Deformation Extrapolation for Improved Initial Predictors in the `imitor` Finite Element Code

Omar Hafez

Background

This document serves to implement the work of Rashid[1] into the `imitor` code base. The basic premise of that work is to improve upon initial predictors for displacements in the solution of large deformation problems. The standard approach of extrapolating based on a constant velocity field is replaced by extrapolation based on constant stretch and rotation rates. The deformation gradient produced from this extrapolation does not in general create a compatible displacement field. Thus, a quadratic functional must be minimized to calculate the improved initial guess, which is fed into the iterative solution process of finding a zero residual. The entire process is explained in an updated Lagrange framework. The `imitor` code, however, is implemented in a total Lagrange sense. This document lays out the steps from Rashid to be implemented in the total Lagrange finite element code `imitor`.

[1] M. M. Rashid, Deformation extrapolation and initial predictors in large-deformation finite element analysis, Computational Mechanics 16, pp. 281-289, 1995

Deformation gradient extrapolation method

Wish to extrapolate from t^{k-1} to t^{k+1}, subject to boundary conditions on $\partial\kappa^{k-1}$ evaluated at t^{k+1}. In the following, $\hat{(\cdot)}$ denotes deformation from t^{k-1} to t^k, $\overline{(\cdot)}$ denotes deformation from t^{k-1} to t^{k+1}. Superscripts in general imply an evaluation at that time step. Summation convention enforced.

$$\text{Given: } \hat{\mathbf{u}}_a,\ \mathbf{u}_a^k,\ \ \hat{\mathbf{R}},\ \ (t^k - t^{k-1})\mathbf{D} \tag{1}$$

$$F_{ij}^k = \delta_{ij} + u_{ia}^k \frac{\partial N_a}{\partial X_j} \tag{2}$$

$$F_{ij}^{k-1} = F_{ij}^k - \hat{u}_{ia} \frac{\partial N_a}{\partial X_j} \tag{3}$$

$$\hat{\mathbf{F}}^{-1} = \mathbf{F}^{k-1}(\mathbf{F}^k)^{-1} \tag{4}$$

$$\mathbf{D} = \frac{(t^k - t^{k-1})\mathbf{D}}{(t^k - t^{k-1})} \tag{5}$$

$$\overline{\mathbf{U}} = \mathbf{I} + (t^{k+1} - t^{k-1})\mathbf{D} + \frac{1}{2}(t^{k+1} - t^{k-1})^2\mathbf{D}^2 \tag{6}$$

$$\sin\hat{\theta} = \frac{1}{2}(\hat{R}_{ij}\hat{R}_{ij} - \hat{R}_{ij}\hat{R}_{ji})^{1/2} \tag{7}$$

$$\text{if } \sin\hat{\theta} = 0 \ \rightarrow\ \mu_i = 0, \quad \text{else } \rightarrow\ \mu_i = \frac{-1}{2\sin\hat{\theta}}\epsilon_{ijk}\hat{R}_{jk} \tag{8}$$

$$\hat{\theta} = \sin^{-1}(\sin\hat{\theta}) \tag{9}$$

$$\text{if } \operatorname{tr}\hat{\mathbf{F}}^{-1} - 1 < 0 \ \rightarrow\ \hat{\theta} = \pi - \hat{\theta} \tag{10}$$

$$\bar{\theta} = \frac{t^{k+1} - t^{k-1}}{t^k - t^{k-1}}\hat{\theta} \tag{11}$$

$$\overline{R}_{ij} = \delta_{ij} + (1 - \cos\bar{\theta})(\mu_i\mu_j - \delta_{ij}) - \sin\bar{\theta}\epsilon_{ijk}\mu_k \tag{12}$$

$$\overline{\mathbf{F}} = \overline{\mathbf{R}}\overline{\mathbf{U}} \tag{13}$$

Enforcing compatible displacement field

Define $\mathbf{G}$ as

$$\mathbf{G} = (\mathbf{I} + \frac{\partial \bar{\mathbf{u}}}{\partial \mathbf{X}^{k-1}})\bar{\mathbf{F}}^{-1} \tag{14}$$

Constrained minimization problem may be stated as follows: find $\bar{\mathbf{u}}(\mathbf{X}^{k-1})$, $\mathbf{X}^{k-1} \in \kappa^{k-1}$, such that

$$I = \int_{\kappa^{k-1}} \left[(1-\rho/2)\mathrm{tr}\mathbf{G}^T\mathbf{G} + (3\rho/2-1)\mathrm{tr}\mathbf{G}^2 - 2\rho\,\mathrm{tr}\mathbf{G} + 3\rho\right] dV^{k-1} \tag{15}$$

is a minimum, where $\bar{\mathbf{u}}(\mathbf{X}^{k-1})$ satisfies any displacement boundary conditions on $\partial\kappa^{k-1}$ prescribed at time t^{k+1}. Define $R = 1 - \cos\bar{\theta}$ and $S = \mathrm{tr}[(\bar{\mathbf{U}} - \mathbf{I})^2]$. Define ρ as

$$\rho = \frac{2}{\pi}\sin^{-1}\frac{S}{\sqrt{R^2+S^2}} \tag{16}$$

$$\text{if } \rho < 0.1 \;\rightarrow\; \rho = 0.1 \tag{17}$$

$$\text{if } \rho > 0.9 \;\rightarrow\; \rho = 0.9 \tag{18}$$

It can be shown that if $\bar{\mathbf{F}}^{-1}$ is compatible, i.e., $\mathbf{G} = \mathbf{I}$, that the functional $I = 0$, and further that if $I > 0$ for any perturbation of $\mathbf{G}$ from $\mathbf{I}$.

