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Origami and the Structure of Materials

By Huan Liu, Paul Plucinsky, Fan Feng, Arun Soor, and Richard D. James

The world's population is growing approximately linearly by about 80 million individuals per year, leaving less and less space per person on average. Perhaps this growth is responsible for an explosion of interest in origami—the art of paper folding—with applications that range from stents to canoes and even buildings. Origami is basically a fitting game. We already know a lot about the rules for smoothly bending and twisting a sheet of paper, as this is the classic subject of locally isometric mappings in differential geometry. *Continuity* is required for origami — these mappings must fit together at the creases.

Differential geometry *per se* is not quite as helpful for this purpose as one might think. It focuses on quantities that are intrinsic, i.e., that do not depend on parameterization. But in origami design, we usually wish to find the particular parameterization that actually describes the origami structure, which we often fold from a flat sheet with a crease pattern. Ideally, we want the full recipe for the sheet's continuous folding—a homotopy, if it exists—to guarantee that the structure is deployable. A Lagrangian approach is therefore fruitful, especially if we also seek to calculate the forces and moments that contribute to the folding.

Such logic brings origami design surprisingly close to the methods that researchers apply to understand the structure of materials at both the atomistic and continuum levels [7]. At the continuum level, a material's underlying crystal structure imposes a symmetry that phase transformations can break, often by passing to a subgroup. This group-subgroup relation describes a family of symmetry-related distortions that are possible at a phase transformation. It also leads to a fitting problem: How can we fit together the different distortions? Atomistic-level arrangements of atoms—such as quasicrystals—suggest unusual origami designs that highlight undeveloped areas of applied mathematics.

The exploitation of discrete symmetries is a powerful tool for both origami design and the study of phase transformations. To explain the simplest method, consider a discrete group of isometries:

$$g_1 = (\mathbf{Q}_1 | \mathbf{c}_1), \quad g_2 = (\mathbf{Q}_2 | \mathbf{c}_2), \ldots, \quad g_n = (\mathbf{Q}_n | \mathbf{c}_n). \tag{1}$$

Here, $\mathbf{Q}_1, \ldots, \mathbf{Q}_n$ are 3×3 orthogonal matrices, $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are three-dimensional vectors, and the group can be finite or infinite ($n = \infty$). $(\mathbf{I}|0)$ is the identity, $g_1 g_2 = (\mathbf{Q}_1 | \mathbf{c}_1)(\mathbf{Q}_2 | \mathbf{c}_2) = (\mathbf{Q}_1 \mathbf{Q}_2 | \mathbf{c}_1 + \mathbf{Q}_1 \mathbf{c}_2)$ is the multiplication rule, and the

