Discrete Exterior Calculus Tips & Tricks 2:

The Laplacian and Spectral Analysis

GATAS Lab Seminar Series, Fall 2023

Luke Morris

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Discrete Exterior Calculus Tips & Tricks:

All you need is ★ d ∧

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Recap: Finite Difference Methods

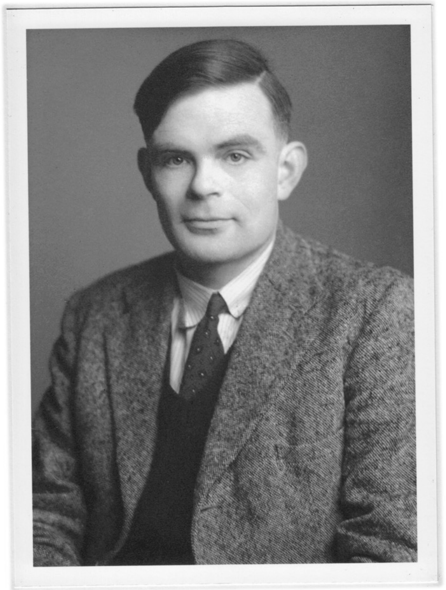
72 A. M. TURING ON THE CHEMICAL BASIS OF MORPHOGENESIS

from one pattern into another, rather than from homogeneity into a pattern. One would like to be able to follow this more general process mathematically also. The difficulties are, however, such that one cannot hope to have any very embracing *theory* of such processes, beyond the statement of the equations. It might be possible, however, to treat a few particular cases in detail with the aid of a digital computer. This method has the advantage that it is not so necessary to make simplifying assumptions as it is when doing a more theoretical type of analysis. It might even be possible to take the mechanical aspects of the problem into account as well as the chemical, when applying this type of method. The essential disadvantage of the method is that one only gets results for particular cases. But this disadvantage is probably of comparatively little importance. Even with the ring problem, considered in this paper, for which a reasonably complete mathematical analysis was possible, the computational treatment of a particular case was most illuminating. The

$$\begin{tikzcd}
\Omega_0 \arrow[r, "d"] \arrow[d, shift right, "\star"'] & \Omega_1 \arrow[r, "d"] \arrow[d, shift right, "\star"'] & \Omega_2 \arrow[r, "d"] \arrow[d, shift right, "\star"'] & \Omega_3 \arrow[d, shift right, "\star"'] \\
\tilde{\Omega}_n \arrow[u, shift right, "\star^{-1}"'] & \tilde{\Omega}_{n-1} \arrow[l, "\tilde{d}"] \arrow[u, shift right, "\star^{-1}"'] & \tilde{\Omega}_{n-2} \arrow[l, "\tilde{d}"] \arrow[u, shift right, "\star^{-1}"'] & \tilde{\Omega}_{n-3} \arrow[l, "\tilde{d}"] \arrow[u, shift right, "\star^{-1}"']
\end{tikzcd}$$

```julia
GrayScott = @decapode begin
  (U, V)::Form0{X}
  (f, k, rᵤ, rᵥ)::Constant{X}

  UV2 == (U .* (V .* V))
  ∂ₜ(U) == rᵤ * Δ(U) - UV2 + f * (1 .- U)
  ∂ₜ(V) == rᵥ * Δ(U) + UV2 - (f + k) .* V
end
```



