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Growing Optimized Anisotropic Microstructures with Reaction/Diffusion

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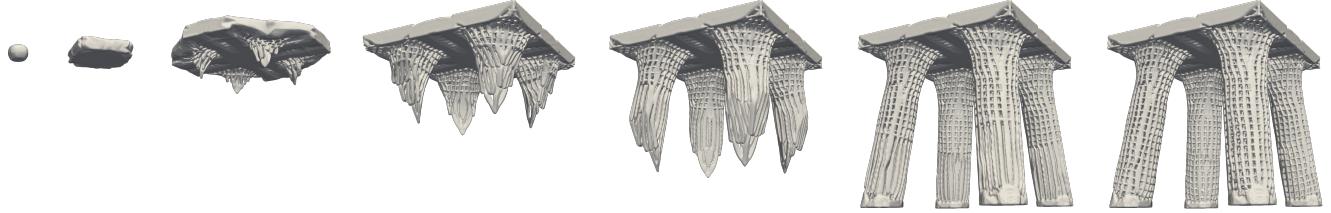


Figure 1: Growth of a lattice-like, stress-aligned, four-legged stool using our adapted Reaction/Diffusion-based approach.

Abstract

Lattice structures can present advantageous mechanical properties while remaining remarkably lightweight. Precise lattice design can however be tricky to set up on arbitrary domain with classical 3D modeling methods as it involves very fine oriented details. Interestingly, natural porous structures can present such lattice-like design which motivates the seek for bio-inspired approaches. In this paper we present a novel method to grow lattice-like structures within an arbitrary shape and aligned along an oriented field using adapted Reaction/Diffusion systems. While not directly computed from a global optimization process our structures still demonstrate remarkable structural properties for which we provide examples with numerical validation.

CCS Concepts

• Computing methodologies → Shape modeling; Volumetric models; Mesh models;

1. Introduction

Recent advances in Additive Manufacturing and 3D Printing allows for high shape complexity that leads to seek for new lightweight designs. Hence there has been a growing interest in design of optimized multi-scale structures [LSZ^{*}14, MDL16, DTZ17, MSDL17, WAWS18, LGC^{*}18, ALSL^{*}18, AK21, SOG^{*}21]. Recent works are mostly built upon Topology Optimization [LHZ^{*}18, PT08, GS18, SPG19, AGDP19, GSA^{*}20, WSG21].

In the field of structural optimization, it is well known that the orientation of orthotropic microstructures has to be locally aligned with the principal stress directions for single-load case stiffness-optimal structure design [Mic04, Ped89, AK93, AJL^{*}19]. Some natural materials show remarkable mechanical performances based on this stress orientation property [Woo60]. In this paper, we describe a novel bio-inspired method to design conforming lattice-like structures. Our method divides into two major steps. The first step proposes to generate intermediate structures with patterns oriented by an underlying tensor field and limited by a prescribed 3D

shape with a growing process. This growth phase is controlled by an anisotropic Reaction/Diffusion model. The second step starts by applying some filter to the different structures to operate on the thickness of the oriented structures before combining them with Boolean operations in a similar way than [GDAP20].

Our contributions are the following:

- A general method for designing field conformal lattice-like structures, compatible with the workflow of topology optimization
- A novel approach based on a classic Reaction/Diffusion model to design global structure using anisotropic growth of microstructures
- A new multi-scale process to design optimized structures which constitute a good trade-off between stiffness property and resistance to buckling despite not being directly an optimizer of these properties

