Atomistically inspired origami

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“land of 10,000 lakes”

Credit: Gerald Brimacombe
Robert J. Lang


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Credit: http://www.langorigami.com/composition/white-rhinoceros-opus-714
Objective structures

\[ S = \{x_{i,j} : i = 1, \ldots, N, j = 1, \ldots, M\} \] is an **objective molecular structure** if there are orthogonal transformations \( \{R_{1,1}, \ldots, R_{N,M}\} \) such that

\[ S = \{x_{i,k} + R_{i,k}(x_{n,m} - x_{1,k}) : n = 1, \ldots, N, m = 1, \ldots, M\} \]

\( S \) is discrete

(no sum over \( k \))

M = 1: **objective atomic structure**

Theorem. After a suitable renumbering of atoms (that allows overlapping molecules), every **objective structure** is the orbit of a finite number of atomic positions under a discrete group of isometries.


Reorient yourself to see the same environment

A helical **objective atomic structure**
Isometry groups

**Theorem**  If one allows for intersecting images, every objective structure is the orbit of a discrete group of isometries on a finite set of points in $\mathbb{R}^3$

$$g = (Q|c), \quad Q \in O(3), \quad c \in \mathbb{R}^3$$

$$g(x) = Qx + c, \quad x \in \mathbb{R}^3$$

$$g_1 = (R_1|c_1) \quad g_2 = (R_2|c_2) \quad g_1g_2 = (R_1R_2|c_1 + R_1c_2)$$

This product rule implies  \[ g_1g_2(x) = g_1(g_2(x)) \]

**Identity**  \[ id = (I|0) \]

The main subject of *The International Tables of Crystallography* are isometry groups containing three linearly independent translations

\[ (I|e_1) \quad (I|e_2) \quad (I|e_3) \]
Examples of Objective Structures

\[ S = \{ x_{i,j} : i = 1, \ldots, N, \; j = 1, \ldots, M \} \]

is an **objective structure** if there are orthogonal transformations \( \{ R_{1,1}, \ldots, R_{N,M} \} \) such that

\[ S = \{ x_{i,k} + R_{i,k}(x_{n,m} - x_{1,k}) : n = 1, \ldots, N, \; m = 1, \ldots, M \} \]
The simplest origami

\[ y : \Omega \rightarrow \mathbb{R}^2, \quad \Omega \in \mathbb{R}^2 \]  

(continuous, \( \Omega \) simply connected)

(Neglect the thickness of the paper)

Paper does not easily stretch:

\[ |\nabla y \cdot e| = 1 \quad \text{for all} \quad |e| = 1 \]

\[ \iff \nabla y \in O(2) = SO(2) \cup SO(2)P \]

\[ P = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]
Compatibility

There is a continuous \( y \) with these gradients if and only if

\[
B - A = a \otimes n
\]

(For complex triangulations, satisfy this at every interface)

Lemma. Given \( A \in SO(2) \) and \( B \in SO(2)P \), there exist \( a, n \in \mathbb{R}^2 \) such that

\[
B - A = a \otimes n
\]

2 x 2 matrices

Notation:

\( \otimes \) means that \( A \) and \( B \) differ by a matrix of rank 1
The simplest origami

2 x 2 matrices

Hence, this holds:

\[ B - A = a_1 \otimes n_1 \]
\[ C - B = a_2 \otimes n_2 \]
\[ D - C = a_3 \otimes n_3 \]
\[ A - D = a_4 \otimes n_4 \]

There are restrictions on the normals
Exactly the same mathematical structure occurs in the study of phase transformations in crystals.
A classic theorem in origami

Theorem. A continuous $y$ satisfies

$\nabla y = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \\ n_4 \end{pmatrix}$

for $A, C$ in $SO(2)$ and $B, D$ in $SO(2)P$ if and only if $\alpha + \beta = \pi$

In all cases there exists a continuous homotopy

$\nabla y_\omega : \Omega \rightarrow \mathbb{R}^3$, \hspace{1cm} -\pi \leq \omega < \pi$

where $\nabla y_\omega \in O(2, 3)$

$\omega$ is the homotopy parameter
Algorithm for determining all planar foldings made with 4-fold nodes

Paul Plucinsky

1. All such configurations that can be folded flat by a continuous homotopy, excluding considerations of self-intersection

2. Extension to the full quarter plane can fail due to an angle between neighboring folds becoming 0 or + or - pi (This implies nonexistence)

