MPM Presentation

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Table of Contents

Table of Contents

Motivation and Key Contributions

- Strong empirical performance; serves as the foundation of MPMNet.
- Introduces a "ghost matrix" formulation for solid–fluid interaction.
- Proposes the B2B0–B0–B1B0 discretization scheme.
- Develops an interface quadrature method for computing boundary integrals.

Table of Contents

Governing Equations

- For domain Ω^k of a coupled solid-fluid system with $k \in \{s, f\}$, the governing equations are

$$\frac{D\rho^k}{Dt} + \rho^k \nabla \cdot \mathbf{v}^k = 0, \quad \mathbf{x} \in \Omega^k \tag{1}$$

$$\rho^k \frac{D\mathbf{v}^k}{Dt} - \nabla \cdot \sigma^k - \rho^k \mathbf{g} = 0, \quad \mathbf{x} \in \Omega^k \tag{2}$$

$$\sigma^k \cdot \mathbf{n}^k = \mathbf{b}, \quad \mathbf{x} \in \partial\Omega^k_N \tag{3}$$

$$\mathbf{v}^k \cdot \mathbf{n}^k = v^k_S, \quad \mathbf{x} \in \partial\Omega^k_S \tag{4}$$

$$\mathbf{v}^k = \mathbf{v}^k_{NS}, \quad \mathbf{x} \in \partial\Omega^k_{NS} \tag{5}$$

where $\mathbf{b}$, v^k_S and $\mathbf{v}^k_{NS}$ are given free surface, slip, and no-slip boundary conditions.

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  where $\mathbf{b}$, v^k_S and $\mathbf{v}^k_{NS}$ are given free surface, slip, and no-slip boundary conditions.

- Also allow free-slip boundary condition **at the interface Γ between Ω^s and Ω^f** by only enforcing the normal velocity continuity

$$(\mathbf{v}^s - \mathbf{v}^f) \cdot \mathbf{n}^s = 0, \quad \mathbf{x} \in \Gamma \tag{6}$$

  and pressure continuity

$$p^s - p^f = 0, \quad \mathbf{x} \in \Gamma. \tag{7}$$

Ghost Matrix for Nonlinear Solids

- View the solid continuum as a combination of a hyperelastic solid component and an air-like massless ghost matrix continuum, which share the same velocity field.
- Solid-fluid interaction is reformulated as the **pressure only interaction** between the matrix and the fluid.
- Express the total energy density as

$$\Psi(\mathbf{F}^s, J^g) = \Psi^s(\mathbf{F}^s) + \Psi^g(J^g), \quad \Psi^g(J^g) = \frac{1}{2}\lambda^g(J^g - 1)^2 \tag{8}$$

where $\Psi^s(\mathbf{F}^s)$ is a standard nonlinear solid constitutive model and $\Psi^g(J^g)$ describes the air-like response of the ghost matrix.

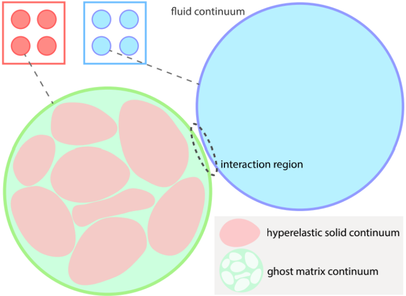

Figure 1: Ghost matrix.

Discretization of Governing Equations of Particles

- Discretize solid momentum conservation equation (2) and ghost matrix pressure evolution equation $\frac{Dp}{Dt} = -\lambda J \nabla \cdot \mathbf{v}$ respectively, we obtain

$$\frac{\rho^{s,n}\mathbf{v}^{s,n+1}}{\Delta t} - \nabla \cdot \sigma^{s,n+1} + \nabla p^{g,n+1} = \frac{\rho^{s,n}\mathbf{v}^{s,n}}{\Delta t} + \mathbf{f}^{fs,n+1}, \tag{9}$$

$$\nabla \cdot \mathbf{v}^{s,n+1} + \frac{p^{g,n+1}}{\lambda^g J^{g,n} \Delta t} = \frac{p^{g,n}}{\lambda^g J^{g,n} \Delta t}, \tag{10}$$

where $\mathbf{f}^{fs,n+1} = h^{n+1}\mathbf{n}^{s,n}$ denotes the normal pressure exerted from fluid to solid.