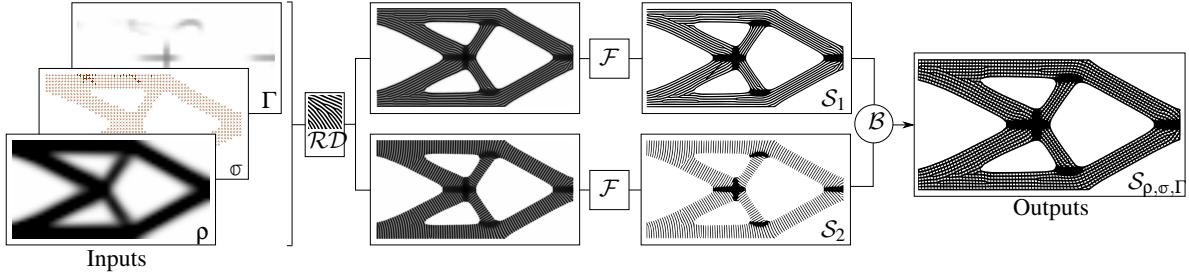


Figure 2: Global pipeline of our method. The first step (\mathcal{RD}) designates the Reaction/Diffusion, the intermediate step (\mathcal{F}) represents a filtering process while the final step (\mathcal{B}) is constituted of boolean operations

35 2. Method

36 2.1. Overview

37 Let us consider a rectangular domain Ω , subset of \mathbb{R}^2 or \mathbb{R}^3 , representing the domain of definition of the three following fields used as
38 inputs of our method as illustrated in Fig.2-left. First the scalar field
39 $p(\mathbf{x} \in \Omega) \in [0, 1]$, describes an initial notion of material density at
40 each position in Ω . For a given isovalue $iso \in]0, 1[$, the domain
41 implicitly defined by $p(\mathbf{x}) > iso$ corresponds to the general appear-
42 ance of the 3D shape where the micro-structure should be syn-
43 thetized, and will be designated as *infill space*. Second, a *tensor field*
44 $\sigma(\mathbf{x} \in \Omega)$ (for instance associated to the stress tensor), whose prin-
45 cipal directions are considered to be the desired local orientation
46 of the microstructures. Third, another scalar field $\Gamma(\mathbf{x} \in \Omega) \in [0, 1]$
47 called *infill map* used to indicate the local regions to infill pref-
48 erentially with solid material instead of lattice microstructures. All
49 inputs and intermediate field values are stored on a discretized grid,
50 and we may pre-process these inputs in up-sampling if needed their
51 values by interpolation to any grid resolution adapted to our ex-
52 pected lattice microstructure.

53 The output of our approach is also described as a scalar field
54 $S_{p,\sigma,\Gamma}(\mathbf{x} \in \Omega) \in [0, 1]$ shown Fig.2-right. The resulting shape sur-
55 face is described as an isovalue of S which can be computed typ-
56 ically using marching cube or dual contouring when a triangu-
57 lar mesh is expected for visualization and manufacturing purpose.
58 This surface represents an hybrid structure mostly filled with lat-
59 tice aligned with both the tensor field directions and the boundary
60 of the *infill space*. More precisely, at the boundary the lattice re-
61 mains oriented according to the tensor field while shaped by the
62 outer shell.

63 The core of our algorithm lies in the two major steps (\mathcal{RD}) and
64 (\mathcal{B}). Step (\mathcal{RD}) is the actual anisotropic Reaction/Diffusion pro-
65 cess allowing to synthesize intermediate scalar fields with locally
66 oriented patterns. We compute 2 (resp. 3) independent processes
67 in 2D (resp. 3D), while considering for each of them one of the
68 principal tensor direction to be the main diffusion direction. The
69 anisotropic Reaction/Diffusion patterns have a linear structure in
70 2D, and a surfacic one in 3D, and are restricted to grow in the re-
71 gions specified by p as explained in Sec. 2.3. Once these interme-
72 diate fields are generated, the final lattice structure is generated in
73 step (\mathcal{B}). To this end, we first apply a filter (\mathcal{F}) on each of the inter-
74 mediate fields in order to steepen the variations of the field as well
75 as thickening or thinning the patterns depending on their direction

77 to optimize the mechanical structure associated to them. The output
78 field S is finally obtained in combining the previous filtered fields
79 using Boolean operations in order to generate a single lattice orga-
80 nization from the individual oriented patterns. These last steps are
81 described in Sec. 2.4.

