Topology Optimization for Interface Defect

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1 Problem Statement

Switchable adhesive materials have been developed as soft grippers for lifting flat surfaces (such as microchips, glasses, solar panels, and other products) of significantly larger dimensions with high energy efficiency, and have potential in lowering manufacturing costs. Importantly, the magnitude of the adhesive force (i.e., the maximal pulling force F_0) is tunable via external stimuli. For example, when a voltage is applied, the percolating conductive propylene-based elastomer (cPBE) phase carrying a current becomes softened due to joule heating, which leads to re-distribution of stress concentration on the contact surface and thus, a decreased maximal pulling force F_1. An ideal gripper should possess large F_0 (to be able to pull up heavy objects) and small F_1 (high tunability), which are influenced by both the material properties and defect patterns on the interface.

This project investigates the topological design of the interface defects that governs the propagation of cracks under pulling, thus achieving high maximal pulling force. Consider the following optimization problem

$$\begin{aligned} \min_{\boldsymbol{\theta}, \{\mathbf{x}_k\}_{k=1}^T, f_0} \quad & f_0 \\ \text{subject to:} \quad & f(\mathbf{x}_k, \boldsymbol{\theta}) - f_0 \leq 0 \\ & \mathbf{x}_{k+1} = \mathbf{T}(\mathbf{x}_k, \boldsymbol{\theta}) \ \forall k = 1, \cdots, K \\ & \mathbf{x}_0 = \mathbf{x}_c \end{aligned} . \tag{1}$$

In the context of crack propagation on the interface, $\mathbf{x}_k$ contains the system states representing particle coordinates and velocity values at time step k; $\boldsymbol{\theta}$ is the defect topology to be designed; $f_k := f(\mathbf{x}_k, \boldsymbol{\theta})$ represents the external force; and f_0 the maximum external force. The state transition $\mathbf{T}(\mathbf{x}_k, \boldsymbol{\theta})$ is governed by the constitutive model of the material, and the initial condition $\mathbf{x}_c$ is given. Details on f and $\mathbf{T}$ will be introduced in Sec. 2. We will model crack propagation as the sequential breaking of bonds between particles, which makes the state transition nonlinear and resemble an explicit solver of a dynamical system. We also choose the fixed time window K to be a large number, so that for any defect topology $\boldsymbol{\theta}$, the set $\{f_k\}_{k=1}^K$ contains the maximum external force, after which the values will drop quickly to zeros as the interface separates.

We denote the partial derivatives of function $f(\mathbf{x}, \cdot)$ with respect to $\mathbf{x}$ as $\nabla_{\mathbf{x}} f$ and the total derivative of $f(\mathbf{x})$ as $d_{\mathbf{x}} f$.

2 The Dynamical Model

The following model of crack propagation is developed based on [?].

Geometry We consider the soft gripper and the object to be lifted as two rectangular blocks with the same cross-sections as shown in Fig. ??. The gripper is set on top of the object. Each is discretized as a stack of particles of dimension 10-by-10-by-10. The interface is then a 2D square with $N = 100$ particles.

Boundary conditions The bottom of the object is fixed to the ground with zero velocity and acceleration. The top of the gripper is set to have a constant upward velocity $\mathbf{v}_0 = 0.5$ and zero acceleration. The four sides of both the gripper and the object are set to have zero velocity and acceleration components in the x-y plane.

State transition The system states concatenates the particle coordinates $\mathbf{s}_k = [s^x_{1,k}, s^y_{1,k}, \cdots, s^x_{N,k}, s^y_{N,k}]^T$ with particle speed $\mathbf{v}_k = [v^x_{1,k}, v^y_{1,k}, \cdots, v^x_{N,k}, v^y_{N,k}]^T$: $\mathbf{x}_k^T = [\mathbf{s}_k^T, \mathbf{v}_k^T]$. For particle i, we denote its neighbours as $\mathcal{N}_i$ and its distances to neighbour j as $d_{ij,0}$. We consider 1st-order neighbours as the four directly adjacent particles, and 2nd-order neighbours as the diagonally adjacent ones. These neighbourhood sets are pre-computed and do not change during the pulling. The change in the distance from $d_{ij,0}$ between particles i and j creates an interaction force $[f^x_{ij,k}, f^y_{ij,k}]^T$ that follows

$$f^l_{ij,k} = \begin{cases} 0 & \text{if } d_{ij,k} < d_{ij,0} \\ (s^l_{j,k} - s^l_{i,k})\bar{f}_k / d_{ij,k} & \text{otherwise} \end{cases} \quad \text{for } l \in \{x, y\}, \tag{2}$$

where

$$\bar{f}_k = 2K_{ij}(d_{ij,k} - d_{ij,0}) + 0.5T_{ij}(\sum_{j' \in \mathcal{N}_i} d_{ij',k} + \sum_{i' \in \mathcal{N}_j} d_{ji',k}) + 0.5(\sum_{j' \in \mathcal{N}_i} d_{ij',k}T_{ij',k} + \sum_{i' \in \mathcal{N}_j} d_{ji',k}T_{ji',k}); \tag{3}$$

K_{ij} and T_{ij} are material properties parameterized by the topology $\boldsymbol{\theta}$. Specifically, $K_{ij} = \frac{2K_{\theta_i a}K_{\theta_j a}}{K_{\theta_i a} + K_{\theta_j a}}$ where θ_i and θ_j take phase values of 0, 1, and 2; subscript $a \in \{1, 2\}$ indicates whether j is a 1st- or 2nd-order neighbour, respectively. $K_{\theta 1} = \frac{E_\theta}{2(1+\mu_\theta)}$ and $K_{\theta 2} = \frac{E_\theta}{4(1+\mu_\theta)}$. And $T_{ij} = \frac{2T_{\theta_i}T_{\theta_j}}{T_{\theta_i} + T_{\theta_j}}$, where $T_\theta = \frac{E_\theta(4\mu_\theta - 1)}{24(1+\mu_\theta)(1-2\mu_\theta)}$.

