The minimization problem is generically defined as **[ABT: place-holder; needs constraints etc.]**

$$\underset{\text{admissible } \omega}{\operatorname{argmin}} \; J(\omega), \tag{1}$$

where J is some deviation metric on the micro structure. Letting S denote the compliance tensor, we choose

$$J(\omega) = \frac{1}{2}\|S^H(\omega) - S^*\|_F^2, \tag{2}$$

for a microstructure with shape ω. There are several other possible choices for the objective functional J, such as deviation of elasticity tensor or error in displacement. In our setting, we are interested in a particular deformation response and compliance becomes the natural measure in this context **[ABT: justify why not displacement itself]**. A nice side effect of defining J as in Eq. (2) is that J is self-adjoint and as a result the shape derivative will have a simple form.

The microstructure boundary $\partial\omega$ is parameterized by a vector $\mathbf{p}$, consisting of, for instance, wire mesh node offsets and thicknesses. The variation of $\partial\omega$ with respect to $\mathbf{p}$

$$\mathbf{v}_{p_\alpha}(\mathbf{y}, \mathbf{p}) = \frac{\partial \mathbf{y}}{\partial p_\alpha} \quad \text{for } \mathbf{y} \in \partial\omega. \tag{3}$$

(with proper assumptions) defines perturbation velocity fields over the boundary. Using $\mathbf{p}$ the minimization problem can be written as

$$\underset{\text{admissible } \mathbf{p}}{\operatorname{argmin}} \; J(\mathbf{p}) \text{ where } J(\mathbf{p}) = \frac{1}{2}\|S^H(\mathbf{p}) - S^*\|_F^2. \tag{4}$$

The derivative of the objective function is then

$$\frac{\partial J}{\partial p_\alpha} = \left[S^H - S^*\right]_{ijkl} \frac{\partial S^H_{ijkl}}{\partial p_\alpha}. \tag{5}$$

The derivative of C^H_{ijkl} with respect to parameter p_a is just $\mathrm{d}C^H_{ijkl}$ evaluated on the $\mathbf{v}_{p_a}$ velocity field. Thus, we can compute the derivative of each homogenized coefficient with respect to each parameter p_a provided that we know the normal velocity scalar field induced by changing p_a, $\mathbf{v}_{p_a} \cdot \hat{\mathbf{n}}$.

In finding a solution to Eq. (4), the shape derivative of a homogenized elasticity tensor is required. The shape derivative of the elasticity tensor for microstructure with shape ω and perturbation $\mathbf{v}$ is defined as the Gâteaux derivative [1]

$$\mathrm{d}C^H[\mathbf{v}] := \lim_{t \downarrow 0} \frac{C^H((1 + t\mathbf{v})\omega) - C^H(\omega)}{t}, \tag{6}$$

where $(1 + t\mathbf{v})\omega := \{\mathbf{x} + t\mathbf{v} : \mathbf{x} \in \omega\}$.

The homogenized elasticity tensor **[ABT: give ref]**, with a bit of manipulation, can be rewritten in the energy form as

$$C^H_{ijkl} = \frac{1}{|Y|}\int_\omega (\mathbf{e}^{ij} + \varepsilon(\mathbf{w}^{ij})) : C^{\text{base}} : (\mathbf{e}^{kl} + \varepsilon(\mathbf{w}^{kl}))\,\mathrm{d}\mathbf{y}. \tag{7}$$

Using this form, the shape derivative of C^H can be readily written as

$$\begin{aligned}\mathrm{d}C^H_{ijkl}[\mathbf{v}] = \frac{1}{|Y|}\int_{\partial\omega} [(\mathbf{e}^{ij} + \varepsilon(\mathbf{w}^{ij})) : C^{\text{base}} \\ : (\mathbf{e}^{kl} + \varepsilon(\mathbf{w}^{kl}))](\mathbf{v} \cdot \hat{\mathbf{n}})\,\mathrm{d}A(\mathbf{y}).\end{aligned} \tag{8}$$

Discretization. If linear finite elements are used, (8) is particularly easy to compute. The energy density term is constant on each boundary element and can be stored as a per-boundary-element tensor C^e_{ijkl}. Then the integral can be computed as:

$$\frac{\partial C^H_{ijkl}}{\partial p_\alpha} = \sum_\alpha \frac{1}{|Y|} C^e_{ijkl} \int_e \mathbf{v}_{p_\alpha} \cdot \hat{\mathbf{n}}\,\mathrm{d}A(\mathbf{y}). \tag{9}$$

If higher order elements are used, we can still approximate either the energy density term or the normal velocity field as piecewise constant. However, to compute the integral exactly requires quadrature over each boundary element.

Computing the compliance tensor. We perform the computation on the flattened tensor representation. Letting F denote the flattening operator **[ABT: needs def]**, the derivative of the compliance tensor $S = C^{-1}$ is given by

$$\frac{\partial S}{\partial p_\alpha} = -S : \frac{\partial F(C)}{\partial p_\alpha} : S. \tag{10}$$

[ABT: check correctness with Julian]

References

[1] JEAN-P Zolésio and MC Delfour. Shapes and geometries: Analysis, differential calculus and optimization. *SIAM, Philadelphia*, 2001.