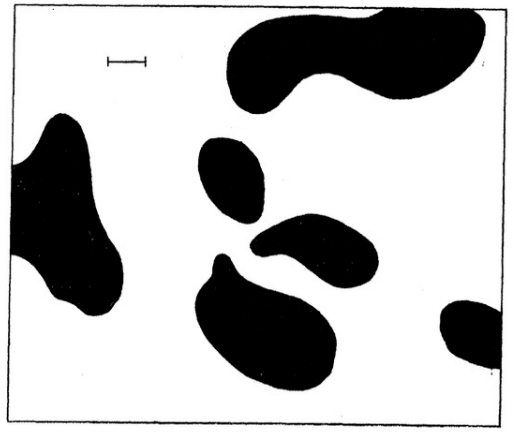
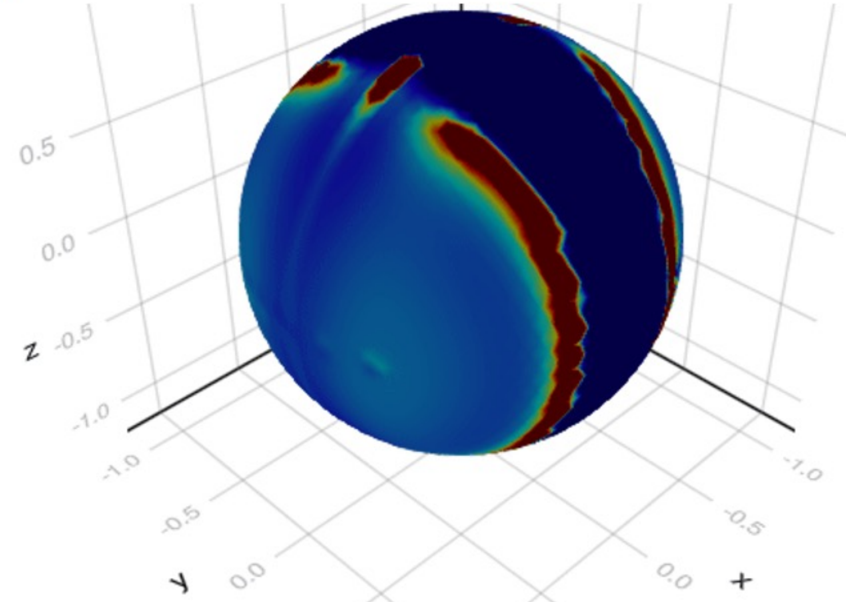


FIGURE 2. An example of a 'dappled' pattern as resulting from a type (*a*) morphogen system. A marker of unit length is shown. See text, §9, 11.



For what else can we use the DEC?

Graph Laplacian

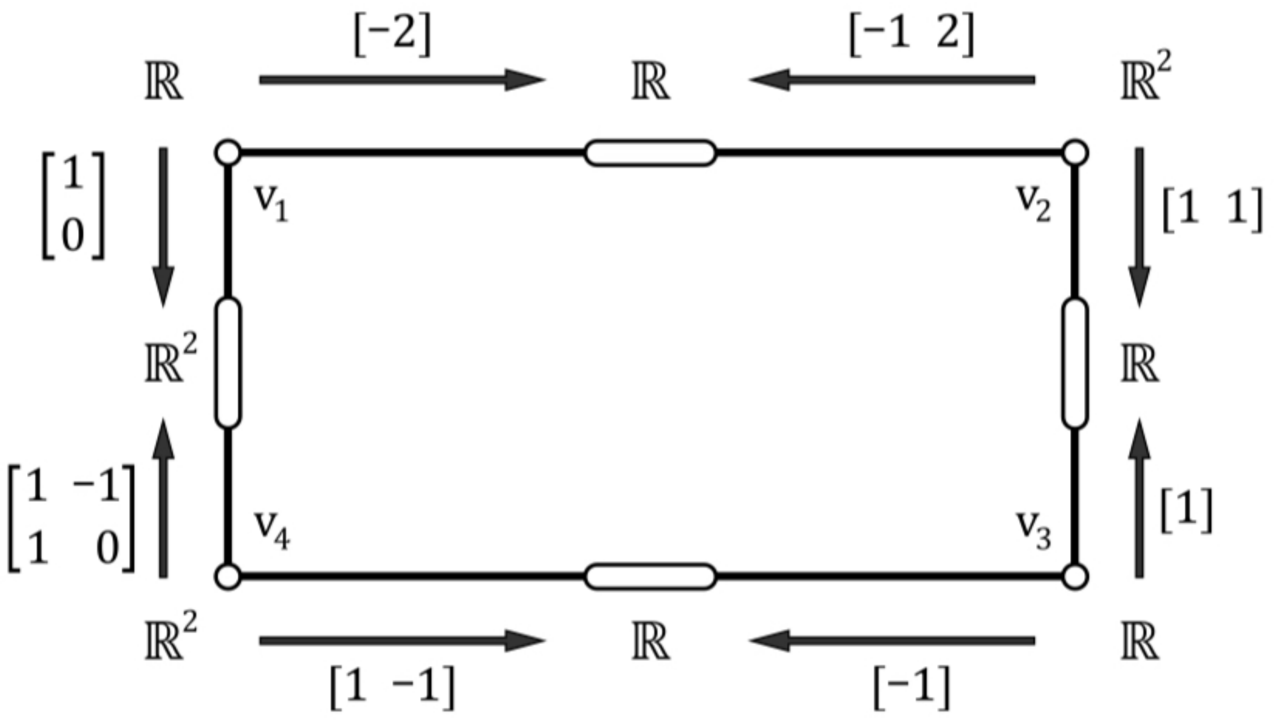
- Given a graph:
  - *Compute the diagonal degree matrix, D*
  - *Compute the adjacency matrix, A*
  - *Take D – A = L.*
- Let's motivate this construction:
  - *L* is the "sum of second derivatives"
  - *L* is the "local deviation from average"
  - *L* is the "divergence of the gradient"