See **Origami** *on page 4*

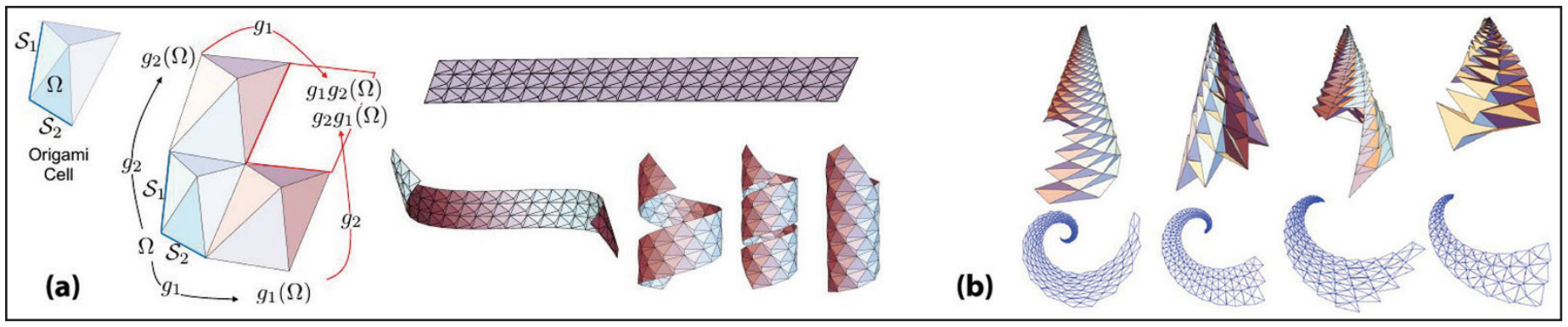

Figure 1. *Group orbit procedure with various tiles and helical/conformal groups.* **1a.** *Group orbit procedure with a Miura tile and helical group.* **1b.** *Group orbit procedure with various tiles and a conformal group. The unfolded crease pattern is shown in blue. Figure 1a adapted from [3], 1b courtesy of the authors.*

Multi-agent Simulations and Vaccine Allocation Strategies

By Jiangzhuo Chen, Stefan Hoops, Parantapa Bhattacharya, Dustin Machi, and Madhav Marathe

Epidemic science pertains to the development of models, technologies, and decision support tools to understand and control the spread of disease. This area of research is especially critical as the COVID-19 pandemic continues to cause significant social, economic, political, and health-related impacts across the globe. In a previous article,[1] we outlined an epidemiological approach that is rooted in network science and data-driven modeling. Here we discuss the challenges of such an approach's implementation during an evolving pandemic in the context of the vaccine prioritization problem, and outline our recent efforts to develop operational models that support policymaking.

We focus on networked models, which consider epidemic spread on an undirected social interaction network $G(V, E)$ over a population V; each edge $e = (u, v) \in E$ implies that individuals (also called nodes) $u, v \in V$ interact. The susceptible-infected-recovered (SIR) model on graph G represents a dynamical process wherein each node is in either an S, I, or R state. Infection can potentially spread from u to v along edge $e = (u, v)$, with a probability of $\beta(e, t)$ at time t after u becomes infected — conditional on node v remaining uninfected until time t. $I(t)$ denotes the set of nodes that become infected at t.

The basic vaccine allocation problem involves deciding *who* to vaccinate and *when* to do so. The objective is to minimize the number of infections, hospitalizations, or deaths [4, 6]. This basic problem is computationally challenging on its own, but it becomes progressively more complex as we consider some of the following real-world constraints [2, 3]:

- **Production Restrictions:** Vaccines are available in limited quantities for a set amount of time. We must thus consider two time-varying processes (epidemic and vaccine production) when prioritizing vaccines.
- **Prioritization:** This problem invites an ethical element. Should vaccine distribution aim to slow disease progression or reduce mortality? The latter usually suggests age- and health-based allocation, while the former implies allocation that targets potential super-spreaders.
- **Immune Profile:** This topic raises several pertinent questions: Who should get the vaccine? What dosage is needed (one or two dose regimens)? Are booster shots necessary? If so, when? And who should receive boosters?
- **Hesitancy:** Some individuals are hesitant about vaccination for various reasons.

Additional complications include lack of timely data, incomplete understanding of disease and immunological processes, social interventions, genomic variations, and vaccine sharing within a country and between countries. The creation of models that assess various vaccine allocation strategies hence becomes a complex system problem that should address five distinct challenges: (i) Most natural problems are

