Max-Planck-**Innovation**

Technology Offer

Shape from Release: Inverse Design and Fabrication of Controlled Release Structures

File no.: MI-1200-6557-GÖ-IT

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Background

Objects with different shapes can dissolve in significantly different ways inside a solution. Predicting different shapes' dissolution dynamics is an important problem especially in pharmaceutics. More important and challenging, however, is controlling the dissolution via shape, i.e., designing shapes that lead to a desired release behavior of materials in a solvent over a specific time. Here, we tackle this challenge by introducing a computational inverse design pipeline.

Technology

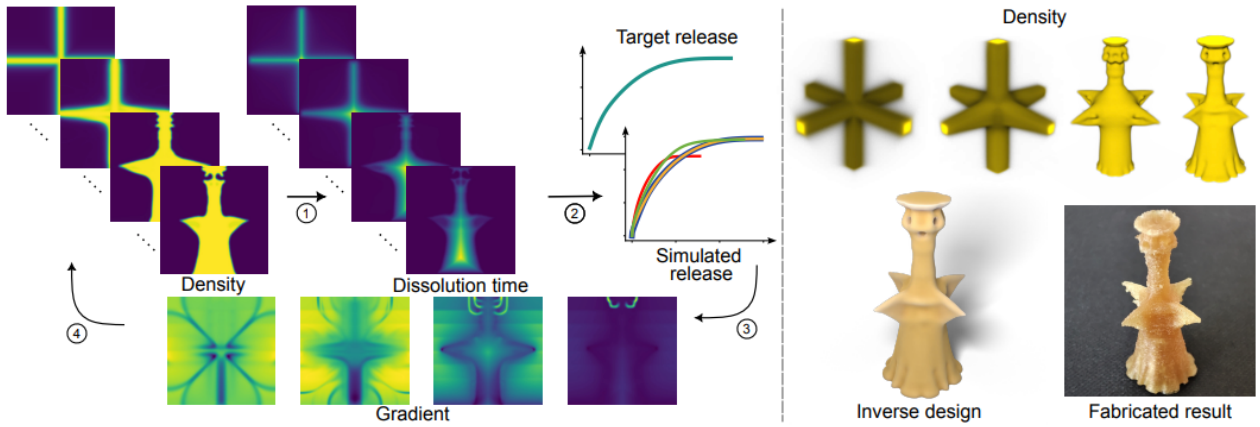

Fig. 1. Our pipeline optimizes for a geometry that achieves a target release curve. Left: starting from the density field at the current iteration, we simulate the release process by ① computing the dissolution time as the solution to a variable-speed Eikonal equation and ② evaluating the release curve by calculating an integral over the domain. The deviation from the target release profile is then measured and differentiated with respect to the density variables ③ to obtain the design objective gradient and update the design ④. Right: visualization of the volumetric density fields describing the evolving 3D design along with the final extracted object and fabricated result.

We propose a gradient-based inverse design framework for the problem of architected release. The backbone of our solution is a simple forward model, based on a geometric abstraction, that is governed by the Eikonal equation. We formulate our problem as a PDE-constrained topology optimization whose objective is to fit the release curve computed from the Eikonal equation solution to the target release profile. We present an exact sensitivity analysis of the discrete fast marching solution and obtain a robust and efficient simulation model with analytical derivatives. Our formulation enables gradient-based optimization for discovering shapes achieving novel release behaviors and exploring trade-offs between release curve closeness and fabricability. A novel image-based measurement setup for acquiring the physical release curves of 3D printed objects is used for testing.

Applications & Advantages

- Suitable for 3D printed pharmaceuticals
- Produces freeform 3D printable geometries
- No additional material needed, no multi-lamination
- Replaces trial & error process with a topology optimization

Patent Information

PCT patent application PCT/EP2023/077032 filed in September 2023, published under WO2024/074417