Competing Perspectives

- There is a:
  - Graph-theoretic interpretation
  - Physical interpretation
  - Geometric interpretation
- We are playing with fire by handling all three at once, but the payoff is worth it
- Studying the Laplacian sits us at the *meet* of these domains

Generalization 1: The Sheaf Laplacian

- Increase the dimension *at each vertex*
- The sheaf Laplacian here is a **block-matrix** version of the graph Laplacian.



An example cellular sheaf from Opinion Dynamics on Discourse Sheaves *from Hansen & Ghrist*

$$\delta = \left[\begin{array}{c|cc|c|cc} -2 & 1 & -2 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & -1 & -1 & 1 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 & 0 \end{array}\right]$$

$$L_{\mathcal{F}} = \delta^T \delta = \left[\begin{array}{c|cc|c|cc} 5 & -2 & 4 & 0 & -1 & 0 \\ \hline -2 & 2 & -1 & -1 & 0 & 0 \\ 4 & -1 & 5 & -1 & 0 & 0 \\ \hline 0 & -1 & -1 & 2 & 1 & -1 \\ \hline -1 & 0 & 0 & 1 & 2 & -1 \\ 0 & 0 & 0 & -1 & -1 & 2 \end{array}\right]$$

Corresponding coboundary and Laplacian matrices from Opinion Dynamics on Discourse Sheaves *from Hansen & Ghrist*

Generalization 2: Weighted Laplacians

- Use weights to *imbue geometry* with the cotan Laplacian

$$w_{v_i} = \sum_{\forall \sigma = \{v_i, v_j, v_k\} \in K_2} \mathcal{A}_\sigma / 3, \qquad w_{e_{ij}} = \frac{1}{2}(\cot \theta_{lij} + \cot \theta_{mij}).$$

$\mathcal{A}_\sigma$ is the area of face σ, and θ_{lij} is the angle at vertex v_l facing the edge $e_{i,j} = \{v_i, v_j\}$.

Weights for the cotan Laplacian from Spectral Coarsening with Hodge Laplacians *from Keros & Subr*

Generalization 3: Hodge Laplacians

- Extend Laplacians on vertices to higher degree simplices
- *i.e. Multiple-dispatch on our definition*

```
Δ(::Type{Val{n}}, s::HasDeltaSet, form::AbstractVector; kw...) where n =
  δ(n+1, s, d(Val{n}, s, form); kw...) + d(Val{n-1}, s, δ(n, s, form; kw...))
Δ(::Type{Val{n}}, s::HasDeltaSet; matrix_type::Type=SparseMatrixCSC{Float64}, kw...) where n =
  δ(n+1,s; matrix_type=matrix_type, kw...) * d(Val{n},s,matrix_type) +
        d(Val{n-1},s,matrix_type) * δ(n,s; matrix_type=matrix_type, kw...)
```