See **Vaccine Allocation** *on page 3*

[1] https://sinews.siam.org/Details-Page/networked-epidemiology-for-covid-19

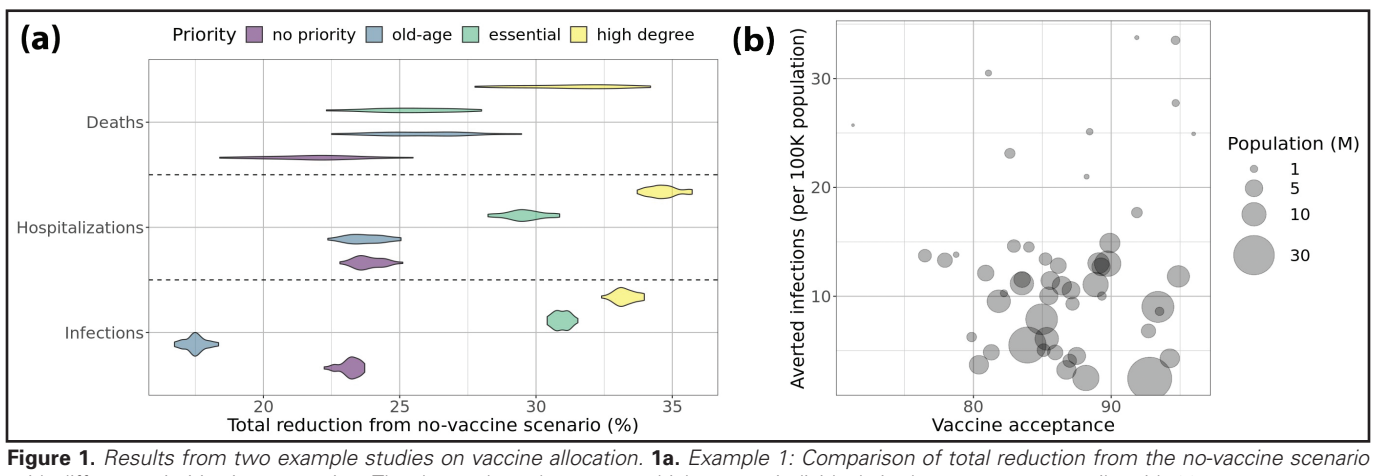

Figure 1. *Results from two example studies on vaccine allocation.* **1a.** *Example 1: Comparison of total reduction from the no-vaccine scenario with different prioritization strategies. The degree-based strategy, which targets individuals in the uppermost quartile with 60 percent accuracy, outperforms the other approaches. The no-priority strategy—which vaccinates randomly selected people—more successfully reduces infections than the old-age strategy, which targets those who are at least 50 years old. However, the opposite is true in the context of death reduction. When it comes to reducing hospitalizations, strategies that target essential workers and high-degree individuals outperform both the no-priority and old-age approaches.* **1b.** *Example 2: Bubble chart that depicts correlations between vaccine acceptance, averted infections, and population size of all 50 U.S. states and Washington, D.C. Although infection aversion does not have an obvious correlation with vaccine acceptance, smaller states seem to have larger (normalized) infection aversions. Figure courtesy of Jiangzhuo Chen.*

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Origami

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notation is traditional. We can apply a group element $g=(\mathbf{Q}\,|\,\mathbf{c})$ to an origami tile $\mathcal{T}$ (or a collection of tiles) in the obvious way: $g(\mathbf{x})=\mathbf{Q}\mathbf{x}+\mathbf{c},\quad \mathbf{x}\in\mathcal{T}$. The apparently unusual group product simply corresponds to a composition of mappings: $g_1g_2(\mathbf{x})=g_1(g_2(\mathbf{x}))$.

Abelian isometry groups are a natural tool for fitting things together. Imagine a tile, a collection of tiles, or any set whatsoever: $(\Omega\subset\mathbb{R}^3)$. Suppose that there are two disjoint subsets of $\mathcal{S}_1,\mathcal{S}_2\in\partial\Omega$, and that two commuting isometries g_1,g_2 satisfy $g_1(\mathcal{S}_1)\subset\partial\Omega$ and $g_2(\mathcal{S}_2)\subset\partial\Omega$. By construction, $g_1(\Omega)$ fits perfectly onto Ω at $g_1(\mathcal{S}_1)$ and $g_2(\Omega)$ fits perfectly onto Ω at $g_2(\mathcal{S}_2)$. But since $g_1g_2=g_2g_1$, $g_1g_2(\Omega)$ thus fits perfectly onto *both* $g_1(\Omega)$ and $g_2(\Omega)$ at $g_1g_2(\mathcal{S}_2)$ and $g_1g_2(\mathcal{S}_1)$ respectively. The Abelian isometry group builds the whole structure by iterating this process. According to the group property, each image of Ω fits together perfectly with its four neighbors. And the tiles are identical, which is a welcome feature for people who actually make and transport the tiles in a real application. Figure 1 (on page 1) illustrates the "group orbit procedure" with Ω as a partly-folded quad origami. The two commuting generators yield a helical group.

