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Optimization of Composite Fracture Properties: Method, Validation, and Applications

A paradigm in nature is to architect composites with excellent material properties compared to its constituents, which themselves often have contrasting mechanical behavior. Most engineering materials sacrifice strength for toughness, whereas natural materials do not face this tradeoff. However, biology's designs, adapted for organism survival, may have features not needed for some engineering applications. Here, we postulate that mimicking nature's elegant use of multimaterial phases can lead to better optimization of engineered materials. We employ an optimization algorithm to explore and design composites using soft and stiff building blocks to study the underlying mechanisms of nature's tough materials. For different applications, optimization parameters may vary. Validation of the algorithm is carried out using a test suite of cases without cracks to optimize for stiffness and compliance individually. A test case with a crack is also performed to optimize for toughness. The validation shows excellent agreement between geometries obtained from the optimization algorithm and the brute force method. This study uses different objective functions to optimize toughness, stiffness and toughness, and compliance and toughness. The algorithm presented here can provide researchers a way to tune material properties for a vast number of engineering problems by adjusting the distribution of soft and stiff materials. [DOI: 10.1115/1.4033381]

1 Introduction

Mechanical defects, which may be introduced during manufacturing, can weaken a material by orders of magnitude, depending on their quantity, location, and size. With imperfections present, a material has diminished strength. In structural design, such strength reductions are not tolerable and defects need to be addressed [1]. As a result, researchers seek to learn from natural materials that have been proven to exhibit high defect tolerance [2–4], i.e., insensitivity to flaws in their microstructure. The presence of structural hierarchy in such natural materials, for example, silk and abalone shells, allows them to achieve properties well beyond those of synthetic materials [5]. Furthermore, natural materials display the ability to combine complementary properties such as brittle and ductile, or soft and stiff. For instance, fish have scales that consist of two distinct phases with contrasting properties that allow them to have enough rigidity to protect themselves from attackers and enough flexibility to move with agility [6]. Nacre, made up 95% of calcite minerals and with only 5% of a compliant biopolymer protein, has a toughness that is 3000 times larger than the brittle minerals alone [2]. Several thorough studies depict natural materials' toughening mechanisms at different

length scales as seen in bone, nacre, and sea sponges [5,7,8]. Due to the complexity of these systems, numerical modeling is needed to enable researchers to investigate material behavior at multiple length scales, which can be difficult to perform through experiments.

While it may be desirable to replicate natural composites' complex designs, they are usually optimized for their own survival, which may involve things such as self-cleaning and obtaining food that lack counterparts in specific engineering applications [9–12]. Such human applications require specific properties, such as stiffness, strength, and lightweight to carry imposed loads economically and reliably, that are not aligned with all the functions that nature requires. This paper discusses a way to evolve a material into an optimized structure through a numerical modeling and optimization approach. Nature's objective function is survival, while for engineering materials, the objectives are human specified material properties. We postulate that we can use nature's design tools to tune and optimize for specific mechanical properties such as toughness and strength. Past efforts have sought to optimize composite materials through ply tailoring, number of plies, and laminate sequence, specifically using genetic algorithms to apply to the design optimization of composite laminate designs [13–16]. In addition, researchers have studied how to optimize composite topology with three materials for thermal conductivity properties [17]. Similarly, topology optimization groups strive to optimize compliance in a structure based on loads and boundary conditions [18–23]. Some research groups have used a form of

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topology optimization to optimize the toughness in a composite [24,25], but limitations to those studies were lack of consideration of either cracks or the presence of multiple materials in the system. To the best of our knowledge, no work thus far has found a method to optimize a material design with a crack using stiff and soft materials for fracture resistant properties. Here, we provide a method to find a distribution of stiff and soft phases, optimized for toughness, in a composite material.

This paper is organized as follows. In Sec. 2, the optimization method will be discussed along with the objective function and finite element method. Section 3 will present case studies on applications using various objective functions with the proposed optimization model. Finally, we summarize our findings and make suggestions for future research.

2 Methods

The optimization method is centered around an algorithm that employs the finite element method to evaluate an objective function based on desired material properties. Validation of the algorithm is carried out using a test suite of cases without cracks to optimize for stiffness and compliance. Geometries obtained from the optimization algorithm optimizing for toughness are compared with brute force method results, which are explained in Sec. 2.3.