The net force on particle i at time step k is

$$\mathbf{F}_{i,k} = \sum_{j \in \mathcal{N}_i} (\mathbf{s}_{j,k} - \mathbf{s}_{i,k})\mathbf{f}_{ij,k} / d_{ij,k}. \tag{4}$$

The acceleration of the particle is $\mathbf{a}_{i,k} = \mathbf{F}_{i,k}/m$, where m is the universal particle mass. For particles other than those with pre-specified states, their velocity and coordinates are updated as

$$\mathbf{v}_{i,k+1} = \mathbf{v}_{i,k} + \mathbf{a}_{i,k}\delta t \tag{5}$$

and

$$\mathbf{s}_{i,k+1} = \mathbf{s}_{i,k} + \mathbf{v}_{i,k}\delta t + 0.5\mathbf{a}_{i,k}\delta t^2. \tag{6}$$

Eq. (5) and Eq. (6) define the state transition. Lastly, the fracture strength is defined as the total net force in the z direction from particles on the top surface of the gripper.

3 Sensitivity Analysis

To solve Eq. (1), we start by noticing that $\{\mathbf{x}_k\}_{k=1}^K$ are inherently functions of $\boldsymbol{\theta}$. Thus we can rewrite the problem as:

$$\begin{aligned} \min_{\boldsymbol{\theta}, f_0} \quad & f_0 \\ \text{subject to:} \quad & f(\mathbf{x}_k, \boldsymbol{\theta}) - f_0 \leq 0 \ \forall k = 1, \cdots, K, \end{aligned} \tag{7}$$

the Lagrangian of which is $L(\boldsymbol{\theta}, f_0, \boldsymbol{\mu}) = f_0 + \sum_{k=1}^K \mu_k (f(\mathbf{x}_k, \boldsymbol{\theta}) - f_0)$, with Lagrangian multipliers $\boldsymbol{\mu}$. The KKT conditions of Eq. (7) are

$$\begin{aligned} & \nabla_{f_0} L = 1 - \sum_{k=1}^K \mu_k = 0 \\ & \nabla_{\boldsymbol{\theta}} L = \sum_{k=1}^K \mu_k d_{\boldsymbol{\theta}} f_k = \mathbf{0} \\ & \boldsymbol{\mu} \geq 0 \\ & f(\mathbf{x}_k, \boldsymbol{\theta}) - f_0 \leq 0 \\ & \mu_k (f(\mathbf{x}_k, \boldsymbol{\theta}) - f_0) = 0, \ \forall k = 1, \cdots, K. \end{aligned} \tag{8}$$

The optimal solution ($\boldsymbol{\theta}^*$ and f_0^*) can be found through a standard algorithm, e.g., sequential quadratic programming, provided that the design sensitivity $d_{\boldsymbol{\theta}} f_k$ is available.

In the following we discuss how this sensitivity can be calculated. Note that $d_{\boldsymbol{\theta}} f_k = \nabla_{\boldsymbol{\theta}} f_k + \nabla_{\mathbf{x}_k} f_k d_{\boldsymbol{\theta}} \mathbf{x}_k$. Here $d_{\boldsymbol{\theta}} \mathbf{x}_k$ can be calculated recursively through

$$\begin{aligned} d_{\boldsymbol{\theta}} \mathbf{x}_k &= \nabla_{\boldsymbol{\theta}} \mathbf{x}_k + (\nabla_{\mathbf{x}_{k-1}} \mathbf{x}_k) d_{\boldsymbol{\theta}} \mathbf{x}_{k-1} \\ & \cdots \\ d_{\boldsymbol{\theta}} \mathbf{x}_2 &= \nabla_{\boldsymbol{\theta}} \mathbf{x}_2 + (\nabla_{\mathbf{x}_1} \mathbf{x}_2) d_{\boldsymbol{\theta}} \mathbf{x}_1 \\ d_{\boldsymbol{\theta}} \mathbf{x}_1 &= d_{\boldsymbol{\theta}} \mathbf{T}_0, \end{aligned} \tag{9}$$

where $\nabla_{\mathbf{x}_k} \mathbf{x}_{k+1} = \nabla_{\mathbf{x}_k} \mathbf{T}_k$ and $\nabla_{\boldsymbol{\theta}} \mathbf{x}_{k+1} = \nabla_{\boldsymbol{\theta}} \mathbf{T}_k$. The analytical forms of $\nabla_{\mathbf{x}_k} f_k$, $\nabla_{\boldsymbol{\theta}} f_k$, $\nabla_{\mathbf{x}_k} \mathbf{T}_k$, $\nabla_{\boldsymbol{\theta}} \mathbf{T}_k$, and $d_{\boldsymbol{\theta}} \mathbf{T}_0$ will be derived using TensorFlow.