In terms of deployability, we want the whole homotopy rather than a single configuration. One component of this ambition is easy. If we consider only piecewise linear, isometric deformations between the creases and perform pairwise fitting at the edges of individual tiles, we can at least hope to conduct the fitting with isometries. Deployability is hence reduced to the question of whether there are sufficiently many free parameters in both the group and unit cell Ω to make the whole structure deformable. Surprisingly, such freedom often exists; Figure 1a (on page 1) illustrates this point with two commuting isometries and a unit cell that collectively allow the structure to be folded continuously from a flat strip to a cylinder. We can also generate this outcome with two commuting conformal transformations: $g_1=(\lambda_1\mathbf{Q}_1\,|\,\mathbf{c}_1)$, $g_2=(\lambda_2\mathbf{Q}_2\,|\,\mathbf{c}_2)$, $\lambda_1,\lambda_2\in\mathbb{R}$. The group product is again a composition of mappings in Figure 1b.

How do these concepts relate to the structure of materials? At the continuum level, we can adapt the aforementioned group orbit procedure. We begin with a deformation $\mathbf{y}:\Omega\to\mathbb{R}^3$, $\Omega\subset\mathbb{R}^3$ (rather than the full homotopy) and consider two Abelian isometry groups; one acts on Ω and the other acts on $\mathbf{y}(\Omega)$. As a simple case, consider $\mathbf{t}\in\mathbb{R}^3$ and a translation group t^i, $i\in\mathbb{Z}$, $t^i(\mathbf{x})=\mathbf{x}+i\mathbf{t}$ that acts on Ω and a circle group $h^i=(\mathbf{Q}^i\,|\,0)$, $i=1,\ldots,n$, $\mathbf{Q}^n=\mathbf{I}$ that acts on $\mathbf{y}(\Omega)$. Suppose that we arrange $h(\mathbf{y}(t^{-1}(\mathbf{x}))=\mathbf{y}(\mathbf{x}),\quad \mathbf{x}\in\mathcal{S}$ on the overlap region $\mathcal{S}=t(\Omega)\cap\Omega$. The groups then build the whole structure for us: $\mathbf{y}(\mathbf{x})=h^i\mathbf{y}(t^{-i}(\mathbf{x}))$, $\mathbf{x}\in t^i(\Omega)$, $i=1,\ldots,n$. To yield a homotopy $\mathbf{y}(\mathbf{x},t)$, we again need sufficient flexibility of the groups and allowable deformations.

Figure 2 illustrates an experimental example with exactly these groups: two variants of a tetragonal phase of a ferromagnetic NiMnGa alloy [5]. It is difficult to experimentally achieve the full homotopy from a rectangular bar in this case; the row of permanent magnets at the top of the figure is instrumental.

How might we achieve Figure 2's reversible phase transformations in nanostructures? One idea involves using two helical groups to generate helical atomic structures, then fitting them together along a helix. We can in fact do so for the green and blue lattices in Figure 3. But the structure is rigid; the interfaces cannot move without slip — i.e., without atoms losing their nearest neighbors. This is always the case when we attempt to fit two helical phases together at a (nondegenerate) helix. On the other hand, inserting the red phase in Figure 3—an exact reflection/"twin" of the blue phase across a horizontal plane and therefore equally stable by the invariance of quantum mechanics—makes the phase transformation possible. Figure 3 illustrates the way in which all atoms retain their nearest neighbors in the process. We suggest that this motion is a viable route to reversible phase transformation in nanotubes.