Quasi-declarative definitions of the Laplace de Rham from
CombinatorialSpaces.jl/src/DiscreteExteriorCalculus.jl

Recall: Spectral Analysis

- Analyze the eigenvalues and eigenvectors of matrices (linear operators)
- Eigenvectors are “principal components”
- Operators with similar spectral subspaces have similar properties

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Eigenvalues and eigenvectors

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"Characteristic root" redirects here. For the root of a characteristic equation, see Characteristic equation (calculus).

In linear algebra, an **eigenvector** (/ˈaɪɡənˌvɛktər/) or **characteristic vector** of a linear transformation is a nonzero vector that changes at most by a constant factor when that linear transformation is applied to it. The corresponding **eigenvalue**, **characteristic value**, or **characteristic root**, often represented by λ, is the multiplying factor.

Geometrically, a transformation matrix rotates, stretches, or shears the vectors it acts upon. The eigenvectors for a linear transformation matrix are the set of vectors that are only stretched, with no rotation or shear. The eigenvalue is the factor by which an eigenvector is stretched. If the eigenvalue is negative, the direction is reversed.[1] The eigenvectors and eigenvalues of a transformation serve to characterize it, and so they play important roles in all the areas where linear algebra is applied, from geology to quantum mechanics.

Eigenvalues and eigenvectors Wikipedia page

Eigenvectors of the Laplacian

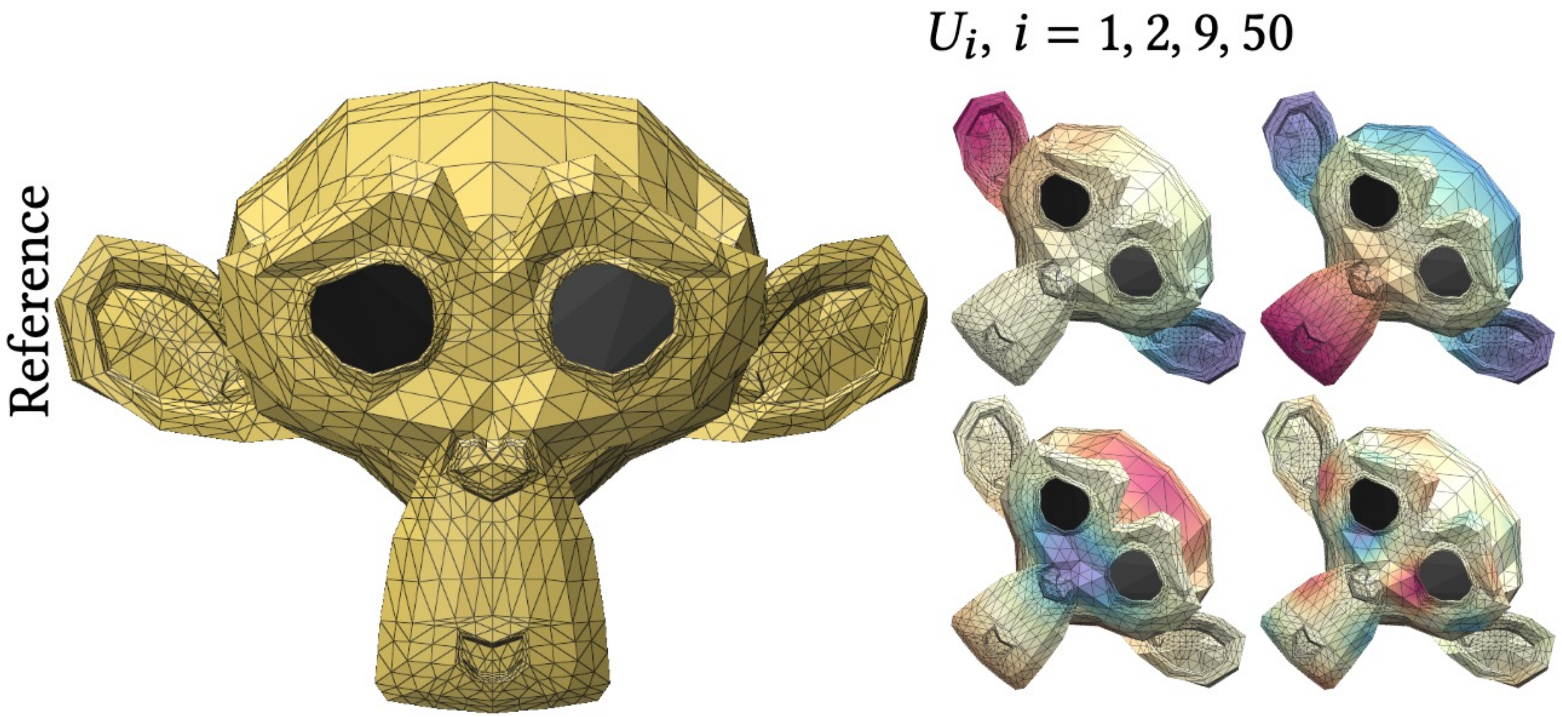
- If the Laplacian is "**local deviation from average**"
- And if the Laplacian is "**imbued with geometry**"
- And if the eigenvectors are "**principal components**"…

