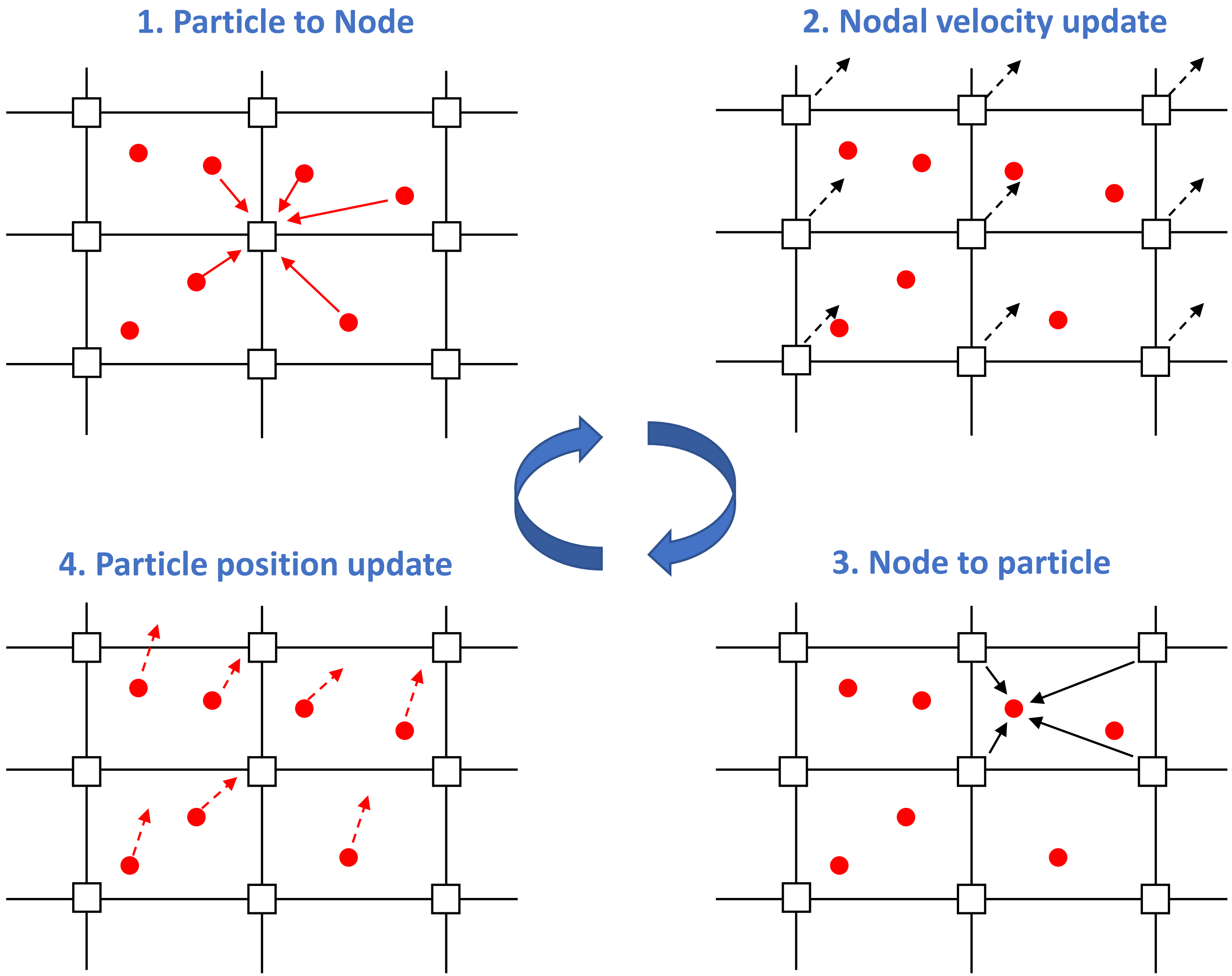


Energy variation with time

Center of mass velocity with time

Excellent match with exact solution, Excellent conservation of total energy

Material Point Method (MPM)



Step 0

- Initialize particle positions, m_p, v_p and σ_p

Step 1

- $m_I^t = \sum_p \phi_I(x_p^t) m_p$
- $(mv)_I^t = \sum_p \phi_I\,(x_p^t)(mv)_p^t$
- $f_I^{\{ext,t\}} = \sum_p \phi_I(x_p) m_p b(x_p)$
- $f_I^{\{int,t\}} = -\sum_p V_p^t\, \sigma_p^t\, \nabla\, \phi_I\,(x_p^t)$

Step 2

- $v_I^{\{t+\Delta\, t\}} = \frac{f_I^{\{ext,t\}} + f_I^{\{int,t\}}}{m_I^t}$

Step 3

- $v_p^{\{t+\Delta t\}} = \alpha\{\, v_p^t + \sum_I \phi_I\,(x_p^t)\left[\Delta v_I^{\{t+\Delta\, t\}}\right]\} + (1 - \alpha)\, \sum_I \phi_I\,(x_p^t)\left[v_I^{\{t+\Delta\, t\}}\right]$

Step 4

- $x_p^{\{t+\Delta\, t\}} = x_p^t + \Delta t\, \sum_I \phi_I(x_p^t) v_I^{\{t+\Delta t\}}$