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- The fluid governing equations can be discretized similarly,

$$\frac{\rho^{f}\mathbf{v}^{f,n+1}}{\Delta t} + \nabla p^{f,n+1} = \frac{\rho^{f}\mathbf{v}^{f,n}}{\Delta t} + \mathbf{f}^{sf,n+1} + \mathbf{f}^{w,n+1}, \tag{11}$$

$$\nabla \cdot \mathbf{v}^{f,n+1} = 0, \tag{12}$$

  where $\mathbf{f}^{sf,n+1} = -h^{n+1}\mathbf{n}^{s,n}$ (implying pressure continuity), and $\mathbf{f}^{w,n+1} = -y^{n+1}\mathbf{n}^{f,n}$ denotes the pressure from the slip boundary.

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- Boundary condition and impenetrability condition are given by

$$\mathbf{v}^{f,n+1}|_{\partial\Omega_S^f} \cdot \mathbf{n}^f = v_S^f, \quad (\mathbf{v}^{s,n+1}|_\Gamma - \mathbf{v}^{f,n+1}|_\Gamma) \cdot \mathbf{n}^{s,n} = 0 \quad (13)$$

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- **Need to be solved for:** $\mathbf{v}^{s,n+1}, \sigma^{s,n+1}, p^{g,n+1}, \mathbf{v}^{f,n+1}, p^{f,n+1}, y^{n+1}, h^{n+1}$.

Operator Splitting

- The **fully coupled constrained nonlinear** system is extremely impractical to solve.
- First advance the solid velocity with a fully nonlinear Newton solve ($\mathbf{v}^{s,n} \to \mathbf{v}^{s,*}$) ignoring the matrix and the fluid:

$$\frac{\rho^{s,n}\mathbf{v}^{s,*}}{\Delta t} - \nabla \cdot \sigma^{s,*} = \frac{\rho^{s,n}\mathbf{v}^{s,n}}{\Delta t}, \tag{14}$$

  where

$$\sigma^{s,*} = \frac{1}{\det(\mathbf{F}^{s,*})}\frac{\partial \Psi^s}{\partial \mathbf{F}}\mathbf{F}^{s,*T} \tag{15}$$

- Then $\mathbf{v}^{s,*}$ replaces $\mathbf{v}^{s,n}$ in Equation (9)

$$\frac{\rho^{s,n}\mathbf{v}^{s,n+1}}{\Delta t} + \nabla p^{g,n+1} - h^{n+1}\mathbf{n}^{s,n} = \frac{\rho^{s,n}\mathbf{v}^{s,*}}{\Delta t}. \tag{16}$$

Weak Form of Governing Equations

- Multiply test functions $\mathbf{q}^s(\mathbf{x}), r^s(\mathbf{x}), \mathbf{q}^f(\mathbf{x}), r^f(\mathbf{x}), u^f(\mathbf{x})$, and $w(\mathbf{x})$ onto the discretized equations and integrate over their corresponding domains.
- Solid momentum conservation equation becomes:

$$\int_{\Omega^s} \frac{\rho^{s,n}\mathbf{q}^s \cdot \mathbf{v}^{s,n+1}}{\Delta t} d\mathbf{x} + \int_{\Omega^s} \mathbf{q}^s \cdot \nabla p^{g,n+1} d\mathbf{x} - \int_{\Gamma} \mathbf{q}^s \cdot \mathbf{n}^{s,n} h^{n+1} ds = \int_{\Omega^s} \frac{\rho^{s,n}\mathbf{q}^s \cdot \mathbf{v}^{s,*}}{\Delta t} d\mathbf{x}, \tag{17}$$

