Worst-Case Stress Relief for Microstructures
Supplementary Material

This document presents detailed derivations of several formulas used in the paper.

1 Shape derivative for model problem

We illustrate the inaccuracy of the traditional formula for shape derivatives in a simpler setting:

$$J(\omega) = \int_\omega j(\nabla u)\ \mathrm{d}\mathbf{x} \qquad \text{where } u \text{ solves } \begin{aligned} -\nabla \cdot (\nabla u + g) &= 0 \text{ in } \omega \\ \mathbf{n} \cdot (\nabla u + g) &= 0 \text{ on } \partial\omega. \end{aligned}$$

Later, we will need the weak form of the constraint PDE:

$$\int_\omega \nabla\phi \cdot (\nabla u + g)\ \mathrm{d}\mathbf{x} = 0 \quad \forall \text{ trial functions } \phi. \tag{A1}$$

Here, g is analogous to the macroscopic strain applied in homogenization.

Computing $\mathrm{d}J[\mathbf{v}]$ in terms of the Eulerian derivative, $\dot{u}$. We seek an expression for $\mathrm{d}J[\mathbf{v}]$, J's initial rate of change as ω is perturbed by velocity field $\mathbf{v}$ into altered shape ω_t. We do this by applying Reynolds Transport Theorem to J, showing a step-by-step derivation of the theorem. Our approach is to express all quantities on the unperturbed reference domain, ω, and then differentiate with respect to "time" t:

$$\mathrm{d}J[\mathbf{v}] \overset{\text{def}}{=} \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \int_{\omega_t} j(\nabla_t u_t)\ \mathrm{d}\mathbf{x}_t = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \int_\omega j(F_t^{-T}\nabla\hat{u}_t)\det(F_t)\ \mathrm{d}\mathbf{x},$$

where $\mathbf{x}_t = \mathbf{x} + t\mathbf{v}$ and ∇_t are the spatial variable and gradient for the perturbed domain, ω_t. We have defined state function u_t on ω_t in terms of function $\hat{u}_t$ defined on the reference domain ($u_t(\mathbf{x}_t) = \hat{u}(\mathbf{x}_t - t\mathbf{v})$). Finally, $F_t = I + t\nabla\mathbf{v}$ is the Jacobian of the mapping from ω to ω_t; it is used to re-express the perturbed domain's gradient operator and volume element in terms of the reference domain quantities.

Now that the integration domain is fixed, we can move the time derivative inside to compute:

$$\mathrm{d}J[\mathbf{v}] = \int_\omega (j') \cdot \left(-(\nabla\mathbf{v})^T\nabla u + \nabla \left.\frac{\partial \hat{u}_t}{\partial t}\right|_{t=0} \right) + j(\nabla u)\nabla\cdot\mathbf{v}\ \mathrm{d}\mathbf{x}, \tag{A2}$$

using the identities $\left.\frac{\partial}{\partial t}\right|_{t=0}(I+\nabla\mathbf{v})^{-T} = -(\nabla\mathbf{v})^T$, $\left.\frac{\partial}{\partial t}\right|_{t=0}\det(I+\nabla\mathbf{v}) = \nabla\cdot\mathbf{v}$, and $\hat{u}_0 = u$. Here, $\left.\frac{\partial\hat{u}_t}{\partial t}\right|_{t=0}$ is the *material derivative* at time $t=0$. We denote it by δu and note its relationship to the Eulerian derivative $\dot{u} \overset{\text{def}}{=} \left.\frac{\partial u_t}{\partial t}\right|_{t=0} = \delta u - \nabla u \cdot \mathbf{v}$. The material derivative's gradient can therefore be written as:

$$\nabla\delta u = \nabla\dot{u} + \nabla(\nabla u\cdot\mathbf{v}) = \nabla\dot{u} + (\mathbf{v}\cdot\nabla)\nabla u + (\nabla\mathbf{v})^T\nabla u. \tag{A3}$$

We use this relationship to simplify (A2). Substituting the rightmost expression for $\nabla\left.\frac{\partial\hat{u}_t}{\partial t}\right|_{t=0}$:

$$\mathrm{d}J[\mathbf{v}] = \int_\omega (j')\cdot\Big(\nabla\dot{u} + (\mathbf{v}\cdot\nabla)\nabla u\Big) + j(\nabla u)\nabla\cdot\mathbf{v}\ \mathrm{d}\mathbf{x}.$$

