Material Point Method for Snow Simulation

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1 Differentiating energy

Given an elasto-plastic energy density function $\Psi(\boldsymbol{F}_E, \boldsymbol{F}_P)$ which evaluates to $\Psi_p = \Psi(\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}}), \boldsymbol{F}^n_{Pp})$ at each particle p using its elastic and plastic parts of the deformation gradient $\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}})$ and $\boldsymbol{F}^n_{Pp}$, we define the full potential energy of the system to be

$$\Phi(\hat{\boldsymbol{x}}) = \sum_p V_p^0 \Psi(\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}}), \boldsymbol{F}^n_{Pp}) = \sum_p V_p^0 \Psi_p,$$

where $\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}})$ is updated as

$$\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}}) = \left(\boldsymbol{I} + \sum_{\boldsymbol{i}} (\hat{\boldsymbol{x}}_{\boldsymbol{i}} - \boldsymbol{x}^n_{\boldsymbol{i}})(\nabla w^n_{\boldsymbol{i}p})^T\right)\boldsymbol{F}^n_{Ep}. \tag{1}$$

For the purposes of working out derivatives, we use index notation for differentiation, using Greek indices $\alpha, \beta, \ldots$ for spatial indices, $\Phi_{,(\boldsymbol{j}\sigma)}$ to indicate partial derivatives on $x_{\boldsymbol{j}\sigma}$, $\Phi_{,(\alpha\beta)}$ to indicate partial derivatives on $F_{E\alpha\beta}$, and summation implied over all repeated indices. The derivatives of $\hat{\boldsymbol{F}}_{Ep}$ with respect to $\boldsymbol{x}_{\boldsymbol{i}}$ are

$$\begin{aligned}
\hat{F}_{Ep\alpha\beta} &= \left(\delta_{\alpha\gamma} + (x_{\boldsymbol{i}\alpha} - x^n_{\boldsymbol{i}\alpha}) w^n_{\boldsymbol{i}p,\gamma}\right) F^n_{Ep\gamma\beta} \\
\hat{F}_{Ep\alpha\beta,(\boldsymbol{j}\sigma)} &= \delta_{\alpha\sigma} w^n_{\boldsymbol{j}p,\gamma} F^n_{Ep\gamma\beta} \\
\hat{F}_{Ep\alpha\beta,(\boldsymbol{j}\sigma)(\boldsymbol{k}\tau)} &= 0
\end{aligned}$$

With these, the derivatives of Φ with respect to $\boldsymbol{x}_{\boldsymbol{i}}$ can be worked out using the chain rule

$$\begin{aligned}
\Phi &= V_p^0 \Psi_p \\
\Phi_{,(\boldsymbol{j}\sigma)} &= \sum_p V_p^0 \Psi_{p,(\alpha\beta)} \hat{F}_{Ep\alpha\beta,(\boldsymbol{j}\sigma)} \\
&= \sum_p V_p^0 \Psi_{p,(\sigma\beta)} w^n_{\boldsymbol{j}p,\gamma} F^n_{Ep\gamma\beta} \\
\Phi_{,(\boldsymbol{j}\sigma)(\boldsymbol{k}\tau)} &= \sum_p (V_p^0 \Psi_{p,(\sigma\beta)} w^n_{\boldsymbol{j}p,\gamma} F^n_{Ep\gamma\beta})_{,(\boldsymbol{k}\tau)} \\
&= \sum_p V_p^0 \Psi_{p,(\sigma\beta)(\tau\kappa)} w^n_{\boldsymbol{j}p,\gamma} F^n_{Ep\gamma\beta} w^n_{\boldsymbol{k}p,\omega} F^n_{Ep\omega\kappa}
\end{aligned}$$

These can be interpreted without the use of indices as

$$-\boldsymbol{f}_{\boldsymbol{i}}(\hat{\boldsymbol{x}}) = \frac{\partial \Phi}{\partial \hat{\boldsymbol{x}}_{\boldsymbol{i}}}(\hat{\boldsymbol{x}}) = \sum_p V_p^0 \frac{\partial \Psi}{\partial \boldsymbol{F}_E}(\hat{\boldsymbol{F}}_{Ep}(\hat{\boldsymbol{x}}), \boldsymbol{F}^n_{Pp})(\boldsymbol{F}^n_{Ep})^T \nabla w^n_{\boldsymbol{i}p} \tag{2}$$

and

$$-\delta \boldsymbol{f}_{\boldsymbol{i}} = \sum_{\boldsymbol{j}} \frac{\partial^2 \Phi}{\partial \hat{\boldsymbol{x}}_{\boldsymbol{i}} \partial \hat{\boldsymbol{x}}_{\boldsymbol{j}}}(\hat{\boldsymbol{x}}) \delta \boldsymbol{u}_{\boldsymbol{j}} = \sum_p V_p^0 \boldsymbol{A}_p (\boldsymbol{F}^n_{Ep})^T \nabla w^n_{\boldsymbol{i}p} \tag{3}$$

where

$$\boldsymbol{A}_p = \frac{\partial^2 \Psi}{\partial \boldsymbol{F}_E \partial \boldsymbol{F}_E}(\boldsymbol{F}_E(\hat{\boldsymbol{x}}), \boldsymbol{F}^n_{P_p}) : \left(\sum_{\boldsymbol{j}} \delta \boldsymbol{u}_{\boldsymbol{j}} (\nabla w^n_{\boldsymbol{j}p})^T \boldsymbol{F}^n_{Ep}\right). \tag{4}$$

and the notation $\boldsymbol{A} = \boldsymbol{\mathcal{C}} : \boldsymbol{D}$ is taken to mean $A_{ij} = \mathcal{C}_{ijkl} D_{kl}$ with summation implied on indices kl.

2 Differentiating constitutive model

For integration, we need to compute $\frac{\partial \Psi}{\partial \boldsymbol{F}_E}$ and $\frac{\partial^2 \Psi}{\partial \boldsymbol{F}_E \partial \boldsymbol{F}_E} : \delta \mathcal{D}$. In this section, we will omit the subscripts E.

$$
\begin{aligned}
\Psi &= \mu \|\boldsymbol{F} - \boldsymbol{R}\|_F^2 + \frac{\lambda}{2}(J-1)^2 \\
\delta\Psi &= \delta\left(\mu \|\boldsymbol{F} - \boldsymbol{R}\|_F^2 + \frac{\lambda}{2}(J-1)^2\right) \\
&= \mu\delta\big(\|\boldsymbol{F} - \boldsymbol{R}\|_F^2\big) + \lambda(J-1)\delta J \\
&= \mu\delta\big(\mathrm{tr}(\boldsymbol{F}^T\boldsymbol{F})\big) - 2\mu\delta\big(\mathrm{tr}(\boldsymbol{R}^T\boldsymbol{F})\big) + \mu\delta\big(\mathrm{tr}(\boldsymbol{R}^T\boldsymbol{R})\big) + \lambda(J-1)\delta J \\
&= 2\mu\boldsymbol{F} : \delta\boldsymbol{F} - 2\mu\delta(\mathrm{tr}(\boldsymbol{S})) + \lambda(J-1)J\boldsymbol{F}^{-T} : \delta\boldsymbol{F} \\
&= 2\mu\boldsymbol{F} : \delta\boldsymbol{F} - 2\mu\,\mathrm{tr}(\delta\boldsymbol{S}) + \lambda(J-1)J\boldsymbol{F}^{-T} : \delta\boldsymbol{F} \\
\boldsymbol{F} &= \boldsymbol{R}\boldsymbol{S} \\
\delta\boldsymbol{F} &= \delta\boldsymbol{R}\boldsymbol{S} + \boldsymbol{R}\delta\boldsymbol{S} \\
\mathrm{tr}(\delta\boldsymbol{S}) &= \mathrm{tr}(\boldsymbol{R}^T\delta\boldsymbol{F}) - \mathrm{tr}(\boldsymbol{R}^T\delta\boldsymbol{R}\boldsymbol{S}) \\
&= \mathrm{tr}(\boldsymbol{R}^T\delta\boldsymbol{F}) - (\boldsymbol{R}^T\delta\boldsymbol{R}) : \boldsymbol{S} \\
&= \mathrm{tr}(\boldsymbol{R}^T\delta\boldsymbol{F}) \\
&= \boldsymbol{R} : \delta\boldsymbol{F}
\end{aligned}
$$

Note that since $\boldsymbol{R}^T\boldsymbol{R} = \boldsymbol{I}$, $\boldsymbol{R}^T\delta\boldsymbol{R}$ must be skew-symmetric. Since $\boldsymbol{S}$ is symmetric, $(\boldsymbol{R}^T\delta\boldsymbol{R}) : \boldsymbol{S} = 0$. Finally,

$$
\begin{aligned}
\delta\Psi &= 2\mu\boldsymbol{F} : \delta\boldsymbol{F} - 2\mu\,\mathrm{tr}(\delta\boldsymbol{S}) + \lambda(J-1)J\boldsymbol{F}^{-T} : \delta\boldsymbol{F} \\
&= 2\mu\boldsymbol{F} : \delta\boldsymbol{F} - 2\mu\boldsymbol{R} : \delta\boldsymbol{F} + \lambda(J-1)J\boldsymbol{F}^{-T} : \delta\boldsymbol{F} \\
\frac{\partial\Psi}{\partial\boldsymbol{F}} : \delta\boldsymbol{F} &= \big(2\mu\boldsymbol{F} - 2\mu\boldsymbol{R} + \lambda(J-1)J\boldsymbol{F}^{-T}\big) : \delta\boldsymbol{F} \\
\frac{\partial\Psi}{\partial\boldsymbol{F}_E} &= 2\mu(\boldsymbol{F}_E - \boldsymbol{R}_E) + \lambda(J_E-1)J_E\boldsymbol{F}_E^{-T}
\end{aligned}
$$

Note that Cauchy stress $\boldsymbol{\sigma}$ and first Piola-Kirchhoff stress $\boldsymbol{P}$ are related to $\frac{\partial\Psi}{\partial\boldsymbol{F}_E}$ by

$$
\boldsymbol{\sigma} = \frac{1}{J}\frac{\partial\Psi}{\partial\boldsymbol{F}_E}\boldsymbol{F}_E^T = \frac{2\mu}{J}(\boldsymbol{F}_E - \boldsymbol{R}_E)\boldsymbol{F}_E^T + \frac{\lambda}{J}(J_E-1)J_E\boldsymbol{I} \qquad \boldsymbol{P} = \frac{\partial\Psi}{\partial\boldsymbol{F}_E}\boldsymbol{F}_P^{-T}
$$

The second derivatives require a bit more care but can be computed relatively easily.

$$
\begin{aligned}
\frac{\partial^2\Psi}{\partial\boldsymbol{F}\partial\boldsymbol{F}} : \delta\boldsymbol{F} &= \delta\left(\frac{\partial\Psi}{\partial\boldsymbol{F}}\right) \\
&= \delta(2\mu(\boldsymbol{F} - \boldsymbol{R}) + \lambda(J-1)J\boldsymbol{F}^{-T}) \\
&= 2\mu\delta\boldsymbol{F} - 2\mu\delta\boldsymbol{R} + \lambda J\boldsymbol{F}^{-T}\delta J + \lambda(J-1)\delta(J\boldsymbol{F}^{-T}) \\
&= 2\mu\delta\boldsymbol{F} - 2\mu\delta\boldsymbol{R} + \lambda J\boldsymbol{F}^{-T}(J\boldsymbol{F}^{-T} : \delta\boldsymbol{F}) + \lambda(J-1)\delta(J\boldsymbol{F}^{-T})
\end{aligned}
$$

Since $J\boldsymbol{F}^{-T}$ is a matrix whose entries are polynomials in the entries of $\boldsymbol{F}$, $\delta(J\boldsymbol{F}^{-T}) = \frac{\partial}{\partial\boldsymbol{F}}(J\boldsymbol{F}^{-T}) : \delta\boldsymbol{F}$ can readily be computed directly. That leaves the task of computing $\delta\boldsymbol{R}$.

$$
\begin{aligned}
\delta\boldsymbol{F} &= \delta\boldsymbol{R}\boldsymbol{S} + \boldsymbol{R}\delta\boldsymbol{S} \\
\boldsymbol{R}^T\delta\boldsymbol{F} &= (\boldsymbol{R}^T\delta\boldsymbol{R})\boldsymbol{S} + \delta\boldsymbol{S} \\
\boldsymbol{R}^T\delta\boldsymbol{F} - \delta\boldsymbol{F}^T\boldsymbol{R} &= (\boldsymbol{R}^T\delta\boldsymbol{R})\boldsymbol{S} + \boldsymbol{S}(\boldsymbol{R}^T\delta\boldsymbol{R})
\end{aligned}
$$

Here we have taken advantage of the symmetry of $\delta\boldsymbol{S}$ and the skew symmetry of $\boldsymbol{R}^T\delta\boldsymbol{R}$. There are three independent components of $\boldsymbol{R}^T\delta\boldsymbol{R}$, which we can solve for directly. The equation is linear in these components, so $\boldsymbol{R}^T\delta\boldsymbol{R}$ can be computed by solving a 3×3 system. Finally, $\delta\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{R}^T\delta\boldsymbol{R})$.