A HYBRID LAGRANGIAN-EULERIAN METHOD FOR TOPOLOGY OPTIMIZATION

ABSTRACT

We propose LETO, a new hybrid Lagrangian-Eulerian method for topology optimization. At the heart of LETO lies in a hybrid particle-grid Material Point Method (MPM) to solve for elastic force equilibrium. LETO transfers density information from freely movable Lagrangian carrier particles to a fixed set of Eulerian quadrature points. The quadrature points act as MPM particles embedded in a lower-resolution grid and enable sub-cell resolution of intricate structures with a reduced computational cost. By treating both densities and positions of the carrier particles as optimization variables, LETO reparameterizes the Eulerian solution space of topology optimization in a Lagrangian view. LETO also unifies the treatment for both linear and non-linear elastic materials. In the non-linear deformation regime, the resulting scheme naturally permits large deformation and buckling behaviors. Additionally, LETO explores contact-awareness during optimization by incorporating a fictitious domain-based contact model into the static equilibrium solver, resulting in the discovery of novel structures. We conduct an extensive set of experiments. By comparing against a representative Eulerian scheme, LETO’s objective achieves an average quantitative improvement of 20% (up to 40%) in 3D and 2% in 2D (up to 12%). Qualitatively, LETO also discovers novel non-linear functional structures and conducts self-contact-aware structural explorations.

Keywords topology optimization · material point method · nonlinear elasticity

1 Introduction

Topology optimization is experiencing a rapid advance over the past few years, thanks to the collision of waves between next-generation computing infrastructure and high-performance simulation software. A surge of recent work has been creating various computing infrastructures, capable of accommodating topology optimization applications with a super-scale resolution—millions to one billion of material voxels—on parallelizable data structures (e.g., [1, 2]). These density-based approaches naturally fall into the category of Eulerian methods, owing to their geometric representation of the material evolution on a fixed grid. Levelset-based [3] methods are also Eulerian due to an implicit representation of the topology on grid nodes. On the other hand, Lagrangian geometries are increasingly attracting attention. For example, particles (e.g., in SPH [4]) can explicitly track the structural evolution by evolving a set of particles under the guidance of material derivatives. Tracking explicit meshes is also a promising direction thanks to the advent of high-performance meshing software [5].

1.1 Hybrid representation

Despite extensive research, Eulerian approaches have limited capability in capturing intricate structures, especially when the problem requires fine features that are hierarchical, codimensional, and can emerge from a nihil. On the other hand, Lagrangian representations suffer from lower computational performance. Analogous to their computational physics
counterparts (e.g., in computational fluid dynamics), Eulerian approaches are not naturally adaptive to small features, whereas Lagrangian methods face challenges in establishing differential stencils that are geometrically symmetric and numerically accurate.

Additionally, computational physics researchers are facing the same dilemma regarding the choice of data structures and the corresponding numerical stencils when simulating large-scale fluids and solids. This dilemma further triggered the invention of a bank of hybrid Lagrangian-Eulerian methods, such as PIC/FLIP methods [6] and MPM [7], which are featured by a Eulerian background grid as a scratch pad and a set of Lagrangian particles moving on top of it to track geometry and topology. By conducting data transfers between the two representations, a hybrid Lagrangian-Eulerian scheme can typically leverage the merits on both sides, enabling flexible and robust numerical solutions that outperform a single representation [6,7].

Motivated by such a design philosophy underpinning PIC/FLIP and MPM, we propose a novel hybrid Lagrangian-Eulerian topology optimization method—LETO that optimizes material distributions over a design domain by evolving a set of material carrier particles on a background Cartesian grid. For the physical constraints, we leverage MPM as an efficient numerical solver that can solve the static equilibrium states to satisfy the force equilibrium. For the optimization search, we evolve a particle system with each particle carrying a temporally varying density to achieve a Lagrangian representation of material distribution. The Lagrangian-Eulerian nature of our framework enables the communication between the moving particles and the fixed background MPM quadrature points by transferring the density values through interpolation functions. More specifically, as the carrier particles move and change their densities, the density values on the quadrature points are updated accordingly, naturally providing sub-cell resolution with the same simulation cost as a traditional FEM solver. For the numerical implementation, a newly designed density mapping function is applied for the transfer of the density between the quadrature points and the carrier particles. The sharpness of the mapping helps to approximate the original 0-1 integer programming problem better.

### 1.2 Nonlinear elasticity

Another long-standing challenge of topology optimization is to optimize structures undergoing large deformations, which requires a nonlinear elasticity model and thus the nonlinear equilibrium constraints. This has become increasingly meaningful with the increasing need for material and structural design in soft robotics, wearable devices, and even space antennas, etc. The state-of-the-art approaches have been facing three major hurdles toward a versatile and robust nonlinear structural optimizer. Given a nonlinear scenario with large deformation, not only is the force equilibrium much harder to solve as it often leads to numerical instabilities, but also the optimization itself will converge slower. Existing works [8,9,10] concentrate on optimizing linearized compliance to capture large displacement but limited to scenarios with only moderate deformation. Additionally, the structure can even self-intersect under large deformation, making the optimization not meaningful. To the best of our knowledge, none of the existing research has explicitly discussed this issue.

Our hybrid Lagrangian-Eulerian method provides a unified formulation of linear and fully nonlinear compliance optimization, together with the unified discretization provided by MPM. In LETO, we apply a line search based projected Newton method to ensure convergence to force equilibrium with high accuracy, enabling our fully nonlinear topology optimization with the highly nonlinear neo-Hookean elasticity to produce more intricate structure and significantly lower compliance than nonlinear SIMP, especially for cases with large force load. We further explore contact-aware topology optimization by enhancing the simulation with a fictitious domain-based contact model. With the inversion-free line search, we ensure local injectivity between material and world spaces, demonstrating that self-contact can be consistently taken into account for both simulation and optimization.

For nonlinear elasticity, we show that LETO is robust to handle both small and large deformation scenarios. We also compare LETO with the nonlinear extension of the state-of-the-art linear topology optimization method on four 3D examples. The experiments show that our approach achieves lower structural compliance with improvements up to 18%. To further demonstrate the advantage of LETO, we conduct an extensive benchmark study of numerical experiments in both two dimensions (14 examples) and three dimensions (8 examples) using linear elasticity. The results also demonstrate the efficacy of our approach by comparing the achieved structural compliance against the state-of-the-art methods, wherein LETO provides an average improvement of 20% in 3D and 2% in 2D, up to 40% and 12% respectively. During the nonlinear experiments, we identified the existence of material self-intersection issues. With a fictitious domain-based approach, we conduct a preliminary exploration of self-contact-aware topology optimization. We show that the optimizer can indeed generate structures that make use of contact forces, which are meaningful in reality.
1.3 Summary

In summary, we propose a novel hybrid Lagrangian-Eulerian framework for general topology optimization with MPM. The resulting scheme can generate thin structures with outstanding mechanical performances that rival conventional methods at a comparable computational cost. Our framework provides a unified treatment for both linear and nonlinear topology optimization and supports optimizing fully nonlinear compliance, which enables robust and accurate optimization of structures undergoing large deformation. Empowered by a unified grid-based treatment of (self-)contact, our nonlinear topology optimization can be contact-aware, which potentially opens up a new avenue for computational fabrication.

2 Related Work

2.1 Topology Optimization

Topology optimization has demonstrated its efficacy in creating structural designs with complex functional in various engineering problems (see [11][12][13] for surveys). A topology optimization algorithm iteratively removes and redistsributes material over a design domain to evolve the structure of the target design by minimizing a design objective (e.g., structural compliance). Topology optimization can be generally classified into Eulerian methods and hybrid Lagrangian-Eulerian methods based on the discretization data structures for geometry. Density [14] and implicit interface [15] are the two most commonly used material discretizations in Eulerian approaches. Hybrid methods use explicit geometry descriptors but still solve the equilibrium equation on a fixed background grid. In the following sections, we provide a brief overview of each category of data structures together with the underlying high-performance material simulators. We further review the existing methods that handle nonlinear elasticity material to capture large displacements.

2.1.1 Eulerian Methods

Level Set Based Approaches Originated from Osher and James [3], level set methods use implicit functions to represent the geometry, which is flexible to handle topological changes such as splitting and merging. Traditionally, the evolution of level sets is performed by solving the “Hamilton-Jacobi-type” equations [15][16]. While topological changes, including merging and splitting, are well-defined, opening up holes on the shape is yet a separate step that might affect the convergence behavior due to potential inconsistencies [17]. Additionally, the initial configuration in level set based methods can have a large bias on finding the local optima [16]. On the other hand, convergence and regularization of level set based methods are also of major consideration. Using a smoothed Heaviside function can speed up the convergence by sacrificing boundary sharpness [18]. Despite the current endeavors, achieving a great level of geometry details while maintaining the control of the spatial gradient remains challenging. We refer to the review articles [19][17] for more details.

Solid Isotropic Material with Penalization Method (SIMP) SIMP [20][21] is one of the most popular methods in topology optimization. It approximates the integer programming formulation of topology optimization by introducing the concept of local material density that smoothly varies from 0 to 1 to represent material distribution on an Eulerian grid. By employing the power-law method, SIMP assumes Young’s modulus of each grid cell to be a polynomial of the material density on that cell, which effectively makes the results more binarized. Specifically, the material stiffness $E(\rho)$ is defined as $\rho^p E_0$ for each cell, where $E_0$ is the base Young’s modulus of the solid material and, $p = 3$ is usually used for reducing the intermediate density values; when $p = 1$, the problem becomes convex. Studies have been established in applying homotopy optimization that first solves the convex problem to acquire a coarse but more global solution and then gradually increases the power to reduce intermediate values and search for local minima that better approximates the integer programming solution. This approach is known as parameters continuation [9][22][8][23], which can effectively improve optimization convergence. LETO directly applies the power-law approach with $p = 3$, but with an additional design of a family of density mapping functions to further help the integer programming approximation via homotopy optimization; see Section [4.2]. The optimization proposed by SIMP is mesh-independent; namely, the number of iterations required to converge does not increase with the resolution of the Eulerian grid. However, the objective proposed by SIMP could have a local minimum that is with checkerboard patterns, which are not meaningful for manufacturing. Therefore, different types of smoothing filters [22][24][25] are applied to the gradient during the search to avoid checkerboard patterns. LETO applies an SPH kernel for transferring density between carrier particles and MPM quadratures, where its smoothing effect plays a similar role to the filtering strategy. Recently, several works [2][1] create various computing infrastructures that accommodate SIMP with a superscale resolution to obtain results with rich geometry features and smooth boundaries. Similarly, to push forward the resolution limitation, we explore sub-cell resolution with MPM by allowing multiple densities within every single cell and introducing Lagrangian...
degrees-of-freedom, enabling our hybrid Lagrangian-Eulerian method to generate more intricate structure at the same simulation cost.