3. Algorithmic complexity is "polynomial time":

\[(\# \text{ rows}) \times (\# \text{ columns}) \times (\# \text{ computed configurations})\]

Typical time of a simulation: 20 x 20 array, including video output of the folding process = 5 sec. on a laptop

4. Output includes an explicit formula for the mapping

\[y(x, t), \quad x \in \Omega\]
Example

... Actuate every other column by:

\[ \theta_a = -0.8\pi \]

\[ \mathcal{E}_{Bend} \sim |\theta - \theta_a|^2 \]

Global energy minimizer is Configuration 210
Example
Compatibility of 1-node Miura pattern

Comaptibility condition:

\[ R_2(\eta)R_3(\xi)R_4(\omega)t_1 = t_1 \]

\[ \iff \cos \eta = \cos \omega \quad (i.e., \eta = \pm \omega). \]

\[ \xi = \xi^\pm(\omega) \quad \text{explicit function} \]

\[ y(x) = \begin{cases} 
    x, & x \cdot e_3 = 0, x \cdot n_2 < 0, x \cdot n_1 \geq 0, \\
    R_2(\eta)x, & x \cdot e_3 = 0, x \cdot n_3 < 0, x \cdot n_2 \geq 0, \\
    R_2(\eta)R_3(\xi)x, & x \cdot e_3 = 0, x \cdot n_4 < 0, x \cdot n_3 \geq 0, \\
    R_2(\eta)R_3(\xi)R_4(\omega)x, & x \cdot e_3 = 0, x \cdot n_1 < 0, x \cdot n_4 \geq 0.
\end{cases} \]

Notice: \( \omega \) and the choice + or - are the only free parameters
Helical Miura-ori

Two isometries $g_1 = (R_1 | c_1)$ and $g_2 = (R_2 | c_2)$, $g_1 g_2 = g_2 g_1$

$$G = \{ g_1^p g_2^q : p, q \in \mathbb{Z} \}$$

$$g_1 = (R_{\theta_1} | \tau_1 e_1 + (I - R_{\theta_1}) z_1)$$

$$g_2 = (R_{\theta_2} | \tau_2 e_2 + (I - R_{\theta_2}) z_2)$$

Parameters $\theta_i, \tau_i, e_i, z_i, i = 1, 2$ are functions of $(\omega, \varphi)$ and a choice of $\pm$

$\omega$ is the folding angle.

$\varphi$ relates to the direction of rotation axis of cylinder
Caveat: nondiscrete groups

Choose isometries $g_1$ and $g_2$ “out of thin air” and arrange that they commute

$$\{ g_1^i g_2^j(x) : i, j \in \mathbb{Z} \}$$

Classic example in nature: microtubule

Atomistic inspiration: to make realistic structures with nondiscrete groups, just restrict the powers $i$ and $j$ (A helical canoe?)

Interesting connections to work of Reidun Twarock (York) on virus receptors, literature on quasicrystals

F. Bassen et al. Scientific Reports, 31723 (2016)
Discrete groups of isometries have a special structure

- Theorem: If a discrete group of isometries does not contain a translation and is not a point group, it is expressible in one of the forms

A \{h^p : p \in \mathbb{Z}\},
B \{h^p f^m : p \in \mathbb{Z}, m = 1, 2\},
C \{h^p g^q : p \in \mathbb{Z}, q = 1, \ldots, n\},
D \{h^p g^q f^m : p \in \mathbb{Z}, q = 1, \ldots, n, m = 1, 2\},

where

1. \( h = (R_\theta | \tau e + (R_\theta - I)x_0) \), \( R_\theta e = e \), \( |e| = 1 \), \( x_0 \cdot e = 0 \), \( e, x_0 \in \mathbb{R}^3 \), \( \tau \neq 0 \), and \( \theta \) is an irrational multiple of 2\( \pi \).
2. \( g = (R_\psi | (R_\psi - I)x_0) \), \( R_\psi e = e \), is a proper rotation with angle \( \psi = 2\pi/n \), \( n \in \mathbb{Z} \), \( n \neq 0 \).
3. \( f = (R | (R - I)x_1) \), \( R = -I + 2e_1 \otimes e_1 \), \( |e_1| = 1 \), \( e \cdot e_1 = 0 \) and \( x_1 = x_0 + \xi e \), for some \( \xi \in \mathbb{R} \).