Finally, we apply the integration by parts $\int_\omega (j)\nabla\cdot\mathbf{v}\ \mathrm{d}\mathbf{x} = -\int_\omega(\mathbf{v}\cdot\nabla)j\ \mathrm{d}\mathbf{x} + \int_{\partial\omega}(j)\mathbf{v}\cdot\mathbf{n}\ \mathrm{d}A(\mathbf{x})$ to arrive at the simplified formula by cancellation:

$$\boxed{\mathrm{d}J[\mathbf{v}] = \int_\omega j'(\nabla u)\cdot\nabla\dot{u}\ \mathrm{d}\mathbf{x} + \int_{\partial\omega} j(\nabla u)\mathbf{v}\cdot\mathbf{n}\ \mathrm{d}A(\mathbf{x}).} \tag{A4}$$

Solving for $\dot{u}$. Formula (A4) requires $\dot{u}$, which we find by differentiating both sides of the constraint's weak form, (A1). We do this using a second step-by-step application of Reynolds Transport Theorem (first re-expressing the weak form for ω_t on reference domain ω):

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} \int_\omega (F_t^{-T} \nabla \phi) \cdot (F_t^{-T} \nabla \hat{u}_t + g) \det(F_t) \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi,$$

and manipulating this equation into a PDE for $\dot{u}$. Here, we defined shape functions on the perturbed domain by evaluating ω's shape functions, ϕ, at the material coordinates; in the discrete setting, this definition coincides with the shape functions one would construct on the perturbed finite element mesh (without remeshing). Following the same steps as for differentiating J, we obtain:

$$\int_\omega -\big((\nabla \mathbf{v})^T \nabla \phi\big) \cdot (\nabla u + g) - \nabla \phi \cdot (\nabla \mathbf{v})^T \nabla u + \nabla \phi \cdot \nabla \delta u + \nabla \phi \cdot (\nabla u + g) \nabla \cdot \mathbf{v} \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi. \tag{A5}$$

We apply (A3) to express this as an equation for $\dot{u}$:

$$\int_\omega \nabla \phi \cdot \Big(- \nabla \mathbf{v} (\nabla u + g) - \cancel{(\nabla \mathbf{v})^T \nabla u} + \big[\nabla \dot{u} + (\mathbf{v} \cdot \nabla) \nabla u + \cancel{(\nabla \mathbf{v})^T \nabla u}\big] + (\nabla u + g) \nabla \cdot \mathbf{v} \Big) \, \mathrm{d}\mathbf{x} = 0 \quad \forall \phi.$$

Applying integration by parts to the last integrand, the left-hand side becomes:

$$\int_\omega \nabla \phi \cdot \Big(- \nabla \mathbf{v} (\nabla u + g) + \nabla \dot{u} + (\mathbf{v} \cdot \nabla) \nabla u \Big) - (\mathbf{v} \cdot \nabla) \Big(\nabla \phi \cdot (\nabla u + g) \Big) \, \mathrm{d}\mathbf{x} + \int_{\partial \omega} \nabla \phi \cdot (\nabla u + g)(\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A(\mathbf{x})$$

Simplifying, we arrive at the PDE for $\dot{u}$ in weak form:

$$- \underbrace{\int_\omega \nabla (\nabla \phi \cdot \mathbf{v}) \cdot (\nabla u + g) \, \mathrm{d}\mathbf{x}}_{I} + \int_\omega \nabla \phi \cdot \nabla \dot{u} \, \mathrm{d}\mathbf{x} + \int_{\partial \omega} \nabla \phi \cdot (\nabla u + g)(\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A(\mathbf{x}) = 0 \quad \forall \phi. \tag{A6}$$

To obtain the traditional boundary integral formula for the shape derivative, we must drop term I. Indeed, provided $(\nabla \phi \cdot \mathbf{v})$ lies is the space of test functions, this term vanishes because u solves (A1). However, *this is precisely the term that does not vanish* for our Lagrange finite elements. For the moment, we will drop it to show how to arrive at the traditional shape derivative formula:

$$\int_\omega \nabla \phi \cdot \nabla \dot{u} \, \mathrm{d}\mathbf{x} + \int_{\partial \omega} \nabla \phi \cdot (\nabla u + g)(\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A(\mathbf{x}) = 0 \quad \forall \phi. \tag{A7}$$