2.1.2 Hybrid Lagrangian-Eulerian Methods

Moving Morphable Components (MMC) MMC method aims to substantially reduce the number of design variables by optimizing component-wise distributions. It is first introduced to represent structures with superellipse level set, a low dimensional morphable component that has the capability of moving, deforming, and overlapping to track topology changes \[26\]. Aside from level sets, Zhang et al. \[27\] proposed to use structural components of linearly varying thicknesses within MMC. MMC can produce results with sharp features; however, its performance and computation are significantly more efficient than traditional approaches. Thus, to acquire solutions with sophisticated geometry features, a more significant number of components, i.e., design variables, is still necessary.

The Moving Node Approach (MNA) MNA \[28\] represents shape with a set of mass nodes, of which the positions are optimized to find optimal structure. In MNA, compliance and force equilibrium is computed by the element-free Galerkin method, wherein the quadrature is a set of regularly sampled discretization nodes, on which the density is computed according to the clustering of mass nodes. Similar to SIMP, a lower bound of density on the discretization node is required to avoid singularity during static solve. However, such an approach can result in a lot of isolated mass nodes from the main structure, which can only be cleaned up in an extra post-processing step. Inspired by the potential of this idea on consistently resolving arbitrarily more complex geometry and topology given larger numbers of particles, we designed LETO that treats both position and density as optimization variables, resulting in a fast and consistent topology optimization framework without the need of any special treatment to regularize the results.

2.1.3 Nonlinear Topology Optimization

Modeling nonlinear material responses plays an increasingly important role in our contemporary life with the rapid development of soft robotics, wearable devices, space antennas, wind turbine blades, compliant mechanism applications, and crashworthiness design. In the infinitesimal displacement analysis, the mean structural compliance is the first-order approximation of elastic potential \[29,30\]. However, existing works \[8,10,31,32,33\] mainly consider this mean compliance as objective function for nonlinear topology optimization. They handle large displacements well but are still limited to small strains since the first-order approximation gets much less accurate to the strain energy when deformation becomes large. Swan and Kosaka \[34\] consider strain energy as objective function but still use small strain formulation, since they only focus on geometrically linear deformations. Another challenge of nonlinear topology optimization is the numerical instability introduced by low-density elements. The severe distortion of these elements usually results in an ill-conditioned stiffness matrix that could even become negative definite, leading to unreasonable search directions during static solve. Several works proposed various solutions to address this issue. As indicated by Zhou et al. \[35\], merely removing these elements will cut off the ability of reappearance of them and can bias the results. Bruns et al. \[9\] construct a Gaussian-weighted density measure, which compensates density for these elements and solves the force equilibrium on the smoother density field, which was later shown to be case dependent by Buhl et al. \[8\], where they instead remove these low-density elements when computing the stopping criteria for Newton iterations while still including them for evaluating the objective function and its gradient. Later, Bruns et al. \[36\] propose a removal and reintroduction pipeline as narrow-band simulation. Additional works were also proposed to model these elements with a better-posed elasticity energy: Wang et al. \[37\] models low-density and high-density elements with linear and nonlinear elasticity respectively, Luo et al. \[38\] use the Yeoh hyperelastic material for low-density elements, and Chen et al. \[39\] perform linear sensitive analysis first and pass the result into the following nonlinear pipeline.

Instead, we directly optimize the strain energy, which is fully nonlinear, and consistently model all elements with the same hyperelastic constitutive model, avoiding the numerical instability issue by projecting every Hessian stencil to symmetric positive semi-definite during the static solve and meanwhile applying an inversion-free line search filter to ensure both robustness and accuracy; see Section 4.4.

2.2 Elasticity Simulation

When applying the adjoint method on topology optimization, elasticity simulation is required, in each iteration, to obtain the nodal displacement under force equilibrium given material distribution and the force load. Since no dynamic information is needed here, static solve is directly conducted. While traditional topology optimization methods often apply uniform grid-based FEM, we novelty apply the MPM for the static setting with the sub-cell resolution achieved by assigning different densities for each quadrature. From the variational point of view, we solve the static equilibrium
with optimization approaches robustly and accurately. We also propose a convenient way to model contact within the static solve to explore contact-aware topology optimization preliminarily.

**Spatial Discretization** Traditional topology optimization methods, including both density-based approaches [20, 8] and level set-based approaches [26, 15], often apply grid-based finite element discretization for the static solve. In FEM, the same material density is assigned for all the quadrature within every single cell. Therefore, the domain boundaries are formed with jagged finite element edges, and even plotting zero-level contour still results in jagged boundaries [17].

To alleviate these artifacts, a higher resolution grid is often required, which is expensive. MPM is a hybrid Lagrangian-Eulerian method widely used in different fields of research, e.g., computer graphics [40, 41], civil engineering [42, 43], mechanical engineering [7, 44, 45]. With the capability of handling large deformation, topology changes, and different material coupling, MPM has been considered as one of the top choices in physics-based simulation, including fracture [44, 41], viscoelastic and elastoplastic solids [46], snow [40, 47, 43], and mixtures [50, 51]. In MPM, Lagrangian particles, which are also known as material points, are used to track quantities like mass, momentum, and deformation gradient, whereas a regular Eulerian grid is built at each time step to evaluate force and update velocity. Particle quantity is then updated from the interpolation of nodal quantities.

LETO applies the MPM spatial discretization and derives a static formulation for directly solving the force equilibrium, which allows us to define quadrature-wise density per cell to take advantage of the sub-cell resolution. As will be shown in our experiments, LETO achieves a comparable convergence speed with lower structural compliance.

**Optimization and Nonlinear Integrators** Numerical integration of partial differential systems can often be reformulated variationally into an optimization problem. These methods can often achieve improved robustness, accuracy, and performance by taking advantage of well-established optimization approaches. In computer graphics, simulation methods are increasingly applying this strategy to simulate both fluid [52] and solid [53] dynamics, which often enable large time step sizes.

As static solve simply corresponds to infinitely large time step size in a dynamic time-stepping point-of-view, we thus also take advantage of optimization integrators to robustly solve our static equilibrium to high accuracy.

For nonlinear optimization problems, Newton-type methods are generally the standard mechanism because it can deliver quadratic convergence when close to the local optima. However, when the initial configuration is far from a local optimum, which is often true in static solves, Newton’s method may fail to provide a reasonable search direction as the Hessian can be indefinite [54, 55, 56]. Teran et al. [57] thus propose a positive definite fix to project the Hessian to a symmetric positive definite form to guarantee that a descent direction can be found. We refer to this method as projected Newton (PN) throughout the paper and apply it for our static solve. Each PN iteration requires solving a linear system.

For MPM simulations which often contain a large number of degrees-of-freedom, Krylov iterative linear solvers such as conjugate gradient (CG) are often more favorable than direct factorizations. To improve CG convergence, different preconditioning options exist. We apply AMGCL [58], a general algebraic multigrid preconditioned CG solver, to solve our systems. AMGCL generally performs well in our examples; but for extremely hard cases, extensive parameter tuning is still required to work well. Therefore, we switch to direct Cholesky factorization in Eigen [59] on those hard examples when AMGCL fails to converge in a reasonable amount of time.

**Self-Contact** Computational contact mechanics is a fundamental topic that has been long studied in diverse perspectives such as engineering, robotics, and computer graphics [60, 61, 62, 63]. However, it has never been explored or applied in topology optimization as none of the existing works optimizes structure under extreme deformation conditions that could lead to self-intersection. Contact problem combines enforcement of challenging intersection-free constraints with the resolution of a force equilibrium, including possibly nonlinear elasticity and external forces. In this paper, we focus on the recently emerged fictitious domain methods [64, 65, 66, 67, 68] that resolves contact in a convenient way.

Fictitious domain methods offer a promising alternative to traditional contact algorithms that defines constraints between surface elements and solves the constrained optimization via sequential quadratic programming, which is expensive and can hardly guarantee interpenetration-free. In fictitious domain methods, motivated by global injectivity conditions [69], voided space is separately discretized by a compatible discretization, sometimes called an air-mesh [65]. Maintaining a non-negative volume on elements of the air mesh guarantees non-interpenetration. This strategy is well-suited for topology optimization as initially, the structure is often uniformly distributed on the entire design space where regions that later become voided are already discretized in a consistent way. Therefore, we procedurally triangulate/tetrahedralize the grid cells with small density and apply barrier energy to ensure their volume always stays positive. In this way, we easily model self-contact into our static solve in a consistent way as for nonlinear elasticity and enable our topology optimization to take advantage of contact forces.
However, as with locally defined proxy volumes, the globally defined air mesh can potentially introduce increasingly large errors, e.g., shearing, and locking forces, as it distorts with the material mesh. In 2D, this issue can be alleviated by local [65] or global [66] remeshing; however, this is highly inefficient in 3D as it does not provide a continuous constraint representation for optimization, nor, even with remeshing, can it resolve sliding and resting contact where air elements must necessarily be degenerate [70]. In this paper, we apply the fictitious domain methods simply as a feasible solution and hope it can inspire further research in contact-aware topology optimization as we demonstrate how results can stay meaningful and be improved while considering self-contact.

