PRISMS-PF Application Formulation: eshelbyInclusion

This example application implements a simple 3D calculation of the displacement field near a homogenous inclusion.
Consider a strain energy expression of the form:

$$\Pi(\varepsilon) = \int_{\Omega} \frac{1}{2}(\epsilon - \epsilon^0) : C : (\epsilon - \epsilon^0) \ dV \tag{1}$$

where ε is the infinitesimal strain tensor, $C_{ijkl} = \lambda \delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$ is the fourth order elasticity tensor and (λ, mu) are the Lame parameters.

1 Governing equations

Considering variations on the displacement u of the from $u + \alpha w$, we have

$$\delta\Pi = \frac{d}{d\alpha} \int_{\Omega} \frac{1}{2} [\epsilon(u + \alpha w) - \epsilon^0] : C : [\epsilon(u + \alpha w) - \epsilon^0] \ dV \bigg|_{\alpha=0} \tag{2}$$

$$= - \int_{\Omega} \nabla w : C : (\epsilon - \epsilon^0) \ dV + \int_{\partial\Omega} w \cdot [C : (\epsilon - \epsilon^0) \cdot n] \ dS \tag{3}$$

$$= - \int_{\Omega} \nabla w : \sigma \ dV + \int_{\partial\Omega} w \cdot (\sigma \cdot n) \ dS \tag{4}$$

$$= - \int_{\Omega} \nabla w : \sigma \ dV + \int_{\partial\Omega} w \cdot t \ dS \tag{5}$$

where $\sigma = C : (\epsilon - \epsilon^0)$ is the stress tensor, ϵ^0 is the misfit strain (eigenstrain), and $t = \sigma \cdot n$ is the surface traction. In this case, we assume that the diagonal elements of ϵ^0 take the form:

$$\epsilon^0_{ii} = m \left(\frac{1}{2} + \frac{1}{2} \tanh(l(r - a)) \right) \tag{6}$$

where m is the magnitide of the misfit strain inside the inclusion, l determines the thickness of the "interface" between the inclusion and the matrix, r is the distance from the origin, and a is the radius of the inclusion. The off-diagonal elements of ϵ^0 are zero.

The minimization of the variation, $\delta\Pi = 0$, gives the weak formulation of the governing equation of mechanics:

$$\int_{\Omega} \nabla w : \sigma \ dV - \int_{\partial\Omega} w \cdot t \ dS = 0 \tag{7}$$

If surface tractions are zero:

$$R = \int_{\Omega} \nabla w : \sigma \ dV = 0 \tag{8}$$

2 Residual expressions

In PRISMS-PF, two sets of residuals are required for elliptic PDEs (such as this one), one for the left-hand side of the equation (LHS) and one for the right-hand side of the equation (RHS). We solve $R = 0$ by casting this in a form that can be solved as a matrix inversion problem. This will involve a brief detour into the discretized form of the equation. First we derive an expression for the solution, given an initial guess, u_0:

$$0 = R(u) = R(u_0 + \Delta u) \tag{9}$$

where $\Delta u = u - u_0$. Then, applying the discretization that $u = \sum_i w^i U^i$, we can write the following linearization:

$$\frac{\delta R(u)}{\delta u} \Delta U = -R(u_0) \tag{10}$$

The discretized form of this equation can be written as a matrix inversion problem. However, in PRISMS-PF, we only care about the product $\frac{\delta R(u)}{\delta u} \Delta U$. Taking the variational derivative of $R(u)$ yields:

$$\frac{\delta R(u)}{\delta u} = \frac{d}{d\alpha} \int_\Omega \nabla w : C : \left[\epsilon(u + \alpha w) - \epsilon^0\right] \ dV \Bigg|_{\alpha=0} \tag{11}$$

$$= \int_\Omega \nabla w : C : \frac{1}{2} \frac{d}{d\alpha} \left[\nabla(u + \alpha w) + \nabla(u + \alpha w)^T - \epsilon^0\right] \ dV \Bigg|_{\alpha=0} \tag{12}$$

$$= \int_\Omega \nabla w : C : \frac{d}{d\alpha} \left[\nabla(u + \alpha w) - \epsilon^0\right] \ dV \Bigg|_{\alpha=0} \quad \textit{(due to the symmetry of C)} \tag{13}$$

$$= \int_\Omega \nabla w : C : \nabla w \ dV \tag{14}$$

In its discretized form $\frac{\delta R(u)}{\delta u} \Delta U$ is:

$$\frac{\delta R(u)}{\delta u} \Delta U = \sum_i \sum_j \int_\Omega \nabla N^i : C : \nabla N^j dV \ \Delta U^j \tag{15}$$

Moving back to the non-discretized form yields:

$$\frac{\delta R(u)}{\delta u} \Delta U = \int_\Omega \nabla w : C : \nabla(\Delta u) dV \tag{16}$$

Thus, the full equation relating u_0 and Δu is:

$$\int_\Omega \nabla w : \underbrace{C : \nabla(\Delta u)}_{r_{ux}^{LHS}} dV = -\int_\Omega \boldsymbol{\nabla} w : \underbrace{\sigma}_{r_{ux}} \ dV \tag{17}$$

The above values of r_{ux}^{LHS} and r_{ux} are used to define the residuals in the following input file:
$applications/eschelbyInclusion/equations.h$