Eigenvectors of the Laplacian

- If the Laplacian is "**local deviation from average**"
- And if the Laplacian is "**imbued with geometry**"
- And if the eigenvectors are "**principal components**"…

- Then, we can study the principal ways in which we deviate from local position???

Eigenvectors of the Laplacian



Eigenvectors of the Laplacian on Blender's "Suzanne" mesh from Spectral Coarsening with Hodge Laplacians *from Keros & Subr*

Spectral Coarsening with Hodge Laplacians

Spectral Coarsening with Hodge Laplacians

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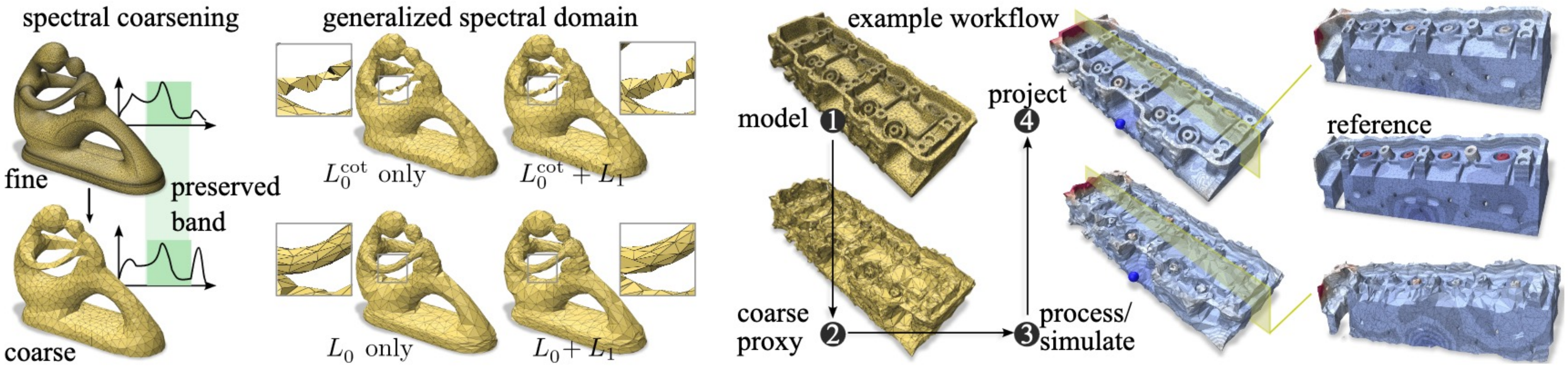

Title and workflow diagram from Spectral Coarsening with Hodge Laplacians *from Keros & Subr*

For what else more can we use the DEC?

