

PRISMS-PF

Mechanics (Infinitesimal Strain)

Consider a elastic free energy expression of the form:

$$\Pi(\varepsilon) = \int_{\Omega} \frac{1}{2} \varepsilon : C : \varepsilon \, dV - \int_{\partial\Omega} u \cdot t \, dS \quad (1)$$

where ε is the infinitesimal strain tensor, given by $\varepsilon = \frac{1}{2}(\nabla u + \nabla u^T)$, $C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$ is the fourth order elasticity tensor, (λ, μ) are the Lamé parameters, u is the displacement, and t is the surface traction.

1 Governing equation

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

$$\delta\Pi = \frac{d}{d\alpha} \left(\int_{\Omega} \frac{1}{2} \varepsilon(u + \alpha w) : C : \varepsilon(u + \alpha w) \, dV - \int_{\partial\Omega} u \cdot t \, dS \right) \Big|_{\alpha=0} \quad (2)$$

$$= \int_{\Omega} \nabla w : C : \varepsilon \, dV - \int_{\partial\Omega} w \cdot t \, dS \quad (3)$$

$$= \int_{\Omega} \nabla w : \sigma \, dV - \int_{\partial\Omega} w \cdot t \, dS \quad (4)$$

where $\sigma = C : \varepsilon$ is the stress tensor and $t = \sigma \cdot n$ is the surface traction.

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

$$\int_{\Omega} \nabla w : \sigma \, dV - \int_{\partial\Omega} w \cdot t \, dS = 0 \quad (5)$$

If surface tractions are zero:

$$R = \int_{\Omega} \nabla w : \sigma \, dV = 0 \quad (6)$$

2 Terms for Input into PRISMS-PF

In PRISMS-PF, two sets of terms 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 :

$$0 = R(u) = R(u_0 + \Delta u) \quad (7)$$

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

$$\frac{\delta R(u)}{\delta u} \Delta U = -R(u_0) \quad (8)$$

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:

$$\frac{\delta R(u)}{\delta u} = \frac{d}{d\alpha} \int_{\Omega} \nabla w : C : \epsilon(u + \alpha w) dV \Big|_{\alpha=0} \quad (9)$$

$$= \int_{\Omega} \nabla w : C : \frac{1}{2} \frac{d}{d\alpha} [\nabla(u + \alpha w) + \nabla(u + \alpha w)^T] dV \Big|_{\alpha=0} \quad (10)$$

$$= \int_{\Omega} \nabla w : C : \frac{d}{d\alpha} \nabla(u + \alpha w) dV \Big|_{\alpha=0} \quad (\text{due to the symmetry of } C) \quad (11)$$

$$= \int_{\Omega} \nabla w : C : \nabla w dV \quad (12)$$

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

$$\frac{\delta R(u)}{\delta u} \Delta U = \sum_i \sum_j \int_{\Omega} \nabla N^i : C : \nabla N^j dV \Delta U^j \quad (13)$$

Moving back to the non-discretized form yields:

$$\frac{\delta R(u)}{\delta u} \Delta U = \int_{\Omega} \nabla w : C : \nabla(\Delta u) dV \quad (14)$$

Thus, the full equation relating u_0 and Δu is:

$$\int_{\Omega} \nabla w : \underbrace{C : \nabla(\Delta u)}_{r_{ux}^{LHS}} dV = - \int_{\Omega} \nabla w : \underbrace{\sigma}_{r_{ux}} dV \quad (15)$$

The above values of r_{ux}^{LHS} and r_{ux} are used to define the equation terms in the following input file:

`applications/mechanics/equations.cc`