3 Overview

3.1 Problem Statement

The general concern of topology optimization is to seek for a material distribution \( \rho \) (a scalar field representing the density of material distribution at each point), defined on a design domain \( \Omega \), to obtain the minimal structural compliance \( c(\rho, u) \), or equivalently, the least strain energy \( e(\rho, u) \), under force equilibrium between internal elasticity force \( -\nabla \hat{e} \) and external force load \( f \) with displacement \( u \):

\[
\min_{\rho, u} \ c(\rho, u) = e(\rho, u) \quad \text{s.t.} \quad \begin{cases} 
\frac{\partial e}{\partial u}(\rho, u) = f \\
V(\rho) \leq \hat{V},
\end{cases}
\]

(1)

where the volume of material is defined as \( V(\rho) = \int_{\Omega} \rho dX \), and \( \hat{V} \) is an upper bound specified by user [20] to constrain the total usage of material so that meaningful structures with small volume but large strength can be obtained. Usually, we also want \( \rho \) to be close to either 0 or 1 for manufacturing, which potentially makes the problem non-smooth.

The compliance objective depends on both material space structure \( \rho \) and world space displacement \( u \), which is nonlinear even for linear elasticity materials, so does the force equilibrium constraint. Adjoint method [71] is often applied to avoid solving the nonlinear KKT system as in standard equality constrained optimization [22]: it takes \( u \) as a function of \( x \) and cancels out \( \frac{\partial u}{\partial x} \) by considering the searching process to be conducted only on the force equilibrium constraint manifold. Given an intermediate state \( \rho \), a static problem provided by the PDE constraint is required to be solved to obtain \( u \) in each iteration. For linear elasticity materials, each solve is on a linear system, which is the bottleneck of topology optimization, making it expensive to obtain intricate results with lower compliance by increasing resolution [21]. It becomes even more challenging for nonlinear elasticity materials not only because a nonlinear system needs to be solved for each iteration that easily leads to numerical instability and even explosion but also that materials can self-intersect, making the optimization meaningless.

3.2 Hybrid Lagrangian-Eulerian Topology Optimization

To address the aforementioned challenges, we novelly propose a hybrid Lagrangian-Eulerian approach to establish a versatile topology optimization framework to accommodate different elastic models. In particular, LETO optimizes the elastic potential as the compliance objective for both linear and highly nonlinear (e.g., neo-Hookean) elasticity materials. LETO adopts a set of carrier particles to represent the material distribution and evolution, wherein each particle is a moving material sample carrying the information of position \( x^c \), density \( \rho^c \), and supporting radius. This modifies the general formulation in (Eq. 1) from a pure Eulerian representation, which directly optimizes the density field \( \rho \), to a hybrid Lagrangian-Eulerian form, which co-optimizes \( x^c \) and \( \rho^c \) that jointly define the material distribution \( \rho(x^c, \rho^c) \) over the design domain:

\[
\min_{\rho, u} \ c(\rho(x^c, \rho^c), u) = e(\rho(x^c, \rho^c), u) \quad \text{s.t.} \quad \begin{cases} 
\frac{\partial e}{\partial u}(\rho(x^c, \rho^c), u) = f \\
V(\rho(x^c, \rho^c)) \leq \hat{V},
\end{cases}
\]

(2)

Using MPM as the static equilibrium solver (see more details in later sections), we discretize the design domain to a background Eulerian grid together with a set of uniformly sampled quadrature points in each grid cell where every quadrature has its own density value that together form the scalar field \( \rho \). In this way, LETO effectively brings in the sub-cell resolution by sampling multiple quadratures per cell.

We further construct the relation between carrier particles \( (x^c, \rho^c) \) and quadrature points \( (\rho) \) using a smoothed-particle hydrodynamics (SPH) kernel and a sharp density mapping function. Adopting SPH kernel has the same effect as the gradient filter [20] that prevents the checkerboard pattern; however, since LETO is acting on the objective, it avoids performing extra smoothing on the gradient which potentially makes the search and objective inconsistent. Likewise, the novel \( C^1 \) continuous density mapping function helps better approximate the original integer programming problem by making \( \rho \) to be close to either 0 or 1.
It is easy to achieve narrow-band simulation [2] using MPM by filtering out low-density quadratures, which is essentially how zero-mass nodes are filtered out in MPM dynamic simulation. However, note that here we make sure the remaining polluted grid cells form a manifold so to avoid singular stiffness matrices (no mass matrix in static solve). We also get a unified simulation framework for different hyperelastic energies including non-invertible nonlinear elasticities like neo-Hookean. This triggers our design on a unified framework for both linear and nonlinear topology optimization.

We derive the gradient of fully nonlinear compliance under nonlinear elasticity force equilibrium by considering the searching process to be only conducted on the constraint manifold. During the static solve, we use projected Newton and line search to guarantee stability and convergence. With barrier energies defined on the fictitious domain elements, we ensure injectivity between material space and world space by ensuring all these elements will not invert, which effectively provides a contact model on the structure, making sure that the proposed optimization always stays meaningful and affords the structure to take advantage of contact forces for minimizing the compliance.

Using moving asymptotes (MMA) [73] as the optimizer, our optimization pipeline can be summarized as the follows; also see an illustration in Fig. 1:

![Figure 1: Hybrid Lagrangian-Eulerian method pipeline with an MPM solver.](image)

0. **Initialize:** Collocate our carrier particles on the uniformly sampled MPM quadrature points and initialize carrier particle density such that the volume constraint is satisfied; see Section 4.2.

1. **Transfer information from carrier particles to quadrature points (C2P):** Transfer density from carrier particles to quadrature points with a spherical kernel and a sharp density mapping function; see Section 4.2.

2. **MPM Static Solve:** see Section 4.1.

   2.1. **Transfer information from quadrature points to grid (P2G):** Transfer density from quadrature points to grid nodes and construct MPM system matrix $\frac{\partial \mathbf{e}}{\partial \mathbf{u}}$ on the grid.

   2.2. **Solve force equilibrium:** Solve $\frac{\partial \mathbf{e}}{\partial \mathbf{u}} = f$ on MPM grid. Here, only a single linear system solve is required for material with linear elasticity (see Section 4.3), while we apply projected Newton method for nonlinear elasticity (see Section 4.4). We additionally include our contact terms into the solve for contact-aware nonlinear topology optimization (see Section 4.6).

   2.3. **Update quadrature deformation gradient (G2P):** Update the deformation gradient $F_q$ of quadrature points with the solved nodal displacements $\mathbf{u}$.
3. **Compute compliance and the derivatives (P2C):** Evaluate compliance objective (Eq. (7)), compliance derivative (Eq. (26)), volume constraint function (Eq. (21)), and volume constraint derivative (Eq. (22)); see Section 4.3.

4. **Update carrier particle data:** Update $\mathbf{x}^c, \rho^c$ using MMA and evaluate convergence criteria; see Section 4.5. If not converged, go to Step 1 and repeat.

4 Hybrid Lagrangian-Eulerian Method

4.1 MPM Discretization

The structural compliance that we seek to minimize is the elastic potential of the material under certain loads

$$e(\rho, u) = \int_{\Omega_0} \Psi(F) dX,$$

(3)

where $\Omega_0$ is the material space the elastic body lies in, $\Psi$ is the elastic energy density function, and $F$ is the deformation gradient, which, in static setting, is defined as

$$F = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = I + \frac{\partial \mathbf{u}}{\partial \mathbf{X}},$$

(4)

where $\mathbf{x}$ is the world space position of the material space position $\mathbf{X}$, and $\mathbf{u}(\mathbf{X}) = \mathbf{x} - \mathbf{X}$ is the nodal displacement.

In MPM, $\Omega_0$ is discretized as a set of material particles, or quadratures. Each quadrature $q$ has its own density $\rho_q$, Young’s modulus $E_q$, deformation gradient $F_q$, elastic energy density function $\Psi_q$, and volume $V_q$, which is initialized uniformly and fixed. The compliance is defined as the integrated elastic potential from all the quadratures:

$$e(\rho, u) \approx \sum_q \rho_q \Psi_0(F_q) V_q,$$

(5)

In our setting, $\Psi$ could be any elasticity energy, e.g., neo-Hookean:

$$\Psi_{NH}(F) = \frac{\mu}{2} (\text{tr}(F^T F) - d) - \mu \log J + \frac{\lambda}{2} (\log J)^2,$$

(6)

where $J = \text{det} F$, $d = 2$ or 3 is the dimension of the problem, and both of the two lamé parameters, $\mu$ and $\lambda$, are with linear relation to Young’s modulus $E$. Similarly to SIMP, we define Young’s modulus to be scaled by the density of the particle: $E_q = \rho_q^p E_0$, where $E_0$ is the material’s Young’s modulus, so that the stiffness of the material is continuously varying over the domain according to its distribution. Since $\Psi$ is linear w.r.t. Young’s modulus, the compliance can be rewritten as

$$e(\rho, u) \equiv \sum_q \rho_q^p \Psi_0(F_q) V_q,$$

(7)

where $\Psi_0$ is the energy density function with Young’s modulus $E_0$.

Since every quadrature has its own density, and we sample $2^d$ quadratures per grid cell in MPM, we can achieve sub-cell resolution with nearly identical simulation cost compared to traditional methods.