Recall: Winding Number

- How many times has the curve gone around me?
- Use to determine whether you are “inside” or “outside”

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Winding number

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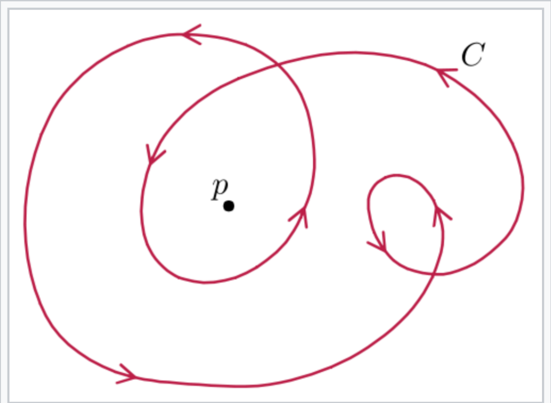
Not to be confused with Map winding number.

In mathematics, the **winding number** or **winding index** of a closed curve in the plane around a given point is an integer representing the total number of times that curve travels counterclockwise around the point, i.e., the curve's number of turns. For certain open plane curves, the number of turns may be non-integer. The winding number depends on the orientation of the curve, and it is negative if the curve travels around the point clockwise.

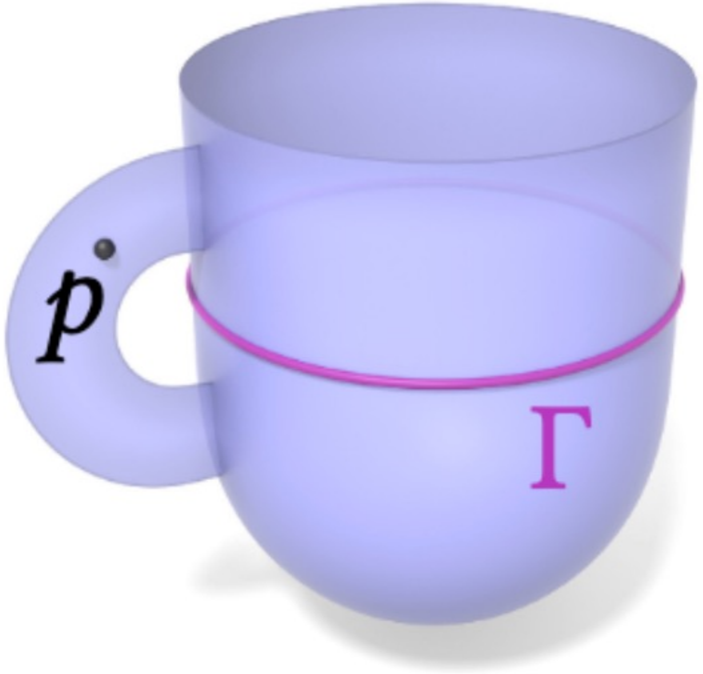


Winding numbers are fundamental objects of study in algebraic topology, and they play an important role in vector calculus, complex analysis, geometric topology, differential geometry, and physics (such as in string theory).

Winding number Wikipedia page

Generalize the Winding Number

- What if you are on the coffee cup?



The inside-outside problem illustrated on a complicated topology from Winding Numbers on Discrete Surfaces *from Feng, Gillespie & Crane*