2.1 Computational Model. We propose an optimization code to generate geometries composed of soft and stiff building blocks by the use of an algorithm combined with existing finite element procedures to solve a particular mechanical problem. The material to be distributed must be either soft or stiff. There is a fixed soft material volume fraction used in the model. The material possesses an edge crack with x -direction tensile loading under mode I failure (Fig. 1). Model parameters include crack geometry, crack location, and loading condition. Different observables from the algorithm are Young's modulus, toughness modulus, compliance, and stress/strain fields. After the unit cell is optimized for a desired application, it can be repeated in a certain orientation to optimize the composite microstructure. This paper will focus on a

single unit cell optimization. The algorithm, along with the finite element solver, optimizes an objective function defined in this section.

The optimization method used is a modified greedy algorithm, which is a mathematical process that looks to create a better solution to a complex problem [26–28]. The algorithm takes as an input a random initial population of soft and stiff elements. From this initial configuration, the objective function for the desired material property is evaluated in order to decide the next best solution for the system. One element at a time is then replaced by its opposite material. For instance, if the element at hand is a soft material, it will be switched to a stiff material. After the first switch, the volume fraction will change. Volume fraction of soft material is kept constant by switching the next best element to the opposite material. For example, if a stiff material is at first switched, the algorithm searches for the best element to switch to a soft material next. This process is continued for all elements in the system, and the corresponding objective function with constraint included is calculated for each switch. From the pool of switches, the switch that obtains the highest objective is kept and used for the next iteration. If the kept objective value is higher than its previous iteration, which for the first iteration is compared to the random initial configuration, it feeds back to replacing each element one at a time. This loop continues until at a certain iteration, the new objective is not higher than its predecessor, which prompts the program to exit and output the final geometry. This overall methodology is depicted in Fig. 2.

The objective function can vary depending on application. Mechanical properties we seek to optimize individually and combined are stiffness, compliance, and toughness moduli. Stiffness is the ability of an object to resist deformation in response to an applied force and is defined in Eq. (1), where E_{eff} is the effective stiffness, N is the number of elements, σ_i is the stress on a given element, and ϵ_i is the strain in a given element. The mean of the stress and strain is calculated because the stiffness distribution is nonhomogeneous. Compliance is defined as the inverse of stiffness. We define toughness modulus as the area underneath the stress–strain curve for a material; it can be understood as the

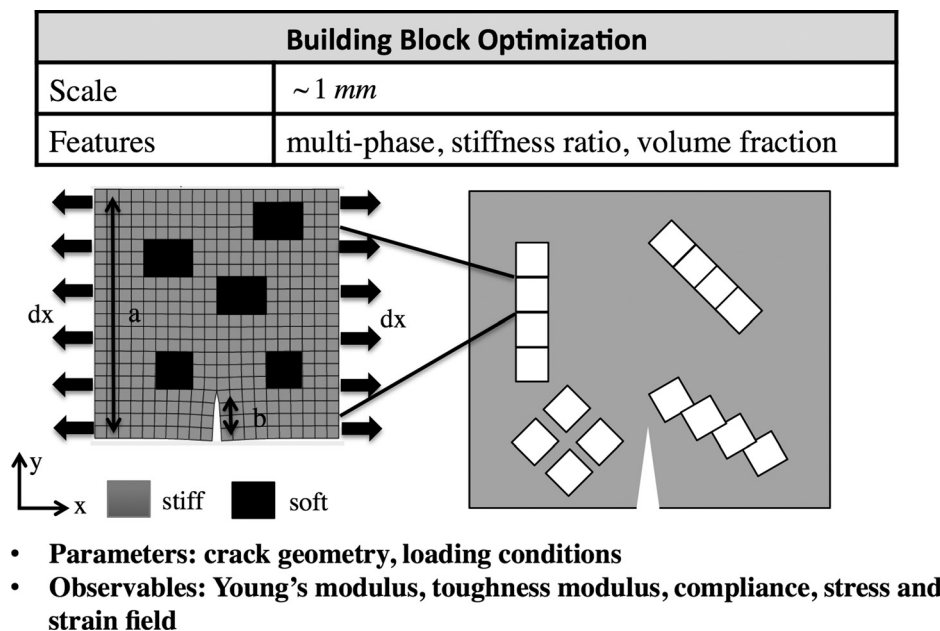


Fig. 1 Model formulation. Targeted material property optimization is performed by algorithmic assignment of stiff and soft elements in a multiphase building block. The prescribed binary distribution of element stiffness defines stiffness and volume ratios for each initial geometry. The material contains an edge crack and undergoes tensile loading under mode I failure with displacement controlled boundary conditions (“dx”). a is the length of the sample (square), and b is the length of the crack.

