Inverse Design of Discrete Interlocking Materials with Desired Mechanical Behavior Supplementary Material

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1 DERIVATIVES FOR COMPUTING STATIC EQUILIBIRUM

We solve the static equilibrium state by minimizing the energy of the system,

$$\min_{\mathbf{q}} E = E_e(\mathbf{q}) + E_c(\mathbf{q}) \,, \tag{1}$$

where $E_c = \mu \sum_{k\in C} s_k b_k$ is the total contact potential summed over all contact pairs in the contact set C with an adaptive barrier stiffness μ, an smooth factor s_k and a log barrier term b_k. E_e denotes the potential via external forces. Solving this minimization problem requires the energy gradient $dE/d\mathbf{q}$ and the hessian $d^2E/d\mathbf{q}^2$. Computing the gradient and hessian for the external potential energy is always easy. For simplicity, we express the k-th contact energy as $E_{c,k} = s \cdot b$, where s and b are the corresponding k-th smooth factor and log barrier term. Therefore, the gradient of the contact potential is

$$\frac{dE_{c,k}}{d\mathbf{q}} = s\frac{db}{dd}\frac{dd}{d\mathbf{q}} + b\frac{ds}{d\mathbf{v}}\frac{d\mathbf{v}}{d\mathbf{q}} \tag{2}$$

with $\mathbf{v} = (d, \lambda)^T$, and the hessian of the contact potential is

$$\begin{aligned}\frac{d^2E_{c,k}}{d\mathbf{q}^2} = &\left(\frac{db}{dd}\frac{dd}{d\mathbf{q}}\right)^T\left(\frac{ds}{d\mathbf{v}}\frac{d\mathbf{v}}{d\mathbf{q}}\right) + s\left(\frac{dd}{d\mathbf{q}}^T\frac{d^2b}{dd^2}\frac{dd}{d\mathbf{q}} + \frac{db}{dd}\frac{d^2d}{d\mathbf{q}^2}\right)\\ &+\left(\frac{ds}{d\mathbf{v}}\frac{d\mathbf{v}}{d\mathbf{q}}\right)^T\left(\frac{db}{dd}\frac{dd}{d\mathbf{q}}\right) + b\left(\frac{d\mathbf{v}}{d\mathbf{q}}^T\frac{d^2s}{d\mathbf{v}^2}\frac{d\mathbf{v}}{d\mathbf{q}} + \frac{ds}{d\mathbf{v}}\frac{d^2\mathbf{v}}{d\mathbf{q}^2}\right)\end{aligned}. \tag{3}$$

Derivatives of Distance. For the gradient and hessian of distance with respect to configuration $\mathbf{q}$, we have

$$\begin{aligned}\frac{dd}{d\mathbf{q}} &= \frac{\partial d}{\partial \mathbf{c}}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial d}{\partial \mathbf{q}}\,,\\ \frac{d^2d}{d\mathbf{q}^2} &= \frac{d\mathbf{c}}{d\mathbf{q}}^T\left(\frac{\partial^2 d}{\partial \mathbf{c}^2}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^2 d}{\partial\mathbf{c}\partial\mathbf{q}}\right) + \frac{\partial d}{\partial \mathbf{c}}\frac{d^2\mathbf{c}}{d\mathbf{q}^2} + \frac{\partial^2 d}{\partial\mathbf{q}\partial\mathbf{c}}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^2 d}{\partial\mathbf{q}^2}\,,\end{aligned} \tag{4}$$

where the derivatives $d\mathbf{c}/d\mathbf{q}$ and $d^2\mathbf{c}/d\mathbf{q}^2$ are unknown. We leverage the state with the minimum distance,

$$\frac{dd}{d\mathbf{c}} = \mathbf{0}\,, \tag{5}$$

as an implicit map between parametric coordinate $\mathbf{c}$ and rigid body configuration $\mathbf{q}$. Any change in configuration $\mathbf{q}$ should lead to a corresponding change in coordinate $\mathbf{c}$ such that we are again at the minimum distance state. Therefore, taking the first-order sensitivity analysis of Equation (5) yields

$$\frac{\partial^2 d}{\partial\mathbf{c}^2}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^2 d}{\partial\mathbf{c}\partial\mathbf{q}} = \mathbf{0}\,, \tag{6}$$

from which we can obtain $d\mathbf{c}/d\mathbf{q}$, the so-called sensitivity matrix, by solving the linear system.