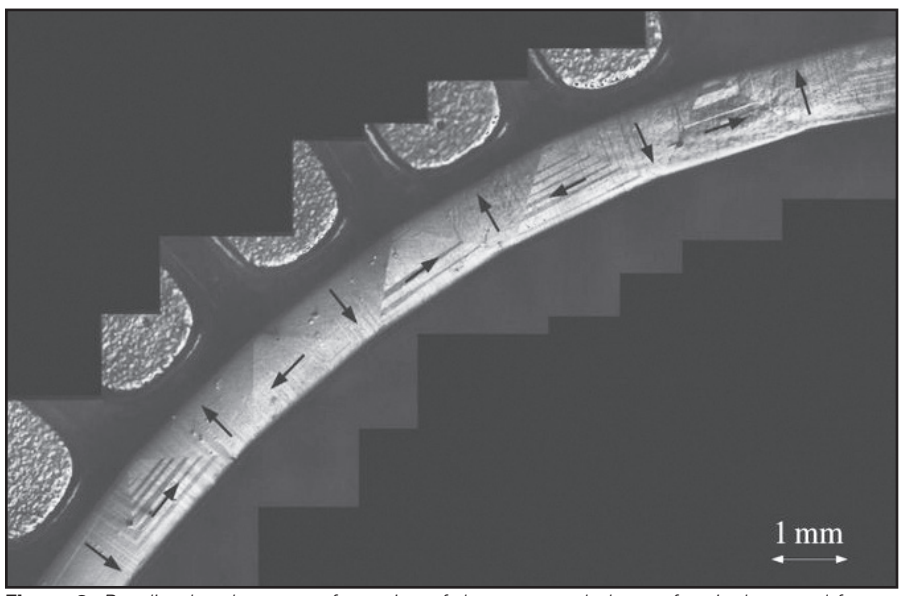

Figure 2. *Bending by phase transformation of the tetragonal phase of a single crystal from a NiMnGa alloy. The arrows depict the direction of magnetization. Figure courtesy of [5].*

Building some elastic energy into an origami structure to bias it towards a particular shape is often a valuable approach [1]. Most elegantly, we can introduce elastic energy by allowing curved, locally isometric mappings between the creases. Again, the Lagrangian approach and group orbit procedure provide powerful methods of synthesis and analysis. The fitting is subtler than before, with careful consideration of the rulings on each side of the crease and exploitation of the additional freedom when the crease itself undergoes a locally isometric mapping. Figure 4 offers some examples that use circle groups for both the reference domain Ω and deformed domain $\mathbf{y}(\Omega)$. We can fold all of these examples isometrically from a flat sheet.[1]

Kirchhoff's nonlinear plate theory—a wonderfully simple and accurate theory—allows us to calculate the elastic energy of these curved origami structures [4]. The finite energy deformations of Kirchhoff's theory are precisely locally isometric mappings.

Can we use the mathematics and inspiration of origami design to suggest completely new kinds of materials? A central idea for material design—and one that is well represented by the periodic table—is that atoms "like to see identical environments." In other words, an isometry can map any atom's full atomic environment to that of any other atom. From a (challenging) mathematical perspective, we can view this property as an intermediate step in the proof of a general crystallization theorem. The property is also evident in the designs of Figures 1 through 4 (excluding Figure 1b); corresponding points on each tile experience the same environment.

A Penrose tiling relaxes this idea. Because there are only two tiles, each node in the tiling sees a finite number of local environments. As the local environment's diameter grows, the number of different local environments grows as well. The presence of a few local environments is an acceptable situation for materials in both energetic and kinetic terms, as evidenced by the existence of quasicrystals. Reidun Twarock and Tom Keef's analysis of virus structure [8] proposes another way to ensure that most atoms in the structure see one of several local environments: use an infinite *non-discrete* isometry group and carefully select elements while avoiding the accumulation points. Since we have minimal knowledge of these non-discrete groups—let alone how to select the elements—there is plenty of room for investigation.