- Ghost matrix pressure evolution equation becomes

$$\int_{\Omega^s} r^s \nabla \cdot \mathbf{v}^{s,n+1} d\mathbf{x} + \int_{\Omega^s} \frac{p^{g,n+1}}{\lambda^g J^{g,n} \Delta t} r^s d\mathbf{x} = \int_{\Omega^s} \frac{p^{g,n}}{\lambda^g J^{g,n} \Delta t} r^s d\mathbf{x}, \tag{18}$$

- Fluid momentum conservation equation becomes:

$$\int_{\Omega^f} \frac{\rho^f \mathbf{q}^f \cdot \mathbf{v}^{f,n+1}}{\Delta t} d\mathbf{x} + \int_{\Omega^f} \mathbf{q}^f \cdot \nabla p^{f,n+1} d\mathbf{x} + \int_{\partial\Omega^f_S} \mathbf{q}^f \cdot \mathbf{n}^f y^{n+1} ds + \int_{\Gamma} \mathbf{q}^f \cdot \mathbf{n}^{s,n} h^{n+1} ds = \int_{\Omega^f} \frac{\rho^f \mathbf{q}^f \cdot \mathbf{v}^{f,n}}{\Delta t} d\mathbf{x}, \tag{19}$$

Weak Form of Governing Equations (Cont'd)

- Fluid incompressibility condition becomes

$$\int_{\Omega^f} r^f \nabla \cdot \mathbf{v}^{f,n+1} d\mathbf{x} = 0, \tag{20}$$

- Boundary and impenetrability conditions become

$$\int_{\partial\Omega^f_S} \mathbf{v}^{f,n+1} \cdot \mathbf{n}^f u ds = \int_{\partial\Omega^f_S} v^f_S u ds, \tag{21}$$

$$\int_{\Gamma} (\mathbf{v}^{s,n+1} - \mathbf{v}^{f,n+1}) \cdot \mathbf{n}^{s,n} w ds = 0 \tag{22}$$

- We will turn these equations into a symmetric linear system **on grid** for unknown quantities $\mathbf{v}^{s,n+1}, p^{g,n+1}, \mathbf{v}^{f,n+1}, p^{f,n+1}, y^{n+1}, h^{n+1}$.

B2B0–B0–B1B0 Discretization Scheme

- Discretize solid velocity and test function with quadratic kernels defined at cell nodes:

$$\mathbf{v}^{s,\{n,n+1\}}(\mathbf{x}) = \sum_i \mathbf{v}_i^{s,\{n,n+1\}} N_i^{s,2}(\mathbf{x}), \tag{23}$$

$$\mathbf{q}^{s}(\mathbf{x}) = \sum_j \mathbf{q}_j^{s} N_j^{s,2}(\mathbf{x}). \tag{24}$$

- Discretize fluid velocity and test function with linear kernels defined at cell centers:

$$\mathbf{v}^{f,\{n,n+1\}}(\mathbf{x}) = \sum_b \mathbf{v}_b^{f,\{n,n+1\}} N_b^{f,1}(\mathbf{x}), \tag{25}$$

$$\mathbf{q}^{f}(\mathbf{x}) = \sum_c \mathbf{q}_c^{f} N_c^{f,1}(\mathbf{x}). \tag{26}$$

- All other scalar pressure-like quantities (p, r, y, u, h, w) are discretized at nodes using $N_i^{s/f,0}(\mathbf{x})$ as piecewise constant fields.
- Satisfy inf-sup stability, prevent kinematic locking, while saving resources and storage.