Similarly, taking the sensitivity analysis for the Equation (6), we can compute the second-order sensitivity matrix $d^2\mathbf{c}/d\mathbf{q}^2$ by solving the following linear system,

$$\frac{d\mathbf{c}}{d\mathbf{q}}\left(\frac{\partial^3 d}{\partial\mathbf{c}^3}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^3 d}{\partial\mathbf{c}^2\mathbf{q}}\right) + \frac{\partial^2 d}{\partial\mathbf{c}^2}\frac{d^2\mathbf{c}}{d\mathbf{q}^2} + \frac{\partial^3 d}{\partial\mathbf{c}\partial\mathbf{q}\partial\mathbf{c}}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^3 d}{\partial\mathbf{c}\partial\mathbf{q}^2} = \mathbf{0}\,. \tag{7}$$

Derivatives of eigenvalue. For the gradient and hessian of the smallest eigenvalue, we assume there is a unique smallest eigenvalue λ with its corresponding eigenvector $\mathbf{e}$ from the hessian matrix $\mathbf{H} = \frac{dd^2}{d\mathbf{c}^2}$. Therefore, its gradient and hessian with respect to configuration $\mathbf{q}$ are, respectively,

$$\frac{d\lambda}{d\mathbf{q}} = \frac{d\lambda}{d\mathbf{H}}\frac{d\mathbf{H}}{d\mathbf{q}}\,, \tag{8}$$

$$\frac{d^2\lambda}{d\mathbf{q}^2} = \frac{d\mathbf{H}}{d\mathbf{q}}^T\frac{d^2\lambda}{d\mathbf{H}^2}\frac{d\mathbf{H}}{d\mathbf{q}^2} + \frac{d\lambda}{d\mathbf{H}}\frac{d^2\mathbf{H}}{d\mathbf{q}^2}\,, \tag{9}$$

with the corresponding items as

$$\frac{d\lambda}{d\mathbf{H}} = \mathbf{e}\mathbf{e}^T\,, \tag{10}$$

$$\frac{d\mathbf{H}}{d\mathbf{q}} = \frac{\partial^3 d}{\partial\mathbf{c}^3}\frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^3 d}{\partial\mathbf{c}^2\partial\mathbf{q}}\,, \tag{11}$$

$$\frac{d^2\lambda}{d\mathbf{H}^2} = (\mathbf{e}\otimes\mathbf{I} + \mathbf{I}\otimes\mathbf{e})\frac{d\mathbf{e}}{d\mathbf{H}}\,, \tag{12}$$

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$$\frac{d\mathbf{e}}{d\mathbf{H}_{k,l}} = \sum_{\lambda_j \neq \lambda} \frac{\mathbf{e}_{(k)}\mathbf{e}_{(l)}}{\lambda - \lambda_j}\mathbf{e}_j \,, \tag{13}$$

$$\frac{d^2\mathbf{H}}{d\mathbf{q}^2} = \frac{d\mathbf{c}}{d\mathbf{q}}^T \frac{\partial^4 d}{\partial^4 \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^3 d}{\partial \mathbf{c}^3} \frac{d^2\mathbf{c}}{d\mathbf{q}^2} + \frac{\partial^4 d}{\partial \mathbf{c}^2 \partial \mathbf{q} \partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial^4 d}{\partial \mathbf{c}^2 \partial \mathbf{q}^2} \,, \tag{14}$$

where $\otimes$ is the Kronecker product operator, $\mathbf{e}_{(k)}$ and $\mathbf{e}_{(l)}$ are the k-th and l-th value in eigenvector $\mathbf{e}$, respectively, and $\mathbf{e}_j$ is the eigenvector associated with eigenvalue λ_j.