**Static Equilibrium** While MPM is commonly used for dynamic time stepping, we here derive a static problem formulation based on MPM spatial discretization. In such a static setting, there is no inertia effect or time-variant variables, meaning that we only have the elasticity and external force term and can directly solve nodal displacement:

$$- \frac{\partial e}{\partial u} (\rho, u) + f = 0,$$

(8)

where $f$ is the external force load (Neumann boundary condition) defined on the quadrature points and then transferred to the grid nodes in the same way as the computation of internal force $- \frac{\partial e}{\partial x}$. Dirichlet boundary conditions can be defined as

$$D \mathbf{u} = 0,$$

(9)

where $D$ is the selection matrix that extracts the Dirichlet grid nodes. From a variational point of view, this is equivalent to solving the following optimization problem

$$\min_u e(\rho, u) - u^T f \quad \text{s.t.} \quad D \mathbf{u} = 0.$$

(10)
In MPM, quadratures are embedded in the background Eulerian grid with a B-spline kernel, meaning that the nodal displacement \( u \) is, in fact, defined on the uniform grid nodes. In our implementation, we choose the linear kernel

\[
N(x) = \begin{cases} 
1 - |x|, & 0 \leq x < 1 \\
0, & 1 \leq x
\end{cases}
\]  (11)

where the weight \( \omega_{iq} \) between grid node \( i \) and quadrature \( q \) is defined by taking the Cartesian product in all dimensions. For example, in 3D, we have

\[
\omega_{iq} = N\left(\frac{1}{h}(x_{q,1} - x_{i,1})\right)N\left(\frac{1}{h}(x_{q,2} - x_{i,2})\right)N\left(\frac{1}{h}(x_{q,3} - x_{i,3})\right).
\]  (12)

The deformation gradient \( F_q \) on quadrature \( q \) is then related to the surrounding grid nodes \( i \) as

\[
F_q = I + \sum_i u_i \nabla^T \omega_{iq},
\]  (13)

which also leads to the elasticity force definition

\[
-\frac{\partial e}{\partial u} = -\sum_q \rho_q^0 V_q^0 \frac{\partial \Psi_0(F_q)}{\partial F_q} \nabla \omega_{iq},
\]  (14)

and the elasticity Hessian (in index notation)

\[
\frac{\partial^2 e}{\partial u_{i\alpha} \partial u_{j\beta}} = \sum_q \rho_q^0 V_q^0 (\nabla \omega_{iq})_{\delta} \frac{\partial^2 \Psi_0(F_q)}{\partial F_q_{\alpha\delta} \partial F_q_{\beta\omega}} (\nabla \omega_{jq})_{\omega}.
\]  (15)

Compared with the MPM formulation for dynamic problems, our static formulation can be seen as only solving for a single “time step,” and the deformation gradient at previous time step, \( F_q^n \), is just the initial undeformed deformation gradient \( F_q^0 = F_q^0 = I \). We demonstrate how to solve the static problem (see Eq. (10)) in Section 4.4.

4.2 Material Distribution Representation

Introducing Lagrangian degrees of freedom by optimizing quadrature positions together with quadrature densities is a straightforward choice. However, arbitrary movements of quadrature may cause large numerical errors especially when degeneration happens. Thus, we introduce another set of moving carrier particles to reparameterize the solution space and at the same time to avoid moving quadratures. Carrier particles are defined in the entire design domain with Lagrangian variables \( \xi = (x^c, \rho^c) \) consists of both position and density. The final material distribution, as well as the elasticity force definition, \( -\frac{\partial e}{\partial u} \) can be approximated, but the optimization problem will be harder to solve. In our experiments, we started with \( k = 1 \) and increased \( k \) by one for every 20 iterations until \( k = 10 \). This procedure can help us take advantage of the stability of

\[
\rho_q = \sum_\alpha \rho_\alpha^c W\left(\frac{|x^c_\alpha - x_q|}{h}\right) V_\alpha,
\]  (16)

where \( W(R) \) is a kernel function, \( h \) is the kernel size, and \( V_\alpha \) is chosen to be \( h^2 \) in 2D and \( h^3 \) in 3D. In this paper, this kernel function with cubic spline is given by

\[
W(R) = \sigma \begin{cases} 
\frac{R^3 - R^2}{2} + \frac{3}{2}, & 0 < R < 1 \\
\frac{R^3}{2}, & 1 < R < 2 \\
0, & \text{otherwise}
\end{cases}
\]  (17)

where \( \sigma \) is a constant of \( \frac{15}{32\pi} \) in 2D and \( \frac{2}{20\pi^2} \) in 3D. To prevent the quadratures’ density from becoming larger than one and make the formulation better approximate the integer programming problem, a density mapping function is further added on top of \( \rho_q \).

We consider a family of density mapping functions \( \{\tilde{\rho}_k\} \) with a parameter \( k \) to control the sharpness or nonlinearity (see Fig. 3). With a larger \( k \), the function becomes sharper and more nonlinear, and a 0-1 step function could be better approximated, but the optimization problem will be harder to solve. In our experiments, we started with \( k = 1 \) and increased \( k \) by one for every 20 iterations until \( k = 10 \). This procedure can help us take advantage of the stability of
Figure 2: **Optimization evolution on carrier and quadrature points.** (a) The position and density changes of carrier particles. (b) The density changes on quadrature points. From top to bottom, we show the state at the 20-th, 40-th, and 132-ed iteration. The left-most column of grid nodes is fixed, while vertical downward forces of total 0.05N are added on the quadrature points at the bottom-right corner. The grid resolution used in this example is $120 \times 40$ with a volume fraction constraint of 40%.

Figure 3: **Density mapping functions.** As $k$ becomes larger, the function becomes steeper and more nonlinear, mapping a larger region of $\tilde{\rho}_c$ to 0 or 1.

lower power to ensure the optimizer find a relatively good local area quickly and obtain better-binarized results when $k$ becomes large. The density mapping functions we consider in this paper are defined as follows:

When $k = 1$,

$$
\hat{\rho}_1(\hat{\rho}) = \begin{cases} 
\hat{\rho}, & 0 \leq \hat{\rho} < 1 - \epsilon \\
\frac{(\hat{\rho} + \epsilon - 1)^2}{4\epsilon} + \hat{\rho}, & 1 - \epsilon \leq \hat{\rho} < 1 + \epsilon \\
1, & \hat{\rho} \geq 1 + \epsilon 
\end{cases}
$$

(18)
where we choose $\epsilon = 0.1$, and when $k > 1$,

$$
\hat{\rho}_{k}(\hat{\rho}) = \begin{cases} 
\frac{1}{2}(2\hat{\rho})^k, & 0 \leq \hat{\rho} < \frac{1}{2} \\
1 - \frac{1}{2}(2 - 2\hat{\rho})^k, & \frac{1}{2} < \hat{\rho} < 1 \\
1, & \hat{\rho} \geq 1.
\end{cases}
$$

(19)

If $\hat{\rho}$ is larger than $1 + \epsilon$, the density mapping function will be 1 and the derivative will be zero. Our design variables are wrapped inside the input variables. By chain rule, the derivatives of design variables will be zero as well, which can prevent particle aggregation. All density mapping functions have $C_1$ continuity, so that their derivatives are well-defined. These functions are crucial in LETO; without them, the gathering of particles can form denser/harder material than the given material, which is physically meaningless.

Finally, the density of each quadrature $q$ is given by,

$$
\rho_q = \hat{\rho}_k(\hat{\rho}),
$$

(20)

and the volume fraction constraint is given by

$$
g(\xi) = \sum_q \rho_q \geq \tilde{V} \leq 0,
$$

(21)

where $q$ belongs to all quadrature points, and its derivative is simply

$$
\frac{dg}{d\xi} = \sum_q \frac{d\rho_q}{d\xi},
$$

(22)

where $q$ denotes quadrature points within the kernel range of $x_o$.

The density of carrier particles are initialized to a uniform scale such that each quadrature’s density is equal to the prescribed volume fraction. Since we started with $k = 1$, we can utilize the linearity of the density mapping function for the initialization by assuming the prescribed volume fraction is $\hat{V}$ and the current quadrature density is $\hat{V}$. We also make sure $V$ lies inside the linear part of $\hat{\rho}_1$, which is easily achieved by initiating carriers’ densities with a very small value. Then the carriers’ densities should be initiated as $\hat{V}$.

For certain design tasks (e.g., the boundary of a wheel), some portion of the material needs to be solid, and parts where the external force is acting on should also be solid. We enforce this constraint by excluding these areas from the volume constraint computation. Since forming stiffer material can lower the compliance, the density of the quadrature points will reach their maximum automatically. Using such a treatment, we obtain a smooth transition along the boundary of the enforced solid region and other parts.

### 4.3 Design Sensitivity Analysis

Here, we derive how to compute derivatives of the compliance objective w.r.t. design variables using the adjoint method by reinterpreting it as performing the searching process only on the force equilibrium constraint manifold.

To compute the derivative of the elastic energy potential function (compliance) w.r.t. an arbitrary set of design variables $\xi^j$ and nodal displacements $u^j$, we have

$$
\frac{de}{d\xi}(\xi^j) = \left[\frac{d\rho}{d\xi}(\xi^j)\right]^T \frac{\partial e}{\partial \rho}(\rho^j, u^j) + \left[\frac{du}{d\xi}(\xi^j)\right]^T \frac{\partial e}{\partial u}(\xi^j, u^j),
$$

(23)

where $\frac{d\rho}{d\xi}$ is very difficult to compute as $u$ and $\xi$ are related by the force equilibrium equation; even the evaluation of $u$ from $\xi$ requires solving a system of equations. However, we can constrain the searching process to be only on the constraint manifold defined by the force equilibrium equation. By differentiating

$$
\frac{\partial e}{\partial u}(\rho^j, u^j) = f,
$$

(24)

where $\rho^j$ are quadratures’ densities determined by $\xi^j$, we have

$$
\left[\frac{d\rho}{d\xi}(\xi^j)\right]^T \frac{\partial^2 e}{\partial \rho \partial u}(\rho^j, u^j) + \left[\frac{du}{d\xi}(\xi^j)\right]^T \frac{\partial^2 e}{\partial u^2}(\rho^j, u^j) = 0.
$$

(25)

By substituting Eq. (25) into Eq. (23), we have

$$
\frac{de}{d\xi}(\xi^j) = \left[\frac{d\rho}{d\xi}(\xi^j)\right]^T \frac{\partial e}{\partial \rho}(\rho^j, u^j) - \left[\frac{d\rho}{d\xi}(\xi^j)\right]^T \frac{\partial^2 e}{\partial \rho \partial u}(\xi^j, u^j) \left[\frac{\partial^2 e}{\partial u^2}(\xi^j, u^j)\right]^{-1} f,
$$

(26)

which is our derivative computation, where the compliance $e$ can be defined by either linear or nonlinear elasticity.
ALGORITHM 1: Projected Newton for Solving Static Equilibrium

Given: material distribution $\rho^j$, external force $f$, and boundary condition $\tau$

Initialize:

1. $\Delta u = 0, u^0 = 0, i = 0$
2. While $||g^*|| \geq \epsilon \sqrt{N}$ or $||\frac{\partial e}{\partial u}(\rho^j, u^i)|| \geq \tau||f||$ do
3. $P \leftarrow$ projectSPD ($\frac{\partial^2 e}{\partial u^2}(\rho^j, u^i)$) // project each Hessian stencil to SPD
4. $\Delta u \leftarrow P^{-1}(f - \frac{\partial e}{\partial u}(\rho^j, u^i))$
5. $\alpha \leftarrow$ LineSearch($u^i, \Delta u$) // Back-tracking line-search
6. $u^{i+1} \leftarrow u^i + \alpha \Delta u$
7. $i \leftarrow i + 1$
8. end
9. $u^j \leftarrow u^i$

Linear Elasticity as a Special Case

Now, we show how our derivation reduces to the linear elasticity case, which is widely recognized in the topology optimization community. The derivative of compliance $e$ w.r.t. the material density function $\rho$ in linear topology optimization under force equilibrium constraint $Ku = f$ is often derived as presented in [20],

$$\frac{de}{d\rho} = -\frac{1}{2} u^T \frac{\partial K}{\partial \rho} u,$$  (27)

where $K$ is the stiffness matrix depending on densities $\rho$. In our formulation, the first Piola-Kirchoff derivative $\frac{\partial^2 e}{\partial F \partial F}$ is constant for linear elasticity, so that the internal elasticity force is linear w.r.t. $u$, and the potential $e$ is quadratic w.r.t. $u$.