82 2.2. Inputs

83 This section describes with more details the automatic computation
84 we followed to generate the input fields p , σ , Γ . While these fields
85 can be provided using arbitrary methods, we will describe them as
86 being automatically computed from a topology optimization as it
87 provides an interesting case of application in the context of struc-
88 tural optimization.

89 **Infill Space p .** The purpose of this input density field is to design
90 the overall shape which will be used as a boundary for lattice ma-
91 terial infill. We adopt a simple approach where this boundary is
92 defined by the optimal distribution of a budget of solid material
93 maximizing the stiffness, given a fix design space with loads and
94 constraints. Hence our desired input density field can be seen as
95 the direct output of the classical compliance topology optimiza-
96 tion problem subject to a global volume constraint, relying on the
97 density-based method colloquially referred to as the *Solid Isotropic*
98 *Material with Penalization* (SIMP) approach described by [BS99].
99 A numerical optimization on a low resolution grid can be conducted
100 following [ACS*11]. The example used as input for Fig.2 is re-
101 ferred to as the *Cantilever* problem, a *de facto* standard test case in
102 the litterature: a load is applied vertically in the middle of the right
103 edge of the design space while the displacement is constrained all
104 along the left edge.

105 **Tensor field σ .** The stress tensor field $\sigma(\mathbf{x} \in \Omega)$ can then be ex-
106 tracted from this preliminary optimization. For each element \mathbf{x} , the
107 tensor is diagonalizable in an orthogonal basis with real eigenval-
108 ues called the principal stresses and their associated eigenvectors
109 form a rotation matrix $\mathbb{R}(\mathbf{x})$ which characterizes the principal stress
110 directions perpendicular to the planes where the principal stresses
111 act.

112 **Infill Map Γ .** The Infill Map indicates the areas to infill with ho-
113 mogeneous material. It can be divided into two sub-maps: $\Gamma(\mathbf{x}) =$
114 $(\Gamma_c \cup \Gamma_\sigma)(\mathbf{x}) = \max(\Gamma_c(\mathbf{x}), \Gamma_\sigma(\mathbf{x}))$. The first one $\Gamma_c(\mathbf{x})$ is given by
115 the designer constraints and the other one $\Gamma_\sigma(\mathbf{x})$ is derived from the
116 previous rotation field. This second map addresses an issue encoun-
117 tered when the input stress field is locally isotropic, or is associated

to very low values. In this case, the ordering and direction of the eigenvalues become meaningless, and the extracted rotation field would exhibit discontinuities. As there is no clear orientation to follow in these regions, we propose to infill them with plain material. To detect these regions, we propose an automatic computation assessing the local consistence of the alignment of all eigenvectors using the value $a(\mathbf{x}) = \frac{1}{|N(\mathbf{x})|d} \sum_{\mathbf{y} \in N(\mathbf{x})} \sum_{1 \leq i \leq d} |\mathbf{v}_i(\mathbf{y}) \cdot \mathbf{v}_i(\mathbf{x})|$ with $N(\mathbf{x})$ the set of neighbours of the element situated in \mathbf{x} . We can then define $\Gamma_\sigma(\mathbf{x}) = (1 - a(\mathbf{x}))\rho(\mathbf{x})$.

2.3. Pattern Growth

The concept of Turing patterns was first introduced by Alan Turing [Tur52] in a foundational paper. The original theory explains pattern formation through a Reaction/Diffusion mechanism and as of this day it remains a major theory in theoretical biology used to model embryonic development as well as skin pigmentation. Here we are only interested in this model as a *tool* to generate smooth oriented patterns through the integration of a PDE. Hence the growth phase of our method is controlled by a two-species Reaction/Diffusion system which is a variant of the Gray-Scott model [GS84, Pea93] where the first species diffuses anisotropically. In this case the evolution of the concentrations $u(\mathbf{x}, t)$ and $v(\mathbf{x}, t)$ of the two reactive chemical species U and V is described by the following set of equations:

$$\begin{cases} \frac{\partial u}{\partial t} = \sigma(\mathbf{x})\nabla^2 u + \gamma f(u, v) \\ \frac{\partial v}{\partial t} = d\nabla^2 v + \gamma g(u, v) \end{cases} \quad (1)$$

where σ represent the anisotropic diffusion tensor, $d = \frac{D_v}{D_u}$ the diffusion ratio between the two species, and γ a parameter which controls the characteristic length of the pattern. In the original model the chemical U is added in the environment at a feed rate F while the chemical V is removed at a kill rate k . Both chemicals diffuse but U diffuses faster than V ($d < 1$) to observe patterns. The reaction kinetics is hence controlled by the following functions:

$$\begin{cases} f(u, v) = -uv^2 + F(1 - u) \\ g(u, v) = uv^2 - (k + F)v \end{cases} \quad (2)$$

Pattern growth can be restricted to a design region $\Omega = \{\mathbf{x}, \rho(\mathbf{x}) > s\}$ (for s chosen in $[0, 1]$) by redefining the term $\gamma g(u, v)$ as

$$\gamma g(u, v)\mathbb{1}_\Omega - \lambda(1 - \mathbb{1}_\Omega)v, \quad (3)$$

where $\mathbb{1}_\Omega(\mathbf{x})$ takes the value 1 if $\mathbf{x} \in \Omega$ and 0 otherwise. We set $\lambda > 0$ and $\lambda \gg F, k$ such that the species of interest ($1 - U$) (i.e. which will generate the intermediate oriented structures) is exponentially "killed" outside the area of interest. We also extend the value k to a space-varying field defined as $k(\mathbf{x}) = k(1 - \alpha\Gamma(\mathbf{x}))$. This allows increase the concentration of V (and so $(1 - U)$) conformly to the *Infill Map*, while the parameter $\alpha \in [0, 1]$ is used to adjusts how much these regions should be infilled.

Our objective is to generate a lattice structure from the synthesized patterns. To this end, we simulate d independent Reaction/Diffusion processes, with $d = \{2, 3\}$ being the dimension of the embedding. Each process $i \in [1, d]$ uses its own diffusion tensor

σ_i favouring one of the main direction of $\sigma = \mathbb{R}\mathbb{A}\mathbb{R}^T$ and defined by:

$$\sigma_i = \frac{1}{\text{Tr}(\mathbb{D}_i)} \mathbb{R}\mathbb{D}_i\mathbb{R}^T \quad (4)$$

where \mathbb{D}_i is a diagonal matrix filled with 1 on the diagonal and $\xi > 1$ the custom anisotropy at the (i, i) position. This will generate patterns oriented along each principal direction of the input tensor field. Gathering all together, each oriented intermediate structures S_i is represented by a (normalized) density field computed from the finite differences integration of each following system:

$$(S_i) \left\{ \begin{array}{l} \frac{\partial u_i}{\partial t} = \sigma_i(\mathbf{x})\nabla^2 u_i + \gamma f(u_i, v_i) \\ \frac{\partial v_i}{\partial t} = d\nabla^2 v_i + \gamma g(u_i, v_i)\mathbb{1}_\Omega - \lambda(1 - \mathbb{1}_\Omega)v_i \\ f(u_i, v_i) = -u_i v_i^2 + F(1 - u_i) \\ g(u_i, v_i) = u_i v_i^2 - [k(1 - \alpha\Gamma(\mathbf{x})) + F]v_i \\ u_i(\mathbf{x}, t=0) = 1, \quad \begin{cases} v_i(\mathbf{x} \in \mathcal{D}_0, t=0) = 1 \\ v_i(\mathbf{x} \notin \mathcal{D}_0, t=0) = 0 \end{cases} \end{array} \right. \quad (5)$$

where \mathcal{D}_0 designates the initial "seed", typically a small disk (in 2D) or sphere (in 3D) included in the *infill space*. This small initial seed was preferred to a large initial and possibly random covering of the infill space, as we noticed experimentally that the Reaction/Diffusion process generates more regular patterns when these are developed as growth through empty space. For the cantilever S_1 and S_2 can be seen Fig.2 (before and after filtering) as the result of an isosurface extraction of the density fields $s_i = 1 - u_i$.