Finite element implementation

Updated Lagrange

Define $\bar{\mathbf{u}} = \bar{\mathbf{u}}_a \phi_a$ on κ^{k-1}, $\mathbf{B}_a \equiv \frac{\partial \phi_a}{\partial \mathbf{X}^{k-1}}$. The tensor $\mathbf{G}$ then becomes

$$\mathbf{G} = \bar{\mathbf{F}}^{-1} + \bar{\mathbf{u}}_a \otimes \mathbf{B}_a \bar{\mathbf{F}}^{-1} \tag{19}$$

Define $\mathbf{A}_a = \bar{\mathbf{F}}^{-T}\mathbf{B}_a$. We then set the derivative of I with respect to free components of $\bar{u}_a$ to zero, i.e., $\frac{\partial I}{\partial \bar{\mathbf{u}}_b} = 0$. The boundaries do not depend on $\bar{u}_{ja}$, so the derivative may be brought inside the integral. Also, it is noted that ρ is not a function of $\bar{\mathbf{u}}_b$.

Upon setting derivatives to zero, the following equation results:

$$\left\{ \int_{\kappa^{k-1}} \left[(2-\rho)(\mathbf{A}_a \cdot \mathbf{A}_b)\mathbf{I} + (3\rho - 2)\mathbf{A}_a \otimes \mathbf{A}_b\right] dV^{k-1} \right\} \bar{\mathbf{u}}_a \tag{20}$$

$$= \int_{\kappa^{k-1}} \left[2\rho \mathbf{A}_b - (2-\rho)\bar{\mathbf{F}}^{-1}\mathbf{A}_b - (3\rho-2)\bar{\mathbf{F}}^{-T}\mathbf{A}_b\right] dV^{k-1} \tag{21}$$

$$\tag{22}$$

or

$$\mathbf{K}_{ba}\bar{\mathbf{u}}_a = \mathbf{f}_b \tag{23}$$

which holds for all nodes b. If we define prescribed displacement BCs as $\tilde{u}_{yz}$, we solve for unknowns $\bar{u}_{ja}$ using the equation:

$$K_{ibja}\bar{u}_{ja} = f_{ib} - K_{ibyz}\tilde{u}_{yz} \tag{24}$$

where summation over direction y for node z applies only for the nodal displacements that are prescribed.

Total Lagrange

Define $\bar{\mathbf{u}} = \bar{\mathbf{u}}_a \phi_a$ on κ, and

$$B_{ia} \equiv \frac{\partial \phi_a}{\partial X_i^{k-1}} = \frac{\partial \phi_a}{\partial X_j}\frac{\partial X_j}{\partial X_i^{k-1}} \tag{25}$$

$$= \frac{\partial \phi_a}{\partial X_j} F_{ji}^{k-1} \tag{26}$$

Or equivalently, $\mathbf{B}_a \equiv (\mathbf{F}^{k-1})^{-T}\frac{\partial \phi_a}{\partial \mathbf{X}}$. $\mathbf{G}$ and $\mathbf{A}_a$ are formed exactly as before.

In general, when integrating the integrand $h(\mathbf{X})$, the following relationship holds:

$$\int_{\kappa^{k-1}} h(\mathbf{X}^{k-1})\ dV^{k-1} = \int_{\kappa} h(\mathbf{X})\ \det\mathbf{F}^{k-1}\ dV \tag{27}$$

After a change of integration variables, where the integrand is now integrated over the reference configuration body:

$$\left\{\int_{\kappa} \left[(2-\rho)(\mathbf{A}_a \cdot \mathbf{A}_b)\mathbf{I} + (3\rho-2)\mathbf{A}_a \otimes \mathbf{A}_b\right] \det\mathbf{F}^{k-1} dV \right\} \bar{\mathbf{u}}_a \tag{28}$$

$$= \int_{\kappa} \left[2\rho\mathbf{A}_b - (2-\rho)\bar{\mathbf{F}}^{-1}\mathbf{A}_b - (3\rho-2)\bar{\mathbf{F}}^{-T}\mathbf{A}_b\right] \det\mathbf{F}^{k-1} dV \tag{29}$$

For the purposes of implementation into `imitor`, the integration points correspond to material points regardless of the configuration of the body, so this essentially amounts to multiplying the integrand for each integration point by $\det\mathbf{F}^{k-1}$.

Once again, after handling of prescribed displacement BCs, the final system to be solved is:

$$K_{ibja}\bar{u}_{ja} = f_{ib} - K_{ibyz}\tilde{u}_{yz} \tag{30}$$

Again, summation over direction y for node z applies only for the nodal displacements that are prescribed.

Finally, once the displacements are solved, the initial guess is assigned as $\hat{\mathbf{u}}_a = \bar{\mathbf{u}}_a - \hat{\mathbf{u}}_a$ to all free DOFs, while prescribed displacements are assigned directly.