Applying the adjoint method. We apply the adjoint method to express $\mathrm{d}J[\mathbf{v}]$ as an explicit differential form, avoiding the need to solve for $\dot{u}$ for every perturbation $\mathbf{v}$. Suppose we can find a scalar field p in our space of test functions so that:

$$\int_\omega (j') \cdot \nabla \psi \, \mathrm{d}\mathbf{x} = \int_\omega \nabla p \cdot \nabla \psi \, \mathrm{d}\mathbf{x} \quad \forall \text{ trial functions } \psi. \tag{A8}$$

Then, taking $\psi = \dot{u}$:

$$\int_\omega (j') \cdot \nabla \dot{u} \, \mathrm{d}\mathbf{x} = \int_\omega \nabla p \cdot \nabla \dot{u} \, \mathrm{d}\mathbf{x} = - \int_{\partial \omega} \nabla p \cdot (\nabla u + g)(\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A(\mathbf{x}),$$

where the last step used (A7) with p replacing ϕ. Plugging this into (A4), we arrive at the standard formula:

$$\boxed{\mathrm{d}J[\mathbf{v}] = \int_{\partial \omega} \Big(j(\nabla u) - \nabla p \cdot (\nabla u + g) \Big) (\mathbf{v} \cdot \mathbf{n}) \, \mathrm{d}A(\mathbf{x}).} \tag{A9}$$

The weak form (A8) corresponds to the adjoint PDE,

$$-\Delta p = -\nabla \cdot j'(\nabla u) \text{ in } \omega, \qquad \frac{\partial p}{\partial \mathbf{n}} = \mathbf{n} \cdot j'(\nabla u) \text{ on } \partial \omega.$$

2 Traditional shape derivative formula for worst-case stress

Now we compute the shape derivative in boundary integral form for our worst-case stress objective. For simplicity, we consider the worst-case Frobenius norm stress measure:

$$J(\omega) = \int_\omega j(\bar{\sigma}^\star(\mathbf{x}) : T^F(\mathbf{x}) : \bar{\sigma}^\star(\mathbf{x}))\ \mathrm{d}\mathbf{x},$$

but the other stress measures' derivations are nearly identical.

To shape-differentiate J, it will be necessary to know how j changes at each $\mathbf{x}$ when the fluctuation strains change. As mentioned in the main text, the worst-case load $\bar{\sigma}^\star$ can be considered constant, but $T^F(\mathbf{x}) = F^T : F$ is a function of the fluctuation strains via (5) from the main text. Furthermore, though the homogenized elasticity tensor $\bar{C}$ is technically a function of the fluctuation strains, it simplifies our derivation to view $\bar{C}$ as an independent parameter of s and then separately compute its shape derivative, (A21). Representing these relationships explicitly, we write:

$$j(s(\mathbf{x})) := j(s(\varepsilon^{pq}, \bar{C}, \mathbf{x})),$$

where ε^{pq} expands to six strain field arguments in 3D. Perturbations $\delta\varepsilon^{kl}$ and $\delta\bar{C}$ of these arguments induce perturbation:

$$\begin{aligned}\delta j &= (j')\frac{\partial s}{\partial \varepsilon^{kl}} : \delta\varepsilon^{kl} + (j')\frac{\partial s}{\partial \bar{C}} :: \delta\bar{C} \\ &= \tau^{kl} : \delta\varepsilon^{kl} + \gamma : \delta\bar{C},\end{aligned}$$

where we defined

$$\tau^{kl} \overset{\text{def}}{=} (j')\frac{\partial s}{\partial \varepsilon^{kl}}, \quad \gamma \overset{\text{def}}{=} (j')\frac{\partial s}{\partial \bar{C}}.$$

2.1 Computing τ^{kl} and γ

First, we compute the rank-two tensor field τ^{kl} expressing the derivative of objective integrand j with respect to fluctuation strain ε^{kl} (holding $\bar{C}$ and thus $\bar{S}$ constant).