2.4. Structure compilation

By merging the different substructures infilled with oriented patterns along the principal stress directions, it is possible to generate a shape with oriented lattice. A filter step is added to adapt the structure thickness before combining them. The result for the cantilever can be seen Fig.2-right.

Magnitude filter. [BK88] introduced the unit-cell with a rectangular hole as it constitutes an optimized microstructure compared to a regular square cell. Following this idea, in order to enhance the structural performance relatively to the mass, one can shift the iso to enlarge the pattern oriented along the first principal stress directions while reducing the width of the others. It can be achieved by redefining the density fields as follow

$$\tilde{s}_i = \text{Normalize}(\max(\min(s_i, s_{\sigma_i} + s_{w\sigma_i}), s_{\sigma_i} - s_{w\sigma_i})) \quad (6)$$

where *Normalize* means that the density field is normalized between 0 and 1, s_{σ_i} denotes the targeted isovalue according to the direction i and $s_{w\sigma_i}$ a parameter which applies a threshold favouring a binary structure while preserving its smoothness.

Boolean Operation. The final structure can be generated through the use of binary merging operators of implicit surfaces, corresponding to the use of min and max functions on their field values:

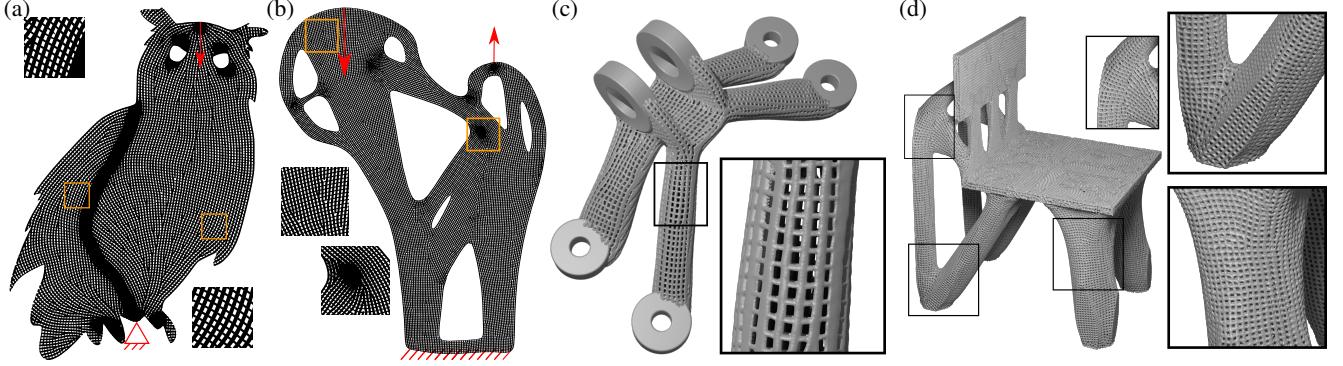


Figure 3: Different results with size of the grid: (a) Owl (752×1024) (b) Optimized Femur Head (2048×2624) (c) Lattice GE Bracket ($302 \times 512 \times 826$) (d) Optimized lattice chair ($504 \times 360 \times 720$)

$$(\mathcal{S}) \left\{ \begin{array}{l} \mathcal{S}_{2D} = \mathcal{S}_1 \cup \mathcal{S}_2 = \max(\tilde{s}_1, \tilde{s}_2) \\ \mathcal{S}_{3D} = \bigcup_{i \neq j} \mathcal{S}_i \cap \mathcal{S}_j = \max_{i \neq j} \left(\min_{i \neq j} (\tilde{s}_i, \tilde{s}_j) \right) \end{array} \right. \quad (7)$$

3. Results and analysis

154 Fixed user-defined 2D shape: Owl. The first result Fig.3a is an
155 example of structure generated from a pre-defined shape given by
156 the designer. The input stress field is computed from topology optimiza-
157 tion considering a fixed load and the final structure is gener-
158 ated by our method.

