Supporting Information: A Topology Optimization Framework for the Inverse Design of Nonlinear Mechanical Metamaterials

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1 | Filtering and interpolation

Two common filters used in density-based TO are implemented in this work. Firstly, the original densities are filtered by solving the Helmholtz-style PDE [1]

$$\int_{\Omega_m} r^2 \nabla\bar{\rho} \cdot \nabla\delta\bar{\rho} + \bar{\rho}\delta\bar{\rho}\, d\Omega_m = \int_{\Omega_m} \rho\delta\bar{\rho}\, \mathrm{d}\Omega_m \tag{1}$$

for the smoothed densities, $\bar{\rho}$, given a filter radius, r. This prevents artifacts such as checkerboarding and aids mesh independence. A filter radius of $r = \frac{1}{112}$ mm was used in this work. The smoothed densities are subsequently passed through a threshold projection scheme [2] which pushes the densities towards zero and one, aiding the formation of "black-and-white" designs. The filtered densities are obtained with the following function

$$\tilde{\bar{\rho}} = \frac{\tanh(\beta\eta) + \tanh(\beta(\bar{\rho} - \eta))}{\tanh(\beta\eta) + \tanh(\beta(1 - \eta))}. \tag{2}$$

in which η defines the threshold above which densities are projected towards 1 and below which densities are projected towards 0, whilst β defines the sharpness of the thresholding. For the volume constraint, the dilated design is calculated by using a value of $\eta = 0.4$ in the threshold projection. It is common to use a continuation scheme to increase β after a certain number of design iterations. This allows for more design freedom in the early iterations whilst also encouraging the formation of black-and-white designs in the later iterations whilst maintaining good convergence. The filtered densities are used to scale the bulk and shear moduli according to

$$K = \gamma K_1 \tag{3}$$

$$G = \gamma G_1 \tag{4}$$

where K_1 is the solid bulk modulus and G_1 is the solid shear modulus. These solid properties can be given by the Young's modulus, E_1, and Poisson's ratio, ν_1, of the solid material using

$$K_1 = \frac{E_1}{3(1 - 2\nu_1)} \tag{5}$$

$$G_1 = \frac{E_1}{2(1 + \nu_1)}. \tag{6}$$

allowing for the density design variables to alter the material properties and affect the microscale behavior. Since the neo-hookean strain energy density function is linear with respect to E_1, the choice of Young's modulus is arbitrary, however, the system is not linear with regard to ν_1 so this must be inputted according to the chosen material. For this work the optimization was performed with $E_1 = 1$ MPa and $\nu_1 = 0.4$.

2 | Continuation Scheme

A continuation scheme is implemented to aid the formation of black-and-white designs. Several parameters are updated every 60 iterations corresponding to a single continuation step, k. There are six continuation steps over the course of the optimization process and at the start of each step the interior point optimizer is warm-started from the continuation before. Table 1 outlines the update rules used for the continuation scheme [3].

TABLE 1 | Continuation scheme used for the update of parameters.

Parameter	Initial value	Update rule	Final value
k	1	$k \leftarrow k + 1$	6
β	2	$\beta \leftarrow 1.2\beta$	4.98
α	0.05	$\alpha \leftarrow \alpha + 0.18$	0.95
ϕ_0	0.35	$\phi_0 \leftarrow \phi_0 - 0.055$	0.075

A relatively small final value of β was used as large values caused numerical instabilities. However, the use of the intermediate density penalty constraint was able to compensate for this and push the design to become black-and-white. It was noted that some solves of the microscale equilibrium problem were unable to converge despite the adaptive solution strategy. In these instances, the optimizer would move to the next continuation step and initialize the optimization with the design possessing the best objective value from the previous continuation step.

3 | Mesh and Initialization

Since strains are applied across the unit cell and the homogenized stress is size agnostic, the dimensions of the mesh for the unit cell for a fixed aspect ratio are arbitrary. In this work a unit square mesh of 1 mm × 1 mm is used with a resolution of 140 × 140 quadrilateral elements. A second order Lagrange vector function space is used for the displacement field, whilst a first order Lagrange function space is used for the density field. The ring-shaped initialization is given by the density field

$$\rho(x_m, y_m) = \sin\left[\left(\frac{5}{2}x_m - \frac{5}{4}\right)^2 + \left(\frac{5}{2}y_m - \frac{5}{4}\right)^2\right]. \tag{7}$$

where x_m and y_m are the microscale local coordinates on the undeformed geometry [3].