Namely, we have

$$e = \frac{1}{2} u^T Ku, \quad \frac{\partial e}{\partial u} = Ku, \quad \frac{\partial^2 e}{\partial u \partial u} = K,$$
$$\frac{\partial e}{\partial \rho} = \frac{1}{2} u^T \frac{\partial K}{\partial \rho} u, \quad \frac{\partial^2 e}{\partial \rho \partial u} = \frac{\partial K}{\partial \rho} u.$$  (28)

Substituting these equations into Eq. (26), we have

$$\frac{de}{d\rho} = \frac{1}{2} u^T \frac{\partial K}{\partial \rho} u - u^T KK^{-1} f = -\frac{1}{2} u^T \frac{\partial K}{\partial \rho} u,$$  (29)

which is exactly the same form derived in traditional linear topology optimization via the adjoint method. For arbitrary design variables $\xi^j$, using the chain-rule, the derivative becomes

$$\frac{de}{d\xi^j}(\xi^j) = -\frac{1}{2} \left[ \frac{d\rho}{d\xi^j}(\xi^j) \right]^T (u^j)^T \frac{\partial K}{\partial \rho}(\rho^j) u^j.$$  (30)

Therefore, for both linear and nonlinear topology optimization, to compute the design sensitivity at $\xi^j$, we first solve the static problem to obtain $u^j$ at the static equilibrium and then use $\xi^j$ and $u^j$ to compute the terms and assemble them together.

4.4 Static Solve with Projected Newton

To solve the equilibrium equation more robustly, we minimize the variational form (Eq. (10)) with projected Newton method [57] as outlined in Algorithm 1. Dirichlet boundary conditions are handled by manipulating the corresponding entries in the matrix and the right-hand-side to keep the problem as unconstrained, which is equivalent to applying Schur complement on the KKT system with linear equality constraints.

Stopping Criteria

Our projected Newton method iterates until either the force residual norm or the characteristic gradient norm (CN) [74] is smaller than a threshold.

The characteristic norm is first introduced by Zhu et al. [74] for properly stopping FEM static solves at consistent accuracy. It is later extended to dynamic [55] and MPM [54] settings. Following [54], we use node-wise CN as the different density values in our optimization are similarly producing heterogeneity. For each quadrature point at its initial
state, we compute the norm of the first Piola-Kirchhoff stress derivative multiplied by a perimeter/area parameter and rasterize this scalar field to grid nodes using per quadrature Young’s modules as a weighting factor. The node-wise CN is computed as the following

\[ C_i = \sum_q E_q \left\| \frac{\partial P}{\partial F} \right\| F \; l_i \omega_{iq}, \]  

where \( l_i = 8\Delta x/24\Delta x^2 \) in 2D/3D, and \( \omega_{iq} \) is the interpolation function between MPM quadrature and grid. The node-wise CN is computed as the following

\[ C_i = \sum_q E_q \left\| \frac{\partial P}{\partial F} \right\| F \; l_i \omega_{iq}, \]  

where \( \otimes \) is block-wise division, such that each block is \( \frac{dE}{du}/C_1 \), \( N \) is number of grid node in the Eulerian mesh grid, and \( \epsilon, \tau \) are chosen to be \( 10^{-7} \) and \( 10^{-2} \).

**Inversion-free Line Search**  Since in each projected Newton iteration, the Hessian has been projected to symmetric positive definite, our search direction \( \Delta u \) is guaranteed to be a descent direction. Therefore, we apply back-tracking line search to ensure \( E(u^{i+1}) < E(u^i) \) after each \( u \) update, which effectively stabilizes the iterations and improves convergence.

However, for the noninvertible elasticity energy (neo-Hookean), projected Newton does not necessarily ensure no deformation gradient inversion along search direction \( \Delta u \). Hence, to further prevent inversion of each \( F_q \), we follow Smith and Schaefer [75] to solve a large feasible step size before each line search by finding the minimum of the smallest positive roots of a family of equations

\[ \{ \det(F_q(u^i + \beta_q \Delta u)) = \epsilon_q \} \],

and then start line search from \( \min_q \beta_q \). Here, we newly use \( \epsilon_q = 0.1 \det(F_q(u^i)) \) to avoid numerical rounding errors, which is more robust than solving with \( \epsilon_q = 0 \) and then shrinking \( \beta \).

4.5 Optimizing Structures with MMA

We use a prominent method, the method of moving asymptotes (MMA) [73], to optimize structures, which co-optimizes the positions and densities of carrier particles. This optimizer is designed for general structural optimization problems with inequality constraints and box constraints. The algorithm approximates the original problem with a series of separable convex optimizations. At each iteration, it sets up two asymptotes for each variable to constrain the searching interval. These asymptotes will be updated according to each sub-optimum. The optimization will be stopped when the relative range of the last ten objective values drop below a given threshold. In our implementation, we adopt an open-source C++ version of MMA.

In order for MMA to perform well, careful parameter tuning is needed, and different examples might have different sets of optimal MMA parameters. With inappropriate parameters, the optimization process can even explode. There are three parameters to tune: \( \text{asyinit}, \text{asyincr}, \text{asydecr} \). In this paper, we borrow a set of parameters used in the original MMC method; these three parameters are set to be 0.02, 1.05, and 0.65, respectively. We use these values throughout all the experiments. To further stabilize and accelerate the optimization in a consistent way, we additionally apply the following regularizations within MMA:

1. We control the step length of each variable by novelly modifying its box constraint at each iteration. In our experiments, we constrain that the change of carrier density cannot exceed 0.5, and the change of carrier position at each dimension cannot exceed 0.025 times the shortest edge length of the design space’s bounding box.

2. Following MMC, we scale the gradient of objective and the volume constraint such that their \( L^\infty \)-norms are both 1. In addition, we also scale the objective and the volume constraint accordingly to make sure the gradients are consistent with the original functions. Our extra scalings allow the volume to get closer to its upper bound and so the structure can utilize as much material as possible.

4.6 Contact-Aware Topology Optimization

With the log barrier term in neo-Hookean elasticity model, static equilibrium is guaranteed to be found in an inversion-free configuration. We similarly use this mechanism to prevent material from self-intersection throughout the optimiza-

[https://github.com/jdumas/mma](https://github.com/jdumas/mma)
We fill in the void area with weak material (small Young’s module). When the boundaries of two solid material get close to each other, the void material will be squeezed and generate arbitrarily large forces depending on the distance. Due to the small Young’s module of the void area, the generated force can be ignored unless the two boundaries become extremely close or faraway to each other. Since the latter case is rarely seen in topology optimization, the force generated here can be safely viewed as a contact force.

However, MPM is based on quadrilateral/hexahedral cells, where the deformation gradients inside one cell are not constant. Making the deformation gradient positive-oriented on all the quadrature does not guarantee inversion-free for other positions in the cell. To address this issue, we use simplex-based FEM to model weak material by dividing each quad/hex cell into two identical triangles in 2D or six identical tetrahedra in 3D.

**Unification of FEM with MPM** The details of the deformation gradient and force computation of simplicial FEM is shown in [76]. To unify these FEM computations into our MPM framework, we derive a new way to compute the deformation gradient and nodal forces of simplex in a compatible fashion with linear MPM.

Given a simplex\(T = \{v_0, ... , v_n\}\), where \(n = 2\) in 2D and \(n = 3\) in 3D, we define the vertex normal as the average of adjacent face-area-weighted face normals. In 2D, the vertex normal of \(v_0\) is defined as

\[
\mathbf{n}_0 = \frac{1}{2}(A_{01}\mathbf{n}_{01} + A_{02}\mathbf{n}_{02}),
\]

where \(A_{ij}\) is the length of edge \(ij\), and \(\mathbf{n}_{ij}\) is the outward unit normal of that edge. In 3D, the vertex normal of \(v_0\) is defined as

\[
\mathbf{n}_0 = \frac{1}{3}(A_{012}\mathbf{n}_{012} + A_{023}\mathbf{n}_{023} + A_{031}\mathbf{n}_{031}),
\]

where \(A_{ij}\) is the area of face \(ijk\), and \(\mathbf{n}_{ijk}\) is the outward unit normal of that face. Let \(\nabla w_i = \frac{\mathbf{n}_i}{V(T)}\), where \(V(T)\) is the volume of \(T\). The deformation gradient \(F(T)\) of \(T\) can be computed as

\[
F(T) = I + \sum_i u_i \nabla w_i^T,
\]

where \(u_i\) is the nodal displacement at vertex \(v_i\). The contribution of interior force of deformed \(T\) to vertex \(v_i\) can be computed as

\[
f_i(T) = -V(T)P(F)\nabla w_i,
\]

where \(P(F)\) is the first Piola-Kirchoff stress on \(T\).

It can be proved that the above formulation is equivalent to which in [76]. Now, we can place a virtual material point at the center of each simplex and use a grid gathering operation to compute the deformation gradient and a particle-to-grid rasterization operation to update grid forces. When implementing this framework, we only need to make sure that these virtual material points only affect the surrounding simplex nodes and modify the weight gradient computation method. The other steps are precisely the same as in our MPM framework.