[1] An animation in the online version of this article shows the full homotopy in the case of a translation group on Ω and a helical group on $\mathbf{y}(\Omega)$.

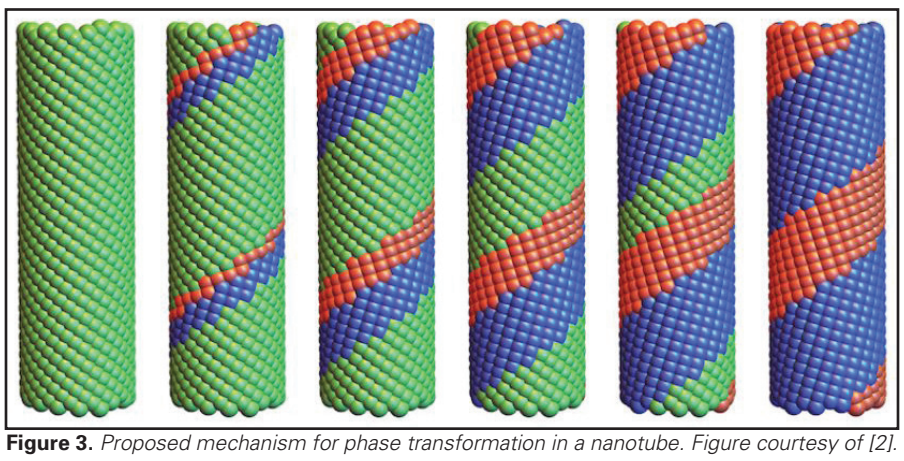

Figure 3. *Proposed mechanism for phase transformation in a nanotube. Figure courtesy of [2].*

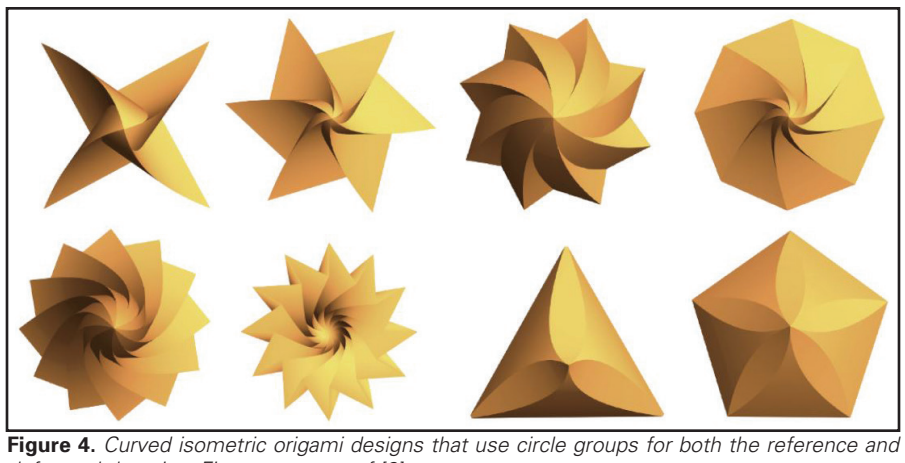

Figure 4. *Curved isometric origami designs that use circle groups for both the reference and deformed domains. Figure courtesy of [6].*

Huan Liu is a graduate student at the University of Minnesota who performs research on the design of materials that both inspire and are inspired by origami. Paul Plucinsky is an assistant professor at the University of Southern California who works on problems at the interface of materials science, mechanics, and applied mathematics. Fan Feng is a postdoctoral researcher at the University of Cambridge who focuses on the geometric evolution and mechanics of liquid crystal elastomers. Arun Soor is a graduate student at the University of Oxford who works on algebraic number theory. Richard D. James is a Distinguished McKnight University Professor in the Department of Aerospace Engineering and Mechanics at the University of Minnesota, where he studies the mathematical design of materials. He can be reached at james@umn.edu.

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