The Winding Number is a Harmonic Function

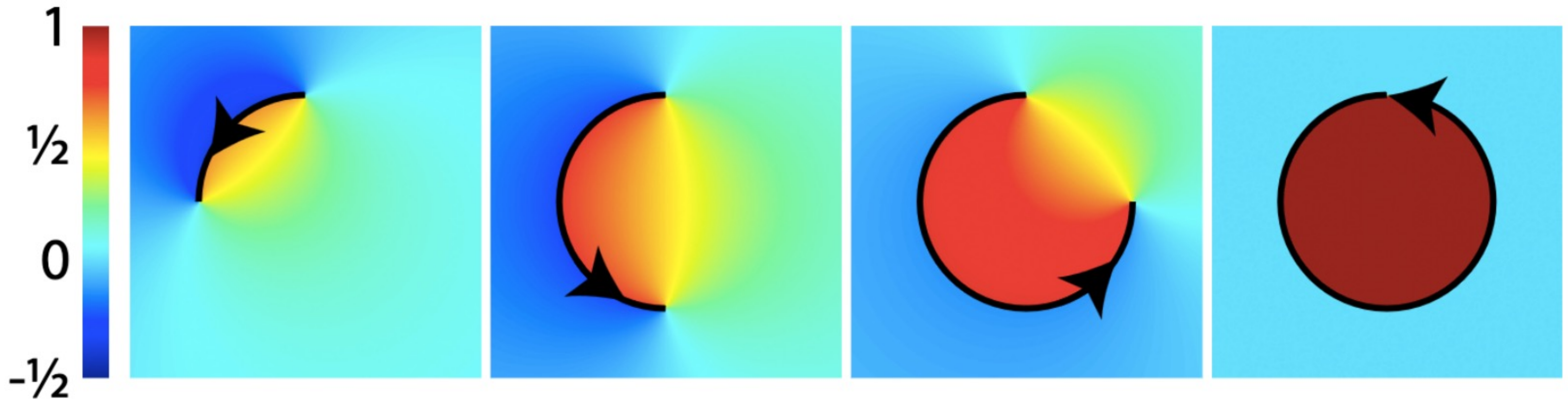


Figure 6: *Left to right: winding number field with respect to an open, partial circle converging to a closed circle. Note the* ± 1 *jump discontinuity across the curve. Otherwise the function is harmonic: smooth with minimal oscillation.*

The generalized winding number on a broken curve from Robust Inside-Outside Segmentation using Generalized Winding Numbers *from Jacobson et al.*

The Winding Number is a Harmonic Function

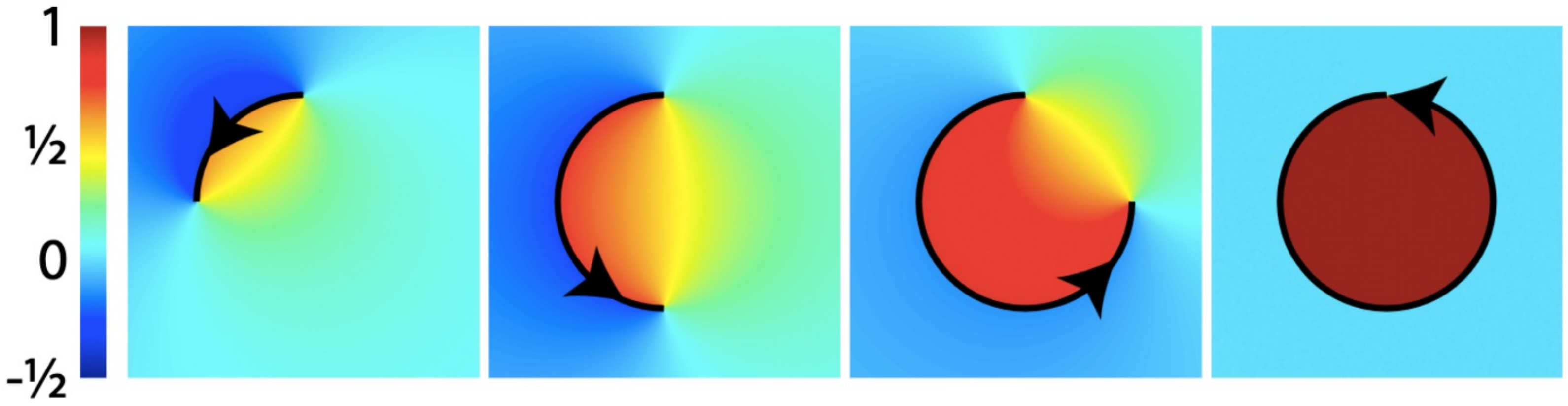


Figure 6: *Left to right: winding number field with respect to an open, partial circle converging to a closed circle. Note the* ± 1 *jump discontinuity across the curve. Otherwise the function is harmonic: smooth with minimal oscillation.*