### 5 Results

As pointed out by Maute and Sigmund [17], albeit a large variety of methods have been explored, they are either not providing substantial novel contributions or lacking comparison with benchmark experiments. It seems hard to identify the practical value if every method is evaluated individually, or even worse, not evaluated at all. With these sharp comments in mind, we compare LETO with the state-of-the-art methods using an extensive benchmark, consisting of various loads, boundary conditions, and volume fraction constraints.

To compare compliances between LETO (hybrid model) and SIMP in a fair setup, we implement both using MPM as the static equilibrium solver. MPM allows particles in one cell to have different densities. However, the FEM-based SIMP uses cells as the smallest unit for physical properties. Hence, in our implementation of SIMP, we maintain that quadratures in each cell have a single density value.

This section is organized as follows. We validate our MPM-based SIMP with the standard FEM-based SIMP on two examplar cases to ensure they work consistently and produce very similar results in Section 5.1. In Section 5.2, we show our nonlinear examples obtained from optimizing the Neo-Hookean elasticity potential directly under different setups and force magnitudes. We also adopt SIMP to optimize the Neo-Hookean elasticity potential directly and compare
Figure 4: FEM SIMP v.s. MPM SIMP. Material distribution obtained by SIMP for the cantilever beam problems. Results with (a)(c) FEM and (b)(d) MPM being the static solver, respectively.

LETO with it. We show LETO’s advantages qualitatively and quantitatively: in Section 5.3 we use our framework on linear topology optimization by comparing LETO with SIMP; the results show LETO achieves much lower compliances with more intricate structures. Finally, in Section 5.4, we preliminarily explore how modeling contact can help construct structures that can take advantage of contact forces and always stay meaningful in reality.

5.1 Validation of MPM-based SIMP

Since we use MPM as our static solver, we need first to validate that MPM-based SIMP is comparable to FEM-based SIMP. In FEM-based SIMP, densities are assigned element-wise. Since we have multiple quadratures per element (grid cell), we enforce every quadrature inside a single grid cell to share the same density. All the other steps in MPM-based SIMP are identical to FEM-based SIMP; we use Optimal Criteria (OC) as the optimizer and perform a mesh-independent gradient filter before density updates.

We compare results on two classic topology optimization setups, see Fig. 4 wherein the results in Figs. 4a and 4c are obtained by the standard 88-line FEM-based SIMP [21], and the results in Figs. 4b and 4d are obtained by our implementation of MPM-based SIMP. For a fair comparison, compliances of the final results are all evaluated using the MPM solver. We show that our MPM-based implementation yields consistent results as the FEM-based implementation, both qualitatively and quantitatively. The Dirichlet boundary conditions and force loads are identical for both implementations. Both experiments are with Young’s modulus of 100 Pa, Poisson’s ratio of 0.3, penalization power of 3, and a volume fraction constraint of 40%.

In the first cantilever beam example (see Figs. 4a and 4b), the left-most column of nodes is fixed, and forces with a magnitude of 0.04N are added on the four grid nodes at the bottom right. The design domain is $3\times 1$ m, discretized with a $120 \times 40$ grid resolution. The final compliance of FEM-based SIMP is $1.145 \times 10^{-4}$, whereas the final compliance of MPM-based SIMP is $1.143 \times 10^{-4}$. The radius of the gradient filter is 3.5 times the grid spacing.

In the second example (see Figs. 4c and 4d), we fix two nodes: one on the top-left corner, and the other on the bottom-left corner. Forces with a magnitude of 0.08N are added on the middle-right six grid nodes. The design domain is $2\times 1$ m, discretized with an $80 \times 40$ grid resolution. The final compliance of FEM-based SIMP is $1.930 \times 10^{-4}$, whereas the final compliance of MPM-based SIMP is $1.927 \times 10^{-4}$. We use 1.5 times the grid spacing for the filter radius.

5.2 Topology Optimization with Nonlinear Elasticity

In this section, we show the results using LETO that optimizes the elastic potential as the compliance objective with the highly nonlinear neo-Hookean elasticity materials. With small force magnitude, which results in small deformation, the optimal structure obtained by LETO can be very similar to the results obtained using linear elasticity materials. As forces become large, the deformation grows, resulting in increasingly different optimal structures, unattainable by optimizing with linear elasticity. We also compare LETO with a SIMP-based nonlinear topology optimization method,
Figure 5: **Wheel Design (linear v.s. nonlinear).** (a) Problem setup; Dirichlet boundaries are rendered in light blue, and force loads are denoted by red arrows. Result obtained using (b) linear elastic material and (c)-(g) nonlinear elasticity. Using relatively small forces (6.575 × 10^{-6} N in total), (c) results using nonlinear elasticity material becomes similar to (b) the ones using a linear elastic material. We increase the magnitude of the forces to 10×, 50×, 100×, and 200× in (d)-(g) compared to (c) the initial scaling while maintaining all the other configurations unchanged.

both optimizing the elastic potential, and demonstrates the advantage of using LETO by obtaining more intricate structures with lower compliance.

### 5.2.1 Different force magnitudes

Different force magnitudes will lead to different optimal structures in nonlinear topology optimization as the displacement at force equilibrium is no longer linearly varying w.r.t. external forces. Here, we show several examples obtained by LETO that optimizes the elastic potential of the neo-Hookean elasticity model. In each case, we only change the magnitudes of the external forces while keeping the volume fraction constraints and the boundary conditions the same. We also show that the results will be similar to those obtained with linear elasticity when forces are small. In the following experiments, the base Young’s modulus is 100 Pa, and the Poisson’s ratio is 0.4.

#### 3D wheel design

In this example, we consider optimal material distributions of a wheel under different magnitudes of external forces; see results in Fig. 5. The wheel has a radius of 1.1m and a thickness of 0.2m, enclosed by a bounding box of 2.2m × 2.2m × 0.2m. The grid resolution is 176 × 176 × 16, with a spacing of 0.0125m for all three dimensions. The design domain is illustrated in Fig. 5a; we fix the grid nodes in the central region within a radius of 0.05m (rendered in blue), and the forces that are perpendicular to the wheel plane (denoted by the red arrows) are evenly added on a thin layer of the outer-most boundary of the wheel. The density of an annulus is fixed, with an inner radius of 0.05m and an outer radius of 0.6m. When the force magnitude is small, the result of nonlinear elasticity is similar to the result of linear elasticity. As the magnitude grows, the optimal structure becomes asymmetric along the normal direction of the wheel and contains increasingly more thin features. The volume fraction constraint is set to 10%.

#### 2D buckling beam

In this example, we explore the modeling of buckling behavior under large deformation when the force magnitude is increasingly large; see results in Fig. 6. The design domain is illustrated in Fig. 6a; it is an 8m × 1m
A Hybrid Lagrangian-Eulerian Method for Topology Optimization

Figure 6: 2D Linear and nonlinear topology optimization. (a) Problem setup with Dirichlet boundary condition (in light blue) and force load (in red). Results obtained using (b) linear elastic material and (c)-(f) nonlinear elasticity. (c) Results using relatively small forces ($1.6 \times 10^{-3} N$). We increase the magnitude of the forces to (d) 5× and (e) 40× that of (c) while keeping all the other configurations fixed.

Figure 7: Nonlinear bridge design 1. (a) Comparison between SIMP and LETO. The problem setup (Dirichlet boundaries in light blue, force loads in red) is shown in the bottom middle. The strain energies evaluated by MPM are shown in the figure. (b) The result of LETO rendered using solid particles.

rectangle, wherein the grid resolution is 800 × 100 with a spacing of 0.01m. The left-most and right-most columns of the grid nodes are fixed. A vertical downward force is loaded at a small region in the middle of the lower boundary. The volume fraction constraint for this example is 40%. Our inversion-free projected Newton with line search allows us to handle large deformation. By considering the full elastic potential, we accurately model buckling behaviors.

5.2.2 Comparison to nonlinear SIMP

As discussed in the related work (see Section 2.1.3), most topology optimization methods for nonlinear elasticity only consider cases with small strains, thus utilize the mean compliance $f^T u$ as the objective function, essentially a linearization of the elastic potential. In contrast, we optimize the total elastic potential energy as the compliance objective to account for the scenarios where the material undergoes large deformation, simultaneously modeling both geometry and material non-linearity within the hyperelastic formulation. Our MPM-based SIMP can easily switch to optimize neo-Hookean elastic potential directly. In this section, we compare LETO with nonlinear SIMP on four 3D examples to show the advantages of our method of obtaining more intricate structures with lower compliance. Following Buhl et al. [8], we use MMA as the optimizer for nonlinear SIMP.

Nonlinear bridge design 1 We show another bridge design example in Fig. 7. The design domain is the entire $4m \times 1m \times 1m$ cuboid. We use a grid resolution of 160 × 40 × 40 with a spacing of 0.025m for all dimensions and set the volume fraction constraint to 20%. We fix the two planes at both ends of the longest dimension and add forces of 0.795N on the bottom plane. The final compliances evaluated with the neo-Hookean elasticity are $3.407 \times 10^{-2}$ and $3.006 \times 10^{-2}$ using SIMP and LETO, respectively. Quantitatively, LETO has an improvement of 11.77% compared to SIMP. Qualitatively, the structure using LETO is essentially different; the result obtained using LETO does not have the central part as in the compared result using SIMP, since the result obtained using LETO distributes these materials for enhancing the connectivity to the two sides that are fixed.
**Nonlinear bridge design 2** In this example, we show different optimal material distributions of a bridge design by SIMP (Fig. 8a) and LETO (Fig. 8b). The design domain is formed by extruding a U shape on the $yz$-plane in $x$-axis. The bounding box is $4m \times 1m \times 1m$, and the simulation grid resolution is $160 \times 40 \times 40$ with a spacing of $0.025m$ for all dimensions. Forces of $1.5 \times 10^{-3}N$ are added on the top plane of the bridge deck, where we fix the four corners of its bottom. The volume fraction constraint is set to $20\%$. Qualitatively, both results using SIMP and LETO contain a pair of arcs connecting the two sides of the bridge, but only LETO is with more support between the arc and the deck with multiple branches at the bottom. Quantitatively, the final compliance evaluated with the neo-Hookean elastic potential energy is $1.478 \times 10^{-6}$ using LETO, much lower than $1.814 \times 10^{-6}$ obtained by SIMP, with an improvement of $18.52\%$.