4 | Solution Strategy

Designing a solution strategy which can efficiently and robustly solve the microscale equilibrium problem for highly nonlinear responses presented a significant challenge. The framework is developed around *Firedrake*'s `solve()` function which implements Newton-like methods through *PETSc*.

A hybrid approach is adopted in which the solution scheme is split into an express solver and an adaptive solver. The express solver described in Algorithm 1 is the faster option as it only solves the microscale equilibrium at the goal applied macrostrains. The *Firedrake* solver at each applied strain is initialized with the microscale displacement fluctuations from the previous design iteration to aid the stability and speed of the solver's convergence. However, the solver may fail to converge if the design changes drastically between optimization iterations or the response experiences severe nonlinearities.

In the event that the express solver is unable to converge for any of the goal point solution attempts, the adaptive solver outlined in Algorithm 2 is called instead. In this approach, the solution strategy begins from the undeformed configuration and incrementally applies macroscale strains in steps of size λ. If a step fails to converge, the step size is halved and the solve is reattempted. If successive steps converge, the step size is doubled. This allows for smaller increments in numerically challenging portions of the solve, such as contact or snap-through, whilst retaining speed in the easier portions.

Algorithm 1 Pseudocode for express solution strategy

```
Express ← TRUE
while Express do
   for i ← [1, N_g] do
      Load previous solution (ũ_m)_i ← (ũ_{m,prev})_i
      Solve microscale equilibrium R(∇_M u*_M)_i = 0
      if SolveConverged then
         Calculate homogenized stress P_M
         Add contribution to objective J
         Save solution (ũ_{m,prev})_i ← (ũ_m)_i
      else
         Express ← FALSE
      end if
   end for
end while
```

Algorithm 2 Pseudo code for adaptive solution strategy

```
Initialize goal index i ← 1
Create successful convergence counter n_c ← 0
while ∇_M u_M ≤ (∇_M u*_M)_{N_g} do
   Step forward ∇_M u_M ← ∇_M u_M + λ(∇_M u*_M)_1
   if ∇_M u_M > (∇_M u*_M)_i then
      Step back to goal point ∇_M u_M ← (∇_M u*_M)_i
   end if
   Solve microscale equilibrium R(∇_M u_M) = 0
   if SolveConverged then
      Update convergence counter n_c ← n_c + 1
      if n_c ≥ 2 then
         Increase step size λ ← 2λ
      end if
      if ∇_M u_M = (∇_M u*_M)_i then
         Calculate homogenized stress P_M
         Add contribution to objective J
         Save solution (ũ_{m,prev})_i ← (ũ_m)_i
         Increase goal index i ← i + 1
      end if
   else
      Step back ∇_M u_M ← ∇_M u_M − λ(∇_M u*_M)_1
      Reset convergence counter n_c ← 0
      Reduce step size λ ← (1/2)λ
   end if
end while
```

5 | Goal points

The goal points outlined in Table 2 were used for the optimization cases of unit cells with pseudo-ductile, monostable with snap-through, and bistable responses. For all cases, the additional goal point in the tensile x-direction was defined with an applied strain of $(\nabla_M \mathbf{u}^*_\mathbf{M})_{xx} = 0.05$ and a goal homogenized stress of $P^*_{M,xx} = 0.05$ MPa.

TABLE 2 | Goal points used for optimization of microstructures.

Response	Strain, $(\nabla_M \mathbf{u}^*_\mathbf{M})_{yy}$	Stress, $P^*_{M,yy}$ [MPa]
Pseudo-ductile	[0.1, 0.25, 0.35]	[0.003, 0.003, 0.003]
Monostable	[0.1, 0.25, 0.35]	[0.003, 0.001, 0.004]
Bistable	[0.1, 0.25, 0.35]	[0.003, −0.001, 0.002]

References

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