The generalized winding number on a broken curve from Robust Inside-Outside Segmentation using Generalized Winding Numbers *from Jacobson et al.*

Discrete Laplacians to the Rescue

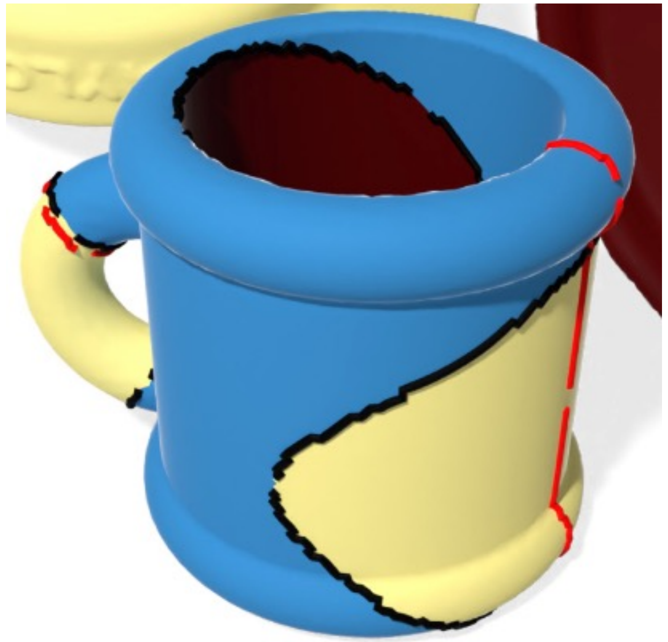
- If we can write the constraints on this harmonic function as a discrete system of equations…

$$\begin{aligned} \Delta u &= 0, && \text{on } M \setminus \Gamma \\ u^+ - u^- &= 1, && \text{on } \Gamma, \\ \partial u^+/\partial n &= \partial u^-/\partial n, && \text{on } \Gamma. \end{aligned}$$

The system of equations describing a generalization of winding number from Winding Numbers on Discrete Surfaces *from Feng, Gillespie & Crane*

Discrete Laplacians to the Rescue

- … we can (literally) run `Problem.solve()`



The "surface winding number" on a coffee cup from Winding Numbers on Discrete Surfaces *from Feng, Gillespie & Crane*

Thanks!

Benjamin Merlin Bumpus

Mathematician & Computer Scientists.

ABOUT

I am Faculty Research Scientist at the University of Florida, working with James Fairbanks in the GATAS lab.

Before that:

- I was a visiting postdoc at the University of Florida, working with James Fairbanks in the GATAS lab.
- I was a postdoc at Eindhoven University of Technology, working with Bart Jansen.
- I completed my PhD supervised by Kitty Meeks at the University of Glasgow in the Formal Analysis, Theory and Algorithms group. You can find *my PhD thesis here*.
- B.SC. (Hons.) Mathematics and its Applications, First-Class; Stirling, Scotland. During my undergrad I worked as a summer research intern with Anthony O'Hare, Jessica Enright and Adam Kleczkowski.

ORGANIZING ROLES

I was the *founder* and *lead organizer of the* e-PCC. This is an online seminar series for PhD students across Europe in discrete mathematics and/or theoretical computer science. (2020)

Thanks!

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My LinkedIn

About me:

I'm a 3rd-year PhD student in the Herbert Wertheim College of Engineering at the University of Florida.

Last summer, I was a research associate at The Topos Institute.

I graduated with my Bachelor's in Computer Science from the University of Kentucky in 2021, *summa cum laude*.

My advisor here in Gainesville is Dr. James Fairbanks of the GATAS Lab.

My Current Research Involves:

- Applied Category Theory
- Opinion Dynamics
- Multiphysics Simulations
- High Performance Computing
- Space Weather