**Nonlinear wheel design** Fig. 9 shows the different optimal structure of a wheel design obtained by optimizing different objective functions. The wheel has a radius of $1.1m$ and a thickness of $0.2m$, enclosed by a bounding box of $2.2m \times 2.2m \times 0.2m$. The grid resolution is $176 \times 176 \times 16$ with a spacing of $0.025m$ for all three dimensions. We fix the grid nodes in the central region within a radius of $0.1m$ rendered in blue. Forces at $6.575 \times 10^{-5}N$ that are perpendicular to the wheel plane denoted by the red arrows are evenly exerted on a thin layer of the outer-most boundary of the wheel. We fix the density of the darkest annulus, which has an inner radius of $1m$, an outer radius of $1.1m$, and a thickness of $0.1m$. The volume constraint is set to $10\%$. Quantitatively, the final compliance using LETO evaluated with the neo-Hookean elastic potential energy is $4.491 \times 10^{-9}$, which is lower than $5.331 \times 10^{-9}$ obtained by SIMP, with an improvement of $15.76\%$. Qualitatively, comparing the structure, LETO reveals more intricate and clustered connections between the center and the annulus.

**Nonlinear chair design** Finally, we show a chair design example in Fig. 10. The design domain is an extruded L-shaped with a bounding box of $2m \times 1.4m \times 1m$. Forces of $0.001N$ and $0.0015N$ are loaded on the back of the chair and the seat plane, respectively. The four corners at the bottom plane are fixed, and we set the volume constraint
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Figure 10: **Nonlinear chair design.** (a) Comparison between SIMP and LETO. The problem setup (Dirichlet boundaries in light blue, force loads in red) is shown in the top middle. The strain energies evaluated by MPM are shown in the figure. (b) The result of LETO rendered using solid particles.

for this example to 20%. Quantitatively, the final compliance evaluated with the neo-Hookean elastic potential energy is $3.720 \times 10^{-5}$ for SIMP, and $3.228 \times 10^{-5}$ for LETO, which shows an improvement of 13.23%. Qualitatively, the main difference of the structure is that the connection on the back of the chair from top to bottom has more and thinner branches using LETO.

5.3 Topology Optimization with Linear Elasticity

In this section, we compare LETO with MPM-based SIMP [20] extensively on a benchmark, consisting of eight 3D examples and fourteen 2D examples. Under the same simulation resolution, LETO obtains more detailed geometry structures and lower compliance at a similar convergence speed. In Section 5.3.1, we start with the 3D benchmark and report the compliance plot, problem setup, and the optimal structures obtained by comparing LETO and MPM-based SIMP. Note that the beginning compliance of SIMP is lower than ours; it is because that we use a different solid enforcement mechanism (as mentioned in Section 4.2)—SIMP sets the densities in fixed areas to be one all the time and are initialized as the same as other areas in LETO. After examining the 3D benchmark, we show plots that summarize the 2D benchmark in Section 5.3.2 quantitatively; selected qualitative results are also reported.

5.3.1 3D Linear Examples

**Torsion rod** We replicate the example of the torsion rod, originally presented by Sigmund et al. [77]. The rod has a length of $2m$ and a diameter of $1m$. We consider only a shell of the rod with an outer radius of $0.5m$ and a thickness of $0.05m$. The grid resolution is $320 \times 160 \times 160$ with a spacing of $0.00625m$ for all dimensions. As shown in light red arrows in Fig. 11 the rod is under pure torsion at the closer end with forces of total magnitude $7.45 \times 10^{-3}N$, and the opposite end annulus highlighted in blue are fixed. The volume fraction constraint is set to 10%. Quantitatively, the final compliances are $4.171 \times 10^{-5}$ and $2.622 \times 10^{-5}$ for SIMP and LETO, respectively; LETO achieves a 37.14% lower compliance. Qualitatively, results obtained using SIMP and LETO reveal distinct structures: the result obtained by SIMP has a net structure, wherein the thickness of each weaving line is the thickness of the hollow rod, and the result obtained by LETO forms a perfect thin shell, wherein the shell consists of only one layer of quadratures. In fact, a thin shell is the optimal solution, as pointed out by Sigmund et al. [77].

**Bridge 1** We demonstrate a design of a 3D bridge; see Fig. 12. The bridge has a length of $6m$, a width of $1m$, and a height of $1m$. The grid resolution is $320 \times 80 \times 80$ with a spacing of $0.0125m$. The two ending planes along the longest axis are fixed (marked in blue), and a plane force of total $1.6N$ is added on the bottom (denoted by red arrows). The volume fraction constraint is set to 20%. Quantitatively, the final compliances are $1.126 \times 10^{-1}$ and $9.836 \times 10^{-2}$ for SIMP and LETO, respectively; LETO achieves a 12.64% lower compliance. Qualitatively, the results obtained by both SIMP and LETO have a curved thick deck that touches the bottom and is connected to the Dirichlet boundaries. However, the result obtained by LETO reveals much more thin supporters under the thick curved deck.

**Bridge 2** We consider a different bridge-like structure by adding a plane force of total $0.2N$ on top of a cuboid; see Fig. 13. The longest edge of the cuboid is $2m$, and the other two dimensions have a length of $1m$. The grid resolution is $160 \times 80 \times 80$ with a spacing of $0.0125m$. We fix the left-most, middle, and the right-most column on the bottom plane. The volume constraint is set to 20%. Qualitatively, while many thick geometry features are formed using SIMP,
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Figure 11: **Torsion rod.** (a) Quantitative compliance plots of SIMP and LETO . (b) Qualitative results of SIMP and LETO , and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles. The cylinder is sliced open to highlight the shell formed by a single layer of quadratures.

Figure 12: **Bridge 1.** (a) Quantitative compliance plots of SIMP and LETO . (b) Qualitative results of SIMP and LETO , and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

Figure 13: **Bridge 2.** (a) Quantitative compliance plots of SIMP and LETO . (b) Qualitative results of SIMP and LETO , and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

various organic supporting fibers emerge using LETO . Quantitatively, the final compliances are $7.148 \times 10^{-4}$ and $6.261 \times 10^{-4}$ for SIMP and LETO , respectively; LETO achieves a 12.41% lower compliance. Since we fix three bar-areas at the bottom, each of the two structures forms two arches. The bridge arches are not entirely solid; there are bars connecting the deck and the bottoms of arches.

**Bridge 3** We design another bridge that possesses a large space for transportation to investigate how the supporting material distribution could be formed; see Fig.14. The design domain is a U shape on the $yz$-plane extending in $x-axis$ with a bounding box of $4m \times 1m \times 1m$. A force of 0.31 N is loaded on the entire plane of the concave region. The grid resolution is $320 \times 80 \times 80$ with a spacing of 0.0125 m. We fix the four corners of the bottom plane. The volume constraint is set to 20%. Quantitatively, the final compliances are $8.253 \times 10^{-2}$ and $7.401 \times 10^{-2}$ for SIMP and LETO , respectively; LETO achieves a 10.33% lower compliance. Qualitatively, a truss structure is formed at each
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Figure 14: Bridge 3. (a) Quantitative compliance plots of SIMP and LETO. (b) Qualitative results of SIMP and LETO, and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

Figure 15: Chair. (a) Quantitative compliance plots of SIMP and LETO. (b) Qualitative results of SIMP and LETO, and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

side of the two bridges. However, truss formed by LETO has much more connecting bars; they are also thinner and very densely distributed.

Chair The optimal distribution of a 3D chair is shown in Fig. 15. The design domain is an extruded L-shaped with a bounding box of $2m \times 1.4m \times 1m$. The grid resolution is $112 \times 160 \times 80$ with a spacing of $0.0125m$. The bottom planes of the four legs are fixed as Dirichlet boundary conditions. Forces of $0.8N$ and $1.2N$ are loaded on the back of the chair and the seat plane, respectively. The volume constraint is set to 20%. Quantitatively, the final compliances are $3.465 \times 10^{-1}$ and $3.174 \times 10^{-1}$ for SIMP and LETO, respectively; LETO achieves a 8.41% lower compliance. Qualitatively, the chair obtained by LETO has much more fibers inside, even in the legs; it also has many thin fibers supporting the seat and the back.

Wheel We revisit the previously discussed wheel design problem, but with linear elastic material; see Fig. 16. The radius and thickness of the wheel are $1.1m$ and $0.2m$, respectively. The grid resolution is $176 \times 176 \times 16$ with a spacing of $0.0125m$. We fix the grid nodes in the central region within a radius of $0.1m$ (rendered in blue), and forces of total $5.26 \times 10^{-5}N$ are loaded on the outer-most boundary of the wheel (denoted by the red arrows), which is perpendicular to the wheel plane. We fix the density of the darkest annulus with an outer radius of $1.1m$ and a thickness $0.2m$. The volume constraint is set to 10%. Quantitatively, the final compliances are $6.078 \times 10^{-3}$ and $4.274 \times 10^{-3}$ for SIMP and LETO, respectively; LETO achieves a 29.68% lower compliance. Qualitatively, the result obtained by LETO has four extra connections from the center to the outside annulus; these four connections have intricate weaving structures.

Rod squeezing We compare SIMP and LETO on a relatively higher volume fraction constraint (40%); see Fig. 17. The design domain is a solid rod with a length of $2m$ and a diameter of $1m$. The grid resolution is $160 \times 80 \times 80$ with a spacing of $0.0125m$. We add normal forces of total $0.157N$ and $0.613N$ on one bottom plane and the entire side surface, respectively. The pressure on the bottom is twice as on the side. The other end plane of the rod is fixed. Quantitatively, the final compliances are $6.029 \times 10^{-4}$ and $5.454 \times 10^{-4}$ for SIMP and LETO, respectively; LETO achieves a 9.53% lower compliance. Qualitatively, cylinders obtained by both SIMP and LETO have formed fibers.
Figure 16: **Wheel.** (a) Quantitative compliance plots of SIMP and LETO. (b) Qualitative results of SIMP and LETO, and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

Figure 17: **Rod squeezing.** (a) Quantitative compliance plots of SIMP and LETO. (b) Qualitative results of SIMP and LETO, and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles. The cylinder is sliced open to highlight the inner structure.