From now on we will choose the group C (the largest Abelian helical group), but we will drop the irrationality of \( \theta \)
Many interesting solutions

“Helical Miura-ori” patterns

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Many bistable cases

Many solutions are bistable: there exist two or more sets of parameters for a helical group and corresponding choices $\omega_1$, $\omega_2$ that give solutions for the same choices $p_1, p_2, p_3, p_4$. 
Generic rigidity

Helical Miura-ori is generically rigid

\[ \eta = \omega \quad \text{and} \quad \eta = -\omega \]
Morphing: atomistic inspiration

1) For helical structures rigidity and bistability are ubiquitous
2) Structures generated by nondiscrete groups (with two commuting elements) are generically flexible

If rigidity is ubiquitous, how do we do morphing?

Give up on rigid isometries? Slight stretching? Phase transformation?

F. Feng, P. Plucinsky, R. James, Phase transformations in helical structures, preprint
How to figure out all compatible helical phases?

1. Formula given earlier for all Abelian helical structures is not good for analyzing compatibility: \((p_1, q_1)\) close to \((p_2, q_2)\) does not imply corresponding atomic positions are close

\[
\{ h^p g^q : p \in \mathbb{Z}, q = 1, \ldots, n \}
\]

2. So, change to nearest neighbor generators. There is a systematic way to do this, under very mild assumptions on the group parameters

New generators \(g_1, g_2\)

\(g_1\) maps red to yellow

\(g_2\) maps red to green

\[
\{ g_1^i g_2^j : i \in \mathbb{Z}, j = 1, \ldots, j^* \}
\]

is the same as Group C above
Now write the formula for the position of the atom \((i,j)\)

\[
y(i, j) = g_1^i g_2^j(x) \\
= Q_{i\psi + j\beta}(x - z) + (im_1 + jm_2)\tau e + z \\
i \in \mathbb{Z}, \quad j = 1, \ldots, j^*
\]

This formula makes perfect sense when \(i\) and \(j\) are real numbers.

A “canonical interpolation” of atomic positions.

Assume two phases, phase a and phase b, and do “continuum mechanics compatibility” with the equation above.
All compatible helical structures
Morphing by phase transformation

Fan Feng and Paul Plucinsky
Microstructure

- Horizontal twin
- Zig-zag twin
- Helical twin
- Helical austenite/martensite
- Supercompatible a/m interface

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F. Feng, P. Plucinsky, R. James, Phase Transformations in helical structures, preprint
Conformal Euclidean group

\[ g_1 = (\lambda_1 \mathbf{Q}_1 | \mathbf{c}_1) \]
\[ g_2 = (\lambda_2 \mathbf{Q}_2 | \mathbf{c}_2) \]
\[ g_1 g_2 = (\lambda_1 \lambda_2 \mathbf{Q}_1 \mathbf{Q}_2 | \mathbf{c}_1 + \lambda_1 \mathbf{Q}_1 \mathbf{c}_2) \]

Oval tesselation,
Robert J. Lang

These structures also expected to interact constructively with Maxwell's equations –
Harry Bateman,
“conformal Lorentz group” (1908)
Twisted waves

\[ E(r, \varphi, z, t) = e^{i(\alpha \varphi + \beta z - \omega t)} \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{n_1 + in_2}{2} & \frac{n_1 - in_2}{2} & 0 \\ \frac{n_2 - in_1}{2} & \frac{n_2 + in_1}{2} & 0 \\ 0 & 0 & n_3 \end{pmatrix} \begin{pmatrix} J_{\alpha + 1}(\gamma r) \\ J_{\alpha - 1}(\gamma r) \\ J_\alpha(\gamma r) \end{pmatrix} \]

\( n = (n_1, n_2, n_3) \) is a (generally complex) vector satisfying \( n \cdot (0, \gamma, \beta) = 0 \)

\( J_\sigma \) is a Bessel function of order \( \sigma \)
\( \omega \) is the frequency
\( \alpha, \beta, \gamma > 0 \) are reals (analogous to \( k \) of plane waves)

\[ \sqrt{\gamma^2 + \beta^2} = \omega/c \]

and the magnetic field is given by
\[ B = -(i/\omega) \text{curl} \ E \]
A twisted wave

Plot of the electric field vectors on a tangent curve (blue) of the Poynting vector:

\[ E(r, \varphi, z, t) = \]

\[ e^{i(\alpha \varphi + \beta z - \omega t)} \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{n_1 + in_2}{2} & \frac{n_1 - in_2}{2} & 0 \\ \frac{n_2 - in_1}{2} & \frac{n_2 + in_1}{2} & 0 \\ 0 & 0 & n_3 \end{pmatrix} \begin{pmatrix} J_{\alpha+1}(\gamma r) \\ J_{\alpha-1}(\gamma r) \\ J_\alpha(\gamma r) \end{pmatrix} \]
General helical objective structure

