Tree-like Processor Architecture for Multiscale, Multi-material and Multi-physics Computation Based on the Material Point Method

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Material Point Method

- Material point method (MPM) is a numerical method solving PDE's.
- It avoids mesh distortion issues of Lagrangian methods, such as the finite element method, and numerical diffusion issues of Eulerian methods, but it is more expensive than both of them.

FEM, (Lagrangian Method)
Cline and Reaugh, J. De. Physique IV, 1991

MPM vs. Eulerian
Applications of material point method

- Problems with extreme material deformation ($\varepsilon >> 100\%$), history dependency, pulverization, and complicated interfaces.

- These types of problems are usually accompanied by high strain rates and non-equilibrium thermodynamics.
MPM and Multi-scale Physics

- Even for thermodynamically non-equilibrium systems, macroscopic equations still hold, provided a correct stress (Irving and Kirkwood, 1950).
- The stress can be calculated (Zhang et al. 2006) from microscopic physics, such as molecular dynamics (MD).
- Need to study macro-micro communications, but the communications are local with MPM.

\[
\sigma_c = \frac{1}{2} \int \sum_i \delta(x - y_i) f_{ij} \otimes r_{ij} P(C_n) dC_n - \rho v' v'
\]

Material point method vs. finite element method

\[
m_i \frac{d \mathbf{v}_i}{dt} = - \int \mathbf{\sigma} \cdot \nabla S_i(x) \, dv + \int \rho g S_i(x) \, dV + \int_{\partial V} S_i(x) \mathbf{\sigma} \cdot \mathbf{n} \, dS,
\]

**FEM**

\[
\int \mathbf{\sigma} \cdot \nabla S_i(x) \, dv = \sum_g w_g J_g \mathbf{\sigma}_g \cdot \nabla S(x_g),
\]

where subscript \( g \) denotes Gauss integration points.

**MPM**

\[
\int \mathbf{\sigma} \cdot \nabla S_i(x) \, dv = \sum_p v_p \mathbf{\sigma}_p \cdot \nabla S(x_p)
\]

where subscript \( p \) denotes material points that move across the Eulerian mesh.

Gauss points are fixed on elements.

Elements are Lagrangian. They can be distorted for large material deformation.

- Both the material points and the Gauss points are Lagrangian and can be used to track deformation history of the material. However, FEM has the difficulty of mesh distortion.
- Material points only communicate with nodes, not among the material points themselves.
MPM and Tree-like Processor Architecture

- We can use a low-speed high accuracy CPU to perform continuum or macroscopic (MPM) calculations.

- For MD calculations we only need statistical quantities, therefore we are more error tolerant, but we need a lot and fast. High-speed MD calculations can be done on GPU's.

- Furthermore, the ideas of coarse graining, super-molecules, and effective force fields, can be used to a hierarchy of length and time scales in a tree-like processor architecture **without inter-branch communications**.