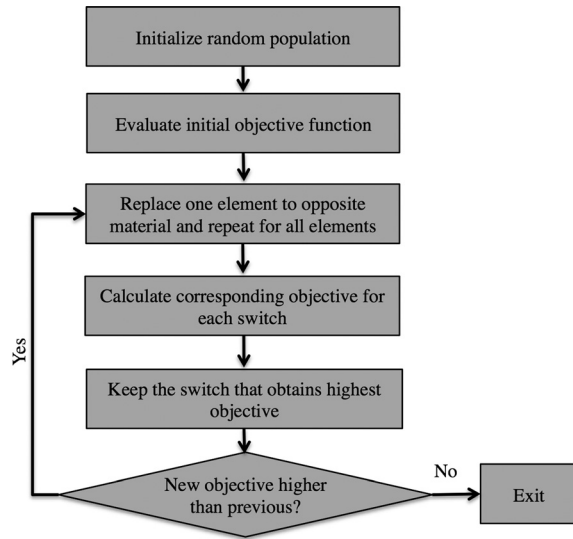


Fig. 2 Algorithm organization. The algorithm takes in as an input a random initial population of soft and stiff elements. At every iteration, an objective function value of the system is calculated for every element when only it is switched. Elements switch from soft to stiff and vice versa. The switch that generates the highest objective value increase is kept for the next iteration. This process is repeated until there is no switch that generates a higher objective value compared to the previous iteration at which point the algorithm exits outputting the final geometry.

energy needed to fracture a system. For our definition of toughness modulus, we solve for the energy to initiate crack propagation and not global composite crack propagation energy. The toughness modulus is defined by Eq. (2) below, where T is the toughness modulus, E_{eff} is the effective stiffness of the material, and ϵ_{tip} is the local element strain of the tip element

$$E_{\text{eff}} = \frac{\frac{1}{N} \sum_{i=1}^N \sigma_i}{\frac{1}{N} \sum_{i=1}^N \epsilon_i} \quad (1)$$

$$T = \frac{1}{2} E_{\text{eff}} \epsilon_{\text{tip}}^2 \quad (2)$$

We use the tip strain element because we assume that the crack will propagate from the crack tip. Material failure is typically controlled by material closest to the crack tip [29–31]. The soft and stiff materials differ in stiffness by a stiffness ratio. The constitutive relation between them is that the soft material has a larger critical strain compared to the stiff material but a lower stiffness with same toughness modulus. This constitutive relation is used because we wanted to look at pure geometry effects of adding soft materials to stiff material instead of material effects. The input values used in the algorithm are stiffness ratio, stiffness modulus of stiff material, length of material, and critical strain for stiff and soft materials and are summarized in Table 1.

Table 1 Inputs to the optimization algorithm used in this study. E_{stiff} is the modulus of the stiff material; E_{soft} is the modulus of the soft material.

| | E_{stiff} | Failure strain of stiff material | Stiffness ratio $E_{\text{soft}}/E_{\text{stiff}}$ | Length of sample |
|-------|--------------------|----------------------------------|--|------------------|
| Value | 1000 | 0.1 | 0.1 | 1 |
| Units | MPa | — | — | mm |

The objective function is evaluated using a finite element method, with four-node elements, each with two degrees-of-freedom. The finite element method is used to obtain the stress and strain field from displacements. A linear elastic model is used because we assume that the dominating mechanisms are controlled by linear elastic mechanisms, which are shown in experimental evidence in additive manufactured materials [32,33]. Displacement boundary conditions are applied in the x -direction. The symmetry of the problem reduces the number of elements by a factor of two. Infinitesimal displacements are assumed, and we stipulate that the toughness modulus is equal for the two different materials. We reiterate that the reason for the toughness equality is to eliminate material effects on change in toughness modulus, so as to make sure it is the geometry that is driving the effects on the change in toughness and not the material used. The failure criterion is strain and we set a critical strain value for both materials, and once the crack tip strain reaches it, the objective function is determined for the given toughness modulus.