Symmetric Linear System of Grid Quantities

- Plug the basis expansion into the weak form equations (17) to (22), we obtain the following linear system, where the unknowns are quantities **on the grid**:

$$\begin{pmatrix} \frac{1}{\Delta t}M^s & G^s & 0 & 0 & 0 & -H^{sT} \\ G^{sT} & -\frac{1}{\Delta t}S^s & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\Delta t}M^f & G^f & B^T & H^{fT} \\ 0 & 0 & G^{fT} & 0 & 0 & 0 \\ 0 & 0 & B & 0 & 0 & 0 \\ -H^s & 0 & H^f & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{v}^{s,n+1} \\ \mathbf{p}^{g,n+1} \\ \mathbf{v}^{f,n+1} \\ \mathbf{p}^{f,n+1} \\ \mathbf{y}^{n+1} \\ \mathbf{h}^{n+1} \end{pmatrix} = \mathbf{r} \tag{27}$$

with $\mathbf{r} = \left(\frac{1}{\Delta t}M^s\mathbf{v}^{s,*}, -\frac{1}{\Delta t}S^s\mathbf{p}^{g,n}, \frac{1}{\Delta t}M^f\mathbf{v}^{f,n}, 0, \mathbf{b}, 0\right)^T$.

- The solid lumped mass matrix, gradient operator, and scaling matrix are given by:

$$M^s_{i_\alpha i_\alpha} = \int_{\Omega^s} \rho^{s,n} N_i^{s,2}(\mathbf{x})d\mathbf{x}, \tag{28}$$

$$G^s_{i_\alpha j} = -\int_{\Omega^s} N_j^{s,0}(\mathbf{x})(\nabla N_i^{s,2}(\mathbf{x}))_\alpha d\mathbf{x}, \tag{29}$$

$$S^s_{ii} = \int_{\Omega^s} \frac{1}{\lambda^g J^{g,n}} N_i^{s,0}(\mathbf{x})d\mathbf{x}. \tag{30}$$

Symmetric Linear System of Grid Quantities (Cont'd)

- The fluid lumped mass, gradient, and boundary operators are given by

$$M^f_{c_\alpha c_\alpha} = \rho^f \int_{\Omega^f} N^{f,1}_c(\mathbf{x}) d\mathbf{x}, \tag{31}$$

$$G^f_{c_\alpha i} = -\int_{\Omega^f} N^{s,0}_i(\mathbf{x}) (\nabla N^{f,1}_c(\mathbf{x}))_\alpha d\mathbf{x}, \tag{32}$$

$$B_{c_\alpha i} = \int_{\partial \Omega^f_S} N^{f,1}_c(\mathbf{x}) N^{f,0}_i(\mathbf{x}) n^f_\alpha ds. \tag{33}$$

- The coupling terms are

$$H^s_{j i_\alpha} = \int_\Gamma N^{s,2}_i(\mathbf{x}) N^{s,0}_j(\mathbf{x}) n^{s,n}_\alpha ds, \tag{34}$$

$$H^f_{j c_\alpha} = \int_\Gamma N^{f,1}_c(\mathbf{x}) N^{f,0}_j(\mathbf{x}) n^{s,n}_\alpha ds. \tag{35}$$

Pressure-Only System

- The coupled system (27) has extremely bad conditioning. We can eliminate the velocity and solve for the pressure variables first:

$$\begin{pmatrix} A_{11} & 0 & 0 & A_{14} \\ 0 & A_{22} & A_{23} & A_{24} \\ 0 & A_{23}^T & A_{33} & A_{34} \\ A_{14}^T & A_{24}^T & A_{34}^T & A_{44} \end{pmatrix} \begin{pmatrix} \mathbf{p}^{g,n+1} \\ \mathbf{p}^{f,n+1} \\ \mathbf{y}^{n+1} \\ \mathbf{h}^{n+1} \end{pmatrix} = \begin{pmatrix} \frac{S^s \mathbf{p}^{g,n}}{\Delta t} - G^{sT}\mathbf{v}^{s,n} \\ G^{fT}\mathbf{v}^{f,n} \\ B\mathbf{v}^{f,n} - \mathbf{b} \\ H^s\mathbf{v}^{s,n} - H^f\mathbf{v}^{f,n} \end{pmatrix} \tag{36}$$