2 DERIVATIVES FOR INVERSE DESIGN

Evaluating the design objectives in Section 3.3 of the main document refers to solving static equilibrium states $\mathbf{y}$ for given design parameters $\mathbf{p}$, where $\mathbf{y} = [\mathbf{q}, \boldsymbol{\varepsilon}]$ for the planar case and $\mathbf{y} = [\mathbf{q}, \boldsymbol{\kappa}]$ for the bending case. According to the periodic boundary conditions and the paraboloid bending condition, we determine an intermediate state of rigid bodies as $\mathbf{q}_B = \mathrm{C}_B(\mathbf{y})$ for computing contacts.

We compute the map between parameters $\mathbf{p}$ and configuration $\mathbf{y}$ again by leveraging the sensitivity analysis of the static equilibrium state,

$$\mathbf{f} = -\frac{dE}{d\mathbf{y}} = -\frac{dE_e}{d\mathbf{y}} - \frac{dE_c}{d\mathbf{y}} = \mathbf{0} \,, \tag{15}$$

which yields

$$\frac{d\mathbf{f}}{d\mathbf{p}} = \frac{\partial \mathbf{f}}{\partial \mathbf{y}} \frac{d\mathbf{y}}{d\mathbf{p}} + \frac{\partial \mathbf{f}}{\partial \mathbf{p}} = \mathbf{0} \,, \tag{16}$$

where $\frac{\partial \mathbf{f}}{\partial \mathbf{y}} = \frac{\partial \mathbf{f}}{\partial \mathbf{q}_B} \frac{\partial \mathbf{q}_B}{\partial \mathbf{y}}$ can be easily computed. Since only the contact force $\mathbf{f}_c$ is a function of design parameters $\mathbf{p}$, we have $\frac{\partial \mathbf{f}}{\partial \mathbf{p}} = \frac{\partial \mathbf{f}_c}{\partial \mathbf{p}} = -\frac{\partial \mathbf{q}_B}{\partial \mathbf{y}}^T \frac{\partial^2 E_c}{\partial \mathbf{q}_B \partial \mathbf{p}}$. In the following derivations, for simplicity, we rewrite the symbol $\mathbf{q}_B$ as $\mathbf{q}$. Therefore, we have

$$\begin{aligned} \frac{\partial^2 E_{c,k}}{\partial \mathbf{q} \partial \mathbf{p}} = s &\left(\frac{\partial d}{\partial \mathbf{q}}^T \frac{d^2 b}{d d^2} \frac{\partial d}{\partial \mathbf{p}} + \frac{db}{dd} \frac{\partial \frac{dd}{d\mathbf{q}}}{\partial \mathbf{p}} \right) + \left(\frac{db}{dd} \frac{\partial d}{\partial \mathbf{q}} \right)^T \left(\frac{ds}{d\mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{p}} \right) \\ &+ b \left(\frac{\partial \mathbf{v}}{\partial \mathbf{q}}^T \frac{d^2 s}{d\mathbf{v}^2} \frac{\partial \mathbf{v}}{\partial \mathbf{p}} + \frac{ds}{d\mathbf{v}} \frac{\partial \frac{d\mathbf{v}}{d\mathbf{q}}}{\partial \mathbf{p}} \right) + \left(\frac{ds}{d\mathbf{v}} \frac{\partial \mathbf{v}}{\partial \mathbf{q}} \right)^T \left(\frac{db}{dd} \frac{\partial d}{\partial \mathbf{p}} \right) \,. \end{aligned} \tag{17}$$

Derivatives of distance. The gradient of distance with respect to the design parameters $\mathbf{p}$ is given by

$$\frac{\partial d}{\partial \mathbf{p}} = \frac{\partial d}{\partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial d}{\partial \mathbf{p}} \,, \tag{18}$$

where $\frac{d\mathbf{c}}{d\mathbf{p}}$ can be computed by solving

$$\frac{\partial^2 d}{\partial \mathbf{c}^2} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^2 d}{\partial \mathbf{c} \partial \mathbf{p}} = \mathbf{0} \,. \tag{19}$$