Figure 18: **Michell sphere.** (a) Quantitative compliance plots of SIMP and LETO. (b) Qualitative results of SIMP and LETO, and the problem setup (Dirichlet boundaries in light blue, force loads in red). (c) The result of LETO rendered by solid particles.

inside, which connect the Dirichlet boundary to the side and the other end. However, the result obtained using LETO has much more and thinner fibers.

**Michell sphere** We reproduce the Mitchell structure\cite{78} in this last example by twisting a 3D sphere shell; see Fig.\cite{18}. The thickness of the shell is 0.02\(m\) with an outer radius of 0.5\(m\). The grid resolution is \(160 \times 160 \times 160\) with a spacing of 0.00625\(m\). We fix a small region centered at one pole while twisting the other. The total force load is \(7.13 \times 10^{-6} N\). The volume constraint is set to \(10\%\). Quantitatively, the final compliances are \(2.794 \times 10^{-11}\) and \(1.659 \times 10^{-11}\) for SIMP and LETO, respectively; LETO achieves a 40.62\% lower compliance. Qualitatively, the result obtained by LETO has more weaving lines. Additionally, extra thin shell structures are formed near the Dirichlet boundary, as highlighted in the solid rendering. Similar to the example of torsion rod, these shells only consist of a single layer of quadratures.
Summary of 3D Linear Examples

We summarize the numerical value of compliances and the improvement of LETO in percentage compared with SIMP; see Table 1. Note that LETO performs much better with shell configurations, wherein thin-shell solutions could be achieved.

| Experiment        | LETO               | SIMP               | Grid Resolution | Improvement (%) |
|-------------------|--------------------|--------------------|-----------------|-----------------|
| Torsion rod       | $2.622 \times 10^{-5}$ | $4.171 \times 10^{-5}$ | $320 \times 160 \times 160$ | 37.14           |
| Bridge 1          | $9.836 \times 10^{-2}$ | $1.126 \times 10^{-1}$ | $320 \times 80 \times 80$  | 12.64           |
| Bridge 2          | $6.261 \times 10^{-4}$ | $7.148 \times 10^{-4}$ | $160 \times 80 \times 80$  | 12.41           |
| Bridge 3          | $7.401 \times 10^{-2}$ | $8.253 \times 10^{-2}$ | $320 \times 80 \times 80$  | 10.33           |
| Chair             | $3.174 \times 10^{-1}$ | $3.465 \times 10^{-1}$ | $112 \times 160 \times 80$ | 8.41            |
| Wheel             | $4.274 \times 10^{-3}$ | $6.078 \times 10^{-3}$ | $176 \times 176 \times 16$ | 29.68           |
| Rod squeezing     | $5.454 \times 10^{-4}$ | $6.029 \times 10^{-4}$ | $160 \times 80 \times 80$  | 9.53            |
| Mitchell sphere   | $1.659 \times 10^{-11}$ | $2.794 \times 10^{-11}$ | $160 \times 160 \times 160$ | 40.62           |

Table 1: Compliance comparisons between SIMP and LETO (ours). Lower compliance is achieved using LETO in all settings, especially the ones with thin-shell solutions.

5.3.2 2D Linear Examples

We further compare LETO with SIMP on fourteen 2D examples. For each example, we run experiments with different volume constraints: 10%, 20%, 30%, and 40%. We show a violin plot of compliance gains grouped by volume constraints in Fig. 19, which includes all 2D data; each violin consists of fourteen samples. These 2D results demonstrate the proposed LETO outperforms SIMP in all tested volume constraints. As the volume constraint decreases, the advantage of using LETO becomes more evident. We show selected rendered results in Table 2.

Table 2: Selected 2D examples to compare LETO and SIMP

| LETO Info                      | SIMP Info                      |
|--------------------------------|--------------------------------|
| Energy: $1.962 \times 10^{-4}$ | Energy: $1.985 \times 10^{-4}$ |
| Volume Fraction: 40%           | Volume Fraction: 40%           |
| Iterations: 134                | Iterations: 169                |
|                                |                                |
| Energy: $4.270 \times 10^{-4}$ | Energy: $4.293 \times 10^{-4}$ |
| Volume Fraction: 40%           | Volume Fraction: 40%           |
| Iterations: 134                | Iterations: 84                 |

Continued on Next Page
Table 2: Selected 2D examples to compare LETO and SIMP

| LETO Info                      | SIMP Info                      |
|-------------------------------|-------------------------------|
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $6.618 \times 10^{-4}$ | Energy: $6.583 \times 10^{-4}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 131               | Iterations: 84                |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $1.276 \times 10^{-4}$ | Energy: $1.293 \times 10^{-4}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 139               | Iterations: 132               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $2.575 \times 10^{-4}$ | Energy: $2.614 \times 10^{-4}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 151               | Iterations: 186               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $5.007 \times 10^{-8}$ | Energy: $5.051 \times 10^{-8}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 98                | Iterations: 48                |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $5.309 \times 10^{-4}$ | Energy: $5.506 \times 10^{-4}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 137               | Iterations: 92                |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $2.056 \times 10^{-3}$ | Energy: $2.143 \times 10^{-3}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 1000 (max_iter)   | Iterations: 132               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $6.487 \times 10^{-5}$ | Energy: $6.504 \times 10^{-5}$ |
| Volume Fraction: 30%          | Volume Fraction: 30%          |
| Iterations: 91                | Iterations: 44                |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $9.780 \times 10^{-4}$ | Energy: $1.043 \times 10^{-3}$ |
| Volume Fraction: 30%          | Volume Fraction: 30%          |
| Iterations: 153               | Iterations: 217               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $4.631 \times 10^{-6}$ | Energy: $4.770 \times 10^{-6}$ |
| Volume Fraction: 20%          | Volume Fraction: 20%          |
| Iterations: 174               | Iterations: 116               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $1.036 \times 10^{-3}$ | Energy: $1.054 \times 10^{-3}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 152               | Iterations: 124               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $6.245 \times 10^{-4}$ | Energy: $6.352 \times 10^{-4}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 136               | Iterations: 138               |
| ![LETO Image]                 | ![SIMP Image]                 |
| Energy: $5.718 \times 10^{-1}$ | Energy: $6.470 \times 10^{-1}$ |
| Volume Fraction: 40%          | Volume Fraction: 40%          |
| Iterations: 197               | Iterations: 221               |
5.4 Contact-Aware Topology Optimization

In this section, we show our preliminary exploration of finding optimal structures that can make use of contact forces; the simulation considers the whole design domain. We use the narrow-band filter to decide whether an area is void. The void area is procedurally tessellated with simplicial complex finite elements with an epsilon Young’s module. To observe contact-aware structures, some areas are set to always stay void intentionally; we call these areas the “always-void” areas. Similar to the previous experiments, some areas always have a 1-valued density. In the following examples, we use neo-Hookean elasticity, and we show the optimized results in both material space and world space.

**Hollow Cuboid**  This example is a shallow cuboid in 3D space; see Fig. 20 for an illustration of the configuration. The design domain is a cuboid of $2m \times 2m \times 0.75m$. The always-void area (in yellow) is another cuboid of $1.4m \times 1.4m \times 0.5m$ in the center of the design domain. The fixed areas (in light blue) are four vertical faces around the cuboid. A downward force of $0.72N$ is loaded evenly on a $1.2m \times 1.2m$ square at the top center, and an upward force of $1N$ is loaded evenly on the whole bottom face. The simulation resolution is $80 \times 30 \times 80$ with grid spacing $0.025m$. The relative minimal Young’s module is $10^{-6}$. To facilitate the formation of contact supporting planes, two always-solid areas (the darker gray area inside the design domain) are setup above and beneath the always-void area. The two always-solid areas are two $1m \times 0.05m \times 1m$ cuboids. Additionally, we also set a thin layer at the top and a thin layer at the bottom (both of height $0.05m$) as always-solid areas.

The optimal structure forms a shell-like structure to connect the top always-solid plane, the bottom always-solid plane, and the fixed areas. Inside the shell, there are two frustum-like structures connecting the contact surfaces and the top/bottom always-solid planes. Furthermore, there is a cavity inside each frustum. In world space, it can be observed that the two contact surfaces contact each other perfectly.

6 Conclusion and Future work

We propose a new hybrid Lagrangian-Eulerian topology optimization method, LETO, that expands the solution space of prior methods while maintaining fast convergence. We use MPM as our static equilibrium solver to enable sub-cell resolution. Our method produces intricate results with comparable and often lower compliance at similar simulation cost compared to Eulerian methods. With a unified treatment, our method optimizes the elastic potential as the compliance objective for both linear and highly nonlinear (e.g. neo-Hookean) hyperelastic materials. Notably, our method robustly captures large deformation and buckling behaviors in nonlinear cases. Modeling self-contact with a fictitious domain-based approach, we perform preliminary explorations of contact-aware topology optimization for finding optimal structures under the influence of self-contact forces.
The finite strain formulation in MPM allows us to construct a unified framework for general hyperelastic materials. With the ability to resolve sub-cell features, LETO can be further extended in future work to optimize anisotropic, heterogeneous, and multi-scale materials. It would also be interesting to apply our framework to optimize different objectives, e.g., compliant mechanism, and task-oriented objectives for designing soft robots.

We have identified self-intersection as an issue during the optimization and proposed a preliminary method based on fictitious domains to take advantage of contact forces so that the resulting structure stays meaningful. However, our contact model is not strictly unilateral, and numerical issues could still happen. We hope our preliminary study can elucidate more research on contact-aware topology optimization and open up a new avenue in computational fabrication.

Last but not least, our method relies on MMA. As mentioned, MMA requires careful parameter tuning to perform well. Even with our general and consistent regularizations for all examples on step length and the relative scaling between constraints and objective, it is still unclear whether the optimization parameters we choose are optimal. For extensions to more complex materials, it is also unclear whether the current MMA parameters can conveniently adapt. Therefore, it would be meaningful to develop a more general and easy-to-setup optimizer for LETO, likely taking advantage of second-order design sensitivity information.

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