  where $A_{11} = \frac{S^s}{\Delta t} + \Delta t G^{sT} M^{s-1} G^s$, $A_{14} = -\Delta t G^{sT} M^{s-1} H^{sT}$,
  $A_{22} = \Delta t G^{fT} M^{f-1} G^f$, $A_{23} = \Delta t G^{fT} M^{f-1} B^T$, $A_{24} = \Delta t G^{fT} M^{f-1} H^{fT}$,
  $A_{33} = \Delta t B M^{f-1} B^T$, $A_{34} = \Delta t B M^{f-1} H^{fT}$,
  $A_{44} = \Delta t (H^s M^{s-1} H^{sT} + H^f M^{f-1} H^{fT})$.
- After solving for pressure variables, **substitute them back into the momentum equation** (system (27)) to get the new velocities.
- Solid deformation gradient is updated as

$$\mathbf{F}_p^{n+1} = (\mathbf{I} + \Delta t(\nabla \mathbf{v}^{n+1}(\mathbf{x}_p)))\mathbf{F}_p^n \tag{37}$$

- Strain of ghost matrix particle is updated as

$$J_p^{g,n+1} = 1 - \frac{p_p^{g,n+1}}{\lambda} \tag{38}$$

  using the interpolated $p_p^{g,n+1}$ and the relationship $p = -\lambda(J-1)$.

Particle Quadrature for Solid and Matrix

- Discretize all integrals that are only associated with solid and matrix using particle quadratures:

$$M^s_{i_\alpha i_\alpha} = m^s_i = \sum_p m^s_p N^{s,2}_i(\mathbf{x}_p), \tag{39}$$

$$G^s_{i_\alpha j} = -\sum_p V^n_p N^{s,0}_j(\mathbf{x}_p)(\nabla N^{s,2}_i(\mathbf{x}_p))_\alpha, \tag{40}$$

$$S^s_{ii} = s^s_i = \sum_p \frac{1}{\lambda^g_p} V^0_p N^{s,0}_i(\mathbf{x}_p). \tag{41}$$

- The previous time pressure $\mathbf{p}^{g,n}$ in RHS of system (27) is computed by taking volume weighted average over all ghost matrix particles

$$p^{g,n}_i = \frac{\sum_p V^0_p J^{g,n}_p p^{g,n}_p N^{s,0}_i(\mathbf{x}_p)}{\sum_p V^0_p J^{g,n}_p N^{s,0}_i(\mathbf{x}_p)}, \tag{42}$$

where $p^{g,n}_p = -\lambda^g_p(J^{g,n}_p - 1)$.

Interface Quadrature and Fluid Volume Quadrature

- Discretize the boundary integral on Γ through IQ points: Locate solid particles $< 0.5\Delta x$ to fluid particles, and insert an IQ point q with area A_q and normal $\mathbf{n}_q$ for each such solid particle.
- Sample an additional fluid volume quadrature at each IQ point, whose volume = average volume of the fluid particles $< 0.5\Delta x$.
- With IQ, the coupling terms are discretized as

$$H^s_{ji_\alpha} = \sum_q A_q N_i^{s,2}(\mathbf{x}_q) N_j^{s,0}(\mathbf{x}_q) n^n_{q\alpha} ds, \tag{43}$$

$$H^f_{jc_\alpha} = \sum_q A_q N_c^{f,1}(\mathbf{x}_q) N_j^{f,0}(\mathbf{x}) n^n_{q\alpha} ds. \tag{44}$$

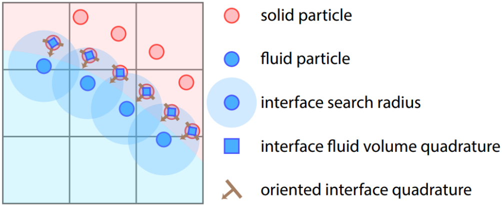

Figure 2: IQ allocation.

