Tech report: augmented MPM for phase-change and varied materials

For our constitutive model we use $\hat{\Psi}_\mu(\boldsymbol{F}) = \Psi_\mu(J^{-\frac{1}{d}}\boldsymbol{F})$, where plasticity does not matter and is ignored for the purposes of computing these derivatives. For convenience, let $a = -\frac{1}{d}$, and μ subscripts are ignored. Then, $\hat{\Psi}(\boldsymbol{F}) = \Psi(J^a\boldsymbol{F})$. We begin by computing $\hat{\Psi}_\mu(\boldsymbol{F})$. We will use index notation for precision during the derivations. Differentiation by the matrix $\boldsymbol{F}_{ij}$ is indicated by enclosing the index pair in parenthesis after a comma, as in $J_{,(ij)}$. Let $\boldsymbol{H} = \boldsymbol{F}^{-T}$. We begin with some preliminary derivatives for J and $\boldsymbol{H}$.

$$\begin{aligned}
H_{ji}F_{jk} &= \delta_{ik} \\
J_{,(ij)} &= JH_{ij} \\
(J^a)_{,(ij)} &= aJ^{a-1}J_{,(ij)} \\
&= aJ^{a-1}JH_{ij} \\
&= aJ^aH_{ij} \\
(H_{ji}F_{jk})_{,(rs)} &= 0 \\
H_{ji,(rs)}F_{jk} + H_{ji}F_{jk,(rs)} &= 0 \\
H_{ji,(rs)}F_{jk} &= -H_{ji}F_{jk,(rs)} \\
H_{ji,(rs)}\delta_{jm} &= -H_{ji}\delta_{jr}\delta_{ks}H_{mk} \\
H_{ji,(rs)} &= -H_{ri}H_{js}
\end{aligned}$$

The derivatives of the quantity $J^a\boldsymbol{F}$ will occur frequently, so we begin by naming them and evaluating them.

$$\begin{aligned}
\mathcal{B}_{kmij} &= (J^aF_{km})_{,(ij)} \\
&= J^aF_{km,(ij)} + (J^a)_{,(ij)}F_{km} \\
&= J^a\delta_{ik}\delta_{jm} + aJ^aF_{km}H_{ij} \\
\mathcal{B}_{kmij}Z_{ij} &= J^a\delta_{ik}\delta_{jm}Z_{ij} + aJ^aF_{km}H_{ij}Z_{ij} \\
\mathcal{B}_{kmij}Z_{ij} &= J^aZ_{km} + aJ^aF_{km}H_{ij}Z_{ij} \\
\mathcal{B} : \boldsymbol{Z} &= J^a(\boldsymbol{Z} + a(\boldsymbol{H} : \boldsymbol{Z})\boldsymbol{F}) \\
Z_{km}\mathcal{B}_{kmij} &= J^a\delta_{ik}\delta_{jm}Z_{km} + aJ^aF_{km}H_{ij}Z_{km} \\
Z_{km}\mathcal{B}_{kmij} &= J^aZ_{ij} + aJ^aF_{km}Z_{km}H_{ij} \\
\boldsymbol{Z} : \mathcal{B} &= J^a(\boldsymbol{Z} + a(\boldsymbol{F} : \boldsymbol{Z})\boldsymbol{H}) \\
\mathcal{B}_{kmij,(rs)} &= (J^a(\delta_{ik}\delta_{jm} + aF_{km}H_{ij}))_{,(rs)} \\
\mathcal{B}_{kmij,(rs)} &= (J^a)_{,(rs)}(\delta_{ik}\delta_{jm} + aF_{km}H_{ij}) + J^a(\delta_{ik}\delta_{jm} + aF_{km}H_{ij})_{,(rs)} \\
\mathcal{B}_{kmij,(rs)} &= aJ^aH_{rs}(\delta_{ik}\delta_{jm} + aF_{km}H_{ij}) + aJ^a(F_{km,(rs)}H_{ij} + F_{km}H_{ij,(rs)}) \\
\mathcal{B}_{kmij,(rs)} &= a\mathcal{B}_{kmij}H_{rs} + aJ^a(\delta_{kr}\delta_{ms}H_{ij} - F_{km}H_{rj}H_{is})
\end{aligned}$$

With the operator $\mathcal{B}$, we can express the relationship between $\hat{\boldsymbol{A}} = \frac{\partial \hat{\Psi}}{\partial \boldsymbol{F}}(\boldsymbol{F})$ and $\boldsymbol{A} = \frac{\partial \Psi}{\partial \boldsymbol{F}}(J^a \boldsymbol{F})$.

$$\begin{aligned} \hat{\Psi}(F_{ij}) &= \Psi(J^a F_{ij}) \\ \hat{\Psi}_{,(ij)} &= \Psi_{,(km)}(J^a F_{km})_{,(ij)} \\ &= \Psi_{,(km)}\mathcal{B}_{kmij} \\ \hat{\boldsymbol{A}} &= \boldsymbol{A} : \mathcal{B} \end{aligned}$$

Finally, we relate $\mathcal{C} = \frac{\partial^2 \Psi}{\partial \boldsymbol{F} \partial \boldsymbol{F}}(J^a \boldsymbol{F})$ to $\hat{\mathcal{C}} = \frac{\partial^2 \hat{\Psi}}{\partial \boldsymbol{F} \partial \boldsymbol{F}}(\boldsymbol{F})$.

$$\begin{aligned} \hat{\Psi}_{,(ij)(rs)} &= (\Psi_{,(km)}\mathcal{B}_{kmij})_{,(rs)} \\ \hat{\Psi}_{,(ij)(rs)} &= \Psi_{,(km)(tu)}\mathcal{B}_{turs}\mathcal{B}_{kmij} + \Psi_{,(km)}\mathcal{B}_{kmij,(rs)} \\ \hat{\Psi}_{,(ij)(rs)} &= \Psi_{,(km)(tu)}\mathcal{B}_{turs}\mathcal{B}_{kmij} + a\Psi_{,(km)}\mathcal{B}_{kmij}H_{rs} + aJ^a\Psi_{,(rs)}H_{ij} - aJ^a\Psi_{,(km)}F_{km}H_{rj}H_{is} \\ \hat{\Psi}_{,(ij)(rs)}Z_{rs} &= \Psi_{,(km)(tu)}\mathcal{B}_{turs}\mathcal{B}_{kmij}Z_{rs} + a\Psi_{,(km)}\mathcal{B}_{kmij}H_{rs}Z_{rs} + aJ^a\Psi_{,(rs)}H_{ij}Z_{rs} - aJ^a\Psi_{,(km)}F_{km}H_{rj}H_{is}Z_{rs} \\ \hat{\mathcal{C}} : \boldsymbol{Z} &= (\mathcal{C} : (\mathcal{B} : \boldsymbol{Z})) : \mathcal{B} + a(\boldsymbol{H} : \boldsymbol{Z})\boldsymbol{A} : \mathcal{B} + aJ^a(\boldsymbol{A} : \boldsymbol{Z})\boldsymbol{H} - aJ^a(\boldsymbol{A} : \boldsymbol{F})\boldsymbol{H}\boldsymbol{Z}^T\boldsymbol{H} \end{aligned}$$