The item $\frac{\partial \frac{dd}{d\mathbf{q}}}{\partial \mathbf{p}}$ in Equation (17) is given as

$$\frac{\partial \frac{dd}{d\mathbf{q}}}{\partial \mathbf{p}} = \frac{d\mathbf{c}}{d\mathbf{q}}^T \left(\frac{\partial^2 d}{\partial \mathbf{c}^2} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^2 d}{\partial \mathbf{c} \partial \mathbf{p}} \right) + \frac{\partial d}{\partial \mathbf{c}} \frac{\partial \frac{d\mathbf{c}}{d\mathbf{q}}}{\partial \mathbf{p}} + \frac{\partial^2 d}{\partial \mathbf{q} \partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^2 d}{\partial \mathbf{q} \partial \mathbf{p}} \,. \tag{20}$$

where computing $\frac{\partial \frac{d\mathbf{c}}{d\mathbf{q}}}{\partial \mathbf{p}}$ requires solving the linear system from the second-order sensitivity analysis of Equation (6),

$$\frac{d\mathbf{c}}{d\mathbf{q}}^T \left(\frac{d^3 d}{d\mathbf{c}^3} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^3 d}{\partial \mathbf{c}^2 \partial \mathbf{p}} \right) + \frac{\partial^2 d}{\partial \mathbf{c}^2} \frac{\partial \frac{d\mathbf{c}}{d\mathbf{q}}}{\partial \mathbf{p}} + \frac{\partial^3 d}{\partial \mathbf{c} \partial \mathbf{q} \partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^3 d}{\partial \mathbf{c} \partial \mathbf{q} \partial \mathbf{p}} = \mathbf{0} \,. \tag{21}$$

Derivatives of eigenvalue. The gradient of smallest eigenvalue λ with respect to design parameters $\mathbf{p}$ is

$$\frac{d\lambda}{d\mathbf{p}} = \frac{d\lambda}{d\mathbf{H}} \frac{\partial \mathbf{H}}{\partial \mathbf{p}} = \frac{\partial \lambda}{\partial \mathbf{H}} \left(\frac{\partial^3 d}{\partial \mathbf{c}^3} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^3 d}{\partial \mathbf{c}^2 \partial \mathbf{p}} \right) \,. \tag{22}$$

The item $\frac{\partial \frac{d\lambda}{d\mathbf{q}}}{\partial \mathbf{p}}$ is given as

$$\begin{aligned} \frac{\partial \frac{d\lambda}{d\mathbf{q}}}{\partial \mathbf{p}} &= \left(\frac{\partial \mathbf{H}}{\partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{q}} + \frac{\partial \mathbf{H}}{\partial \mathbf{q}} \right)^T \frac{d^2 \lambda}{d\mathbf{H}^2} \left(\frac{\partial \mathbf{H}}{\partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial \mathbf{H}}{\partial \mathbf{p}} \right) + \\ \frac{d\lambda}{d\mathbf{H}} &\left(\frac{d\mathbf{c}}{d\mathbf{q}}^T \left(\frac{\partial^2 \mathbf{H}}{\partial \mathbf{c}^2} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^2 \mathbf{H}}{\partial \mathbf{c} \partial \mathbf{p}} \right) + \frac{\partial \mathbf{H}}{\partial \mathbf{c}} \frac{\partial \frac{d\mathbf{c}}{d\mathbf{q}}}{\partial \mathbf{p}} + \frac{\partial^2 \mathbf{H}}{\partial \mathbf{q} \partial \mathbf{c}} \frac{d\mathbf{c}}{d\mathbf{p}} + \frac{\partial^2 \mathbf{H}}{\partial \mathbf{q} \partial \mathbf{p}} \right) \,. \end{aligned} \tag{23}$$