$$\begin{aligned}\tau^{kl}_{ij} =& j'\ \frac{\partial}{\partial \varepsilon^{kl}_{ij}}\left[\bar{\sigma}^\star : F^T : F : \bar{\sigma}^\star\right] = j'\bar{\sigma}^\star : \left[\left(\frac{\partial}{\partial \varepsilon^{kl}_{ij}} F^T\right) : F + F^T : \frac{\partial}{\partial \varepsilon^{kl}_{ij}} F\right] : \bar{\sigma}^\star, \\ =& 2j'\bar{\sigma}^\star : F^T : \left(\frac{\partial}{\partial \varepsilon^{kl}_{ij}} F\right) : \bar{\sigma}^\star,\end{aligned}$$

using the fact that a tensor and its transpose give the same quadratic form. From definition (5) in the main text,

$$\frac{\partial}{\partial \varepsilon^{kl}_{ij}} F_{abcd} = C^{\text{base}}_{abef}\bar{S}_{ghcd}\frac{\partial}{\partial \varepsilon^{kl}_{ij}}(\varepsilon^{gh}_{ef} + e^{gh}_{ef}) = C^{\text{base}}_{abef}\bar{S}_{ghcd}\delta_{gk}\delta_{hl}\delta_{ei}\delta_{fj} = C^{\text{base}}_{abij}\bar{S}_{klcd}.$$

After simplification, we have

$$\tau^{kl} = (2j' C^{\text{base}} : F : \bar{\sigma}^\star)[\bar{S} : \bar{\sigma}^\star]_{kl}. \tag{A10}$$

Next, we compute the rank-four tensor field γ expressing the partial derivative of objective integrand j with respect to the homogenized elasticity tensor $\bar{C}$.

$$\begin{aligned}\delta j &= 2j'\bar{\sigma}^\star : F^T : C^{\text{base}} : G :\ \mathrm{d}\bar{S} : \bar{\sigma}^\star, \\ &= 2j'\bar{\sigma}^\star : F^T : C^{\text{base}} : G : (-\bar{S} :\ \mathrm{d}\bar{C} : \bar{S}) : \bar{\sigma}^\star, \\ &= (-2j'\bar{\sigma}^\star : F^T : F) :\ \mathrm{d}\bar{C} : (\bar{S} : \bar{\sigma}^\star), \\ &= \left[(-2j'\bar{\sigma}^\star : F^T : F) \otimes (\bar{S} : \bar{\sigma}^\star)\right] ::\ \mathrm{d}\bar{C}.\end{aligned}$$

Thus,

$$\gamma = (-2j' F^T : F : \bar{\sigma}^\star) \otimes (\bar{S} : \bar{\sigma}^\star). \tag{A11}$$

Now, applying the Reynolds Transport Theorem to our objective, we find:

$$\begin{aligned} \mathrm{d}J[\mathbf{v}] &= \int_{\partial\omega} (\mathbf{v} \cdot \hat{\mathbf{n}}) j \; \mathrm{d}A(\mathbf{x}) + \int_\omega \tau^{kl} : \varepsilon(\dot{\mathbf{w}}^{kl}[\mathbf{v}]) + \gamma :: \mathrm{d}\bar{C}[\mathbf{v}] \; \mathrm{d}\mathbf{x} \\ &= \int_{\partial\omega} (\mathbf{v} \cdot \hat{\mathbf{n}}) j \; \mathrm{d}A(\mathbf{x}) + \underbrace{\int_\omega \tau^{kl} : \varepsilon(\dot{\mathbf{w}}^{kl}[\mathbf{v}]) \; \mathrm{d}\mathbf{x}}_{I} + \left(\int_\omega \gamma \; \mathrm{d}\mathbf{x} \right) :: \mathrm{d}\bar{C}[\mathbf{v}], \end{aligned} \tag{A12}$$

where $\dot{\mathbf{w}}^{kl}[v]$ is an Eulerian derivative with respect to "time" t under the advection velocity $\mathbf{v}$. The first and third terms are straightforward to evaluate (once we derive a formula for $\mathrm{d}\bar{C}[\mathbf{v}]$), but the middle integral "I" involves the problematic term $\dot{\mathbf{w}}^{kl}[v]$, which measures how the fluctuation displacements change when perturbing the shape with velocity field $\mathbf{v}$.