2.2 Validation of the Algorithm for Effective Stiffness and Compliance.

The algorithm can be applied to a case where the material has no crack. To check the validity of the method, a test case for effective stiffness and compliance was done on a material with no crack and a fixed volume fraction. The volume fraction constraint is used because of the trivial answer that maximum stiffness derives from all stiff elements in a material, and likewise, all soft elements produce a maximum compliance case. Using the same x -direction loading case as the case with a crack in Fig. 1, a volume fraction of 50% soft material and 50% stiff material is used in the composite. Due to the mechanics theory of springs in series and in parallel, the optimized material for stiffness should have in-parallel conditions, while the optimized material for compliance should have in-series conditions, as shown in Fig. 3. The algorithm is capable of obtaining the correct geometries from any random geometry. Additionally, it is observed that there is no single solution for the optimum geometry, but many solutions with the same objective function value. Using the values given for stiffness ratio and modulus (E_{stiff}) in Table 1, the optimized values for these two cases should be $5.5E_{\text{stiff}}$ for maximum stiffness and $0.18E_{\text{stiff}}$ for maximum compliance, and these converged values are shown for a larger grid size system in Fig. 4.

2.3 Validation of the Algorithm Using a Brute Force Method for Toughness.

The validation of a maximum stiffness and compliance solution was shown in Sec. 2.2 using a case where the material has no crack. Since there is no known geometry for optimized toughness with a crack in a material, a brute force method is used for comparison with the proposed algorithm. The generated geometries from the modified greedy algorithm used in this project are compared with geometries using brute force. The brute force method works by checking all the possibilities in a system with a set volume fraction and picking the final solution that obtains the highest toughness modulus. The number of possibilities for this method is determined based on a combinatorial approach taking into consideration the volume fraction of the two materials. For instance, if the grid size is 16 and the volume fraction is 25% soft material (4 soft and 12 stiff elements), there are 1820 possible configurations, and the brute force algorithm evaluates all of them, choosing the best one. This method, though it can guarantee the optimized solution, is very computationally