Table of Contents

Algorithm Pipeline

1. **P2G.** Solid and fluid particles transfer their mass and velocity onto the grid using APIC; ghost matrix particles transfer pressure $p^{g,n}$ onto the grid using (42).
2. **Projected Newton solver.** Solid velocities are integrated from $\mathbf{v}^{s,n}$ to $\mathbf{v}^{s,*}$ considering nonlinear hyperelasticity and collision objects.
3. **Identify IQ.** IQ points with areas and normals are identified, as well as additional fluid volume quadrature points.
4. **Coupled solve.** The coupled pressure-only system (36) is constructed and solved. New velocities are reconstructed using the pressures.
5. **G2P.** Solid and fluid particles update their velocities and advect using APIC; ghost matrix particles update their strain J^g using the interpolated $p^{g,n+1}$.

Table of Contents

MPMNet Workflow

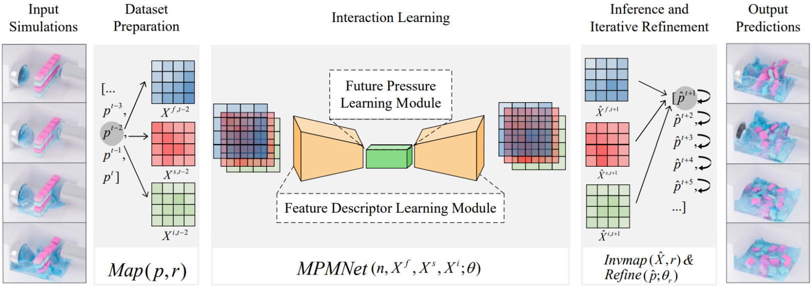

Figure 3: MPMNet framework.

- Major goal: Break computational bottleneck of solving system (36), accelerate pressure prediction using neural network.
- Dataset preparation: Generate training data using IQ-MPM; $\mathbf{p}^{f,t}$ & $\mathbf{y}^{t}$ $\rightarrow \mathrm{X}^{f,t}$, $\mathbf{p}^{s,t}$ $\rightarrow \mathrm{X}^{s,t}$, $\mathbf{h}^{t}$ $\rightarrow \mathrm{X}^{i,t}$.
- Interaction learning: Autoencoder (3D CNN) & ConvLSTM.
- Iterative refinement: $\hat{\mathbf{p}}$ as starting point for solving system (36).

Algorithm

Algorithm 1 Pseudo-code for data processing and MPMNet inference

for t in n **do**
    particle-to-grid transfer
    coupled solve (equation 4)
    get $\boldsymbol{p}^{f,t}$, $\boldsymbol{p}^{s,t}$, $\boldsymbol{y}^{t}$,$\boldsymbol{h}^{t}$ and the corresponding node coordinate $\boldsymbol{r}$ from physical method
    map pressure fields to effective matrices $X^{f,t}$, $X^{s,t}$, $X^{i,t}$; ($X = Map(\boldsymbol{p}, \boldsymbol{r})$)
    normalization procedure (see Sec 4.1)
    grid-to-particle transfer
end for
get MPMNet input $I = [n, X^{f}, X^{s}, X^{i}]$
for t in m **do**
    particle-to-grid transfer
    MPMNet inference and output $\hat{X}^{f,t}$, $\hat{X}^{s,t}$, $\hat{X}^{i,t}$
    map effective matrices to pressure fields $\hat{\boldsymbol{p}}^{f,t}$, $\hat{\boldsymbol{p}}^{s,t}$, $\hat{\boldsymbol{y}}^{t}$, $\hat{\boldsymbol{h}}^{t}$; ($\hat{\boldsymbol{p}} = Invmap(\hat{X}, \boldsymbol{r})$)
    Iterative refinement (see Sec 4.4)
    grid-to-particle transfer
end for

Figure 4: Algorithm.

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Thank you!
Any questions?