2.1.1 Forward version

The "forward" sensitivity analysis determines, for a particular velocity field $\mathbf{v}$, the change in fluctuation displacements $\dot{\mathbf{w}}^{kl}[\mathbf{v}]$ and substitutes them into (A12). We can determine an equation for $\dot{\mathbf{w}}^{kl}[\mathbf{v}]$ by differentiating the weak form of the kl^{th} cell problem. To simplify the derivation, we apply our periodic boundary conditions and no-rigid-translation constraints directly to the space of trial and test functions. Then the cell problem's weak form is just

$$\int_\omega \varepsilon(\phi) : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \; \mathrm{d}\mathbf{x} = 0 \quad \text{(for all } \phi\text{)}, \tag{A13}$$

where $\mathbf{w}^{kl}$ and ϕ are periodic vector fields on the unit cell Y. Differentiating both sides of this equation by naïvely applying Reynolds Transport Theorem (assuming shape functions, ϕ, are independent of ω),

$$\int_{\partial\omega} (\mathbf{v} \cdot \hat{\mathbf{n}}) \Big(\varepsilon(\phi) : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \Big) \; \mathrm{d}A(\mathbf{x}) + \int_\omega \varepsilon(\phi) : C : \varepsilon(\dot{\mathbf{w}}^{kl}[\mathbf{v}]) \; \mathrm{d}\mathbf{x} = 0 \quad \text{(for all } \phi\text{)}, \tag{A14}$$

which is the weak from of a cell problem for $\dot{\mathbf{w}}^{kl}[\mathbf{v}]$. Once we solve this equation for each $\dot{\mathbf{w}}^{kl}[\mathbf{v}]$, we can compute (A12) easily.

2.1.2 Adjoint version

We determine the adjoint equations by noticing the following: suppose we can find an "adjoint solution" $\mathbf{p}^{kl}$ from the same space as ϕ (i.e., a periodic test function for the original PDE) such that

$$\int_\omega \tau^{kl} : \varepsilon(\psi) \; \mathrm{d}\mathbf{x} = \int_\omega \varepsilon(\mathbf{p}^{kl}) : C : \varepsilon(\psi) \; \mathrm{d}\mathbf{x} \quad \text{(for all } \psi\text{)}, \tag{A15}$$

where ψ is from the same space as $\dot{\mathbf{w}}^{kl}$ (i.e., a periodic trial function for the original PDE). Then we can use $\mathbf{p}^{kl}$ to compute integral I as follows:

$$I = \int_\omega \tau^{kl} : \varepsilon(\dot{\mathbf{w}}^{kl}) \; \mathrm{d}\mathbf{x} = \int_\omega \varepsilon(\mathbf{p}^{kl}) : C : \varepsilon(\dot{\mathbf{w}}^{kl}) \; \mathrm{d}\mathbf{x} = -\int_{\partial\omega} (\mathbf{v} \cdot \hat{\mathbf{n}}) \Big(\varepsilon(\mathbf{p}^{kl}) : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \Big) \; \mathrm{d}A(\mathbf{x}).$$

The second step follows by substituting $\dot{\mathbf{w}}^{kl}$ for ψ in (A15), and the third by substituting $\mathbf{p}^{kl}$ for ϕ in (A14). Using this formula, our full shape derivative can be computed efficiently as:

$$\boxed{\mathrm{d}J[\mathbf{v}] = \int_{\partial\omega} \Big(j - \varepsilon(\mathbf{p}^{kl}) : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \Big) \mathbf{v} \cdot \hat{\mathbf{n}} \; \mathrm{d}A(\mathbf{x}) + \left(\int_\omega \gamma \; \mathrm{d}\mathbf{x} \right) :: d\bar{C}[\mathbf{v}],} \tag{A16}$$

summing over kl. We recognize (A15) as the weak form of the adjoint cell problem PDE:

$$\begin{aligned} -\nabla \cdot \sigma(\mathbf{p}^{kl}) &= -\nabla \cdot \tau^{kl} && \text{in } \omega, \\ \sigma(\mathbf{p}^{kl})\hat{\mathbf{n}} &= \tau^{kl}\hat{\mathbf{n}} && \text{on } \partial\omega, \\ \mathbf{p}^{kl} \text{ periodic}, & && \int_\omega \mathbf{p}^{kl} \, \mathrm{d}\mathbf{x} = 0. \end{aligned}$$