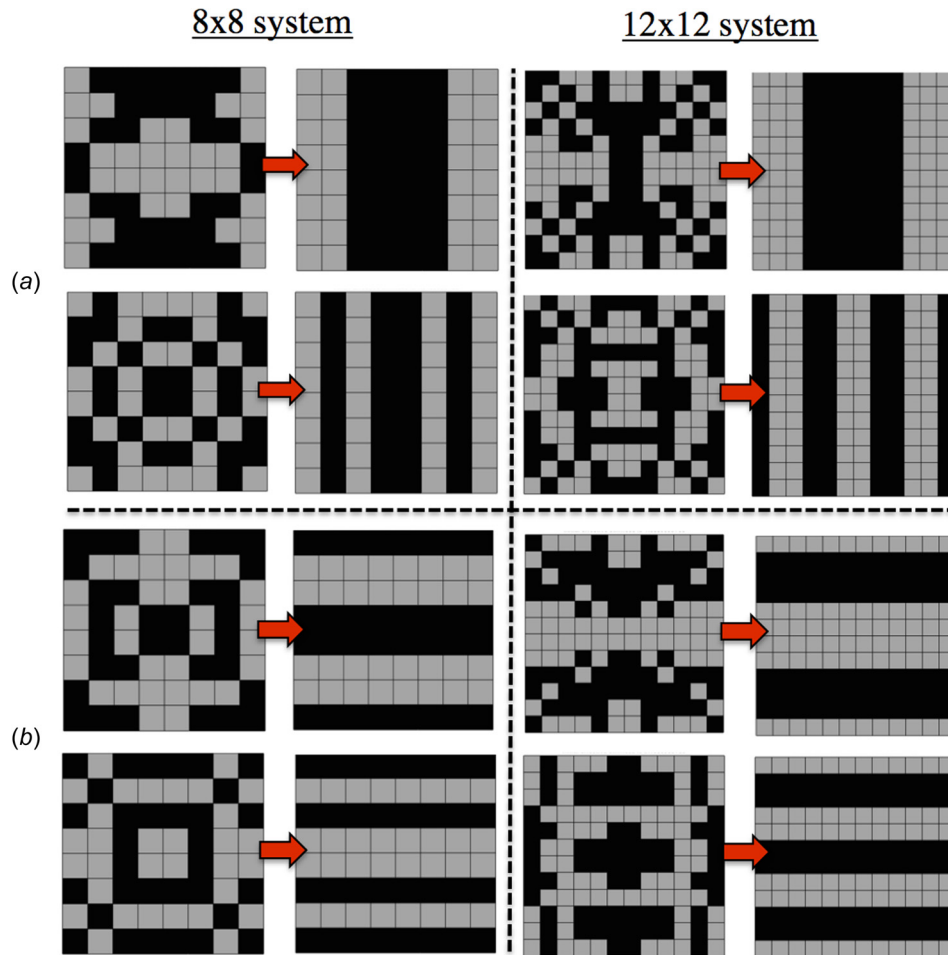


Fig. 3 Optimized solutions for maximizing effective compliance and effective stiffness for 8×8 and 12×12 grid size systems. (a) The maximum compliance solution is a geometry in which the soft (black) and stiff (gray) materials are in series with the loading conditions. From different initial random geometries, the algorithm leads to the optimized design of in-series materials. (b) The maximum stiffness solution is a geometry in which the soft and stiff materials are in parallel. Similarly, the algorithm leads to the optimized design starting from random initial geometries. These final geometries show that there is no single optimum solution for these problems, but many optimal solutions solving the same objective function.

expensive. For two test cases of 8×8 and 10×10 discretizations, respectively, with set volume fractions and crack sizes shown in Fig. 5, our algorithm was able to obtain the exact same solution as brute force, but orders of magnitude faster. This performance shows that our proposed algorithm is reliable and efficient.

3 Results and Discussion

3.1 Case Studies. For different applications, optimization parameters may vary. Here, we show different case studies for (1) optimizing toughness alone (f_T), (2) optimizing toughness and stiffness (f_{TS}), and finally (3) optimizing toughness and compliance (f_{TC}). The objective functions are shown in the following equations:

$$f_T = \left(\frac{T}{T_0} \right) \quad (3)$$

$$f_{TS} = \frac{E_{\text{eff}}}{E_0} \left(\frac{T}{T_0} \right) \quad (4)$$

$$f_{TC} = \frac{E_0}{E_{\text{eff}}} \left(\frac{T}{T_0} \right) \quad (5)$$

where T is the toughness, T_0 is the initial population toughness, E_0 is the effective stiffness of the initial population, and E_{eff} is the effective stiffness. Using a 20×20 grid size and a crack size of 20% of the length of the material, we generated geometries based on different objective functions. In addition, a volume fraction of 20% soft material is used. For the objective function of optimizing for toughness alone, the geometry that we generated is shown in Fig. 6. Soft material starts to surround the crack tip area to mitigate the local stress. For the objective function of optimizing toughness and stiffness, the geometry is shown in Fig. 6. Now, more material wants to be in parallel to the direction of loading compared to the case in which only toughness is optimized. Softer materials that were originally not aligned with the loading conditions moved so that the material could be stiffer. In the case for which toughness and compliance are simultaneously optimized, the opposite is true. More elements tend to be in series to the direction of loading, and a more columnar structure perpendicular to the direction of loading results.

3.2 Strain Delocalization. To observe the strain field of a tougher material design, a more refined 40×40 system geometry for case study 1 is compared to a homogenous stiff solution in Fig. 7. In the homogenous solution, strain concentrates at the crack tip. The resultant geometry mitigates strain at the crack tip