160 Optimized 2D shape: Femur Head. Fig.3b gives an example of a
161 structure optimized inside the the overall shape of a femur head.

162 3D Optimized GE Bracket. Fig.3c shows our version for the GE
163 Bracket scenario [Gra13] in case of a single load.

164 3D Optimized Chair. We propose to compare our result with the
165 previous work from Wu et al. [WWG21] that proposed an opti-
166 mized lattice chair generated using a Topology Optimization with
167 oriented homogenized material followed by a parameterization op-
168 timization algorithm to design the lattice. Using the same under-
169 lying tensor field, the growth lattice obtained using our method is
170 shown Fig.3d. Our result shows more lattice regularity especially
171 near the surface of the object due to the aptitude of the Reac-
172 tion/Diffusion to smoothly grow along the overall 3D shape.

173 Non-linear Structural Analysis. We run a general non-linear anal-
174 ysis in Abaqus 2021 to compare two design variants for the MBB
175 Beam scenario and retrieve the force-displacement curves shown in
176 Fig. 4. The two design variants have the same mass and are obtained
177 with a classical compliance-based topology optimization (TO de-
178 sign) and with the proposed Reaction-Diffusion approach (RD de-
179 sign). The force-displacement curves of both design initially start
180 with a roughly linear portion with the steeper slope indicating that
181 the TO design achieves a higher stiffness, which is to be expected
182 because it was specifically optimized for maximum stiffness. How-
183 ever, at a load magnitude of approximately 140 kN the TO design
184 undergoes in-plane buckling and collapses. In contrast, the RD de-
185 sign shows near-linear deformation up to a load magnitude of 200

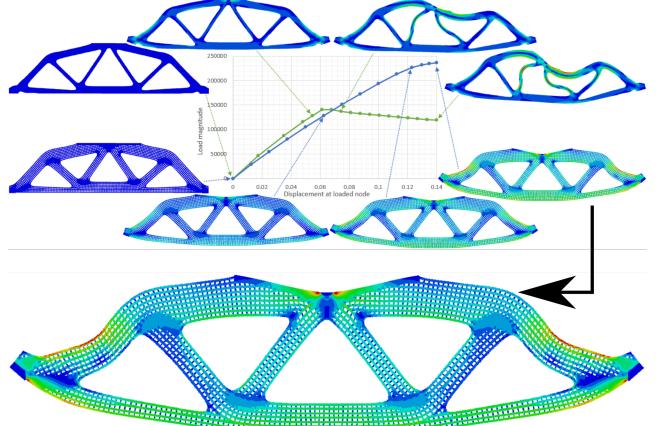


Figure 4: Force-Displacement curves for TO design variant (in green) and the RD design (in blue) in an MBB Beam scenario, with a zoom on RD design variant at peak load in the non linear analysis.

186 kN, and supports a peak load approximately 70% higher than the
187 TO design.

4. Conclusion

The present work proposed a novel approach to design conforming lattice-like structures, inspired by morphogenesis. Our method finds its main application in the design of optimized microstructures oriented by inputs which can be provided by a stress field or an anisotropic material orientation field inside a structurally optimized shape. In this context, our lattice-like structures come as a good trade-off between pure stiffness property and resistance to buckling despite they are not the output of an optimizer of these properties. Due to its multiscale nature, our method is fast and scalable to high resolution designs. Moreover, the microstructure generation is completely local, allowing the designer to dynamically interact with the growing structure, by erasing or modifying some parts and letting it evolve. Additionally, the aptitude of the Reaction/Diffusion to smoothly grow along the overall 3D shape ensure to generate structures with high lattice regularity, which is desirable both for aesthetics and mechanical performance considerations.

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