3 Accurate discrete formulation (volume form)

Since we consider straight-edged finite elements, the perturbation velocity $\mathbf{v}$ is a piecewise linear vector field and is represented as a perturbation vector on each mesh vertex:

$$\mathbf{v} = \sum_i \lambda_i \delta\mathbf{q}_i \ ,$$

where λ_i is vertex i's linear shape function (barycentric coordinates) and $\delta\mathbf{q}_i$ is its perturbation. Unfortunately, the most straight-forward approach to computing shape derivatives of plugging this piecewise linear $\mathbf{v}$ into a discretized version of (A16) leads to wildly inaccurate results for the high L_p norms needed to prevent stress concentrations.

It turns out that the Reynolds Transport Theorem and the Eulerian derivatives used in (A12) are the source of the error. As in the model problem, where proceeding from (A5) to (A7) introduced an error, the analogous step for our objective is problematic. We avoid this step by keeping everything in terms of material derivatives.

3.1 Discrete sensitivity of the objective

The analog to (A2) in our setting is:

$$\begin{aligned} \mathrm{d}J[\mathbf{v}] &= \int_\omega j\nabla \cdot \mathbf{v} + \tau^{kl} : D[\varepsilon(\mathbf{w}^{kl})] + \gamma :: d\bar{C}[v] \, \mathrm{d}\mathbf{x} \\ &= \int_\omega j\nabla \cdot \mathbf{v} + \underbrace{\tau^{kl} : \varepsilon(D[\mathbf{w}^{kl}])}_{II} - \tau^{kl} : \mathrm{sym}(\nabla \mathbf{w}^{kl} \nabla \mathbf{v}) \, \mathrm{d}\mathbf{x} + \left(\int_\omega \gamma \, \mathrm{d}\mathbf{x} \right) :: \mathrm{d}\bar{C}[\mathbf{v}], \end{aligned} \tag{A17}$$

where $D[\cdot]$ denotes the material derivative, and we use ∇ applied to a vector field to denote the Jacobian (not its transpose). Note that $D[\cdot]$ and $\varepsilon(\cdot)$ do not commute, but the following identity holds for any linear combination, $\mathbf{w}$, of shape functions, ϕ:

$$D[\varepsilon(\mathbf{w})] = \varepsilon(D[\mathbf{w}]) - \mathrm{sym}(\nabla \mathbf{w} \nabla \mathbf{v}). \tag{A18}$$

Again, II is the difficult term to compute.

3.1.1 Discrete Forward Sensitivity of $\mathbf{w}^{kl}$

We can determine $D[\mathbf{w}^{kl}]$, the material derivative of the fluctuation displacements, by differentiating the weak form (A13). First, we define microscopic stress $\sigma^{kl} \stackrel{\text{def}}{=} C : \left[\varepsilon(\mathbf{w}^{kl}) + e^{kl}\right]$ to simplify notation. Then, differentiating both sides of the weak form:

$$\begin{aligned} \forall\phi: \quad 0 &= \int_\omega \left(\varepsilon(\phi) : \sigma^{kl}\right) \nabla \cdot \mathbf{v} + D\left[\varepsilon(\phi) : C : \left[\varepsilon(\mathbf{w}^{kl}) + e^{kl}\right]\right] \, \mathrm{d}\mathbf{x} \quad (\text{for all } \phi), \\ &= \int_\omega \left(\varepsilon(\phi) : \sigma^{kl}\right) \nabla \cdot \mathbf{v} - \mathrm{sym}(\nabla\phi\nabla\mathbf{v}) : \sigma^{kl} + \varepsilon(\phi) : C : \left(\varepsilon(D[\mathbf{w}^{kl}]) - \mathrm{sym}(\nabla \mathbf{w}^{kl} \nabla \mathbf{v})\right) \mathrm{d}\mathbf{x}, \end{aligned} \tag{A19}$$

where we used the fact that $D[\phi] = 0$ because the test functions for straight-edged finite elements are expressed in terms of the mesh's barycentric coordinate functions and thus are tied to material points (i.e. their values advect with the mesh and have zero material derivative). (A19) is the weak form of a PDE solving for $D[\mathbf{w}^{kl}]$, which can be discretized in the straight-forward way: as a vector holding the material derivative of $\mathbf{w}^{kl}$ at each mesh node. Notice that this equation is the analog of (A5).

3.1.2 Discrete adjoint sensitivity

To obtain an explicit representation of the differential form accepting the perturbation velocity fields on ω and outputting a change in the objective, we must apply the adjoint method.

The adjoint equations turn out to be identical to (A15) due to the similarity of integrals I and II; simply substitute $D[\mathbf{w}^{kl}]$ for $\dot{\mathbf{w}}^{kl}$ in the derivation. However, once we have the adjoint solutions $\mathbf{p}^{kl}$, the exact discrete gradient differs from (A16). Instead, we derive it by computing II as follows: First, substitute $D[\mathbf{w}^{kl}]$ for ψ in (A15) to determine:

$$II = \int_\omega \tau^{kl} : \varepsilon(D[\mathbf{w}^{kl}]) \, \mathrm{d}\mathbf{x} = \int_\omega \varepsilon(\mathbf{p}^{kl}) : C : \varepsilon(D[\mathbf{w}^{kl}]) \, \mathrm{d}\mathbf{x}$$

Next, substitute $\mathbf{p}^{kl}$ for ϕ in (A19) to rewrite the first integrand again:

$$II = \int_\omega - \left[\varepsilon(\mathbf{p}^{kl}) : \sigma^{kl}\right] \nabla \cdot \mathbf{v} + \mathrm{sym}(\nabla \mathbf{p}^{kl} \nabla \mathbf{v}) : \sigma^{kl} + \varepsilon(\mathbf{p}^{kl}) : C : \mathrm{sym}(\nabla \mathbf{w}^{kl} \nabla \mathbf{v}) \, \mathrm{d}\mathbf{x}.$$

Finally, the full discrete shape derivative is evaluated as:

$$\boxed{\begin{aligned} \mathrm{d}J_d[\mathbf{v}] = & \int_\omega \left[j - \varepsilon(\mathbf{p}^{kl}) : \sigma^{kl}\right] \nabla \cdot \mathbf{v} + (\nabla \mathbf{p}^{kl} \nabla \mathbf{v}) : \sigma^{kl} + (\varepsilon(\mathbf{p}^{kl}) : C - \tau^{kl}) : (\nabla \mathbf{w}^{kl} \nabla \mathbf{v}) \, \mathrm{d}\mathbf{x} \\ & + \left(\int_\omega \gamma \, \mathrm{d}\mathbf{x}\right) :: d\bar{C}[\mathbf{v}], \end{aligned}} \tag{A20}$$

which gives the exact discrete shape derivative when the piecewise polynomial FEM fields are substituted for $\mathbf{p}^{kl}, \mathbf{w}^{kl}$, and $\mathbf{v}$. We dropped the symmetrization operator $\mathrm{sym}(\cdot)$ since its output is always double contracted with a symmetric tensor.

3.1.3 Discrete Differential Form

It is convenient to express $\mathrm{d}J_d[\mathbf{v}]$ as an explicit inner product with the per-vertex perturbation vector field $\delta\mathbf{q}$. To do this, we must re-express the terms involving $\mathbf{v}$ in terms of $\delta\mathbf{q}$. The easiest is $\nabla \cdot \mathbf{v} = \sum_m \nabla\lambda_m \cdot \delta\mathbf{q}_m$. The terms like $\tau^{kl} : (\nabla \mathbf{p}^{kl} \nabla \mathbf{v})$ take more work. Recalling that we take ∇ to represent the Jacobian when applied to vectors (rather than its transpose),

$$\nabla \mathbf{v} = \sum_m \delta\mathbf{q}_m \otimes \nabla\lambda_m.$$

We can write $\nabla \mathbf{p}^{kl}$ in terms of each *scalar*-valued finite element shape function φ_n and its *vector*-valued coefficient $\mathbf{p}^{kl}_n$ as:

$$\nabla \mathbf{p}^{kl} = \sum_n \mathbf{p}^{kl}_n \otimes \nabla\varphi_n.$$

Plugging these Jacobian expressions into the double contraction we wish to compute:

$$\begin{aligned} \tau^{kl} : (\nabla \mathbf{p}^{kl} \nabla \mathbf{v}) &= \sum_{n,m} \tau^{kl} : \left[(\mathbf{p}^{kl}_n \otimes \nabla\varphi_n)(\delta\mathbf{q}_m \otimes \nabla\lambda_m)\right] \\ &= \sum_m \delta\mathbf{q}_m \cdot \left(\sum_n \left[\nabla\lambda_m \cdot (\tau^{kl}\mathbf{p}^{kl}_n)\right] \nabla\varphi_n \right). \end{aligned}$$

Finally, we make these substitutions in $\mathrm{d}J_d[\mathbf{v}]$ to express the differential form as an inner product with the vertex node perturbations (here summation over vertices, m, and FEM nodes, n, is implied).

$$\boxed{\begin{aligned}\mathrm{d}J_d[\lambda_m \delta\mathbf{q}_m] = &\left(\int_\omega \left[j - \varepsilon(\mathbf{p}^{kl}) : \sigma^{kl}\right] \nabla\lambda_m + \left[\nabla\lambda_m \cdot \left(\sigma^{kl}\mathbf{p}_n^{kl} + (\varepsilon(\mathbf{p}^{kl}) : C - \tau^{kl})\mathbf{w}_n^{kl}\right)\right] \nabla\varphi_n \ \mathrm{d}\mathbf{x}\right) \cdot \delta\mathbf{q}_m \\ &+ \left(\int_\omega \gamma \ \mathrm{d}\mathbf{x}\right) :: d\bar{C}[\mathbf{v}].\end{aligned}}$$

3.1.4 Homogenized Tensor Discrete Shape Derivative

The evaluation is completed once we substitute the discrete formula for $\mathrm{d}\bar{C}$. We start with the "energy form" of the homogenized tensor [1]:

$$\bar{C}_{ijkl} = \frac{1}{|Y|}\int_\omega [\varepsilon(\mathbf{w}^{ij}) + e^{ij}] : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \ \mathrm{d}\mathbf{x}.$$

Applying the analog of (A2) for this expression:

$$\begin{aligned}\mathrm{d}\bar{C}_{ijkl}[\mathbf{v}] = \frac{1}{|Y|}\int_\omega \Big(\sigma^{ij} : C^{-1} : \sigma^{kl}\Big)\nabla\cdot\mathbf{v} + \Big(\varepsilon(D[\mathbf{w}^{ij}]) - \mathrm{sym}(\nabla\mathbf{w}^{ij}\nabla\mathbf{v})\Big) : C : [\varepsilon(\mathbf{w}^{kl}) + e^{kl}] \\ + \Big(\varepsilon(D[\mathbf{w}^{kl}]) - \mathrm{sym}(\nabla\mathbf{w}^{kl}\nabla\mathbf{v})\Big) : C : [\varepsilon(\mathbf{w}^{ij}) + e^{ij}] \ \mathrm{d}\mathbf{x}.\end{aligned}$$

Finally, because $D[\mathbf{w}^{ij}]$ can be written as a linear combination of the shape functions ϕ, the two terms involving it vanish due to (A13) (so no adjoint problem is required). Applying the same manipulations as in the previous section, we arrive at the explicit differential form:

$$\boxed{\mathrm{d}\bar{C}_{ijkl}[\lambda_m\delta\mathbf{q}_m] = \left(\frac{1}{|Y|}\int_\omega \left(\sigma^{ij} : C^{-1} : \sigma^{kl}\right)\nabla\lambda_m - \left[\nabla\lambda_m \cdot \left(\sigma^{kl}\mathbf{w}_n^{ij} + \sigma^{ij}\mathbf{w}_n^{kl}\right)\right] \nabla\varphi_n \ \mathrm{d}\mathbf{x}\right) \cdot \delta\mathbf{q}_m,} \tag{A21}$$

where again summation over m and n is implied.

References

[1] Julian Panetta, Qingnan Zhou, Luigi Malomo, Nico Pietroni, Paolo Cignoni, and Denis Zorin. Elastic textures for additive fabrication. *ACM Transactions on Graphics (TOG)*, 34(4):135, 2015.