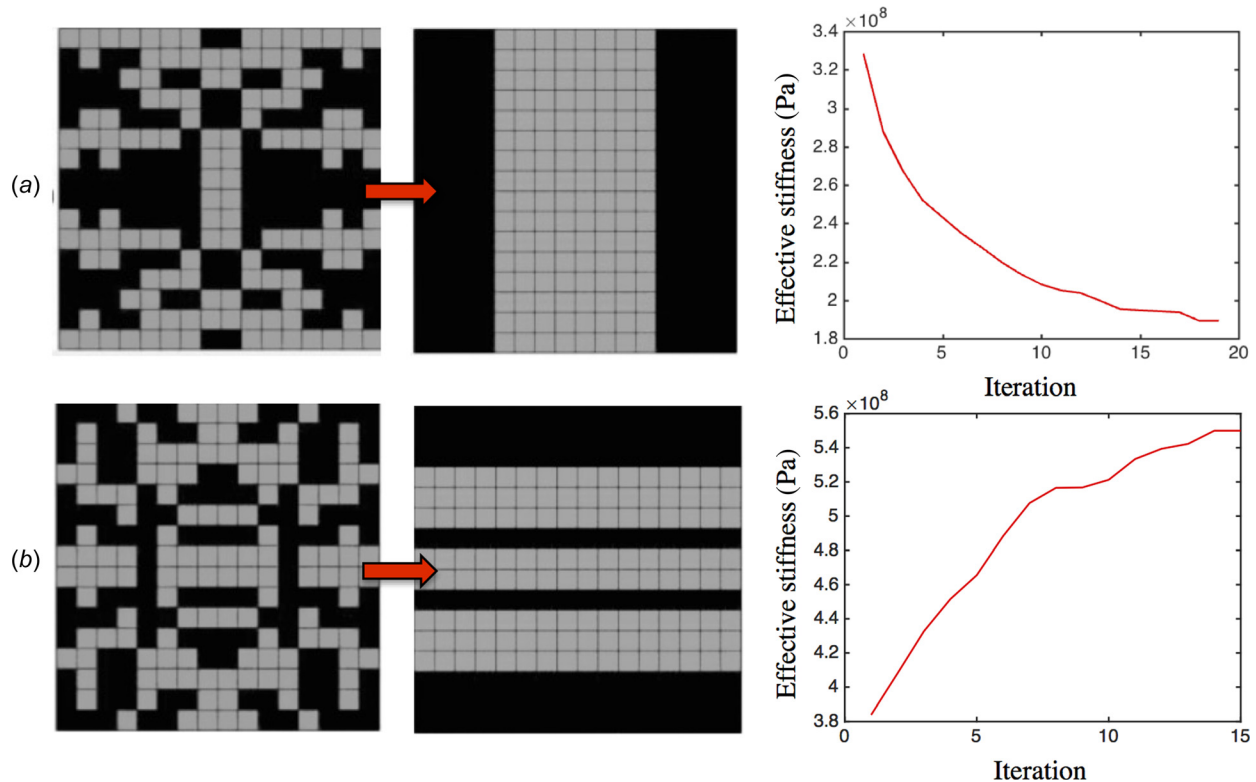


Fig. 4 Larger grid size solutions for minimizing stiffness (maximizing compliance) and maximizing stiffness. Convergence of solutions: (a) For a 16×16 system, the optimal solution obtained from the algorithm remains the same. The graph shows that the initial effective stiffness starts out high and decreases as iteration increases. (b) The optimal solution remains the same for maximizing stiffness and the graph shows an increase in effective stiffness with iteration. These two graphs show the solutions converging to the theoretical optimal values of compliance and stiffness.

| System | A (8x8) | B (10x10) |
|----------------------------------|---------------|---------------|
| Volume fraction of soft material | 25% | 10% |
| Crack size | 0.5a | 0.2a |
| Number of possibilities | ~10 million | ~2 million |
| Time to finish using brute force | 92569 seconds | 23564 seconds |
| Time to finish with algorithm | 7 seconds | 10 seconds |
| T_{brute}/T_{alg} | 1 | 1 |

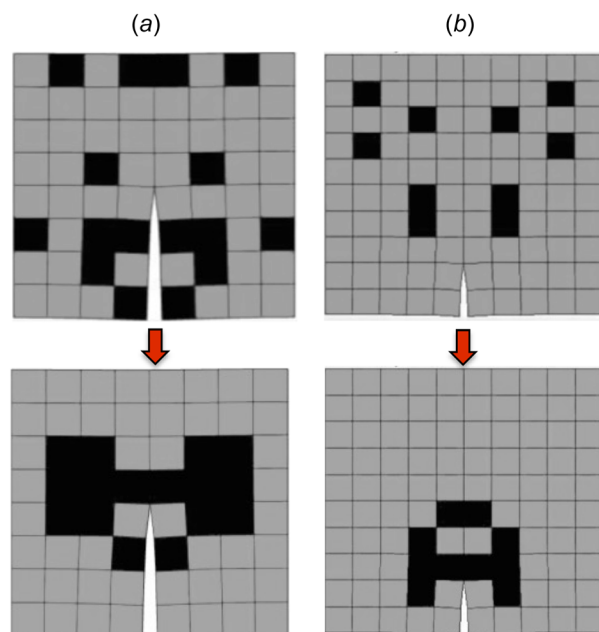


Fig. 5 Solutions from brute force method to validate algorithm when optimizing for toughness. The chart describes the differences between systems A and B. System A has a grid size of 8×8 and an edge crack that is 50% of the system length, with a being the length of the sample. The algorithm begins with a random geometry and generates the solution that exactly matches the solution obtained from brute force (i.e., checking every possible solution and selecting the best). The algorithm, however, is orders of magnitude faster than the brute force method. System B has a grid size of 10×10 and an edge crack that is 20% of the system length. The algorithm also obtains the same solution as the brute force method. T_{brute} is the toughness obtained from the brute force method and T_{alg} is the toughness obtained from our algorithm, and the ratio shows unity. This performance confirms that our algorithm is effective and robust.

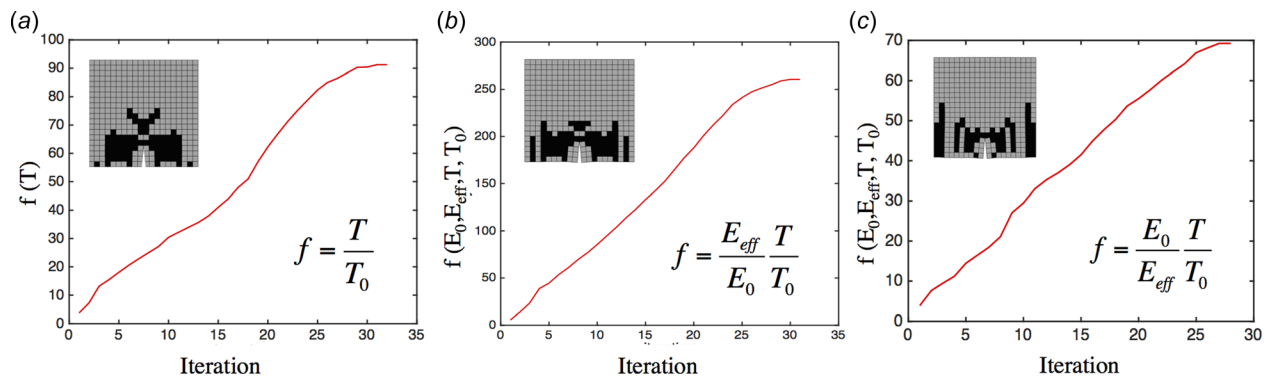


Fig. 6 Various case studies. (a) The geometry for the objective function that optimizes toughness modulus only. (b) The geometry for the objective function that optimizes toughness along with stiffness. More elements need to be in parallel to maintain high stiffness and also toughness. (c) The geometry for the objective function that optimizes toughness along with compliance. More elements are spread out to be in series with each other. Variables: f is the objective function, T is the toughness modulus, T_0 is the initial geometry toughness modulus, E_{eff} is the effective stiffness of the system, and E_0 is the effective stiffness of the initial population.

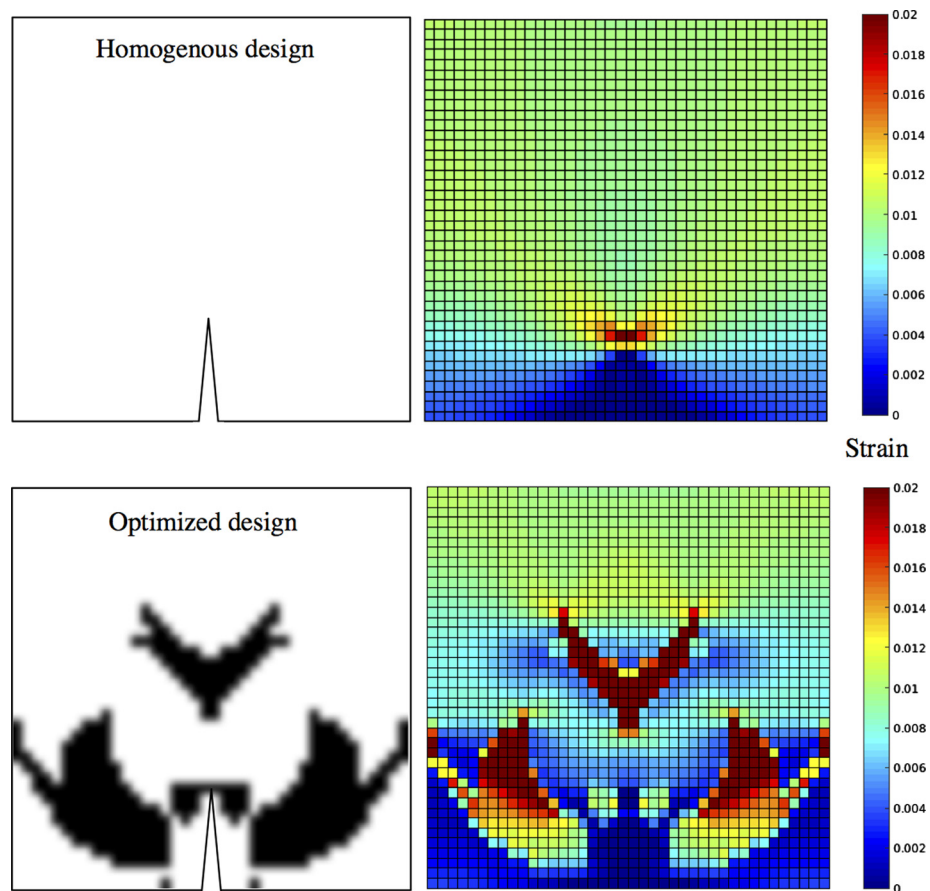


Fig. 7 Strain field for homogenous design compared to optimized design for 40×40 grid size. White space represents the stiff material and black space represents the soft material. Delocalization of strain seen in optimized design from crack tip area to soft material locations.

and increases its fracture energy. The placement of the soft material in relation to the stiff material and the crack tip leads to lower local stress. The role of the soft material is to delocalize the stress. As a result, soft material is placed in the regions circling around the crack tip. The soft material relaxes the stiff material around the crack tip and protects it from high stress concentration; strain will concentrate in the soft material instead of stiff as a result. Another aspect of the geometry is that the soft material follows

the stress contour around the crack tip. The soft material pattern follows the stress gradient, which helps to alleviate the stress concentration with soft material.

3.3 Future Outlook. Now that we have a technique to optimize composites with a crack, we look to manufacture these designs and test them for mechanical properties. These

multimaterial complex designs cannot be synthesized through traditional subtractive manufacturing. It requires a different approach that may be similar to how other researchers synthesize bio-inspired designs from nature such as nacre. Researchers tried to replicate natural material nacre by mimicking the natural layer-by-layer approach to fabricate a hierarchical crystalline multilayer material [34] and used nanoindentation to study its fracture behavior. Others have learned how to create a nanoscale version of nacre with alternating organic and inorganic layers by sequential deposition of polyelectrolytes and clays [35]. Freeze casting of various polymers and ceramics to create the brick and mortar designs proved to have a significant increase in toughness compared to the base materials [36,37].

Most recent are endeavors to emulate the brick-and-mortar structure of nacre using three-dimensional (3D) printing and testing for mechanical properties [32,33,38]. Three-dimensional printing is a tool that does not limit the geometry of the sample. For future work, we plan to use additive manufacturing to manufacture optimized geometries and test them in tension to compare and analyze with simulation predictions.

4 Conclusions

This paper explored the optimization of a composite structure made up of soft and stiff building blocks with an edge crack under uniaxial tension. We used a modified greedy algorithm to find the optimized composite morphology and showed that through iteration, we can achieve a better design compared to the initial configuration. To validate our algorithm, we simulated the material with no crack and a fixed volume fraction to show that the algorithm obtains the optimized solutions for maximum effective stiffness and compliance. Indeed, the algorithm obtains the stripes parallel to the loading conditions for maximizing stiffness and obtains the columnar shapes in series to the loading conditions for maximizing compliance. Additionally, through a brute force method, we were able to validate our algorithm with crack for various grid sizes.

We applied our algorithm to various case studies of optimizing toughness alone, toughness and stiffness, and toughness and compliance. For the case of optimizing toughness alone, soft materials start to surround the crack tip area. For the case of optimizing toughness and stiffness, soft materials move toward the structure that optimizes stiffness, without crack, which align parallel to the loading conditions. Observing the strain field for a larger grid size, the strain is delocalized and the highest strained area is experienced by the soft material. We presented a technique to design and optimize materials for different material properties. Possible next steps include manufacturing these designs and testing them for mechanical properties.

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