Electric field evaluated at the atoms for a tuned twisted wave
Production of twisted waves

\[
E(r, \varphi, z, t) = e^{i(\alpha \varphi + \beta z - \omega t)} \begin{pmatrix} \cos \varphi & -\sin \varphi & 0 \\ \sin \varphi & \cos \varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{n_1 + in_2}{2} & \frac{n_1 - in_2}{2} & 0 \\ \frac{n_2 - in_1}{2} & \frac{n_2 + in_1}{2} & 0 \\ 0 & 0 & n_3 \end{pmatrix} \begin{pmatrix} J_{\alpha+1}(\gamma r) \\ J_{\alpha-1}(\gamma r) \\ J_{\alpha}(\gamma r) \end{pmatrix}
\]

Integral representation of Bessel functions:

\[
J_{\alpha}(\gamma r) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\psi - \gamma r \sin \psi} d\psi
\]

\[
J_{\alpha}(\gamma r) e^{i(\alpha \varphi + \beta z)} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i[\alpha(\psi + \omega) + \beta z - \gamma r \sin \psi]} d\psi
\]

\[
= \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i\alpha \psi} e^{i(R_{\psi} k) \cdot x} d\psi
\]

\[
R_{\psi} = \begin{pmatrix} \cos \psi & -\sin \psi & 0 \\ \sin \psi & \cos \psi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad k = (0, \gamma, \beta) \quad x = (r \cos \varphi, r \sin \varphi, z)
\]
Production of twisted waves

\[ E(r, \varphi, z, t) = e^{i(\alpha \varphi + \beta z - \omega t)} \]

\[
\begin{pmatrix}
\cos \varphi & -\sin \varphi & 0 \\
\sin \varphi & \cos \varphi & 0 \\
0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\frac{n_1 + in_2}{2} & \frac{n_1 - in_2}{2} & 0 \\
\frac{n_2 - in_1}{2} & \frac{n_2 + in_1}{2} & 0 \\
0 & 0 & n_3
\end{pmatrix}
\begin{pmatrix}
J_{\alpha+1}(\gamma r) \\
J_{\alpha-1}(\gamma r) \\
J_{\alpha}(\gamma r)
\end{pmatrix}
\]

Remarkable algebraic fact

\[
e^{i(\alpha \varphi + \beta z)} \begin{pmatrix}
J_{\alpha+1}(\gamma r) \\
J_{\alpha-1}(\gamma r) \\
J_{\alpha}(\gamma r)
\end{pmatrix} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \begin{pmatrix}
e^{i((\alpha+1)\psi - \varphi)} \\
e^{i((\alpha-1)\psi + \varphi)} \\
e^{i\alpha \psi}
\end{pmatrix} e^{i(R_\psi k \cdot x)} d\psi
\]

Hence, an integral formula for a twisted wave:

\[
E(x, t) = \frac{1}{2\pi} e^{-i\omega t} \int_{-\pi}^{\pi} e^{i\alpha \psi} R_\psi n e^{i(R_\psi k \cdot x)} d\psi
\]
Approximate the integral

The trapezoidal rule

\[ E(x, t) \approx e^{-i\omega t} \sum_{j=1}^{N} \frac{1}{N} e^{i\alpha \psi_j} R_{\psi_j} n e^{i(R_{\psi_j} k \cdot x)} \]

Plane waves

- Phases synchronized
- Amplitudes rotate
- Wave vectors rotate by the same angle

Intersection region of the plane waves is the domain of the twisted wave

1/r decay

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Fast convergence with the number of plane waves

<table>
<thead>
<tr>
<th>Plane Waves</th>
<th>Max Normalized Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>1.6</td>
</tr>
<tr>
<td>10</td>
<td>0.01</td>
</tr>
<tr>
<td>15</td>
<td>1.1 x 10^-6</td>
</tr>
<tr>
<td>20</td>
<td>1.5 x 10^-11</td>
</tr>
</tbody>
</table>

Convergence is actually faster than $M a^{-N}$, $N = \#$ plane waves. Trapezoidal rule: approximate expression satisfies the **exact** design equations for a discrete subgroup.

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Scheme for production of this radiation

Concept: