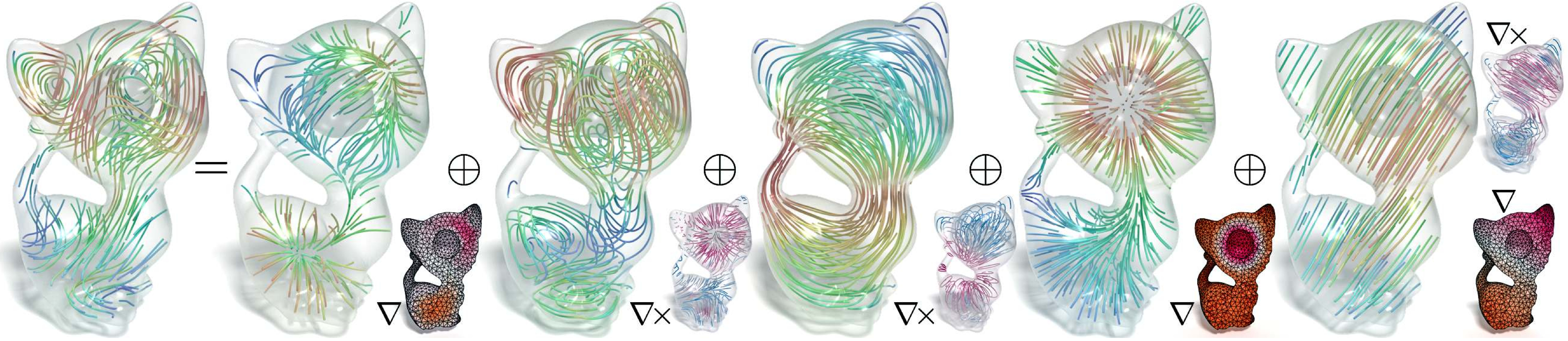
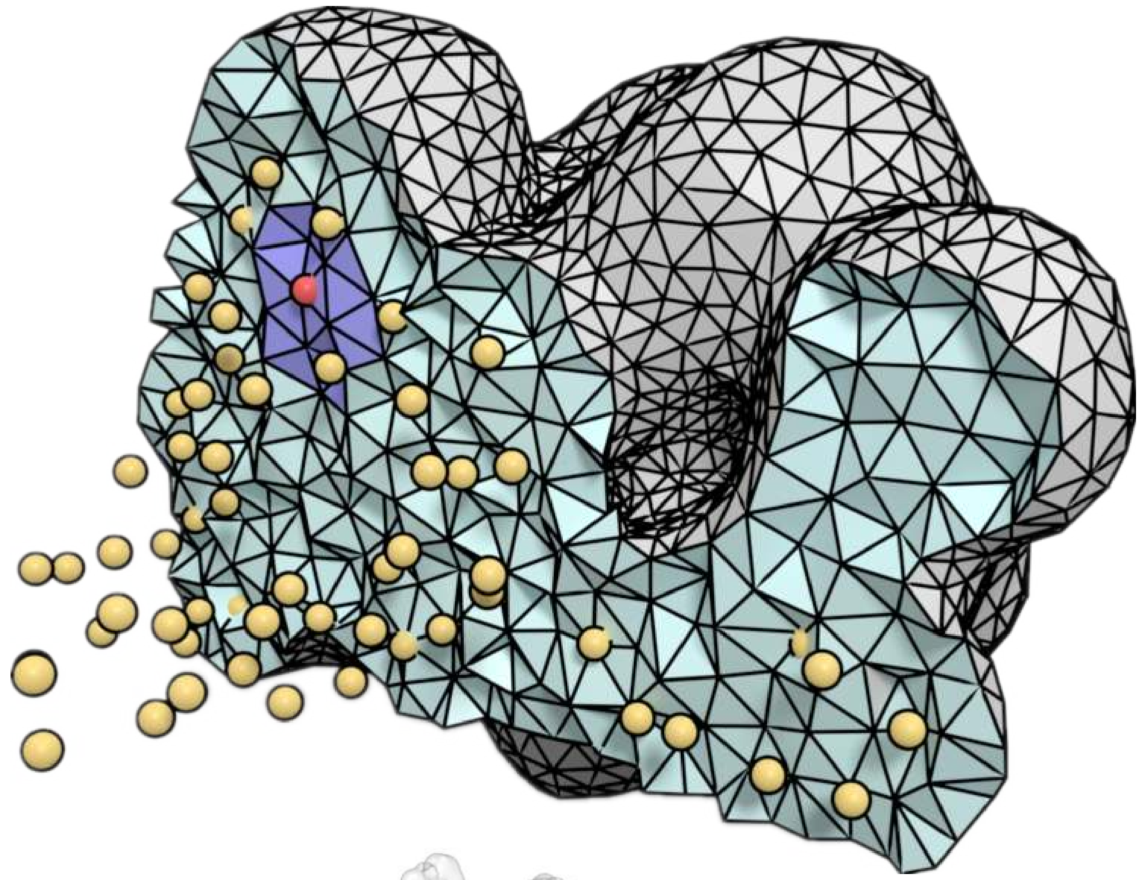
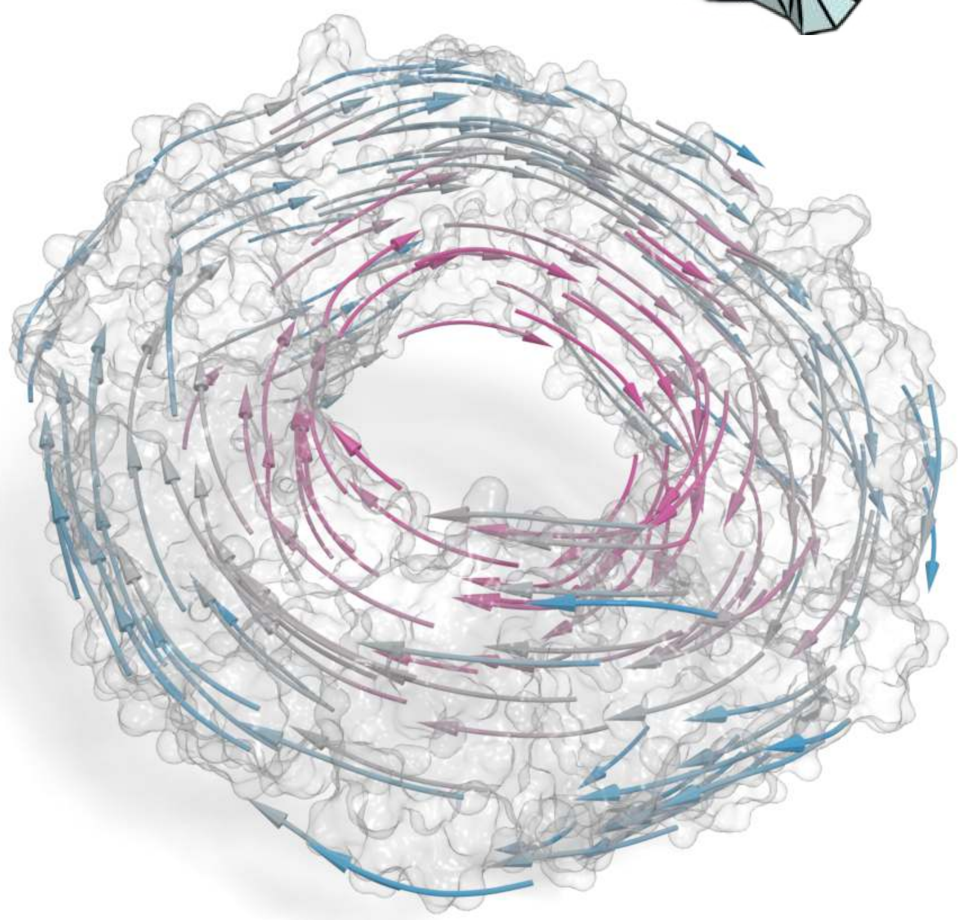


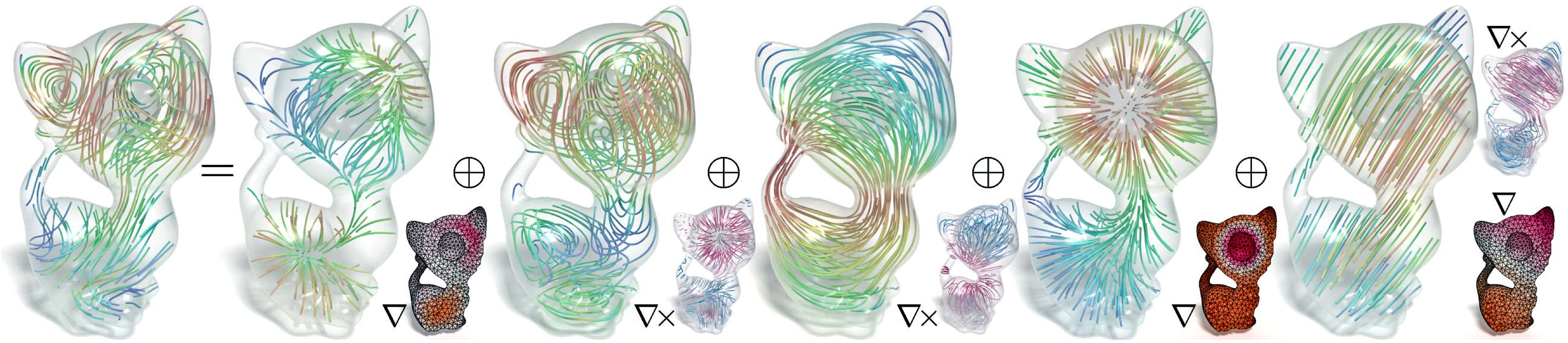
# Discrete de Rham-Hodge Theory and Applications on Geometry & Topology Analysis of Biological Macromolecules





**Jiahui Chen, Rundong Zhao, Yiying Tong, and Guo-Wei Wei**

MICHIGAN STATE UNIVERSITY



# Section I: Overview

# Motivation

- Describing and understanding 3D shapes!

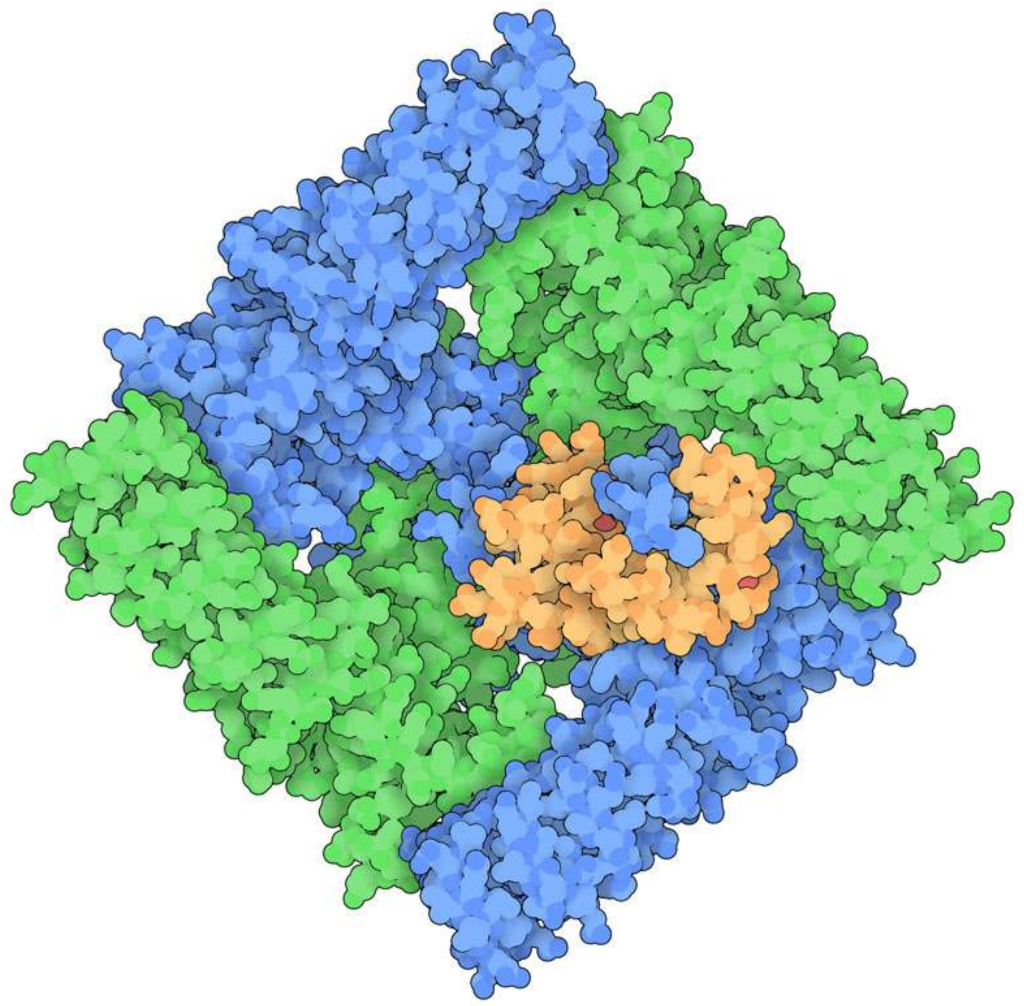
It has 2 major parts, head and body!

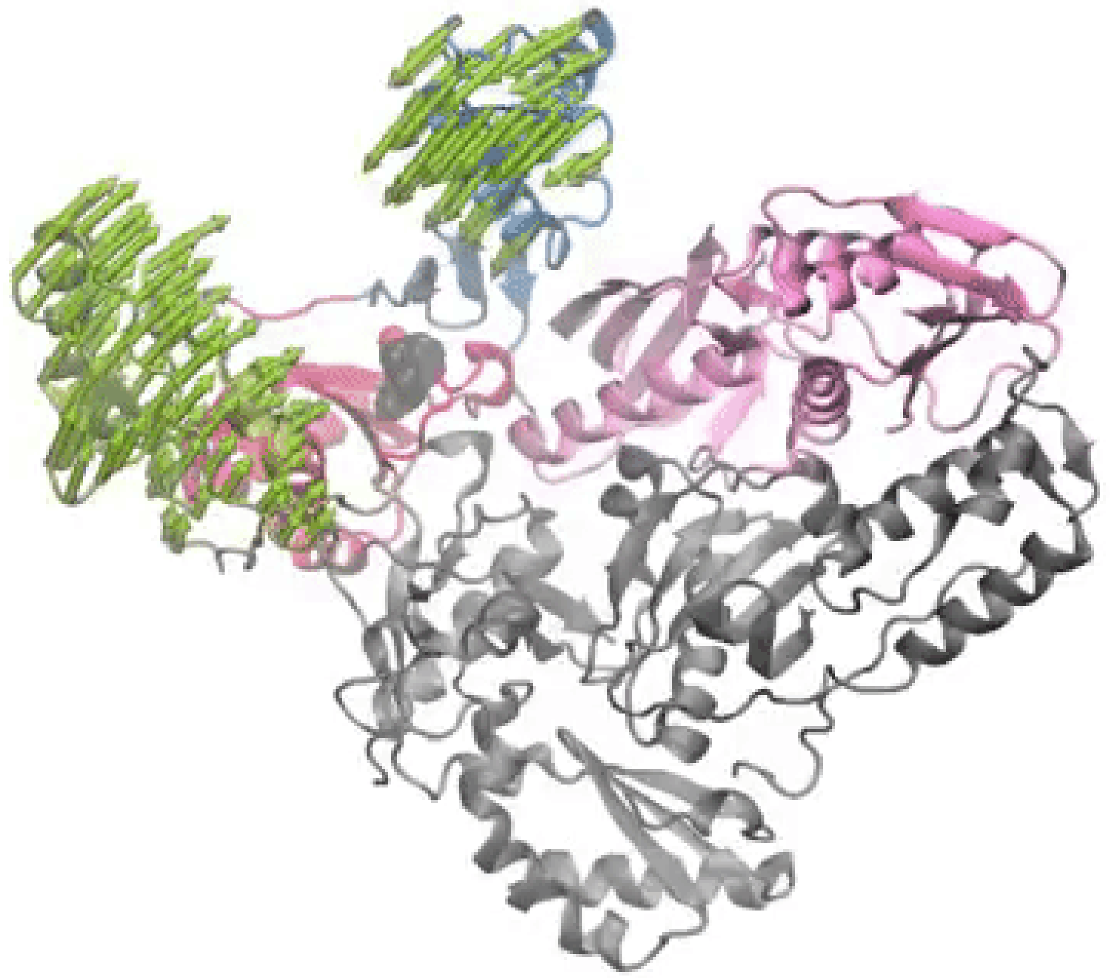
It also has 2 ears!

There is a handle we can grab!

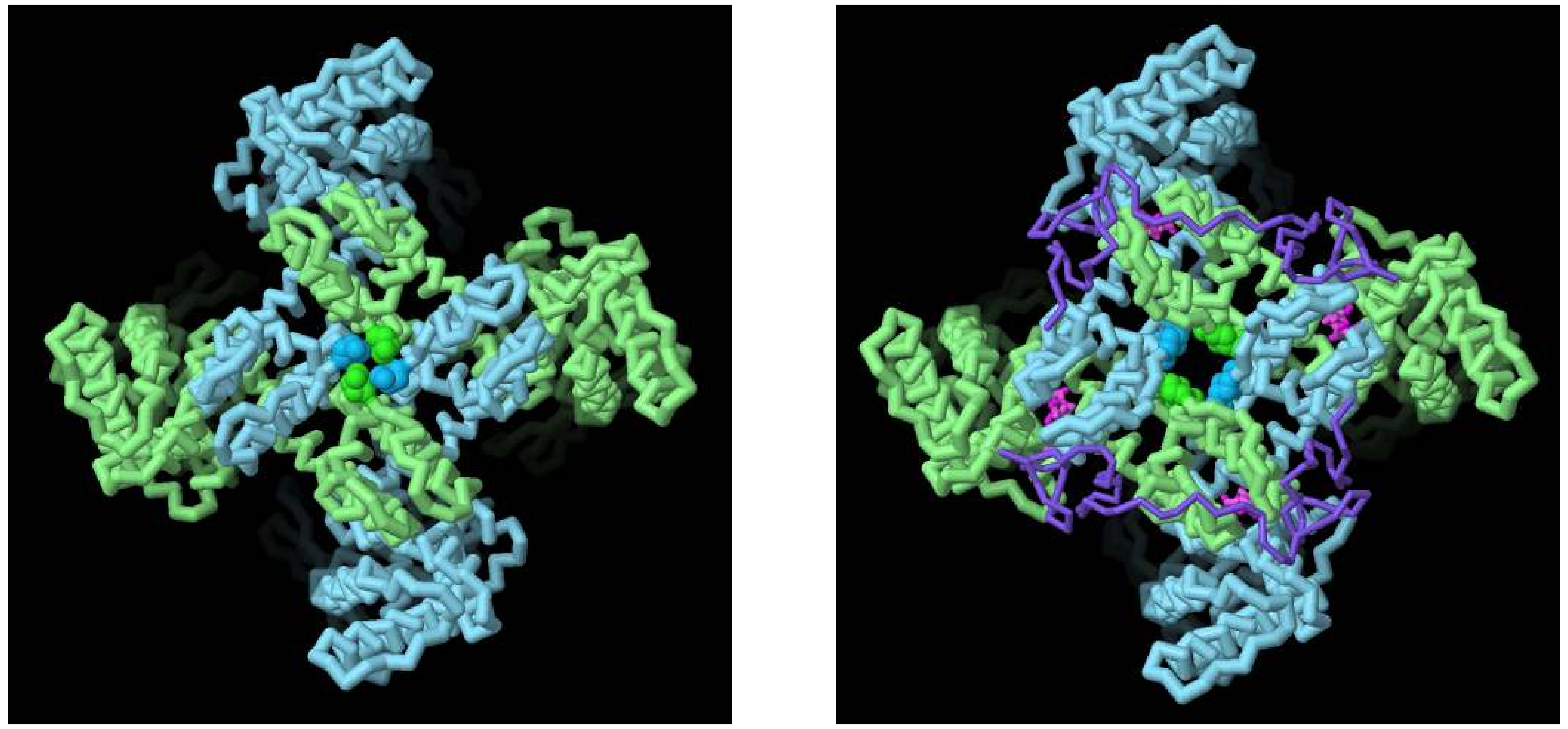
# Motivation

- Describing and understanding 3D shapes!

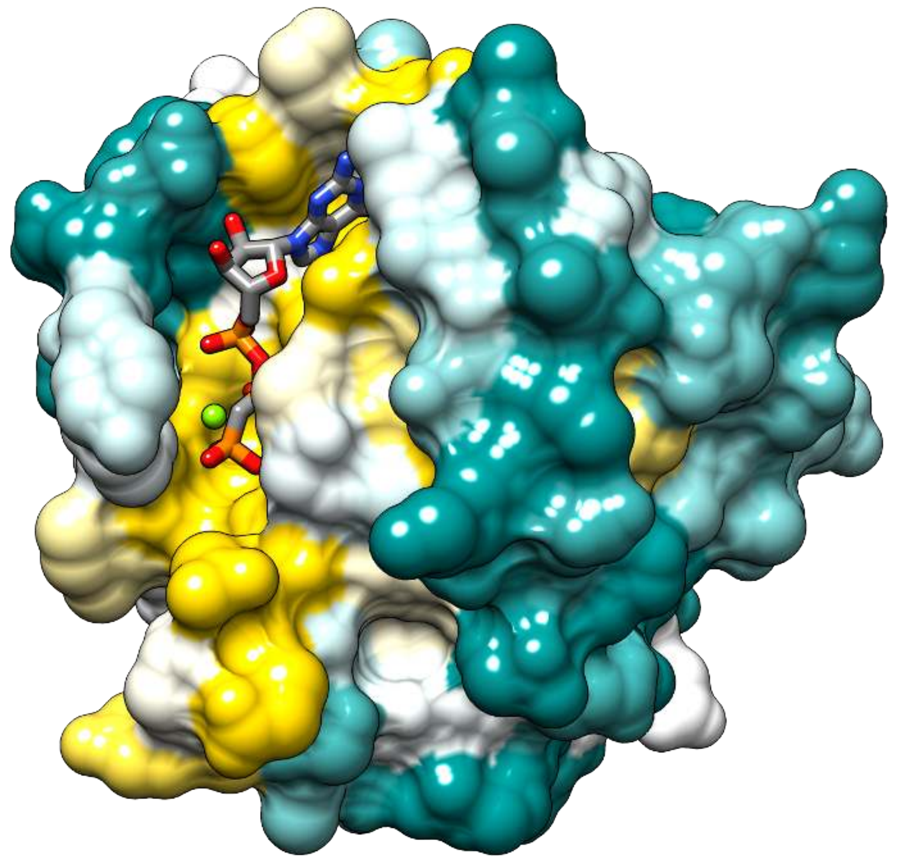




[Bakan et. al. 2011]



[Hughes et. al. 2018]



[Finn et. al. 2008]

# Challenges

- 3D shapes are intrinsically hard to describe.
- 3D shape descriptions are usually ad hoc for specific settings, or even hand crafted.
- There are no approaches to extract both geometry and topology features in a consistent way.

It has 2 major parts, head and body!
It also has 2 ears!
There is a handle we can grab!

Can we get those information with only one shot?

# The Cure

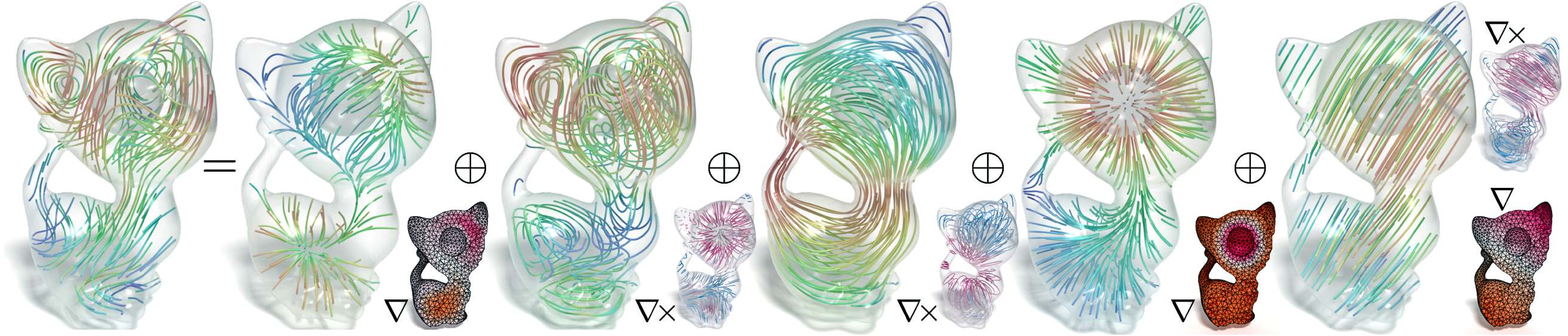
## The de Rham-Hodge Theory

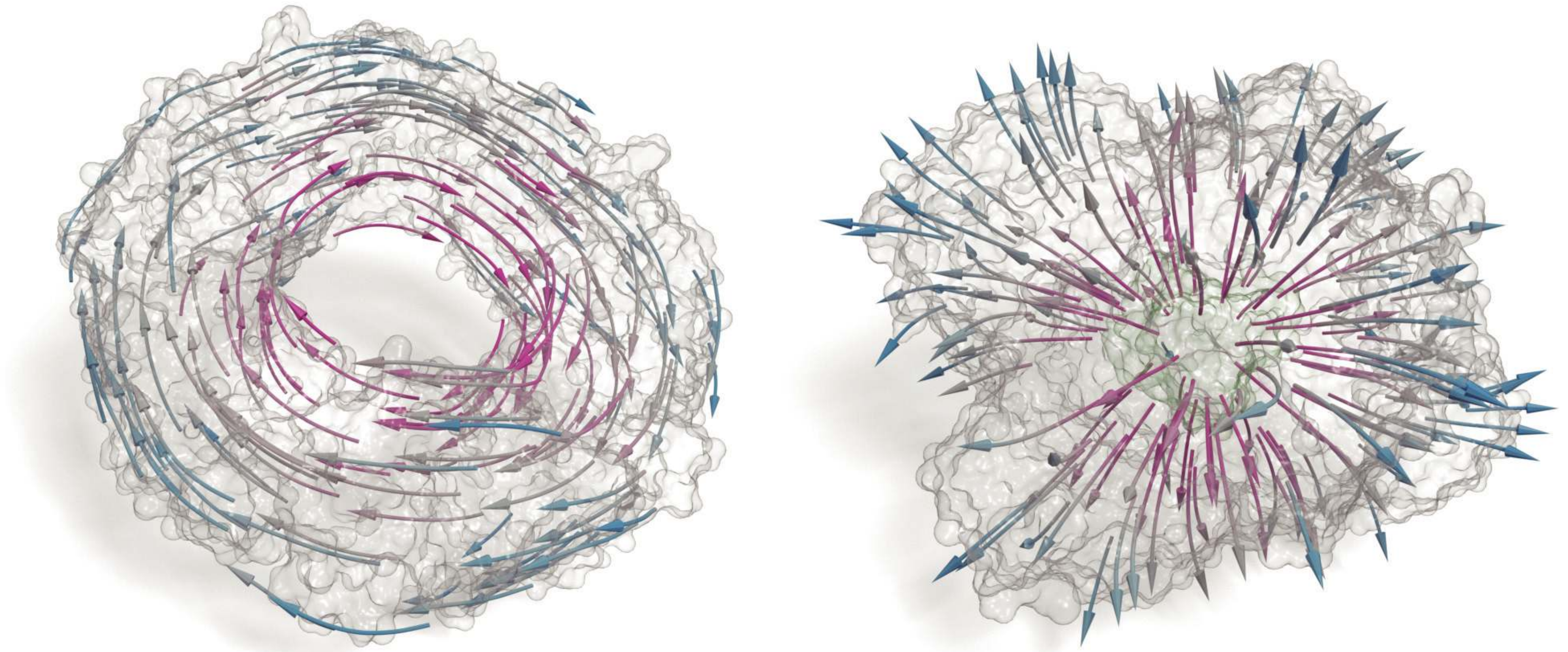
*In retrospect it is clear that the technical difficulties in the existence theorem did not really require any significant new ideas, but merely a careful extension of classical methods.*

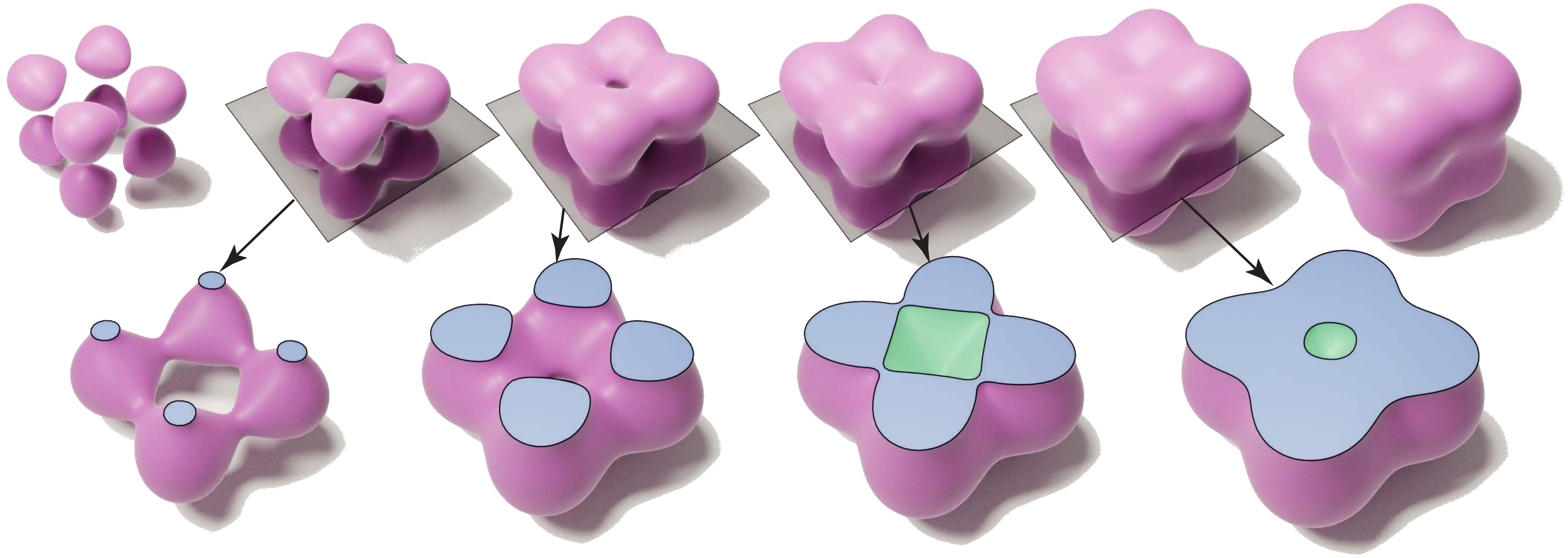
- William Vallance Douglas Hodge

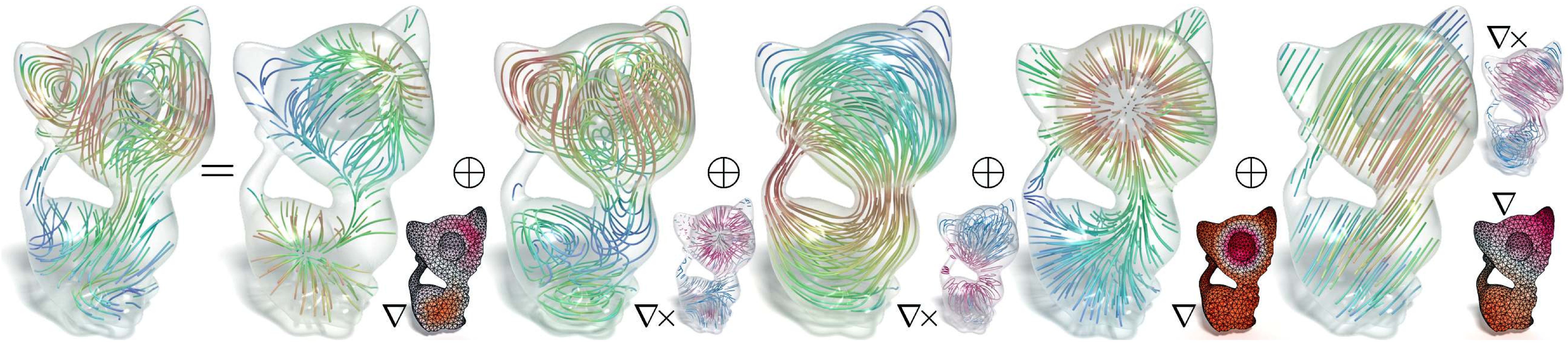
# Contribution

- Discrete de Rham-Hodge Theory by Hodge Decomposition
- Geometry and Topology Analysis for Biological Macromolecules
- Evolutionary de Rham-Hodge Method



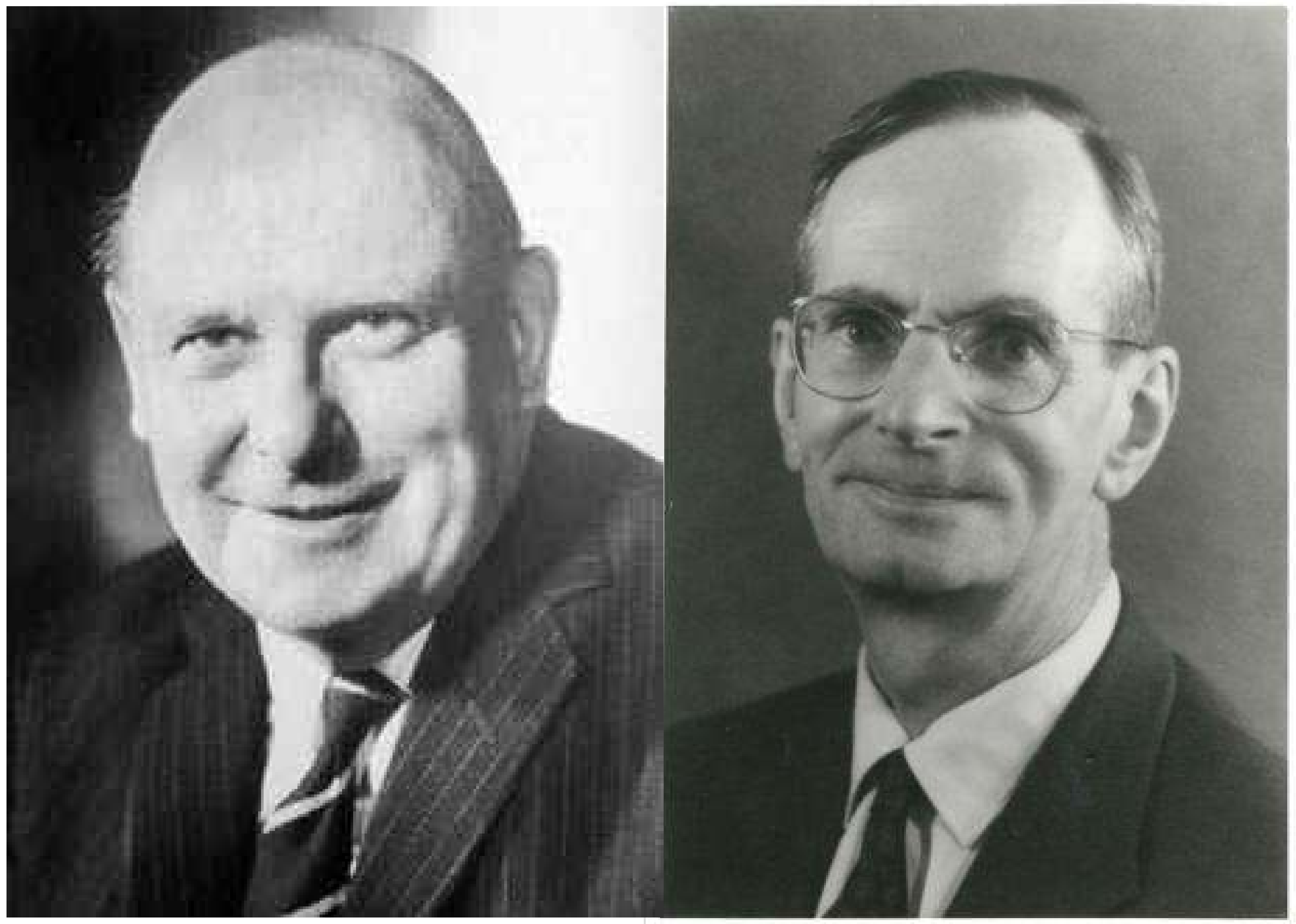





# Section II:
# Discrete de Rham-Hodge Theory

# History of de Rham-Hodge Theory

Every cohomology class has a canonical representative, a differential form which vanishes under the Laplacian operator.



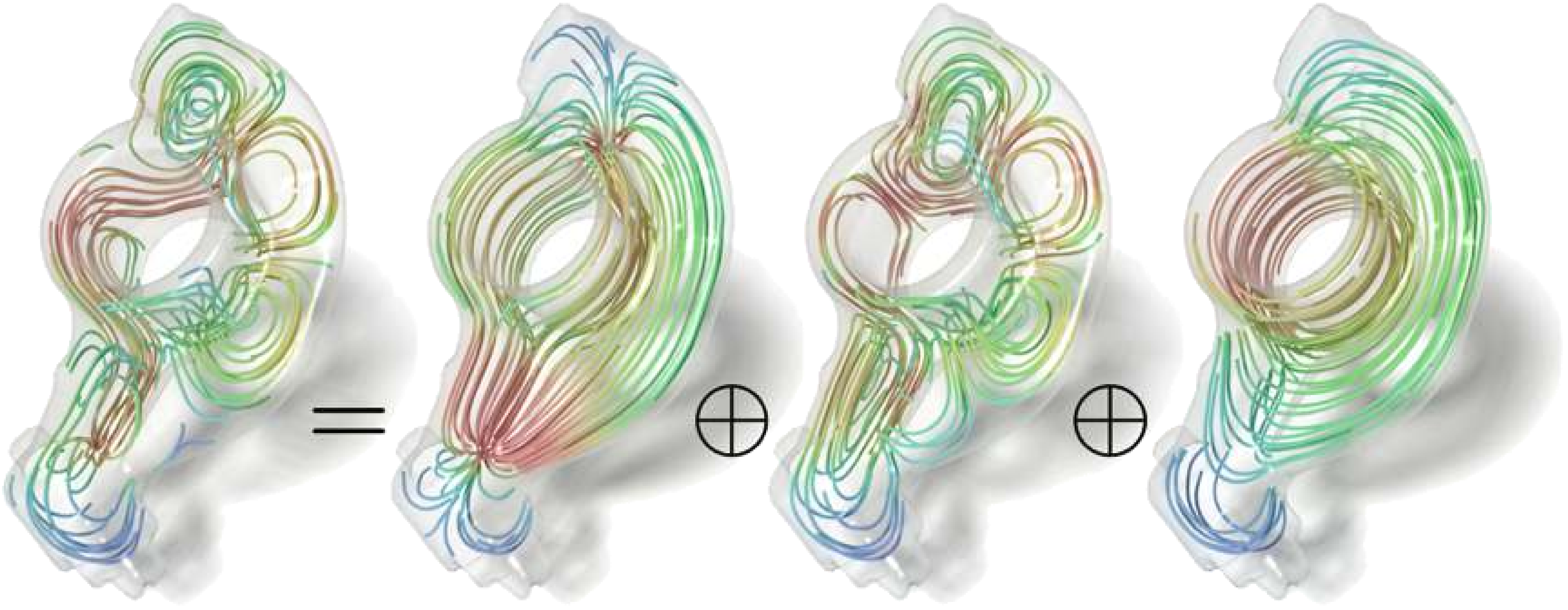
V. W. D. Hodge　　George de Rham

Handle ⟷ Harmonic vector field

# Hodge Decomposition

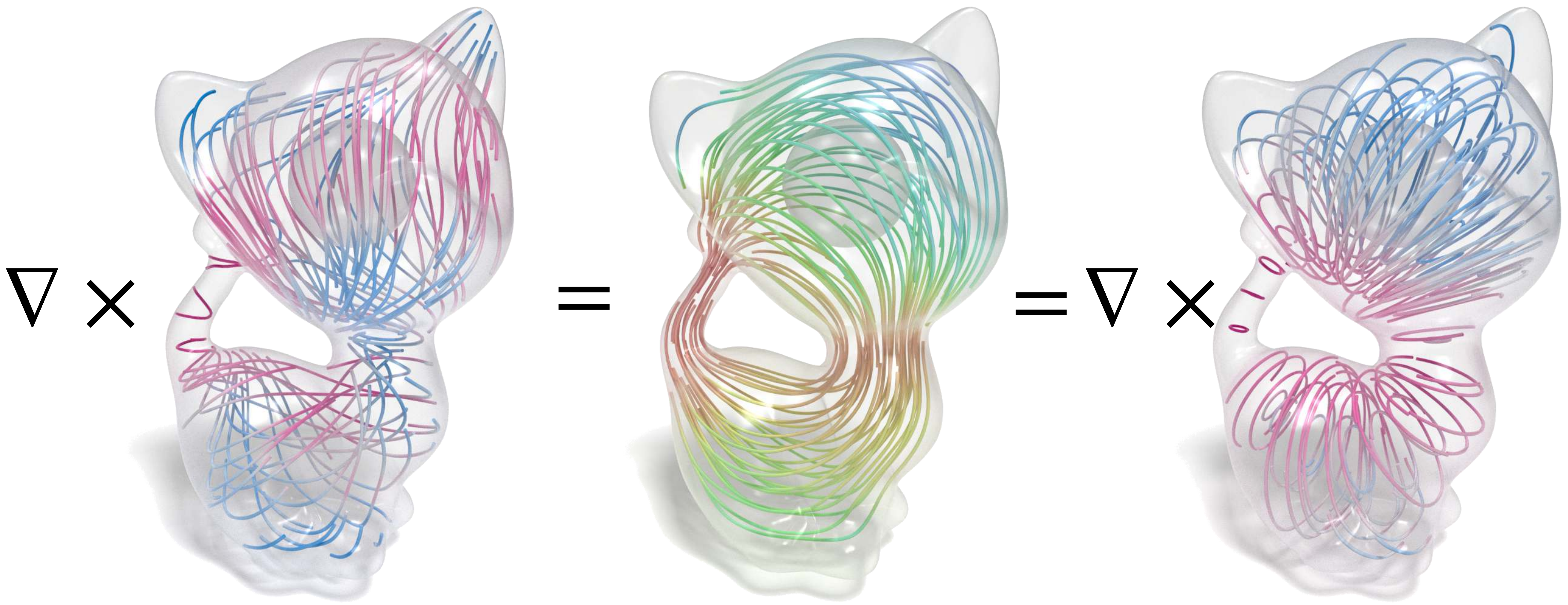
- The heart of de Rham-Hodge theory

- Fundamental in static and dynamical problems
- Need rigorous computational treatment
- 3D domain with arbitrary topology
- Numerical issues from failure to capture proper topology

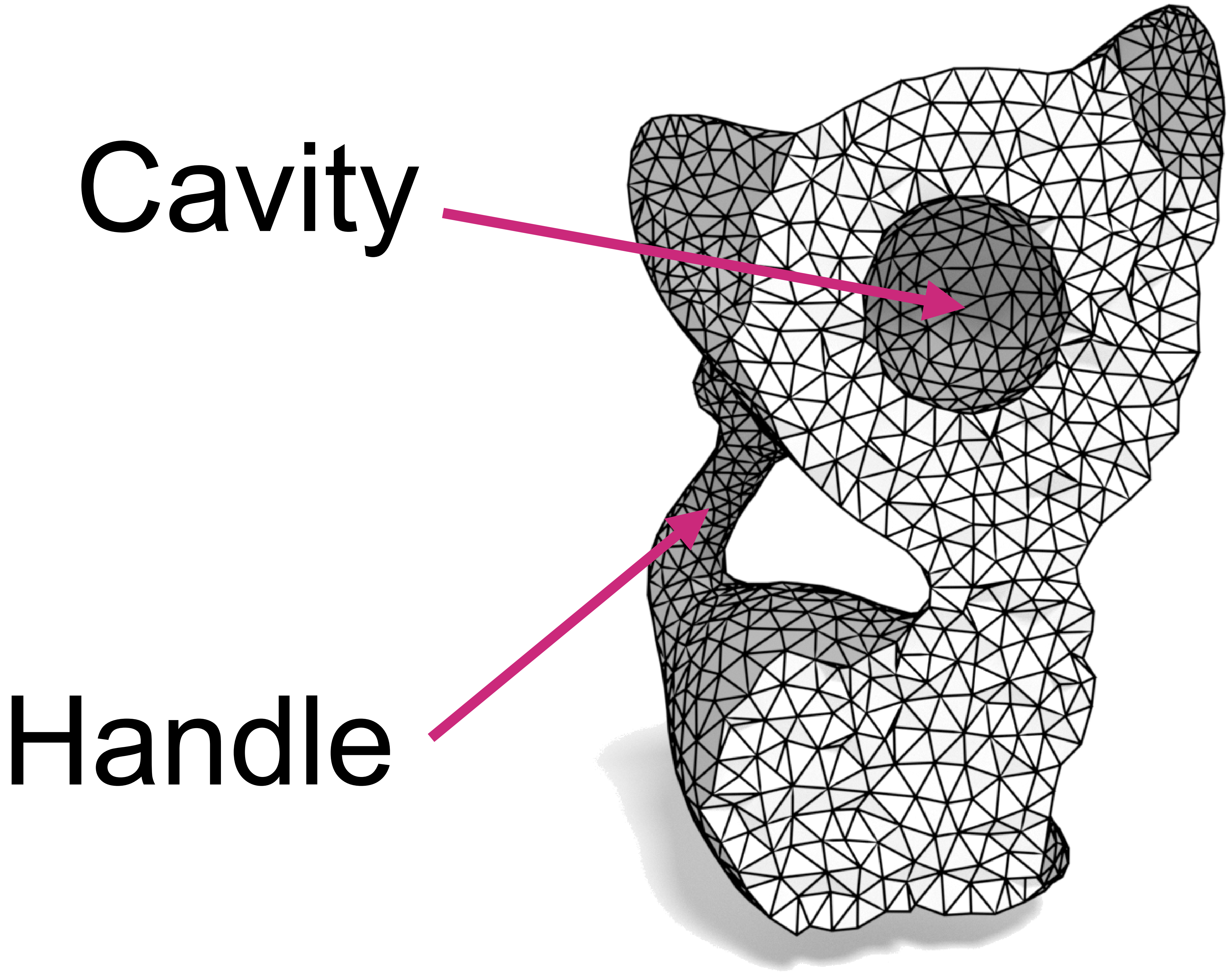


# Previous work - 3D decomposition

- Mathematical Foundation [Hodge 1941] [Shonkwiler 2009]
- A proof of existence [Cantarella et. al. 2002]
  Lack of computational treatment
- A variational approach [Tong et. al. 2003]
  Wrong dimensionality of harmonic space



# Hodge-Morrey-Friedrichs Decomposition

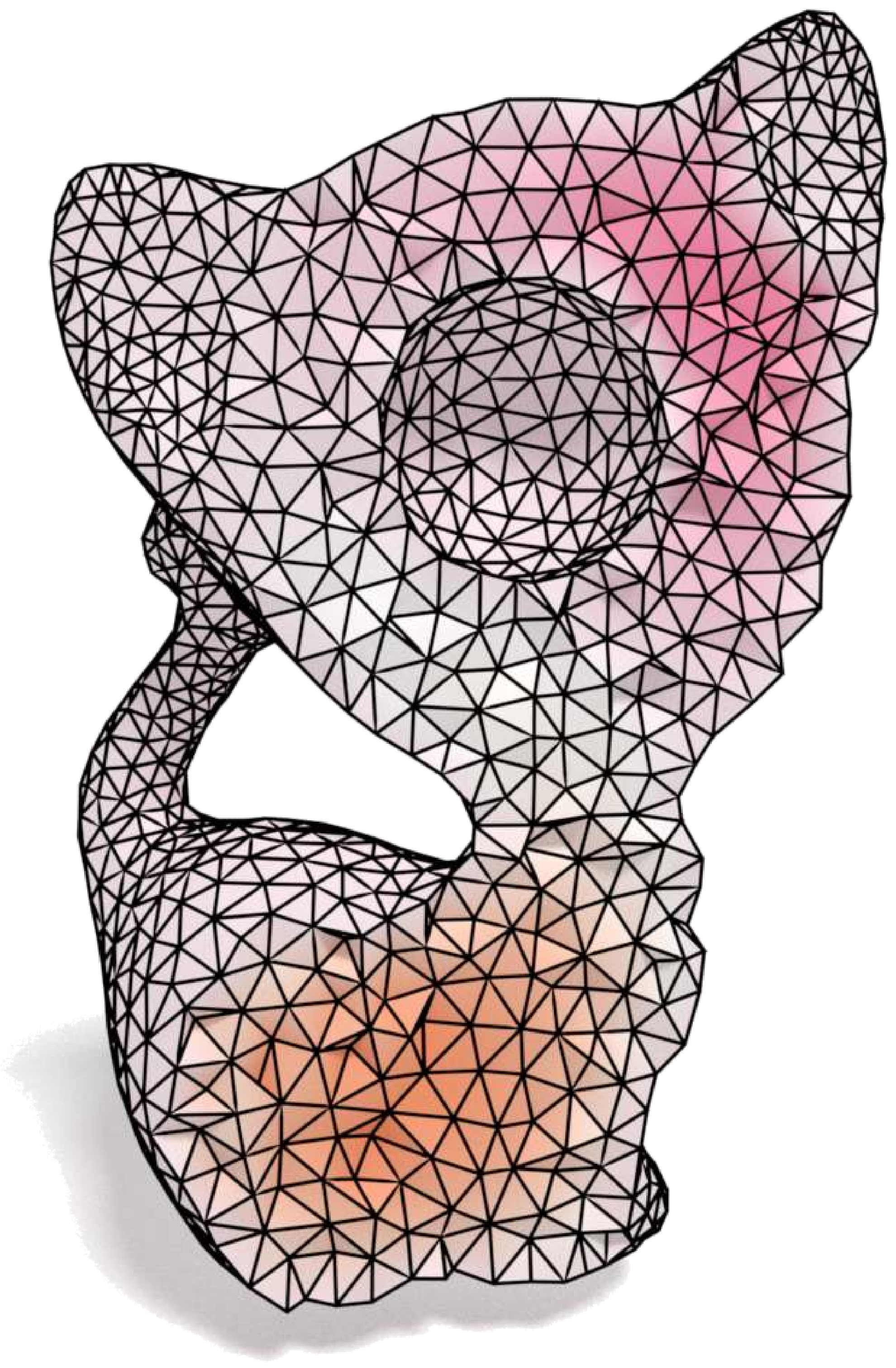



# Hodge-Morrey-Friedrichs Decomposition

$$V = NG \oplus \ldots$$

Normal Gradient Field

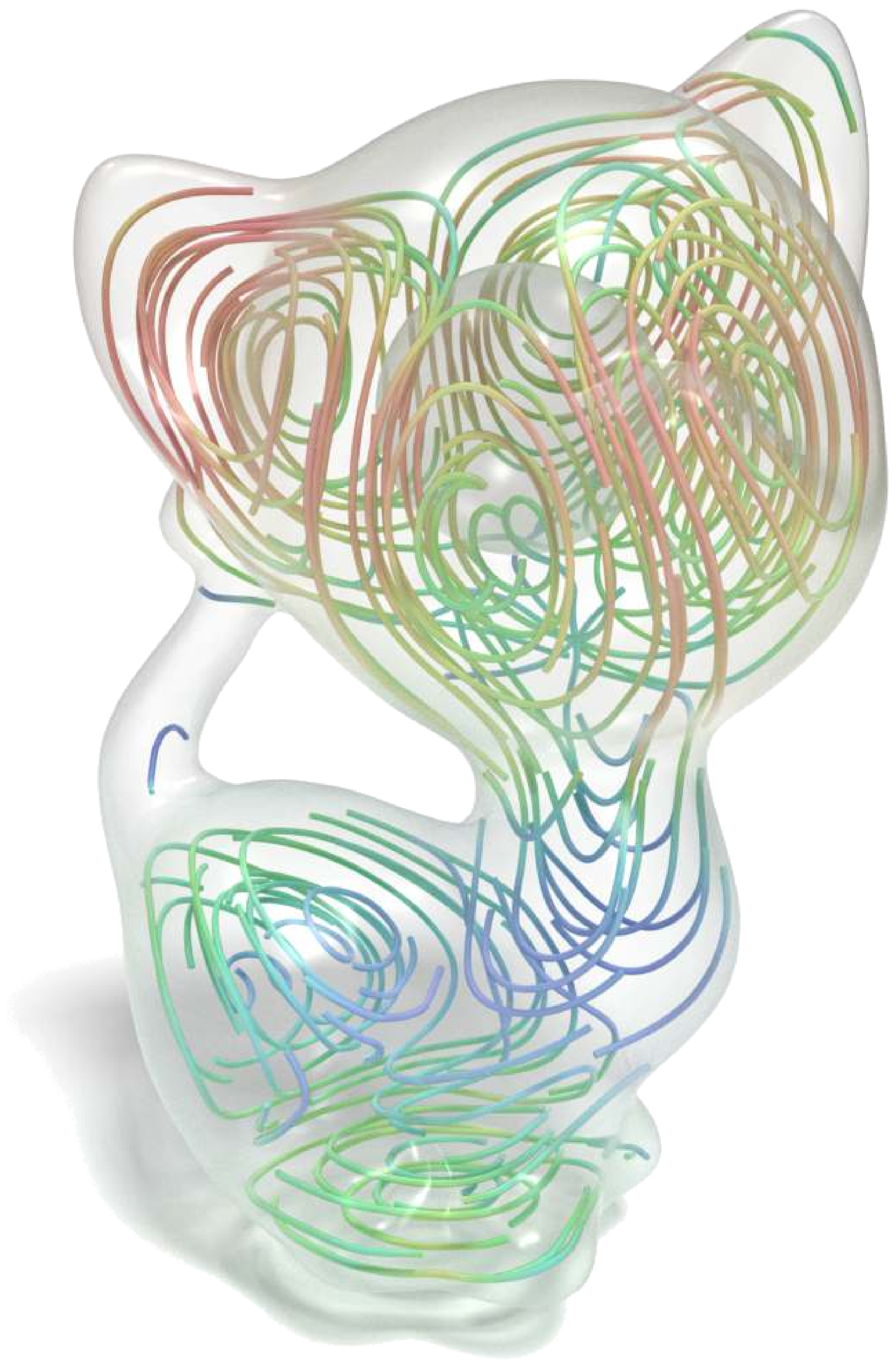
$$= \nabla$$



# Hodge-Morrey-Friedrichs Decomposition

$$V = NG \oplus TC \oplus \ldots$$

Tangential Curl Field



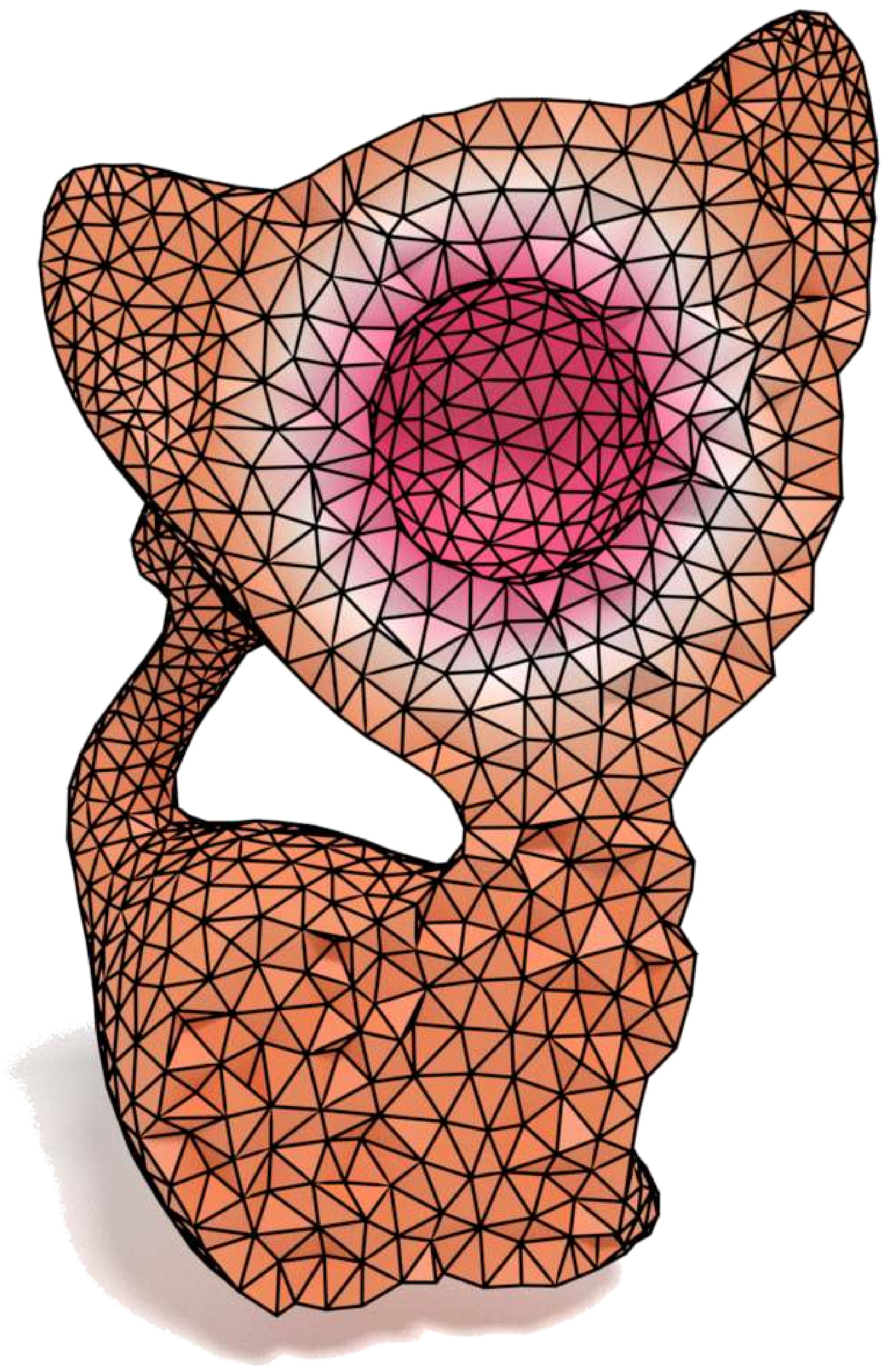
$$= \nabla \times$$

# Hodge-Morrey-Friedrichs Decomposition

$$V = NG \oplus TC \oplus NH \oplus \ldots$$

Normal Harmonic Field

$$= \nabla$$



# Hodge-Morrey-Friedrichs Decomposition

$$V = NG \oplus TC \oplus NH \oplus TH \oplus \ldots$$

Tangential Harmonic Field

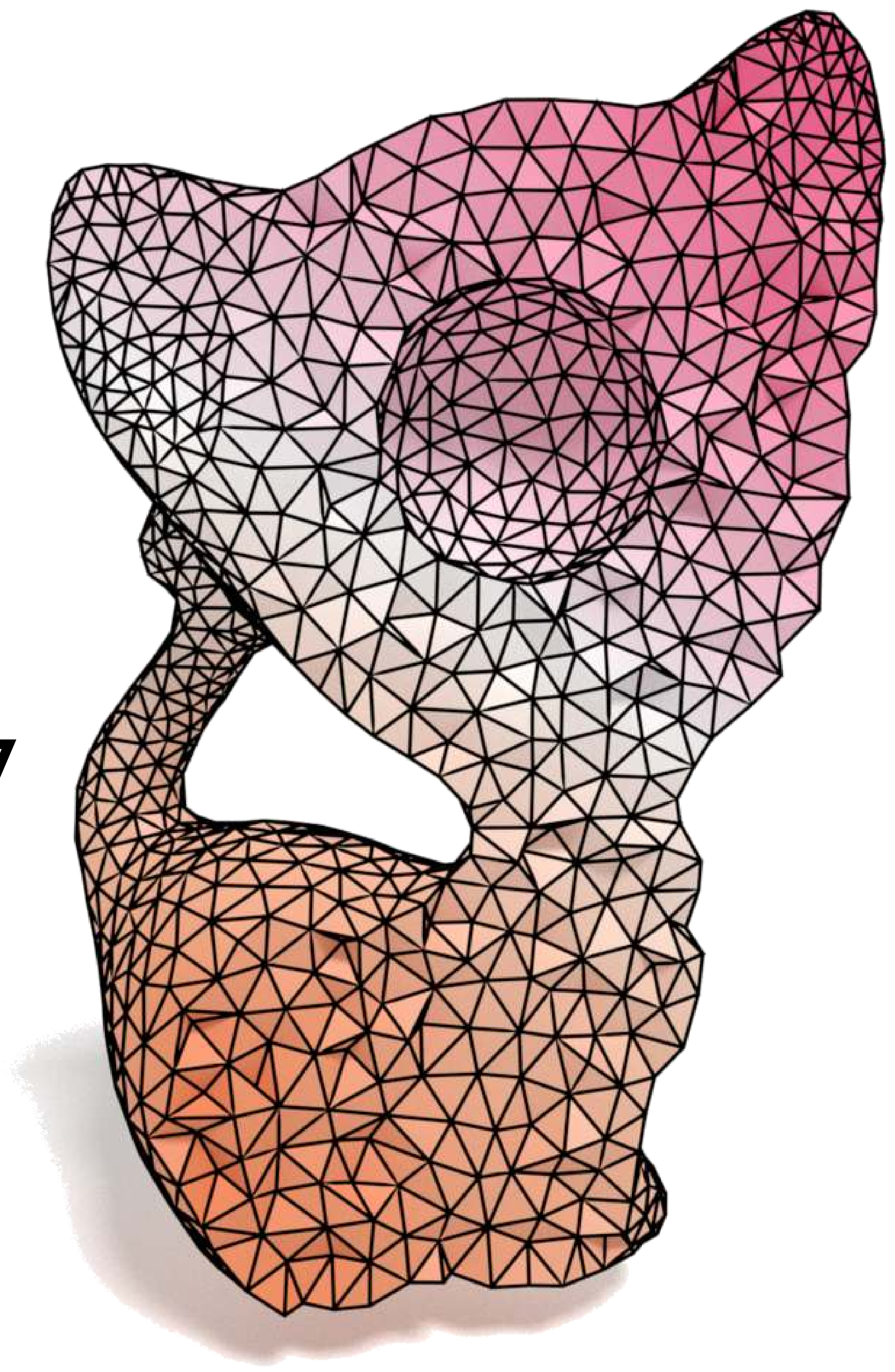
$$= \nabla \times$$

# Hodge-Morrey-Friedrichs Decomposition

$$V = NG \oplus TC \oplus NH \oplus TH \oplus CH$$

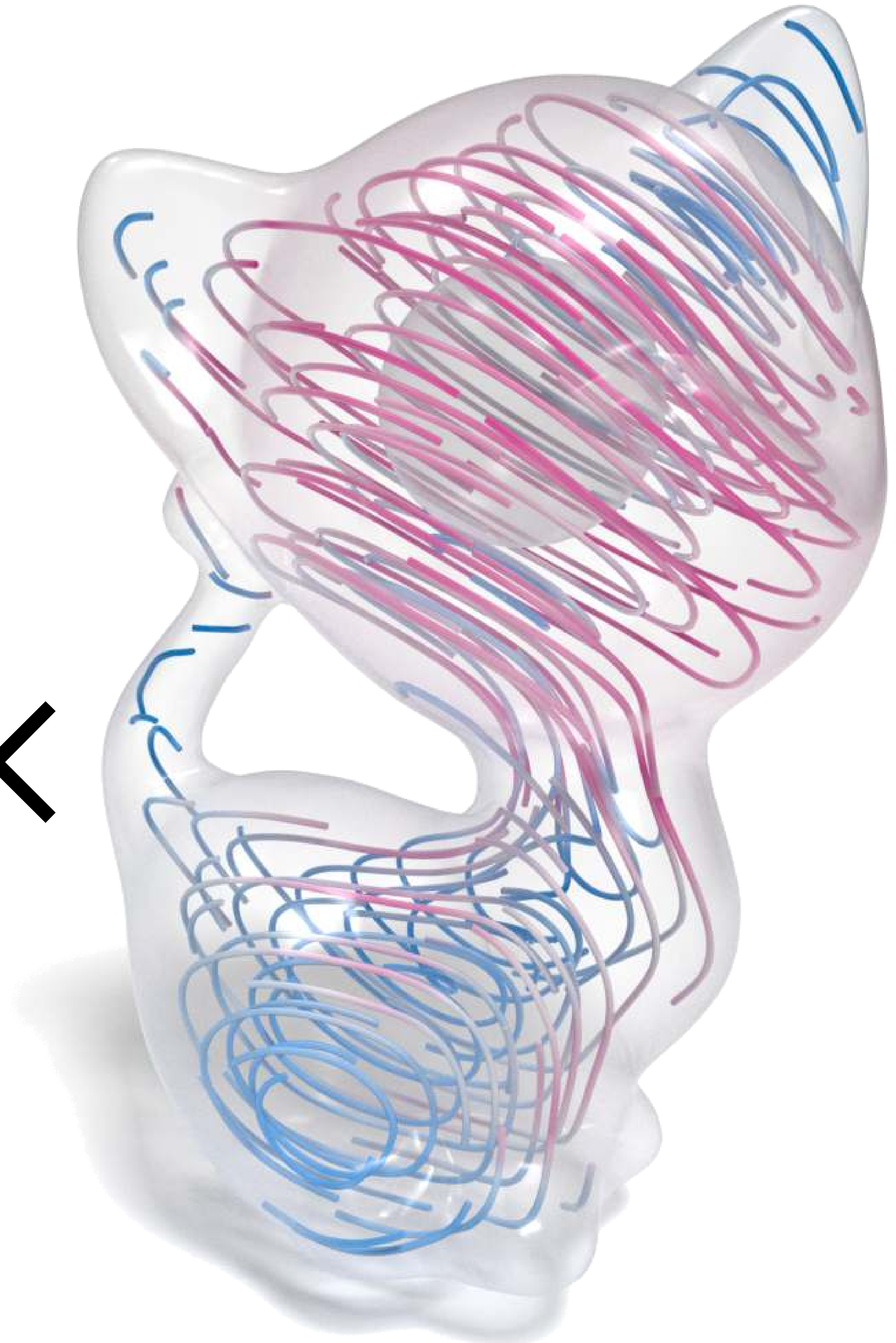
Central Harmonic Field

$\nabla$



$=$

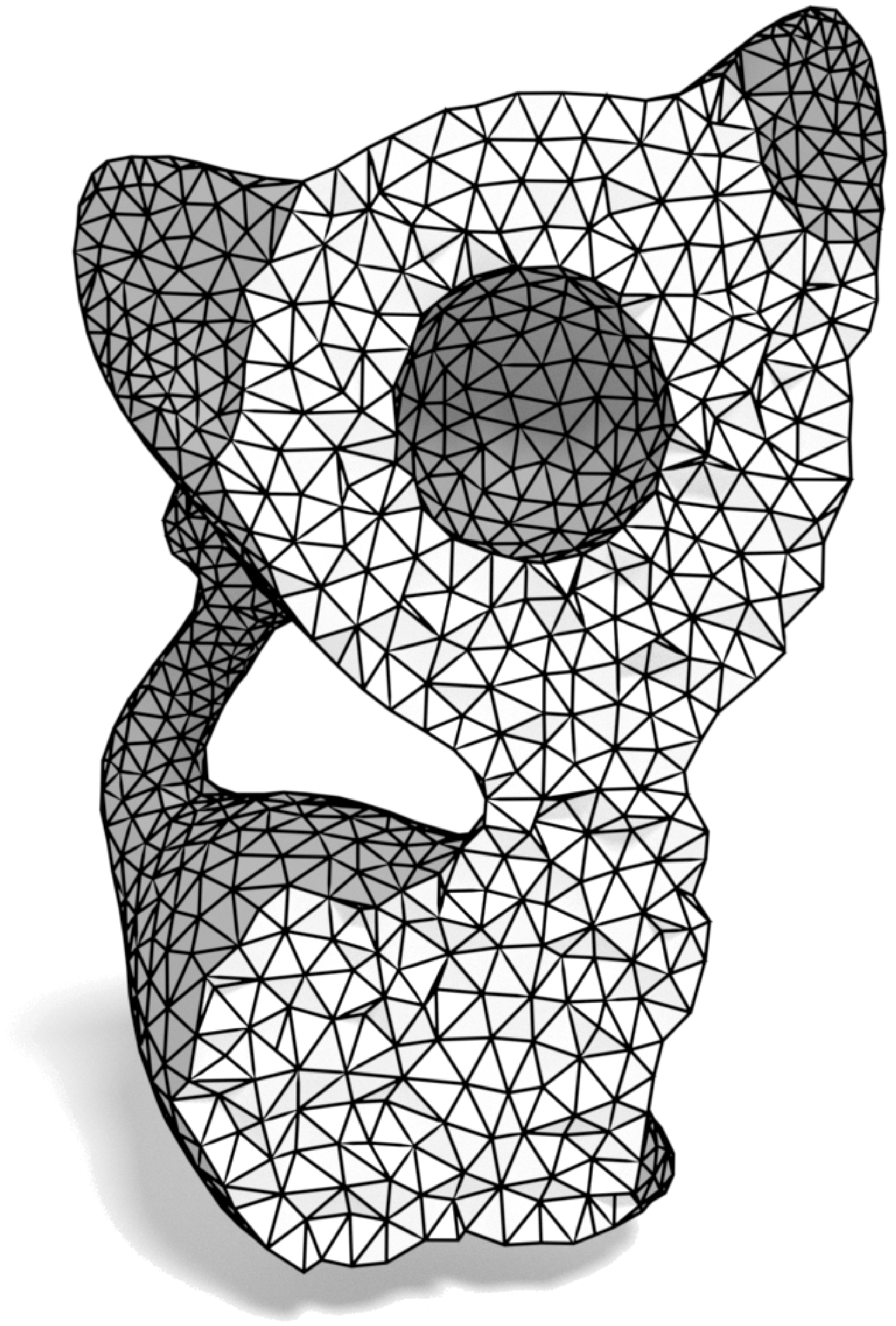
$= \nabla \times$

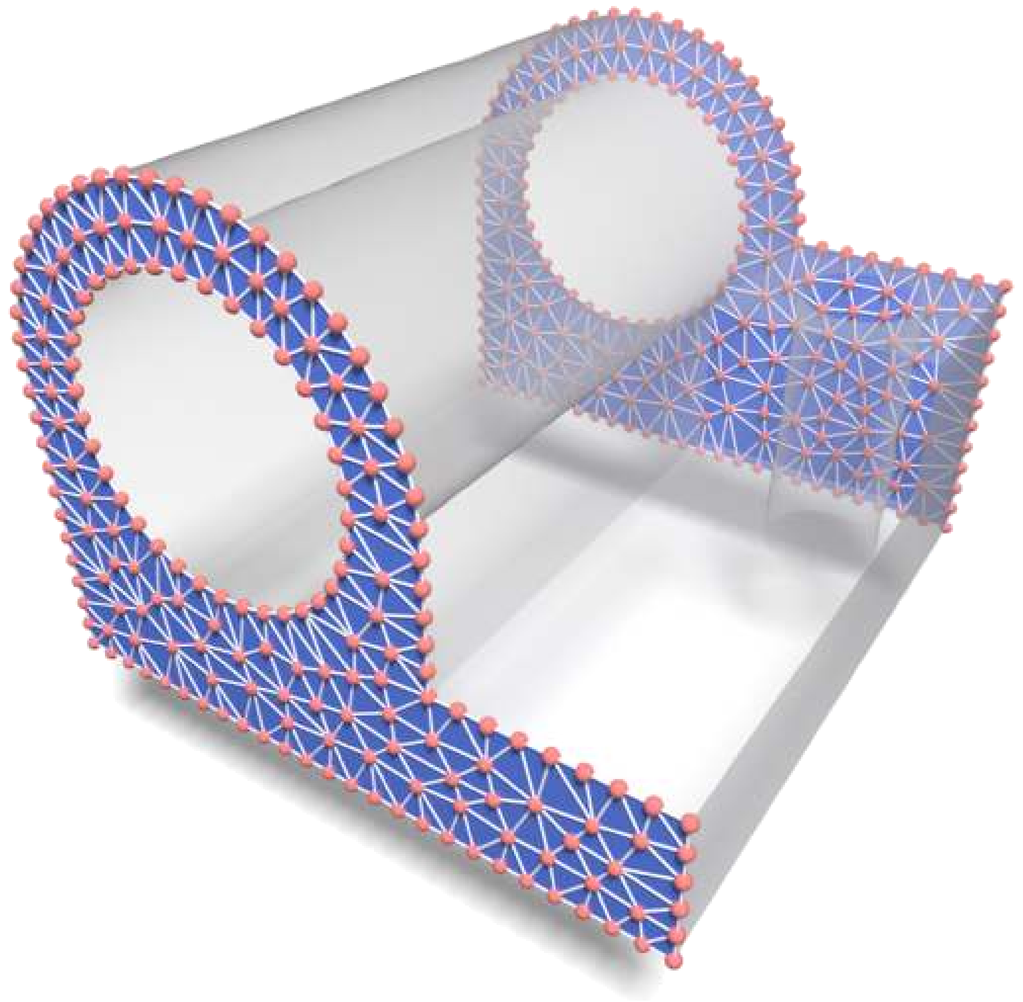


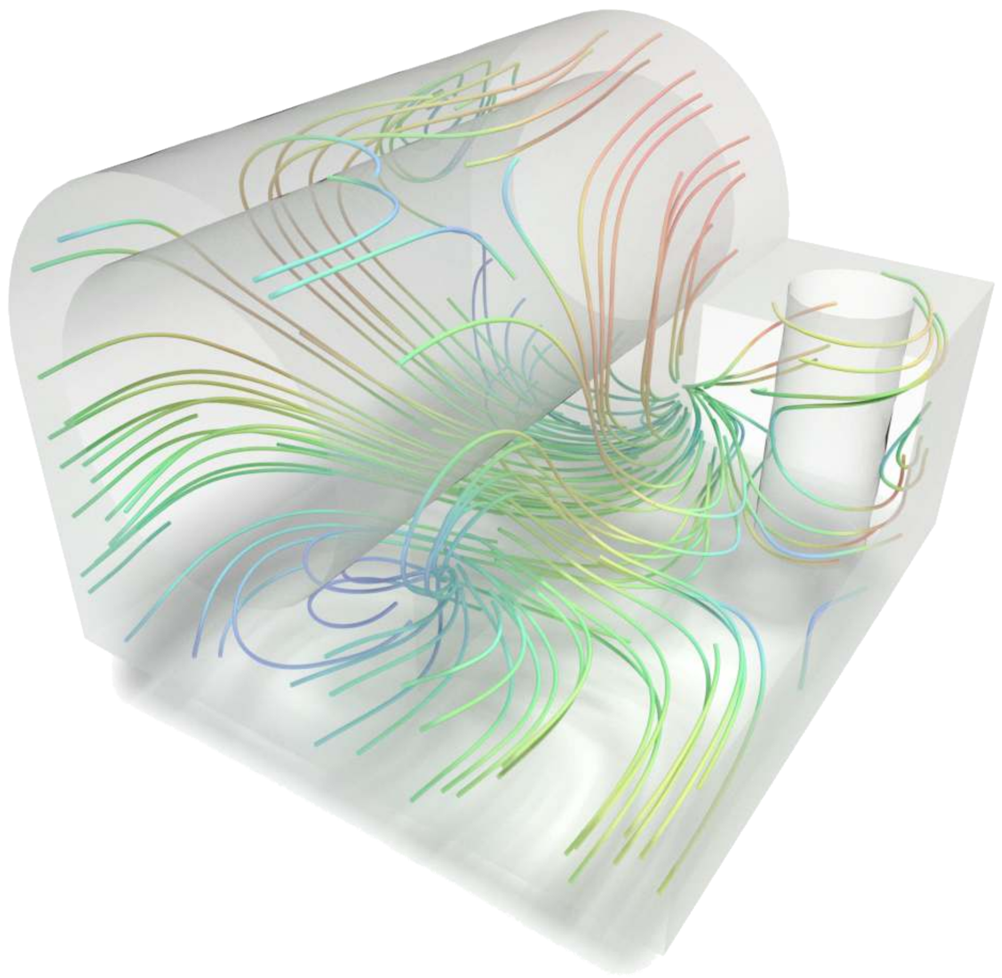
# Contributions at a Glance

- Discrete Exterior Calculus (DEC)-based
- Proper Boundary Condition for 3-Manifold
- Correct Harmonic Space (Cohomology)
- Mixed Boundary Condition
- High Order Basis

Inclusion/exclusion of boundary elements







# Differential Form

- Vector calculus independent of coordinates
- A unified definition of integrands.

0-Form ⟷ Scalar Field

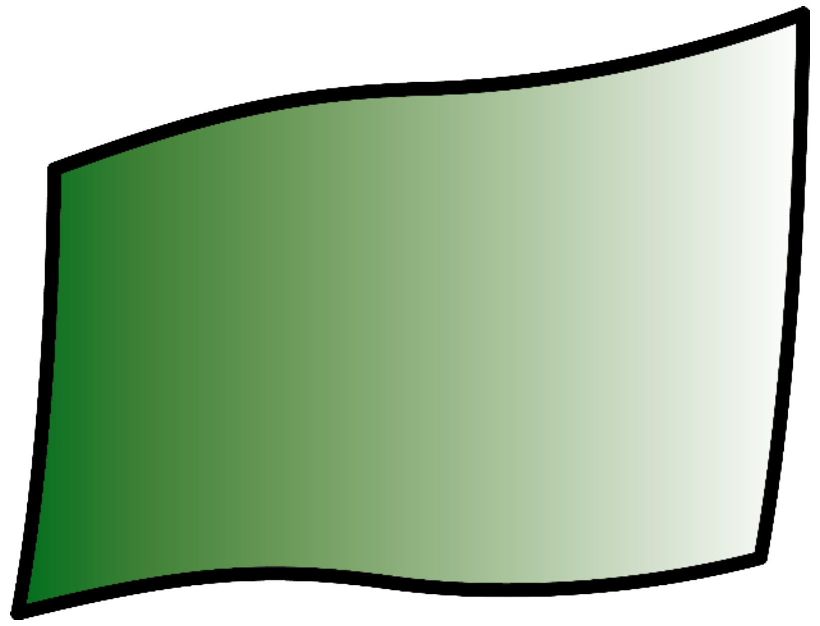
1-Form ⟷ Vector Field

2-Form ⟷ Vector Field

3-Form ⟷ Scalar Field

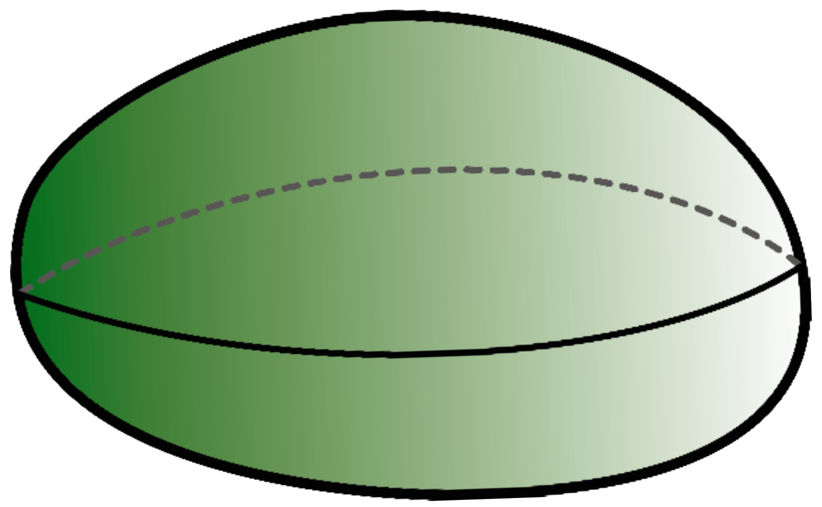
$$\int_L \boldsymbol{v} \cdot d\boldsymbol{L}$$

1-Form



$$\int_S \boldsymbol{v} \cdot d\boldsymbol{S}$$

2-Form



$$\int_V f dV$$

3-Form

# Operators

- Exterior Derivative $d^k$
- Hodge Star $\star^k$
- Codifferential $\delta^k = (-1)^{n(k-1)+1} \star^{n-k+1} d^{n-k} \star^k$

$$\begin{tikzcd}
\text{0-Form} \arrow[r, "d^0", "\nabla"'] & \text{1-Form} \arrow[r, "d^1", "\nabla\times"'] \arrow[l, bend left=60, "\delta^1", "\nabla\cdot"'] & \text{2-Form} \arrow[r, "d^2", "\nabla\cdot"'] \arrow[l, bend left=60, "\delta^2", "\nabla\times"'] & \text{3-Form} \arrow[l, bend left=60, "\delta^3", "\nabla"']
\end{tikzcd}$$

# Operators

- Exterior Derivative $d^k$
- Hodge Star $\star^k$
- Codifferential $\delta^k = (-1)^{n(k-1)+1} \star^{n-k+1} d^{n-k} \star^k$
- Laplacian $\Delta^k = d^{k-1}\delta^k + \delta^{k+1}d^k$

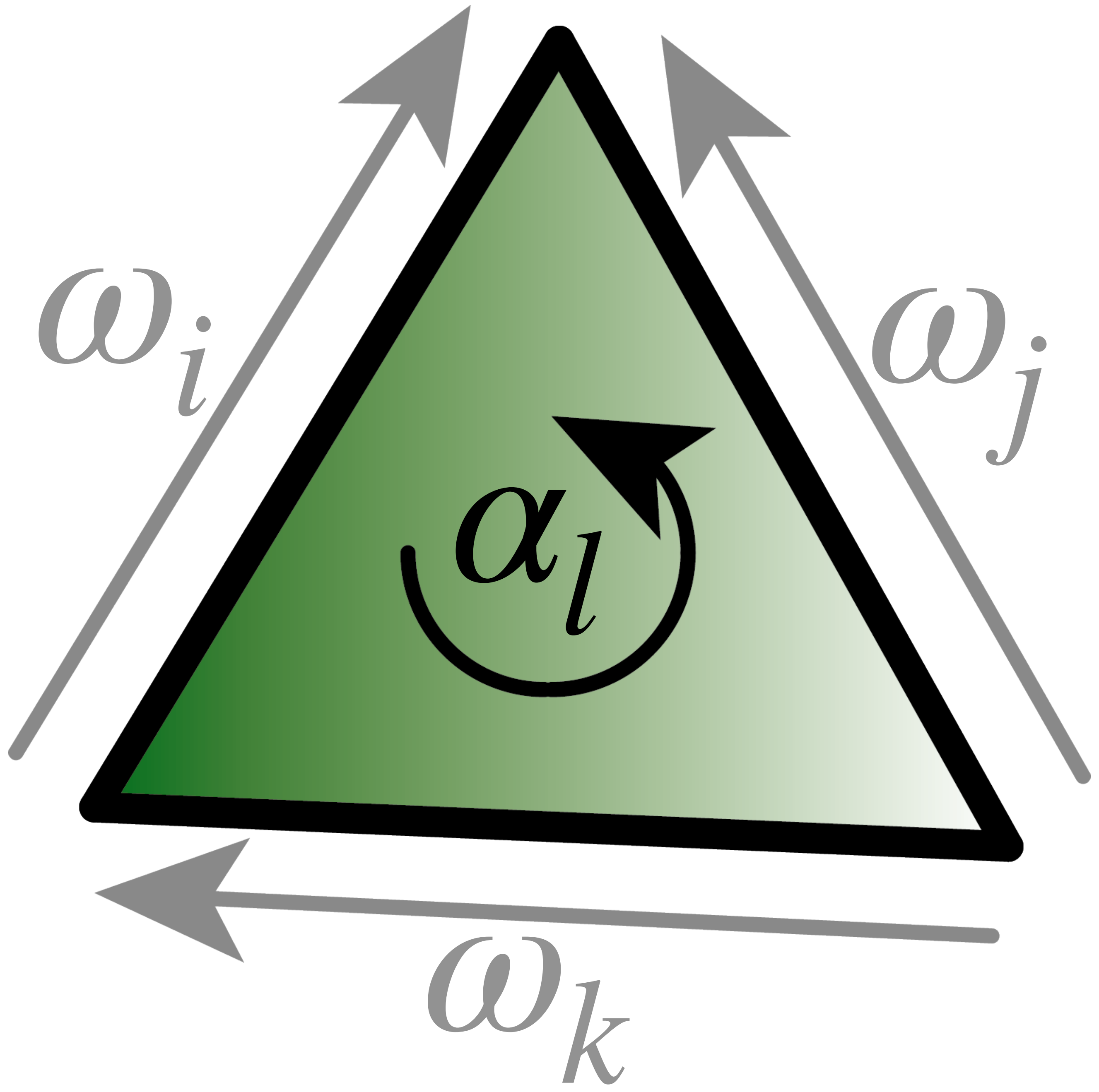
$$\begin{tikzcd}[column sep=huge]
\text{0-Form} \arrow[r, "d^0", "\nabla"'] & \text{1-Form} \arrow[r, "d^1", "\nabla\times"'] \arrow[l, bend left, "\nabla\cdot", "\delta^1"'] & \text{2-Form} \arrow[r, "d^2", "\nabla\cdot"'] \arrow[l, bend left, "\nabla\times", "\delta^2"'] & \text{3-Form} \arrow[l, bend left, "\nabla", "\delta^3"']
\end{tikzcd}$$

$$\Delta^1 = d^0\delta^1 + \delta^2 d^1$$

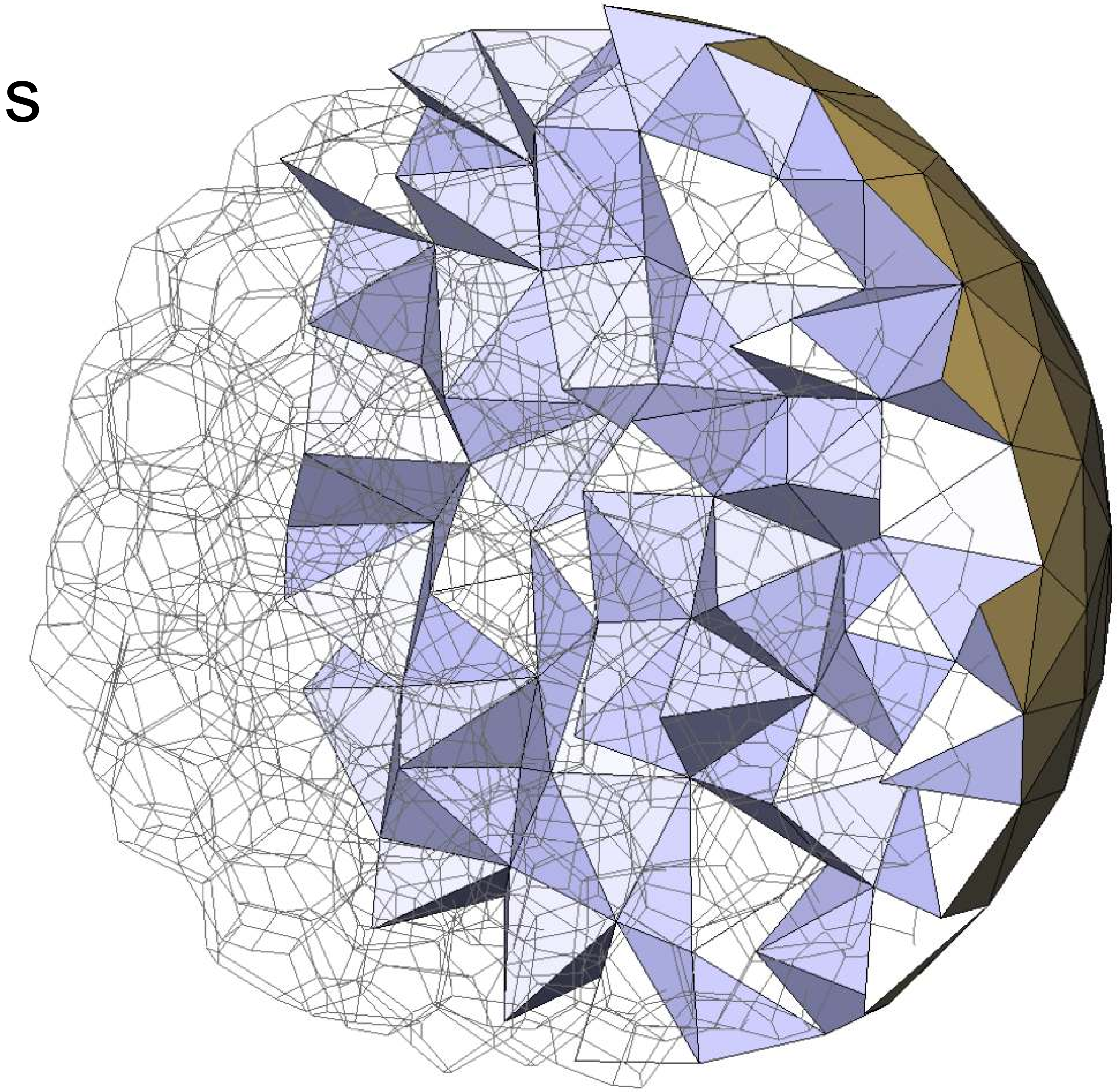
# Into the Discrete World

- Discrete forms are stored on SIMPLICES as column vectors.
- Discrete Exterior Derivative $D_k$

$D_1:$




$$\alpha_l = -\omega_i - \omega_k + \omega_j$$

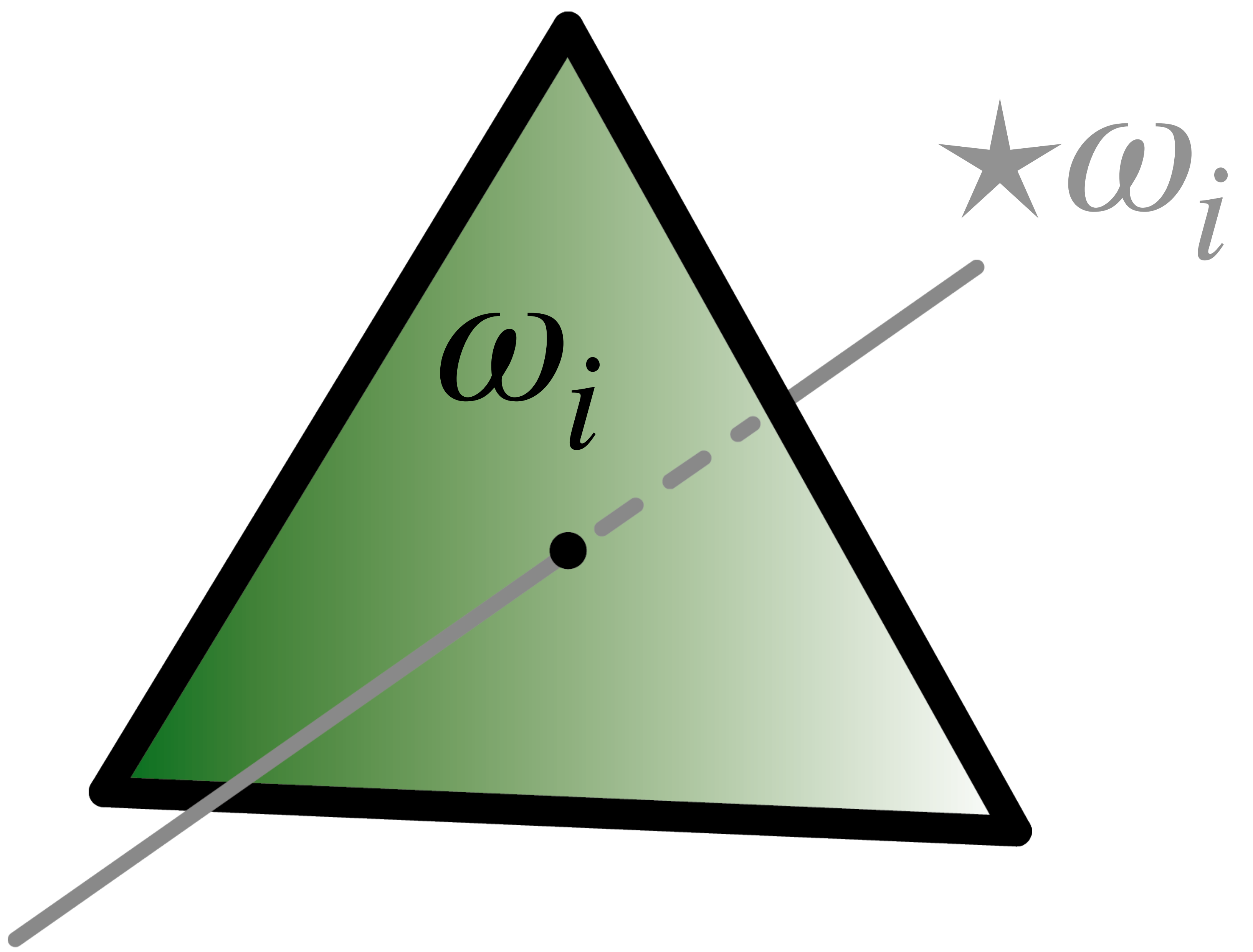


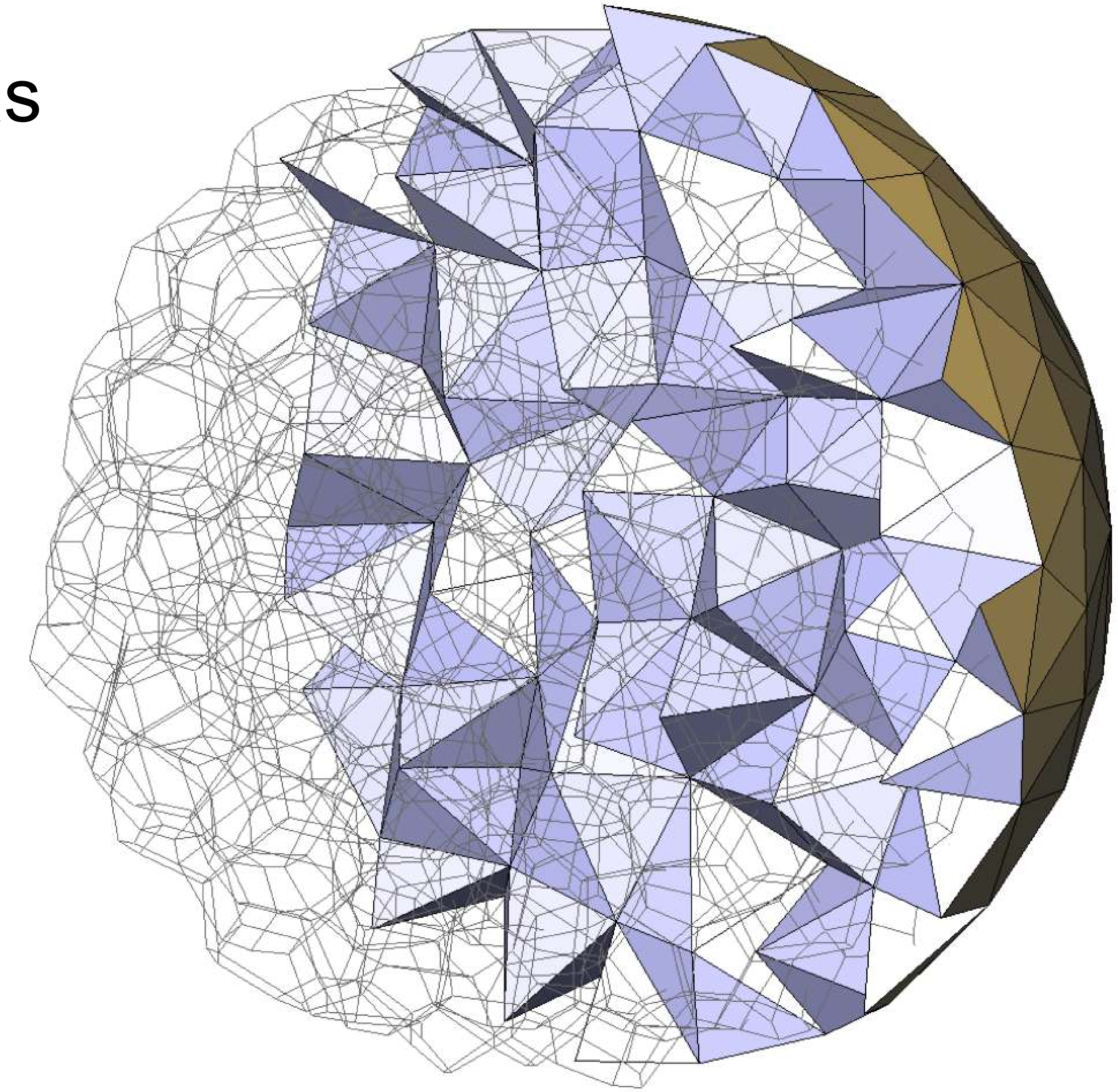
[Mullen et. al. 2011]

# Into the Discrete World

- Discrete forms are stored on SIMPLICES as column vectors.
- Discrete Exterior Derivative $D_k$
- Discrete Hodge Star $S_k$

$S_2$ :

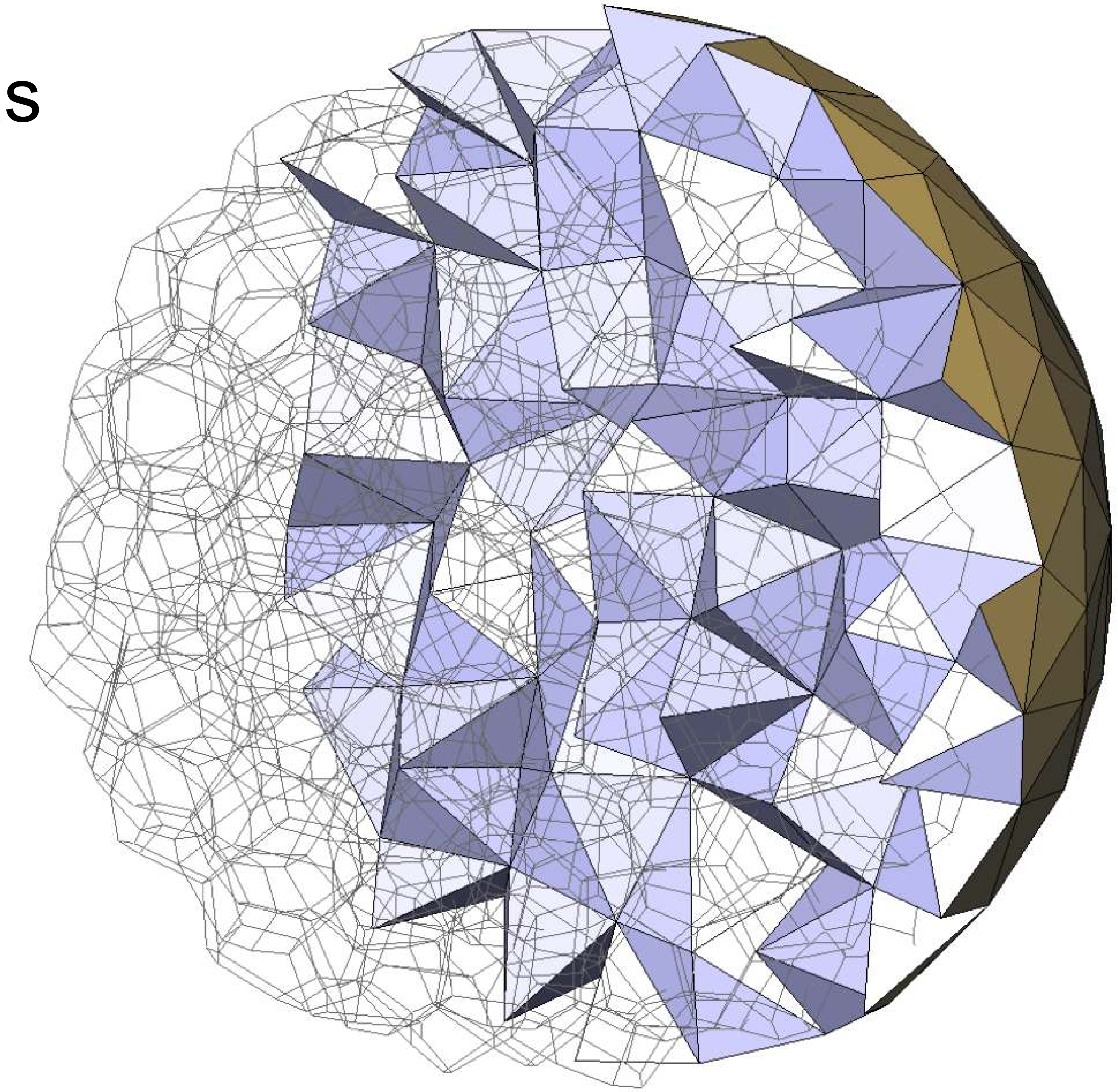




[Mullen et. al. 2011]

# Into the Discrete World

- Discrete forms are stored on SIMPLICES as column vectors.
- Discrete Exterior Derivative $D_k$
- Discrete Hodge Star $S_k$
- Discrete Laplacian $L_k$



[Mullen et. al. 2011]

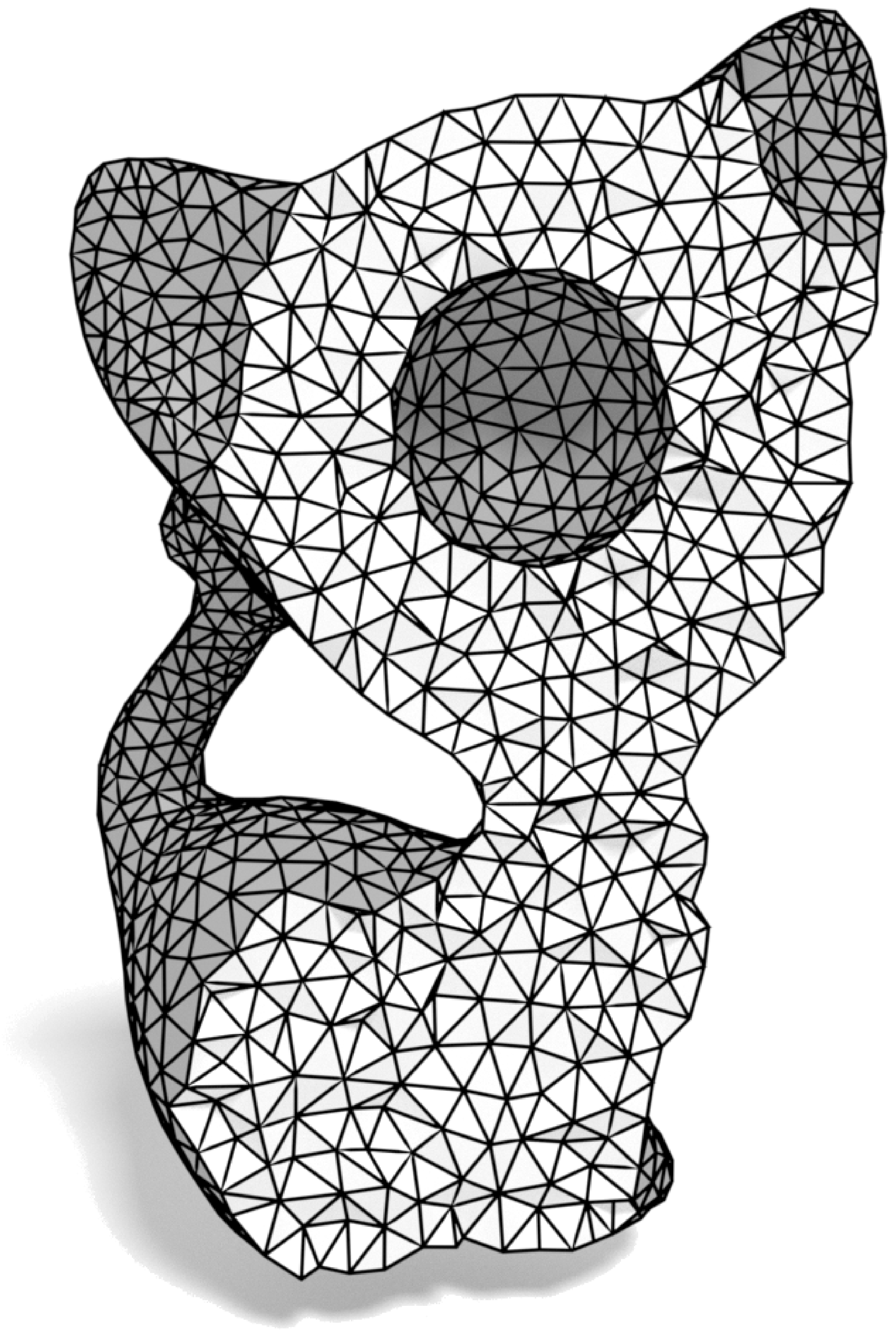
$$L_k = D_k^T S_{k+1} D_k + S_k D_{k-1} S_{k-1}^{-1} D_{k-1}^T S_k$$

Mimicking $\star^k \Delta^k$ to symmetrize discrete operator

# Boundary Condition Treatment

$$L_{k,t} = D_k^T S_{k+1} D_k + S_k D_{k-1} S_{k-1}^{-1} D_{k-1}^T S_k$$

$$L_{k,n} = D_{k,int}^T S_{k+1,int} D_{k,int} + S_{k,int} D_{k-1,int} S_{k-1,int}^{-1} D_{k-1,int}^T S_{k,int}$$



# Boundary Condition Explanation (2-Form)

$L_{2,n}U = b \quad L_{2,n} = D_{2,int}^T S_{3,int} D_{2,int} + S_{2,int} D_{1,int} S_{1,int}^{-1} D_{1,int}^T S_{2,int}$

| | | |
|---|---|---|
| Interior: | Apply Gauge<br>$\nabla \nabla \cdot$ | Capture Vorticity<br>$-\nabla \times \nabla \times$ |
| Boundary: | No-Transfer<br>$\boldsymbol{u} \cdot \boldsymbol{n} = 0$ | Free-Slip<br>$(\nabla \times \boldsymbol{u}) \cdot \boldsymbol{t}_1 = 0$<br>$(\nabla \times \boldsymbol{u}) \cdot \boldsymbol{t}_2 = 0$ |

Missing gauge term means boundary conditions not fully specified.

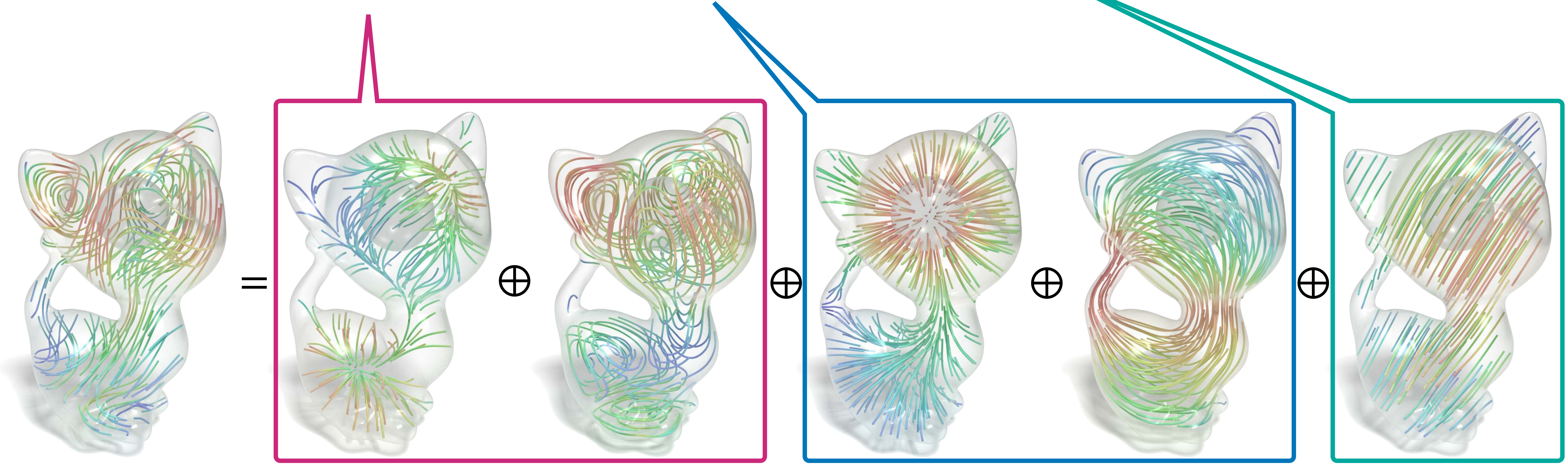
# Duality Structure

$$L_{k,n} \qquad L_{3-k,t}$$

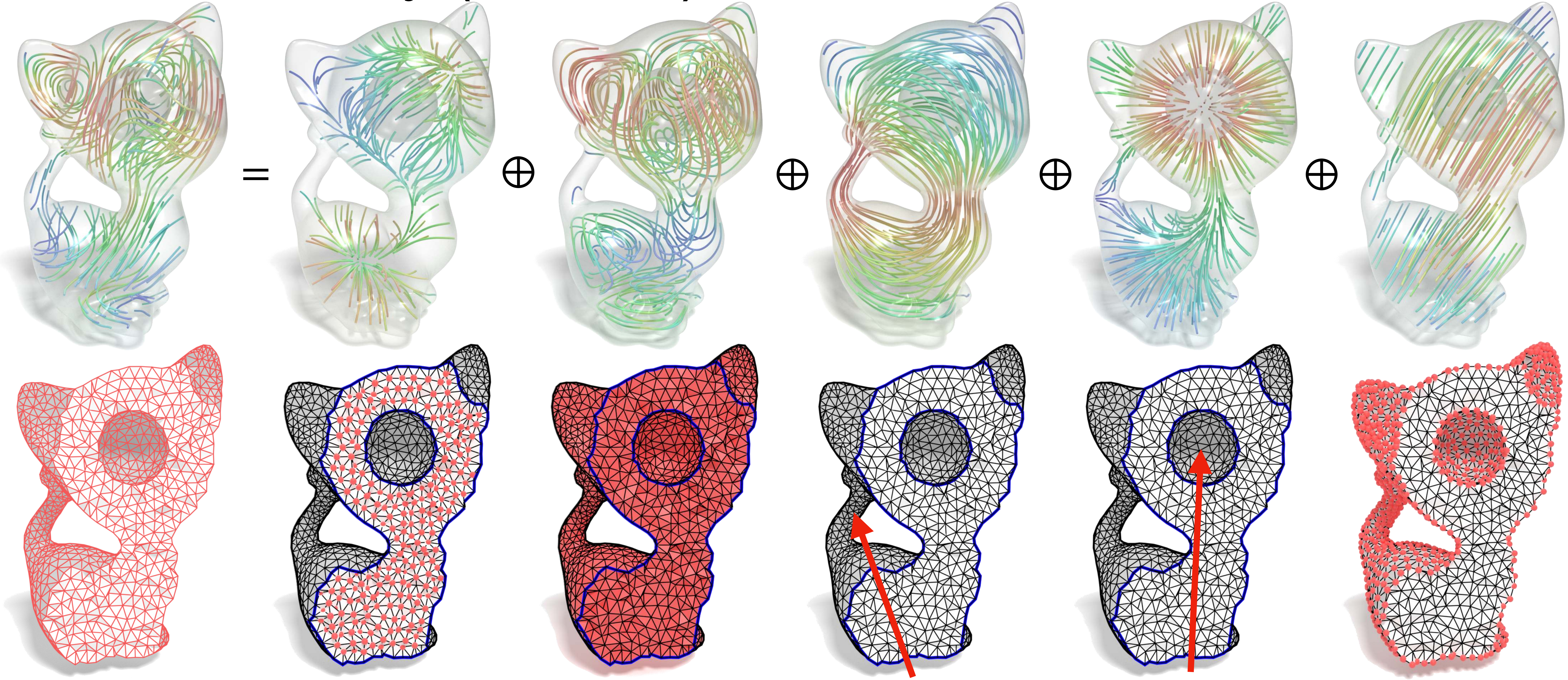
$$L_{2,n} \qquad L_{1,t}$$

# 5-Component Decomposition Realization

- Projection to subspaces with Laplacian spanned by regular basis, harmonic basis and rest.



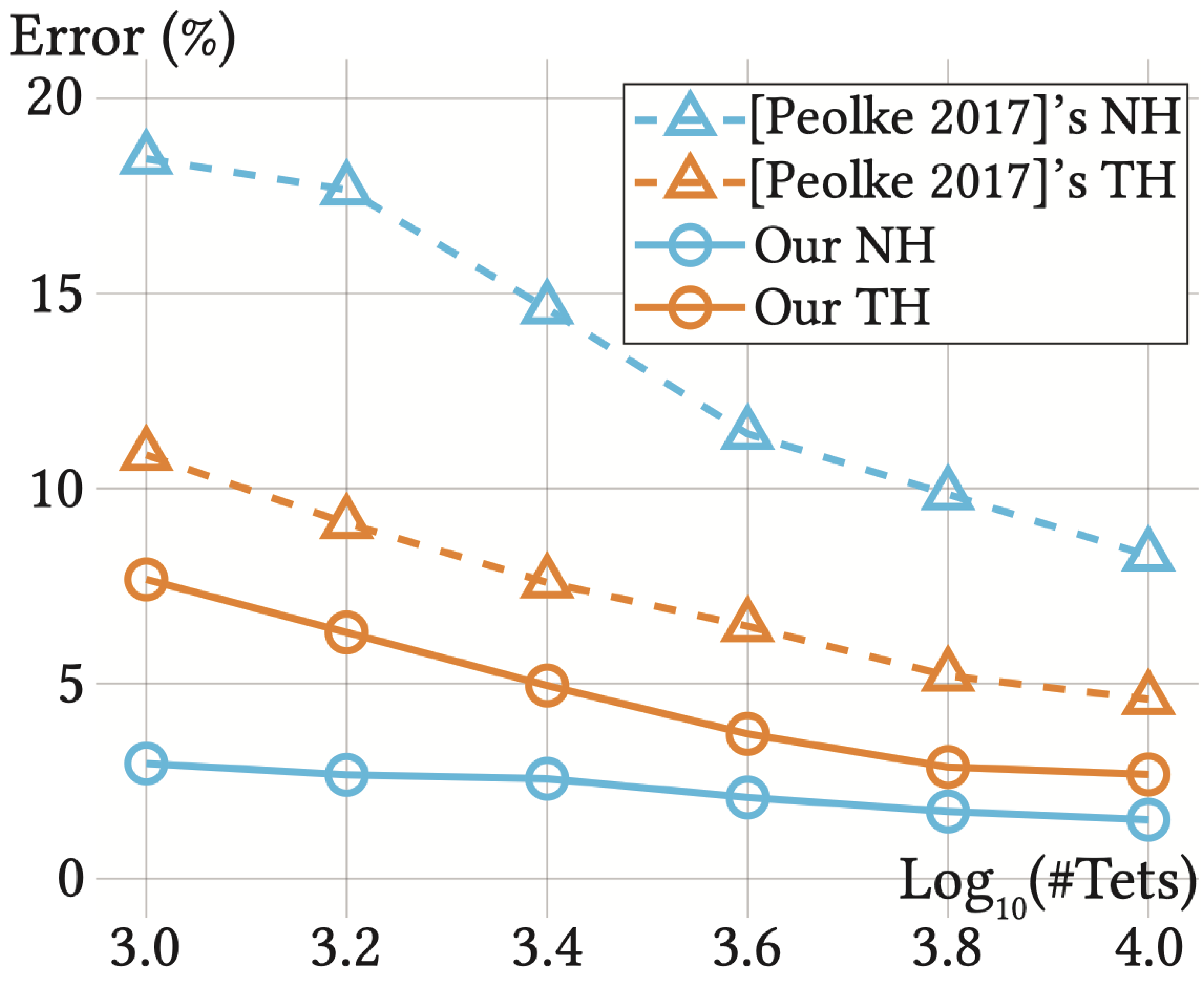
# Dimensionality (1-Form)

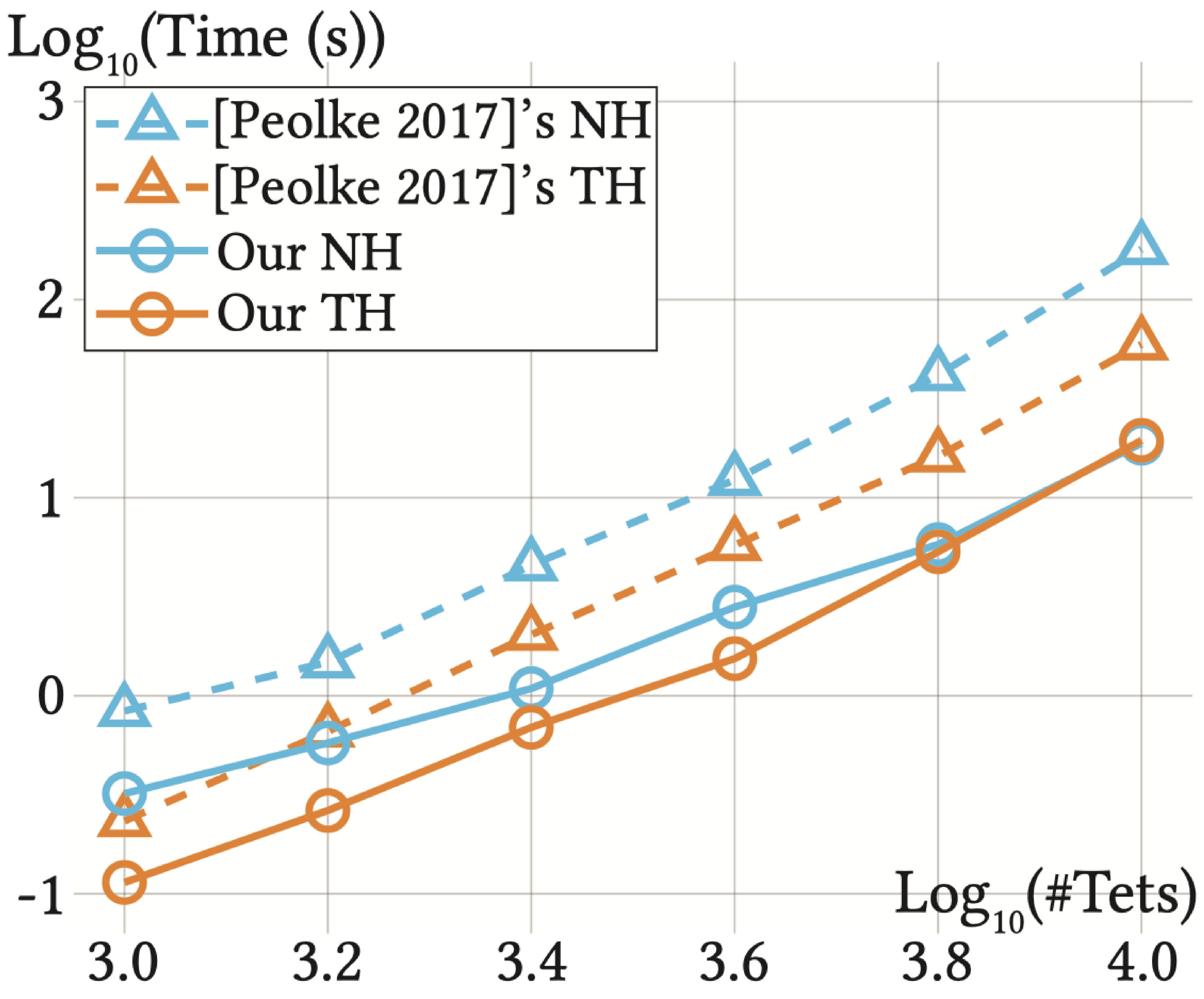


$$(|E|) = (|V_I|) + (|F|-|T|-\beta_2) + (\beta_1) + (\beta_2) + (|V_B|-\beta_2-\beta_0)$$

Poincaré-Euler Formula: $|V|-|E|+|F|-|T| = \beta_0 - \beta_1 + \beta_2$

# Comparisons in NH TH Field

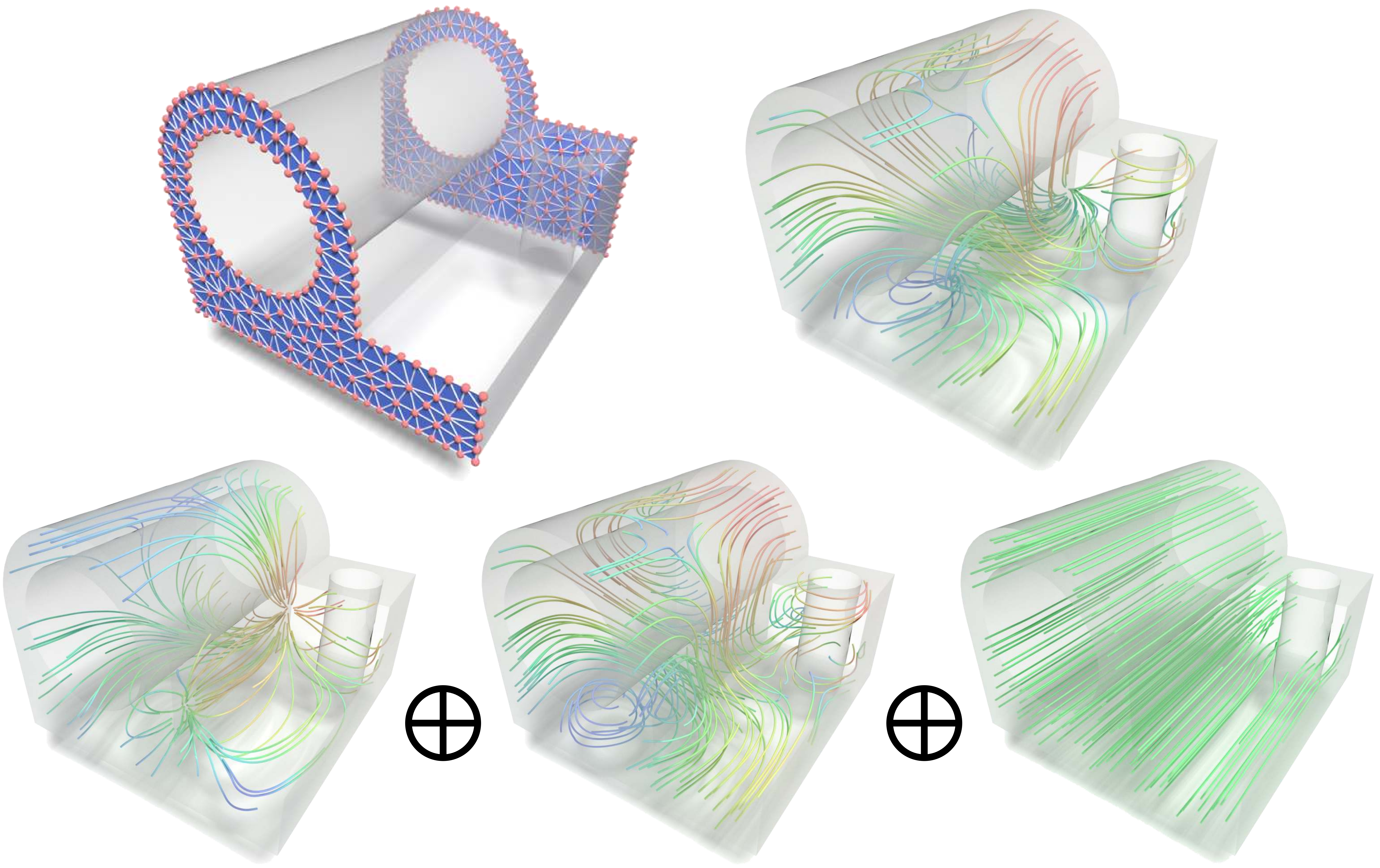



**More Accurate!**

**More Efficient!**

# Mixed Boundary Conditions



# High Order Basis

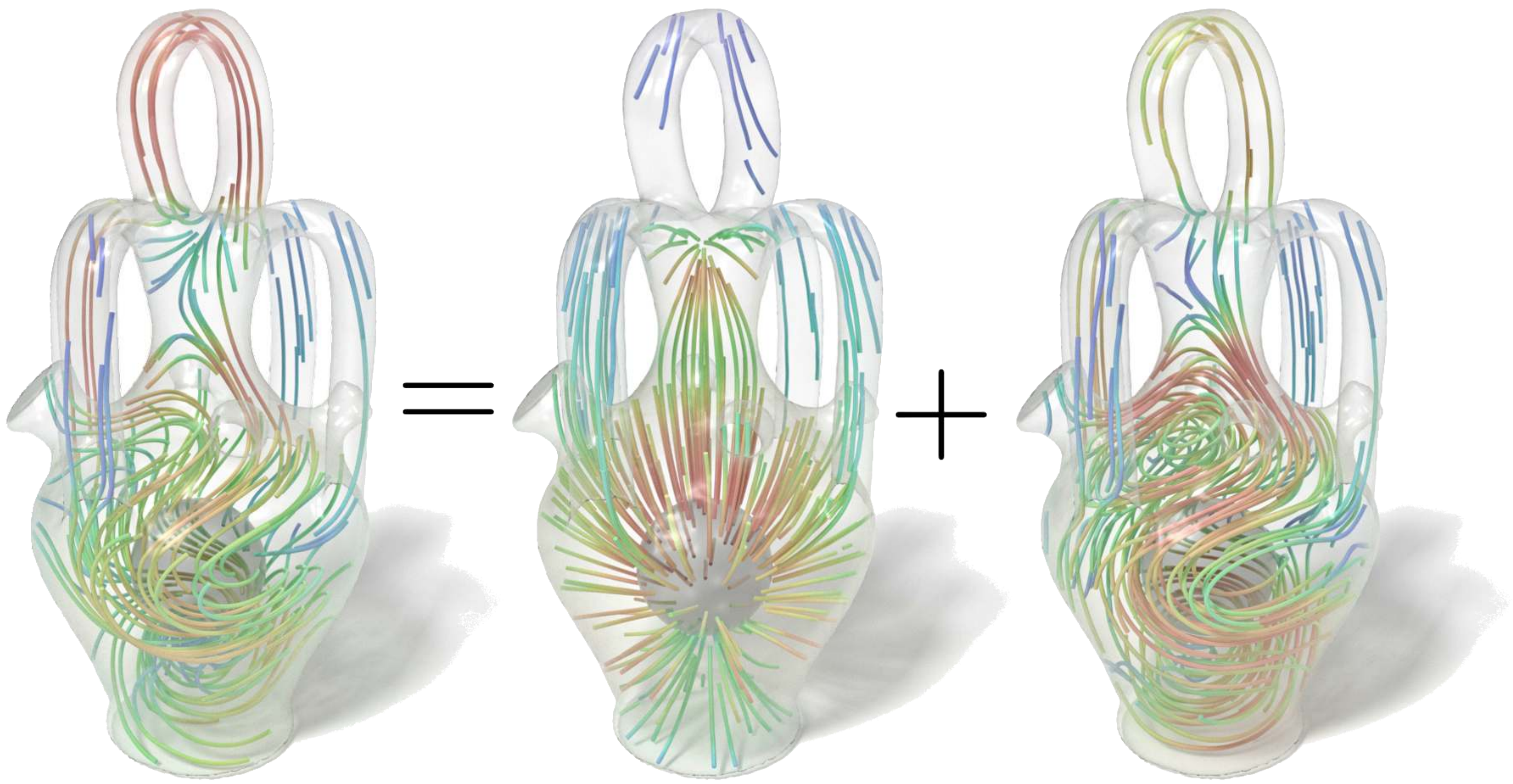
- Problem: S_k is no longer diagonal.
- Principle: Change gauge.

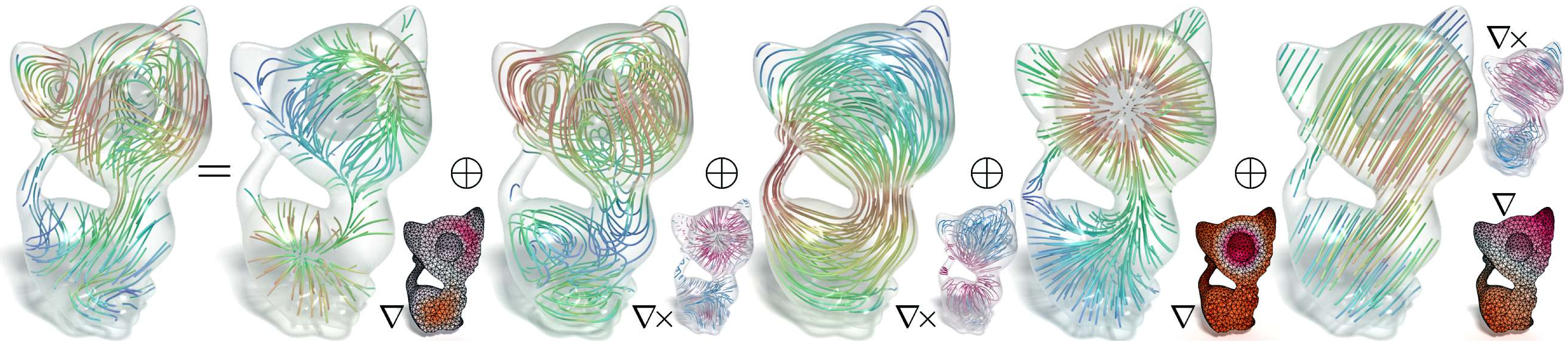
$$L_k\beta = (D_{k+1}^T S_{k+2} D_{k+1} + S_{k+1} D_k S_k^{-1} D_k^T S_{k+1})\beta = S_{k+1} D_k S_k^{-1} \gamma$$

$$L_k\beta = (D_{k+1}^T S_{k+2} D_{k+1} + S_{k+1} D_k \tilde{S}_k D_k^T S_{k+1})\beta = S_{k+1} D_k \tilde{S}_k S_k \gamma$$

# Conclusion

- DEC-Based
- Boundary Condition
  - Exclusion & Inclusion
- Arbitrary Topology
  - Null Space
- Efficient
  - Sparse SPD
- Accurate
  - Precise Sampling
- Versatile
  - Mixed-Boundary
  - High-Order Basis

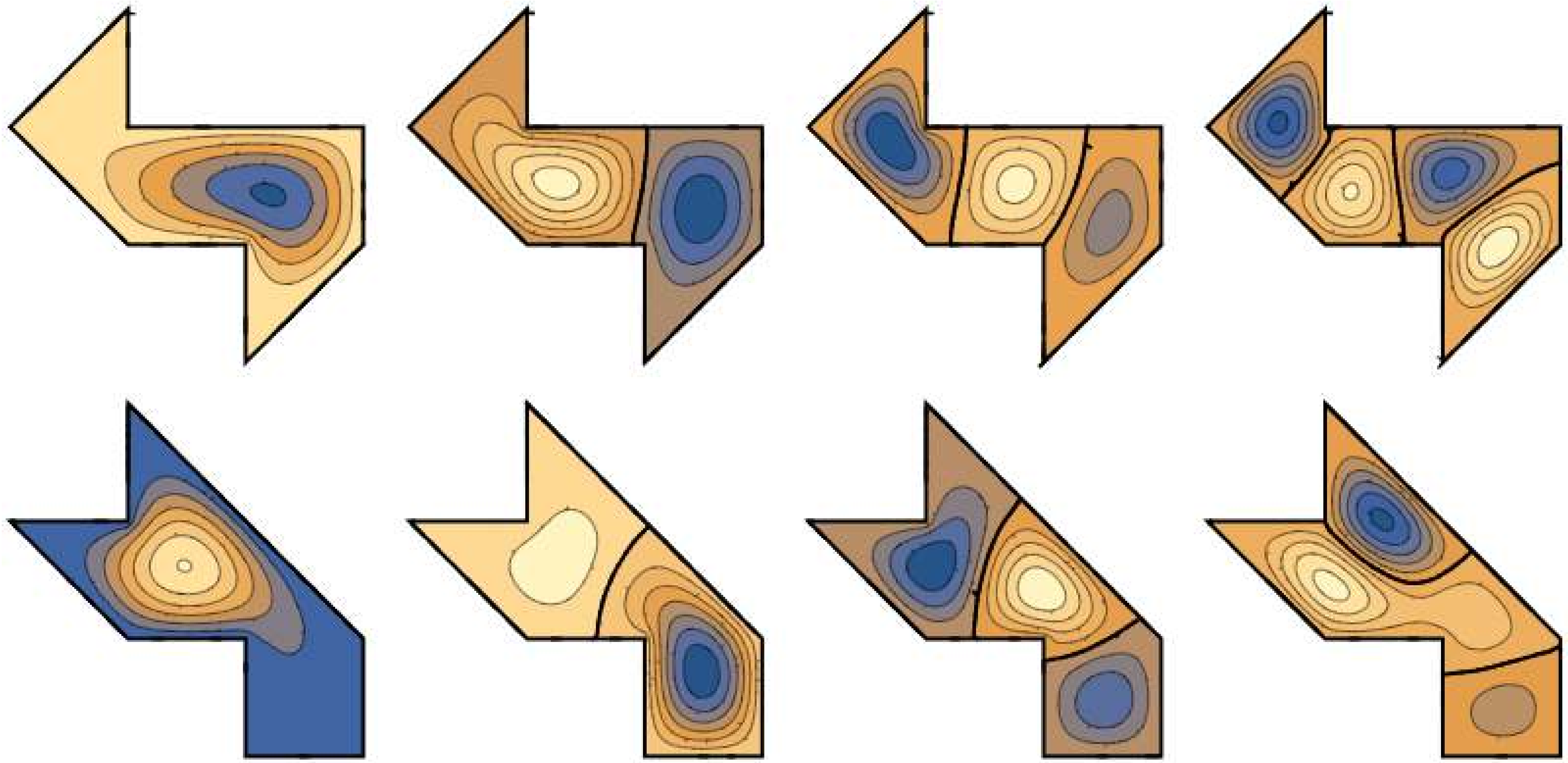





# Section III:
# Geometry and Topology Analysis for Biological Macromolecules

# Motivation

- “Can we hear the shape of a drum?” - Mark Kac 1966



$$L_{0,n}$$

# Laplacian Spectral Analysis

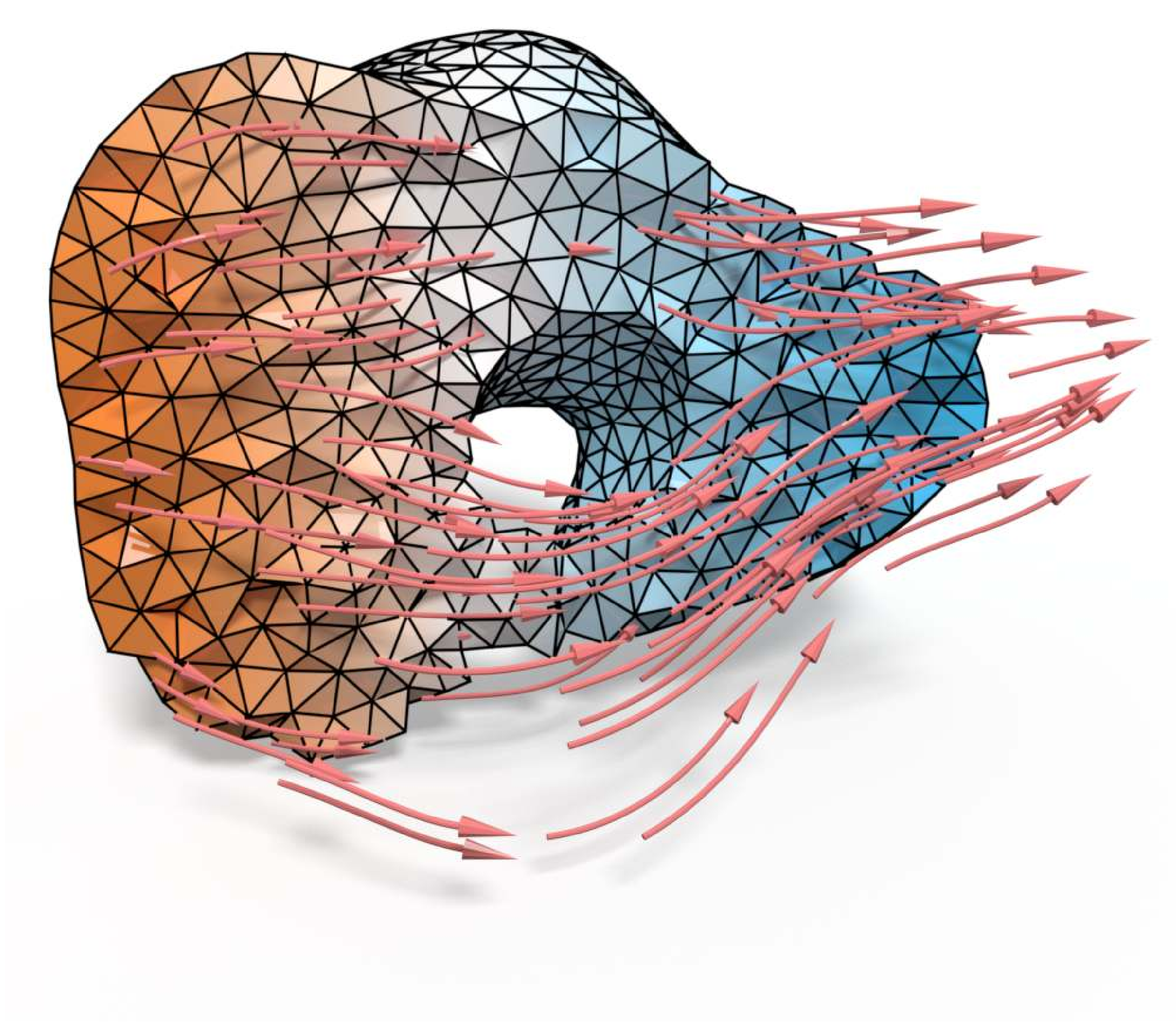
$$L_{0,n} \qquad L_{3,t}$$

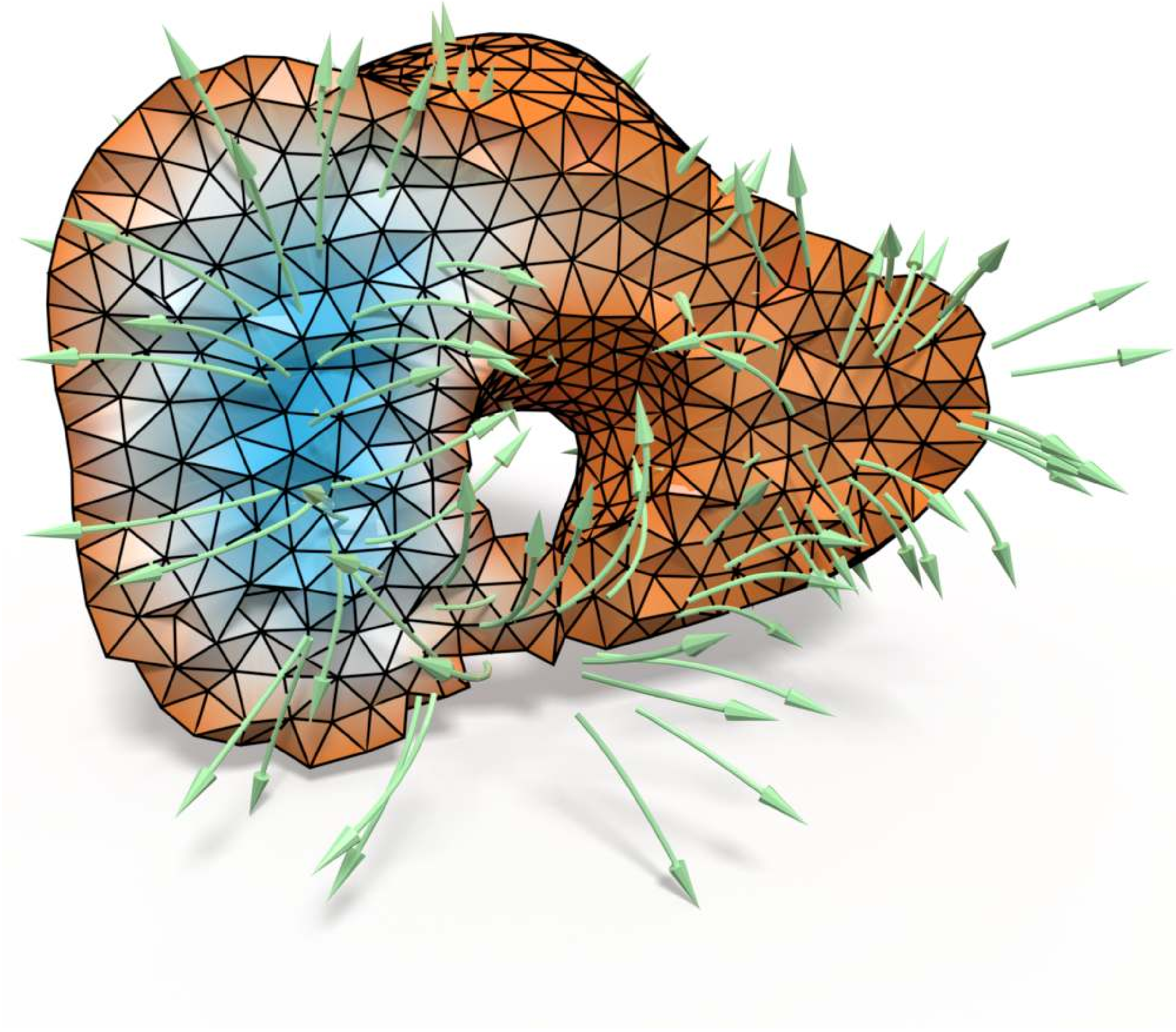
$$L_{1,n} \qquad L_{2,t}$$

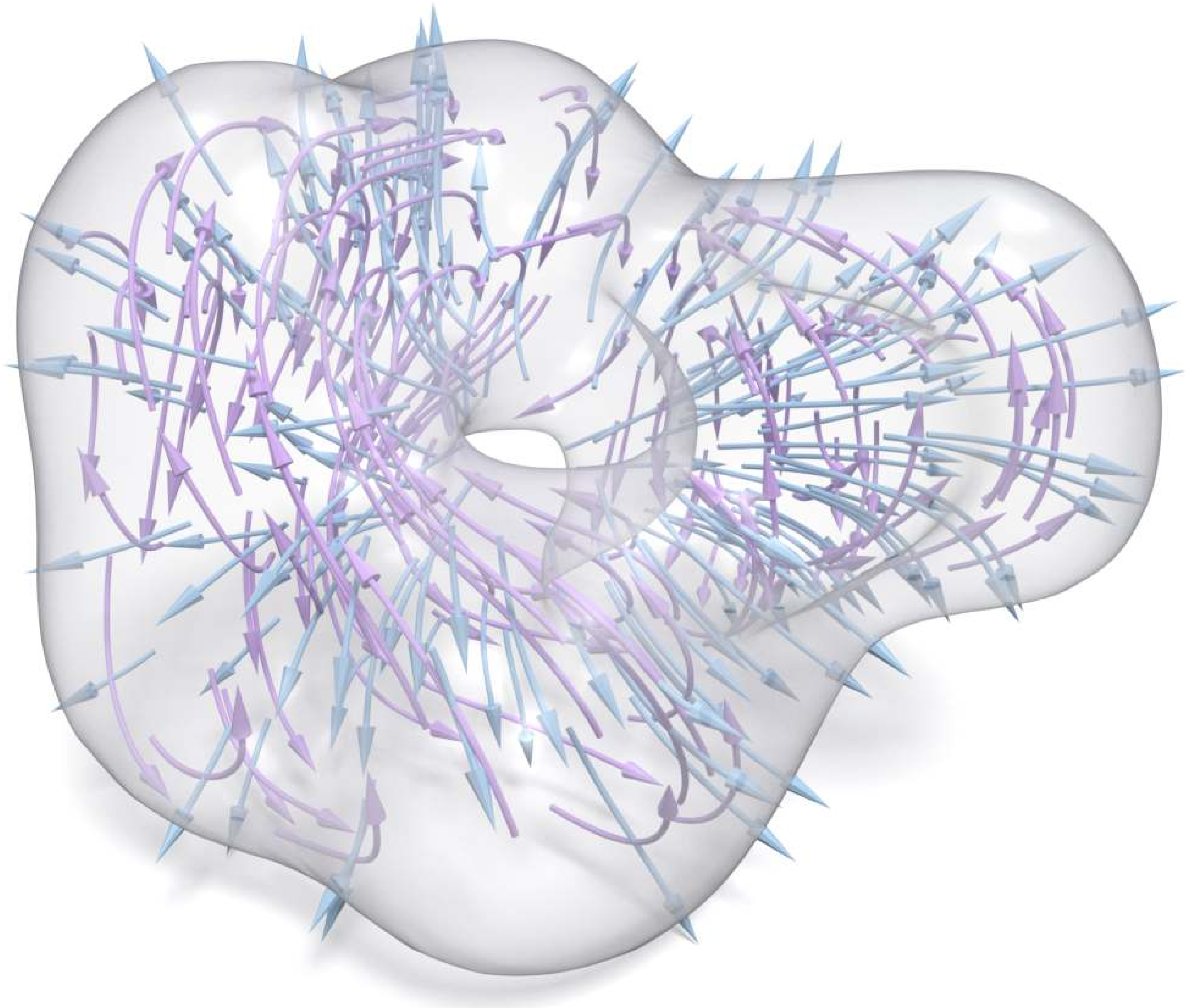
$$L_{2,n} \qquad L_{1,t}$$

$$L_{3,n} \qquad L_{0,t}$$

# Laplacian Spectral Analysis

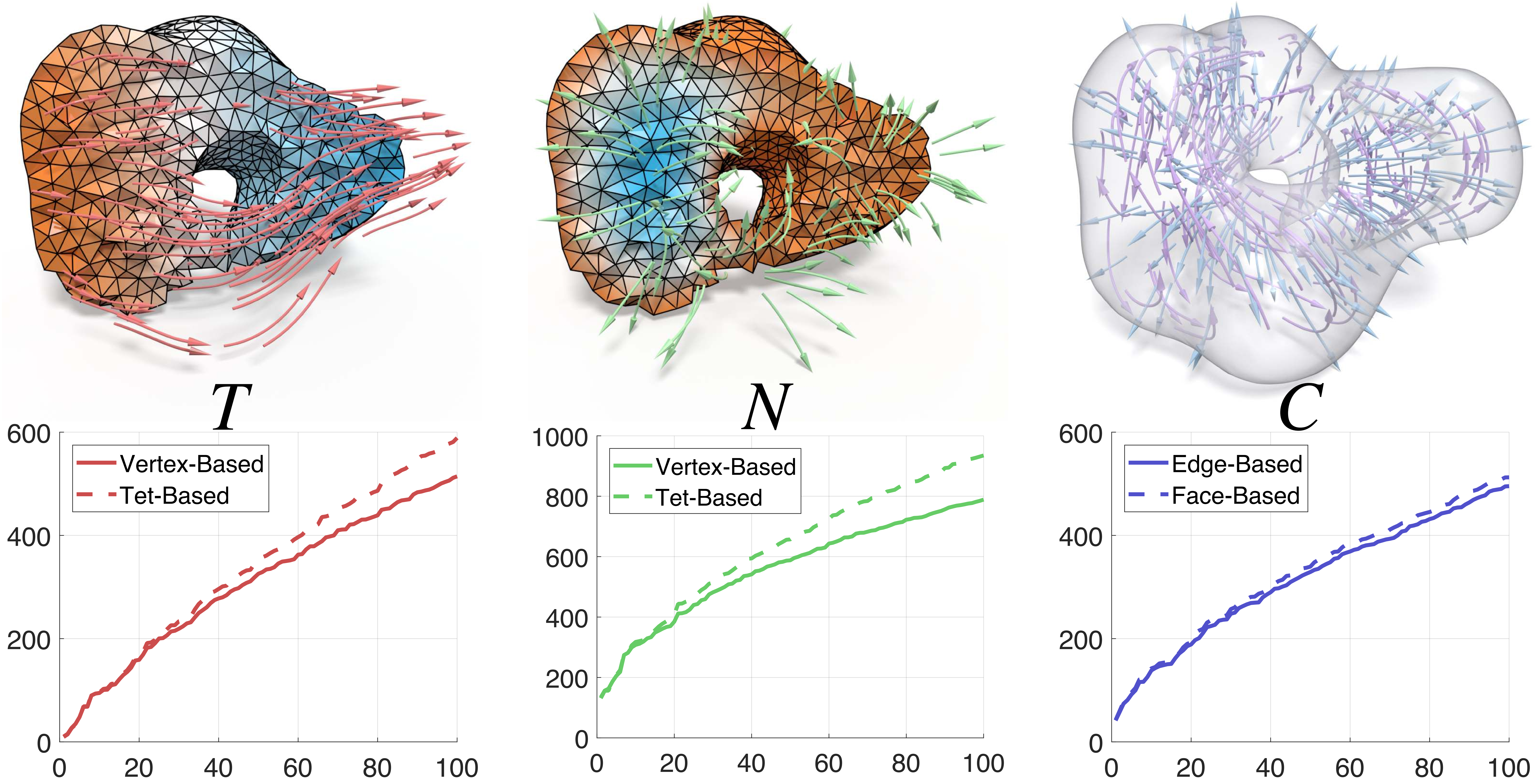




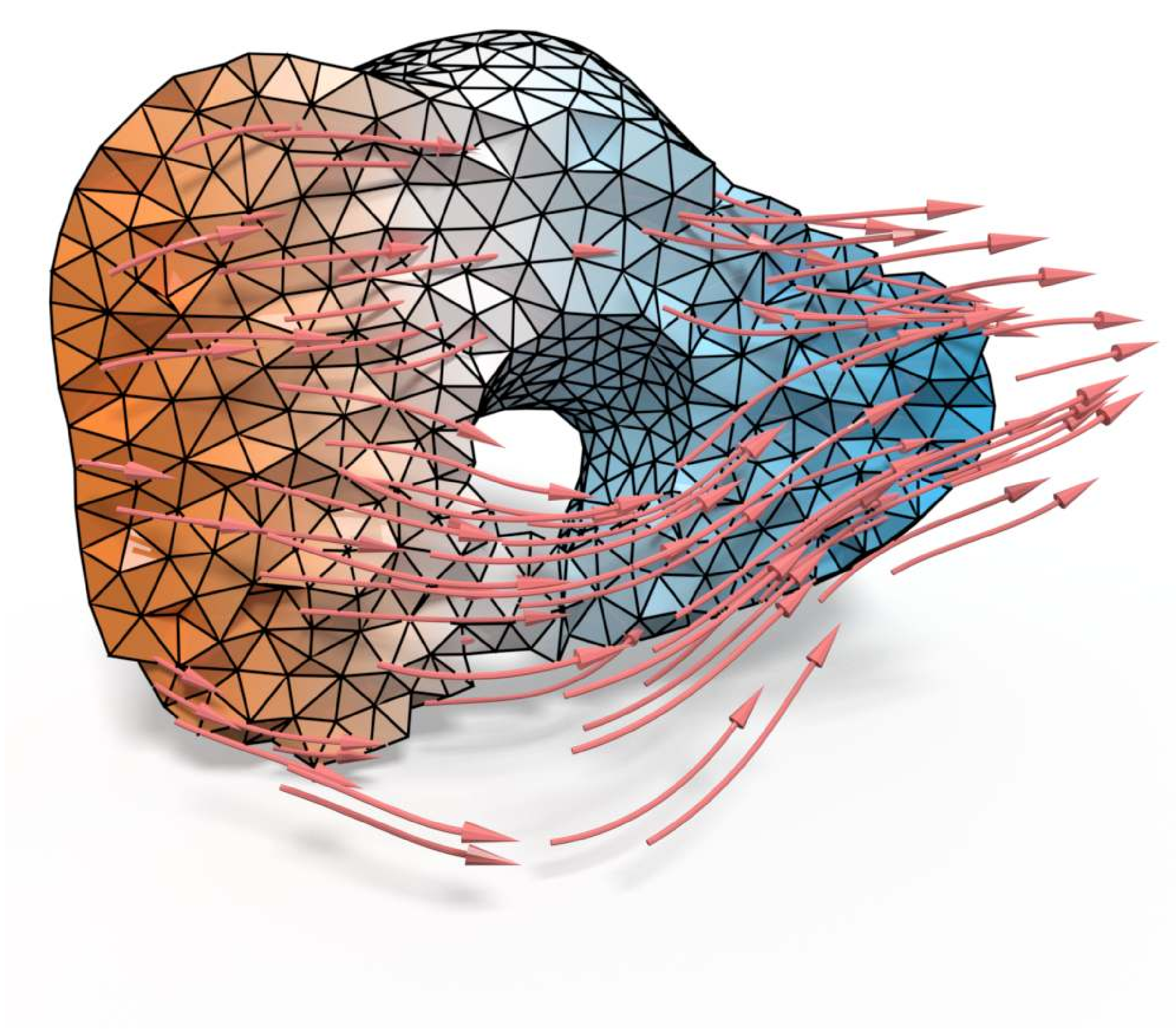


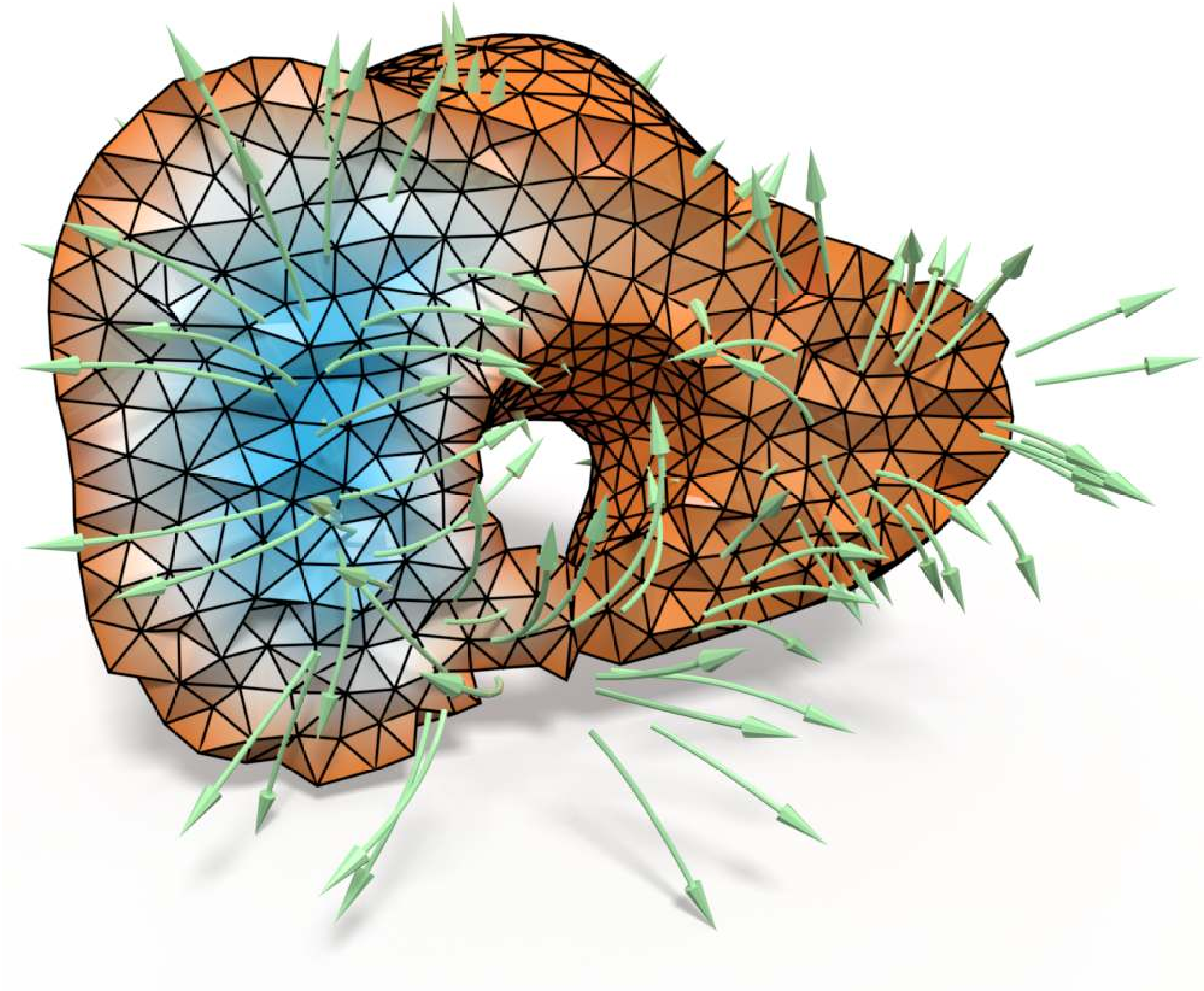
$$\overbrace{L_{0,t}\ \ L^{G}_{1,t}\ \ L^{G}_{2,n}\ \ L_{3,n}}^{T} \qquad \overbrace{L_{0,n}\ \ L^{G}_{1,n}\ \ L^{G}_{2,t}\ \ L_{3,t}}^{N} \qquad \overbrace{L^{C}_{1,t}\ \ L^{C}_{1,n}\ \ L^{C}_{2,t}\ \ L^{C}_{2,n}}^{C}$$

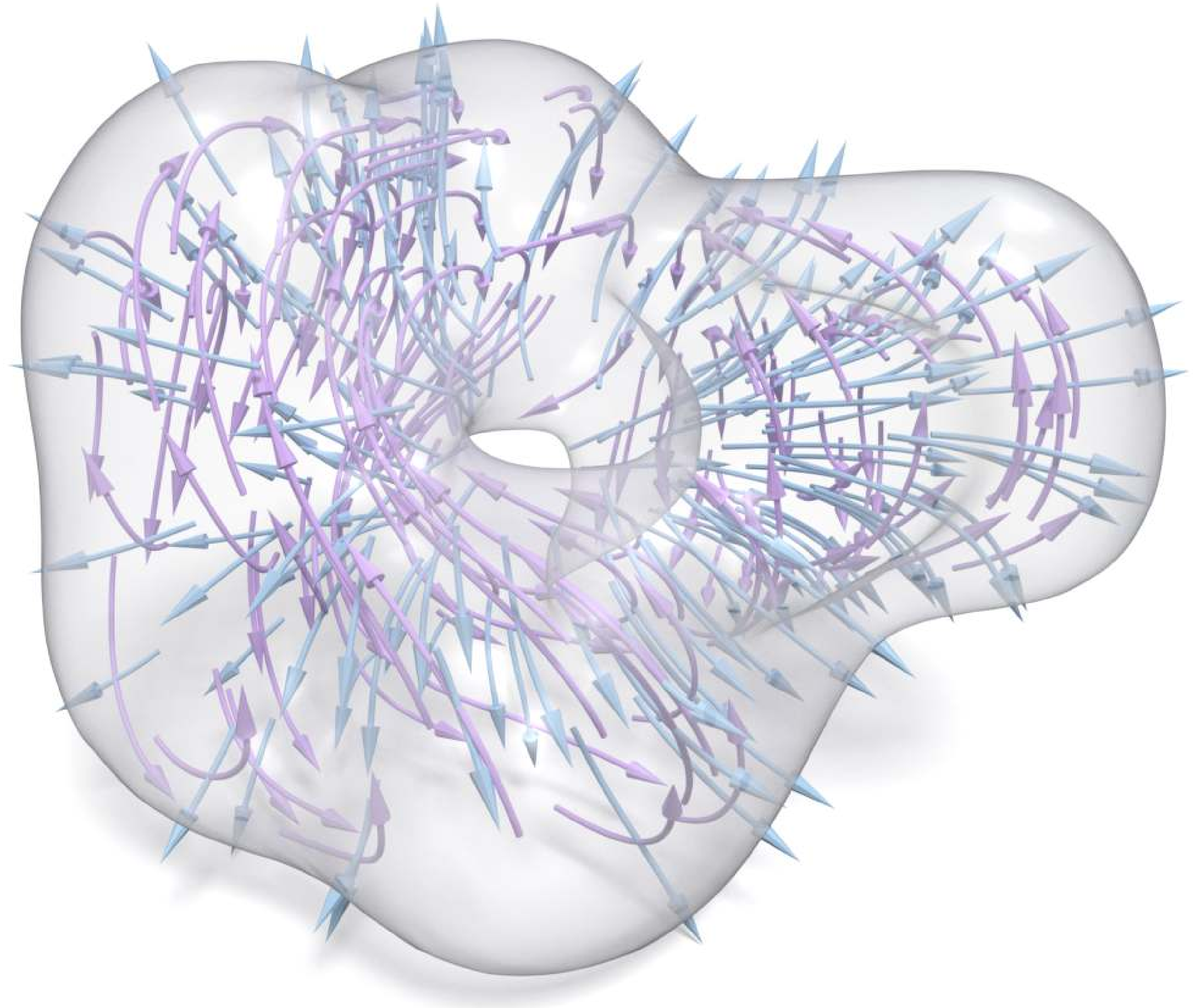
# Laplacian Spectral Analysis

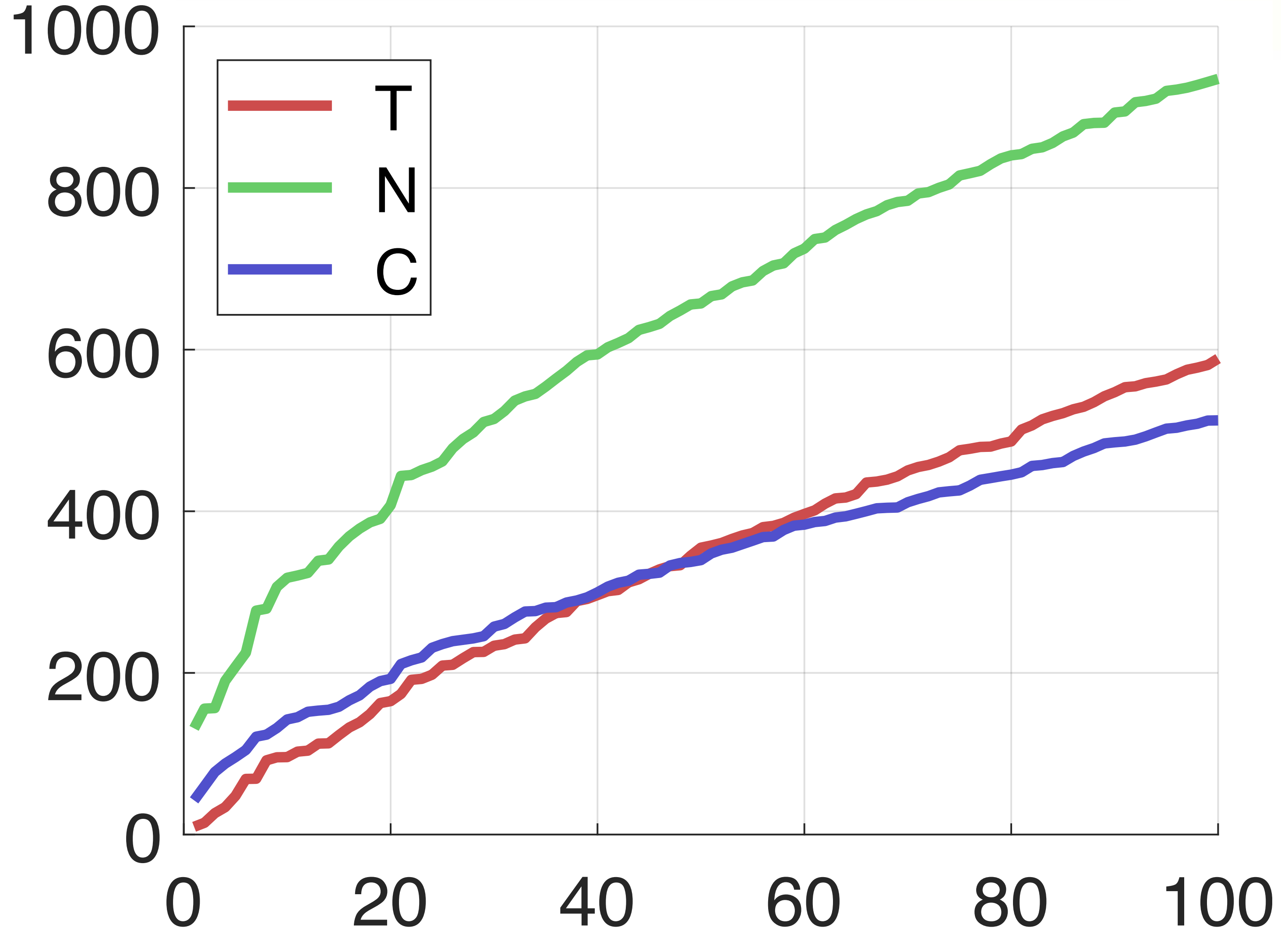


# Laplacian Spectral Analysis

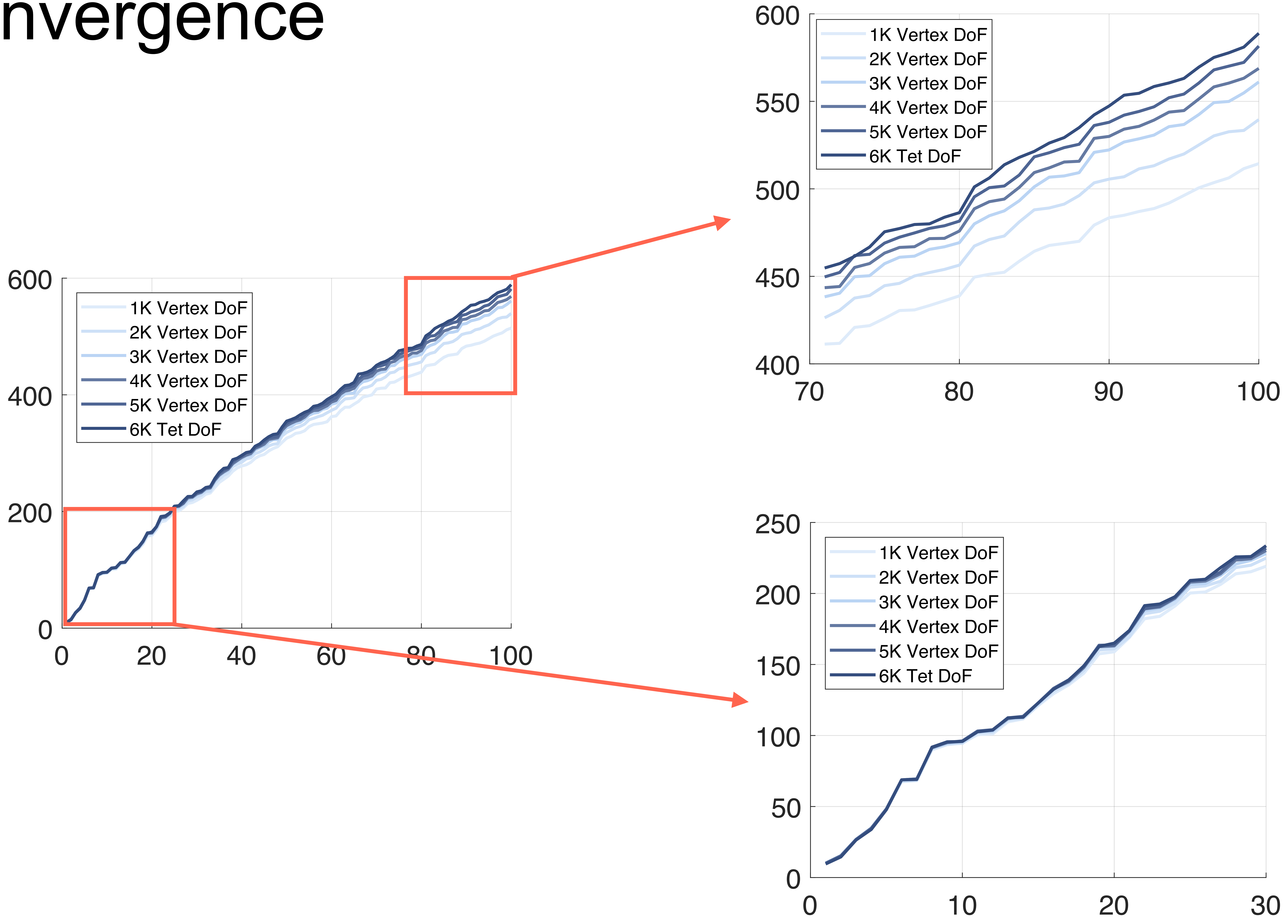




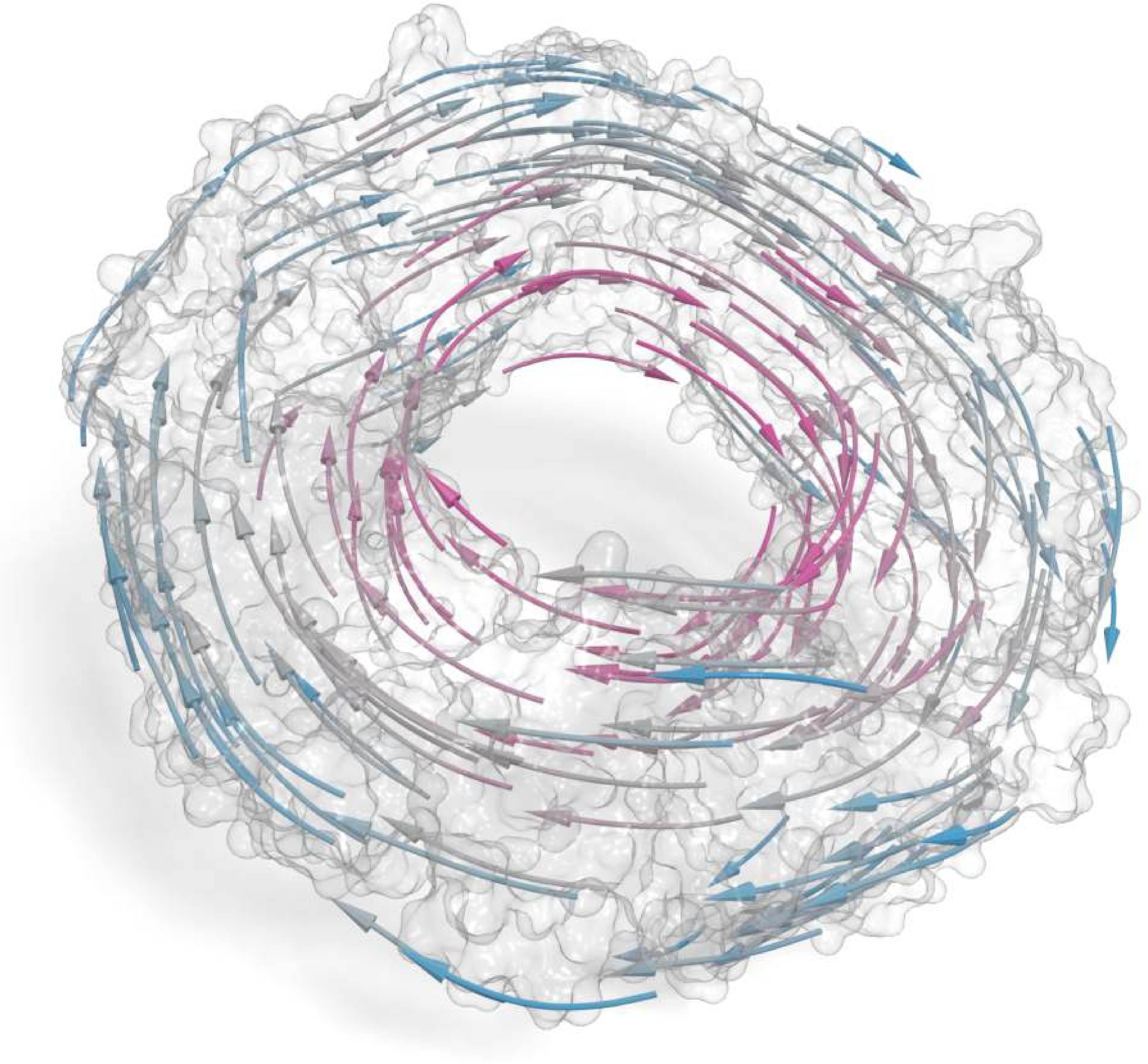




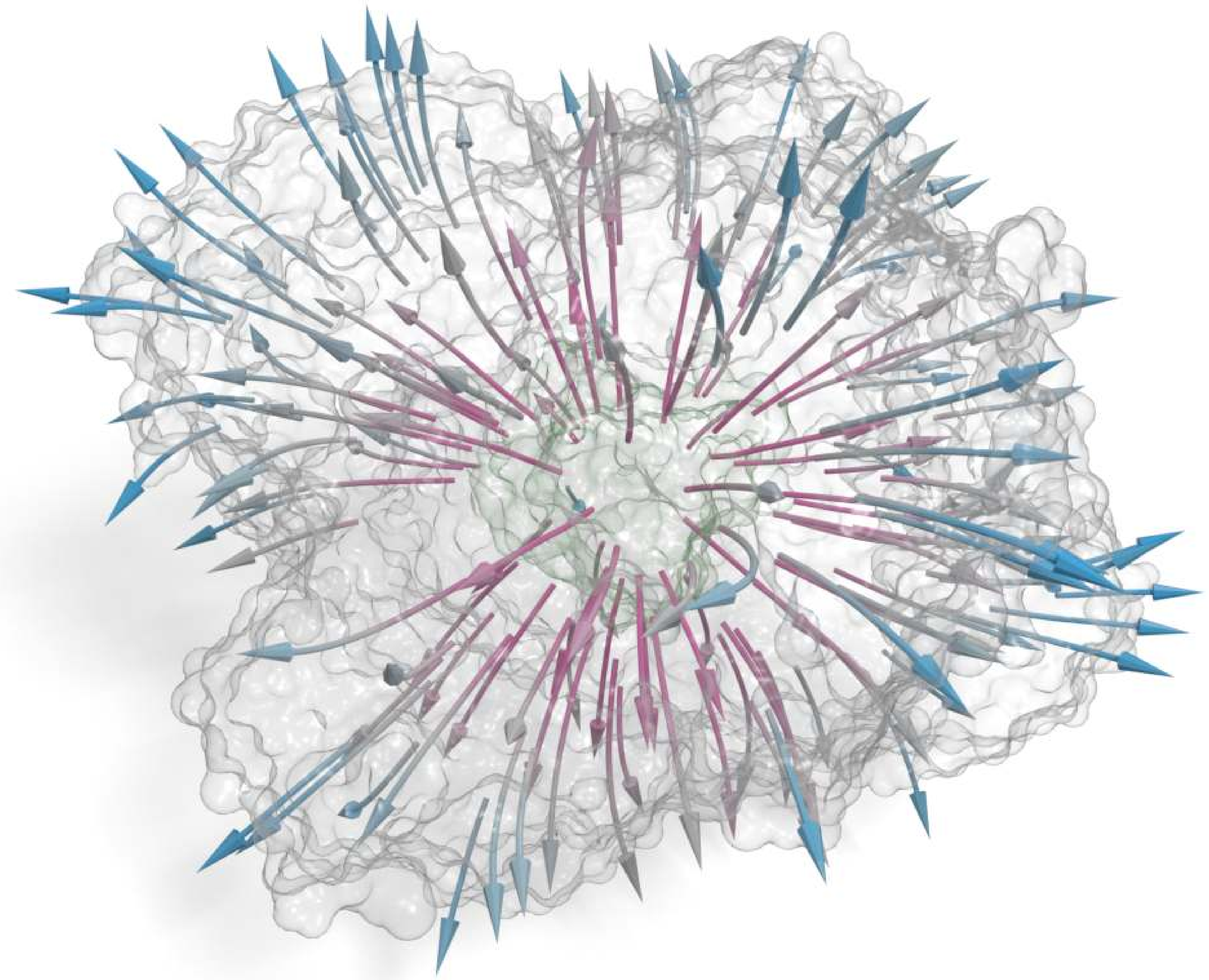
# Convergence



# Topology Descriptor

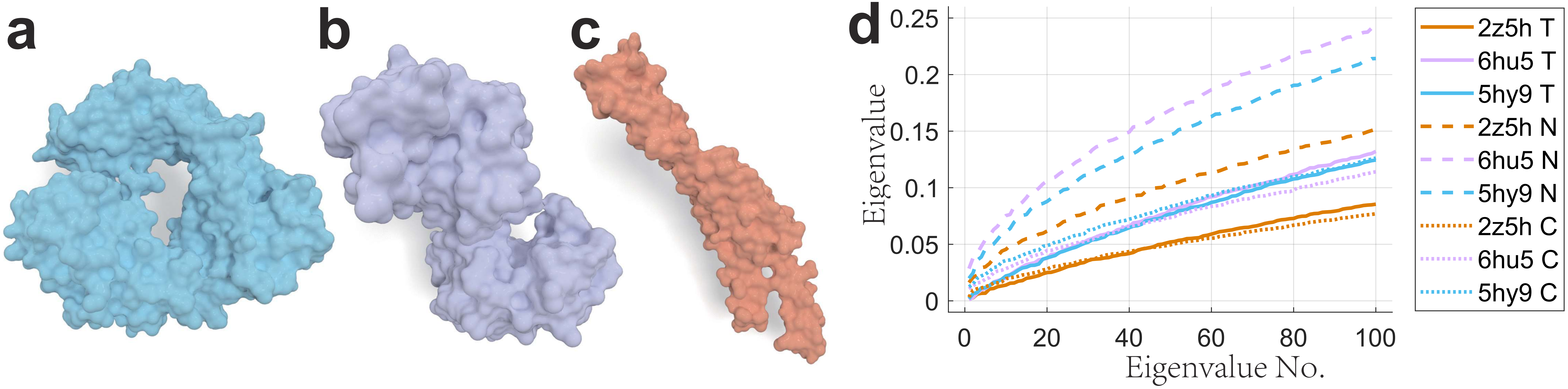


Handle

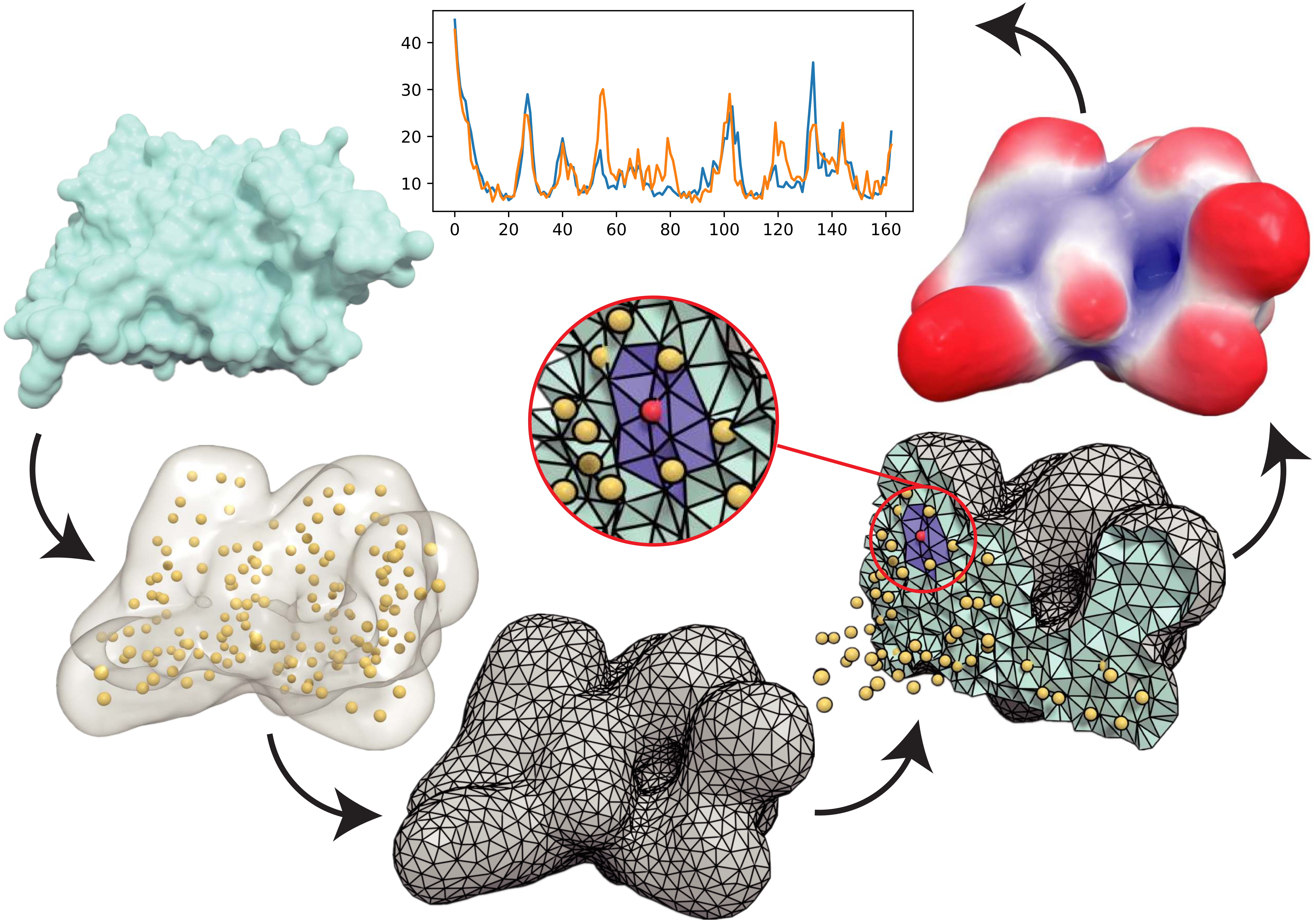


Cavity

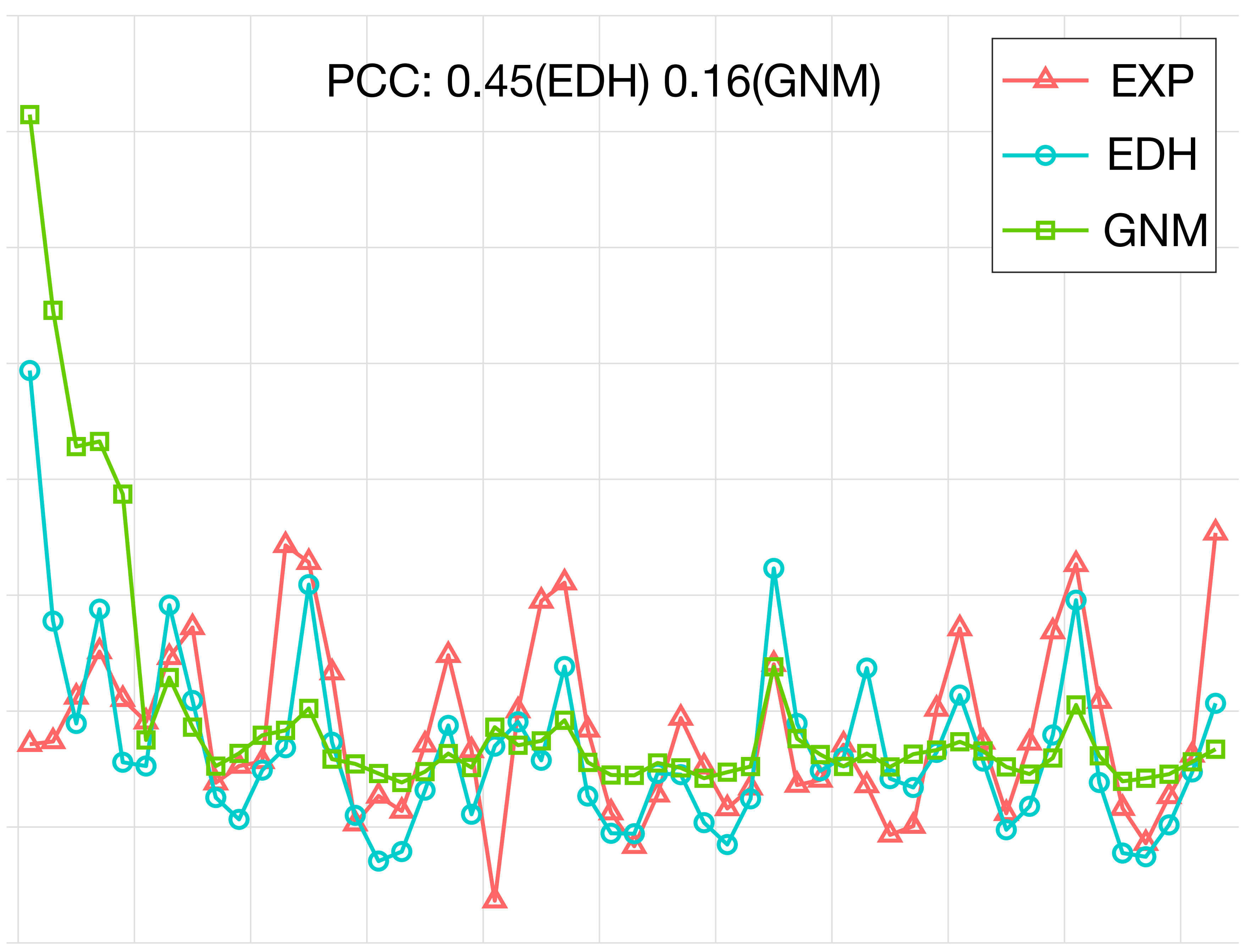
# Geometry Descriptor



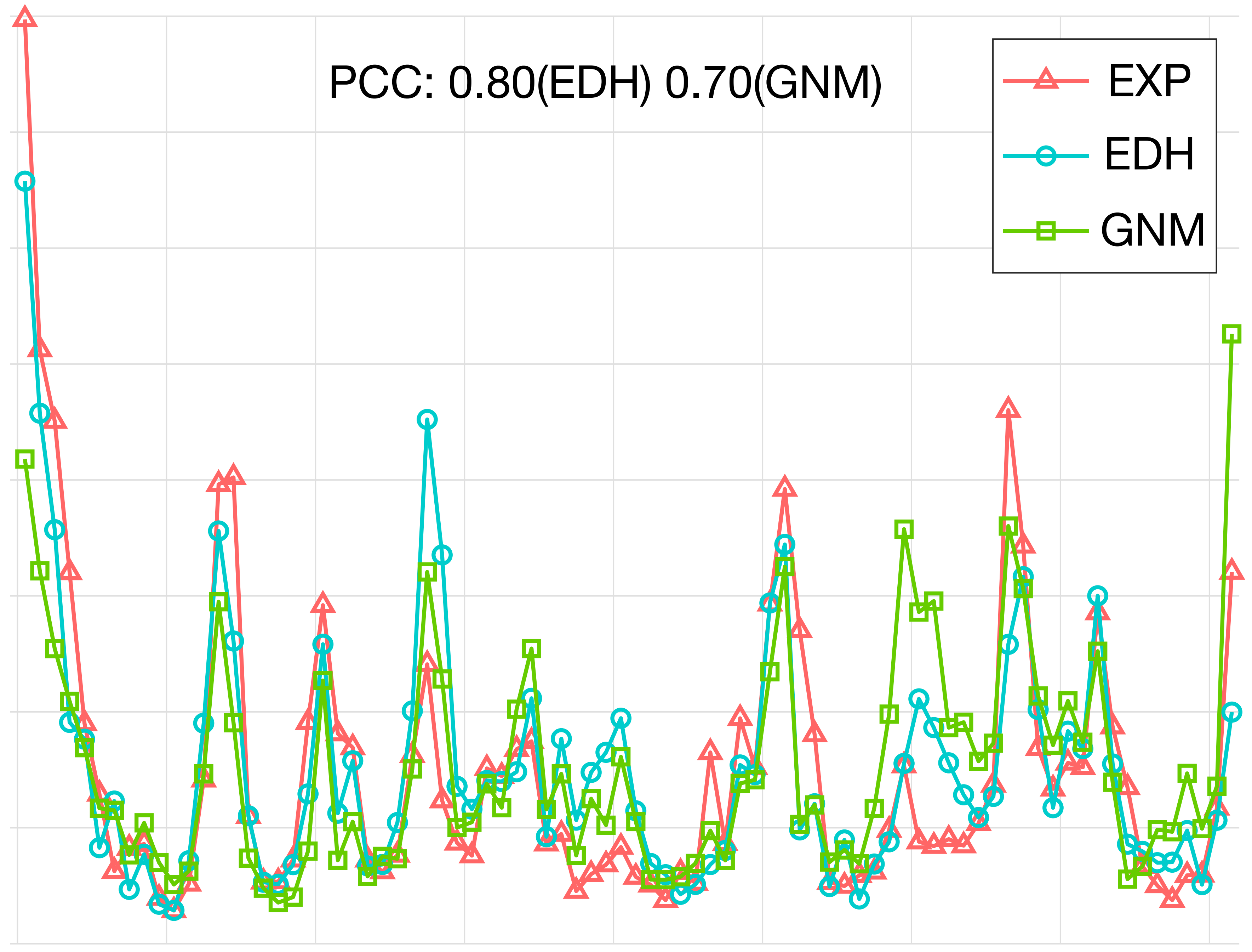
# Application - Flexibility Prediction



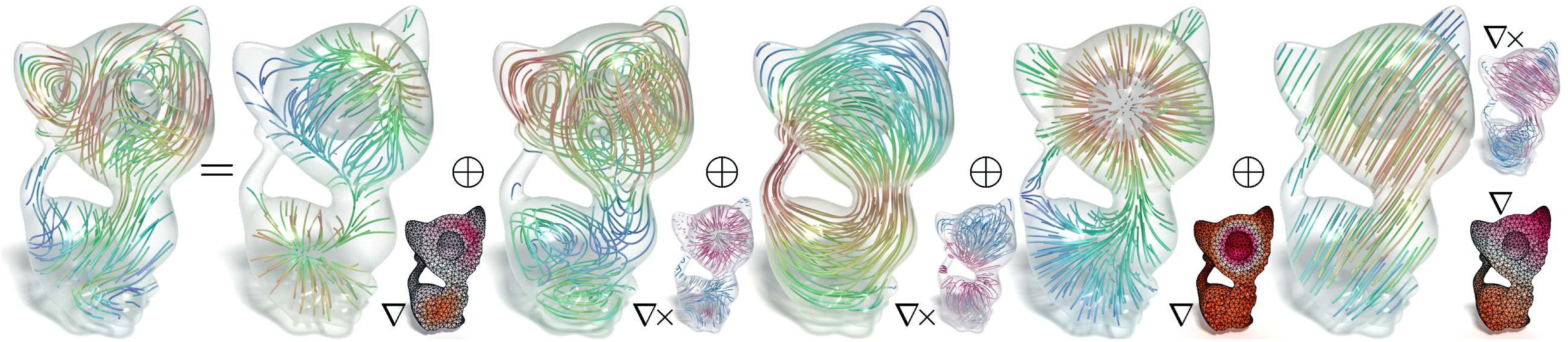
# Application - Flexibility Prediction




Protein ID: 1V70



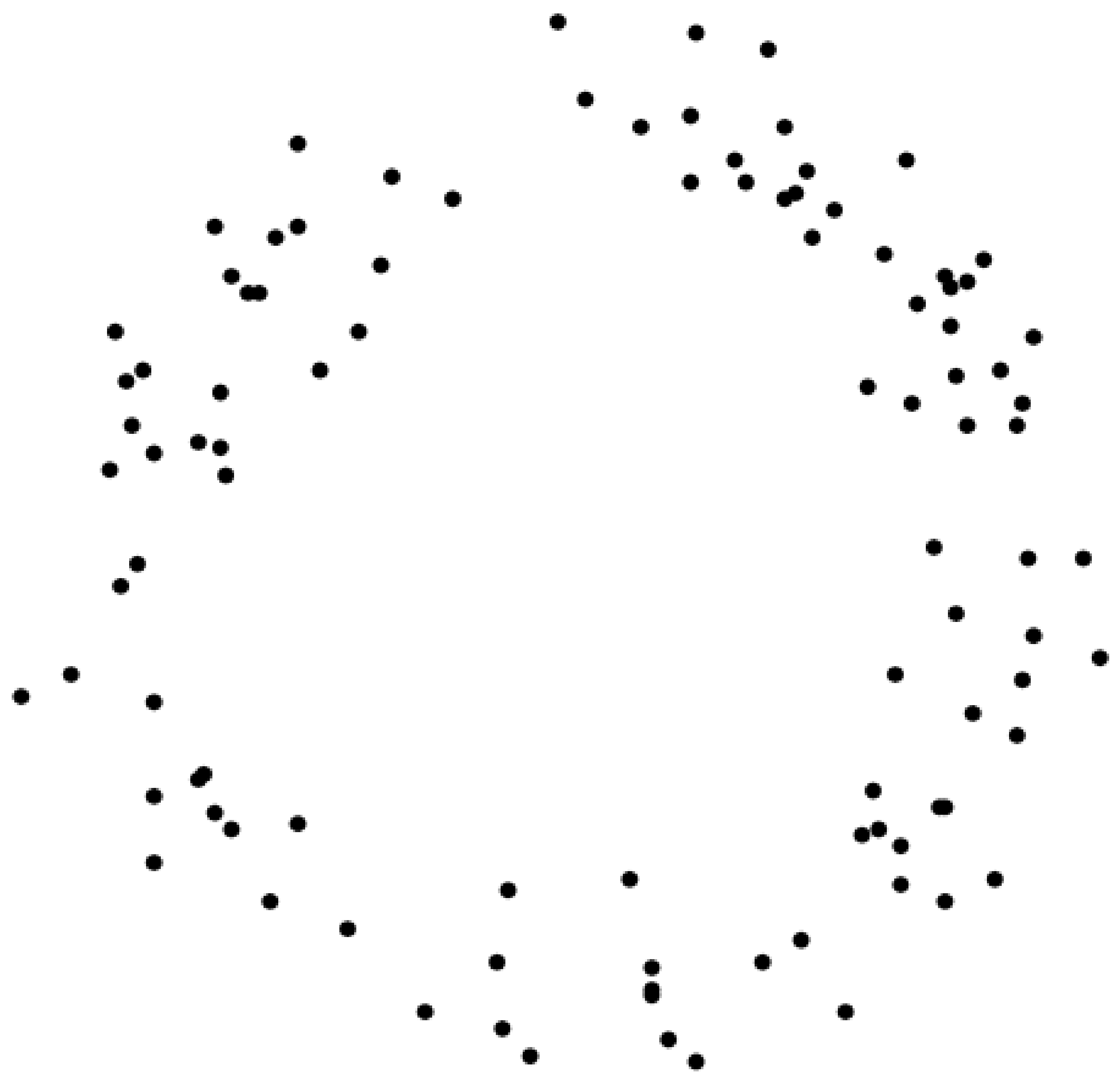

Protein ID: 3VZ9




# Section IV:
# Evolutionary de Rham-Hodge Method

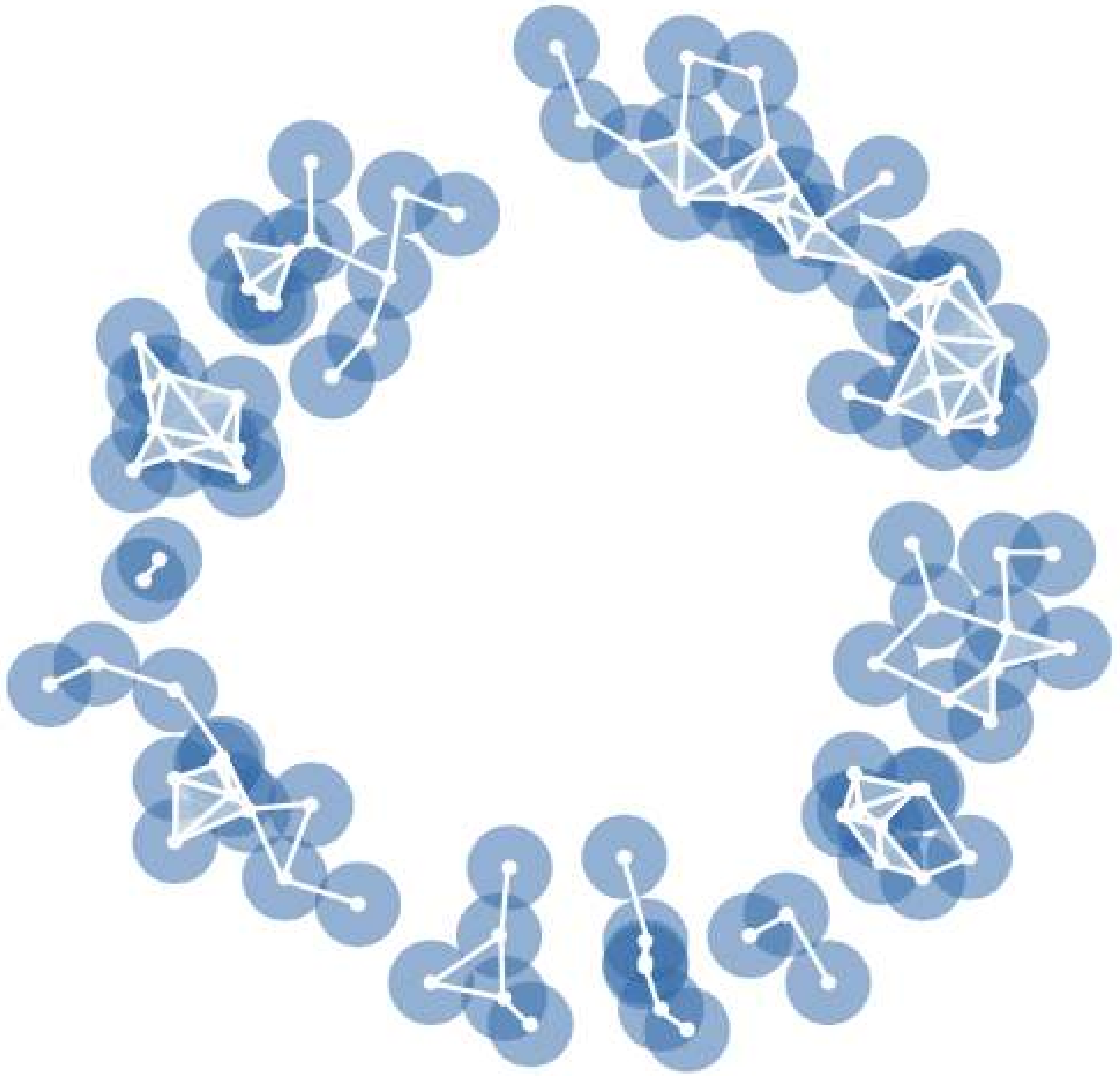
# Motivation - from Persistent Homology

- How can we get most significant feature in geometric data?

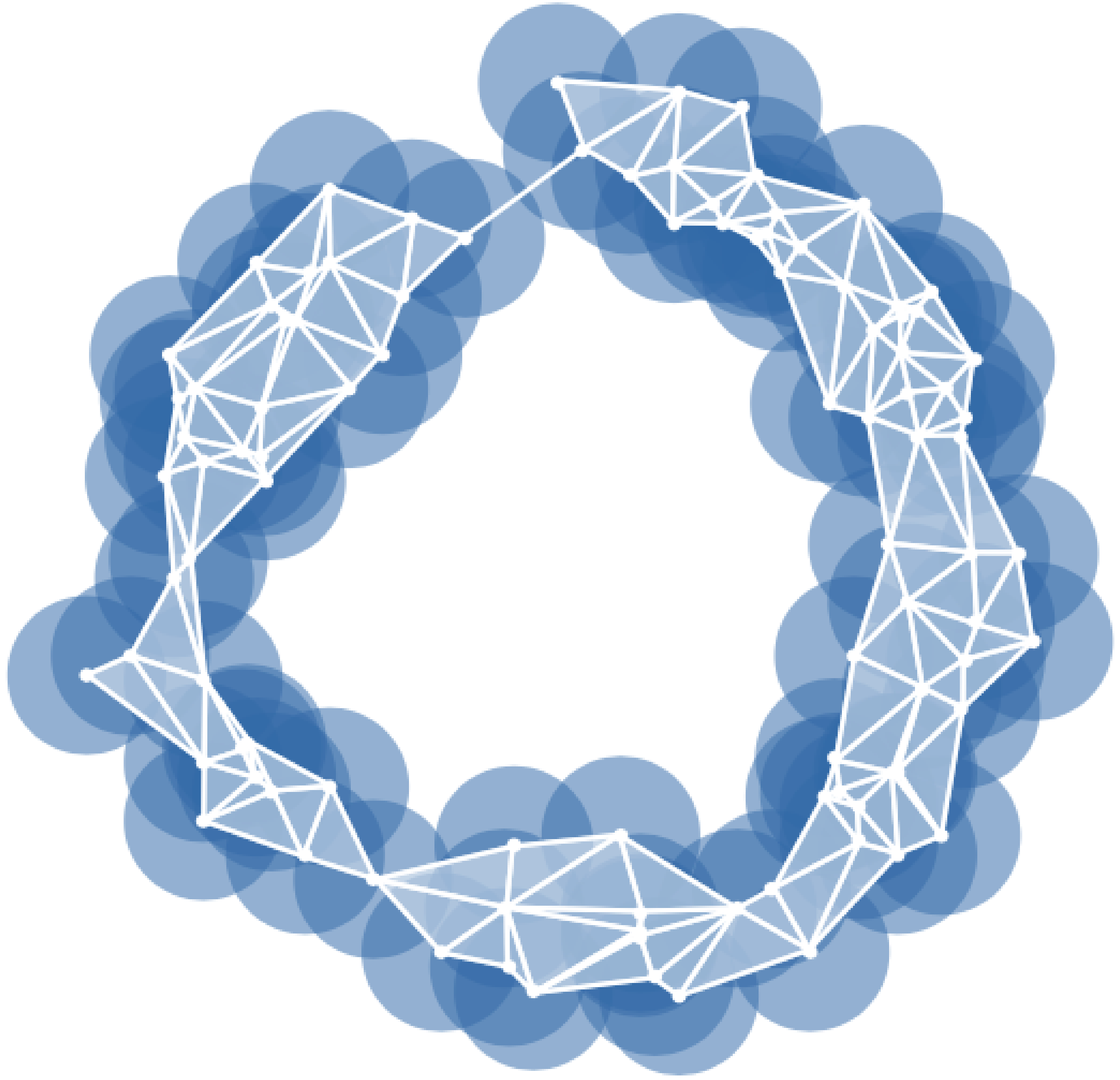


[Bauer 2019]

# The Idea of Persistence

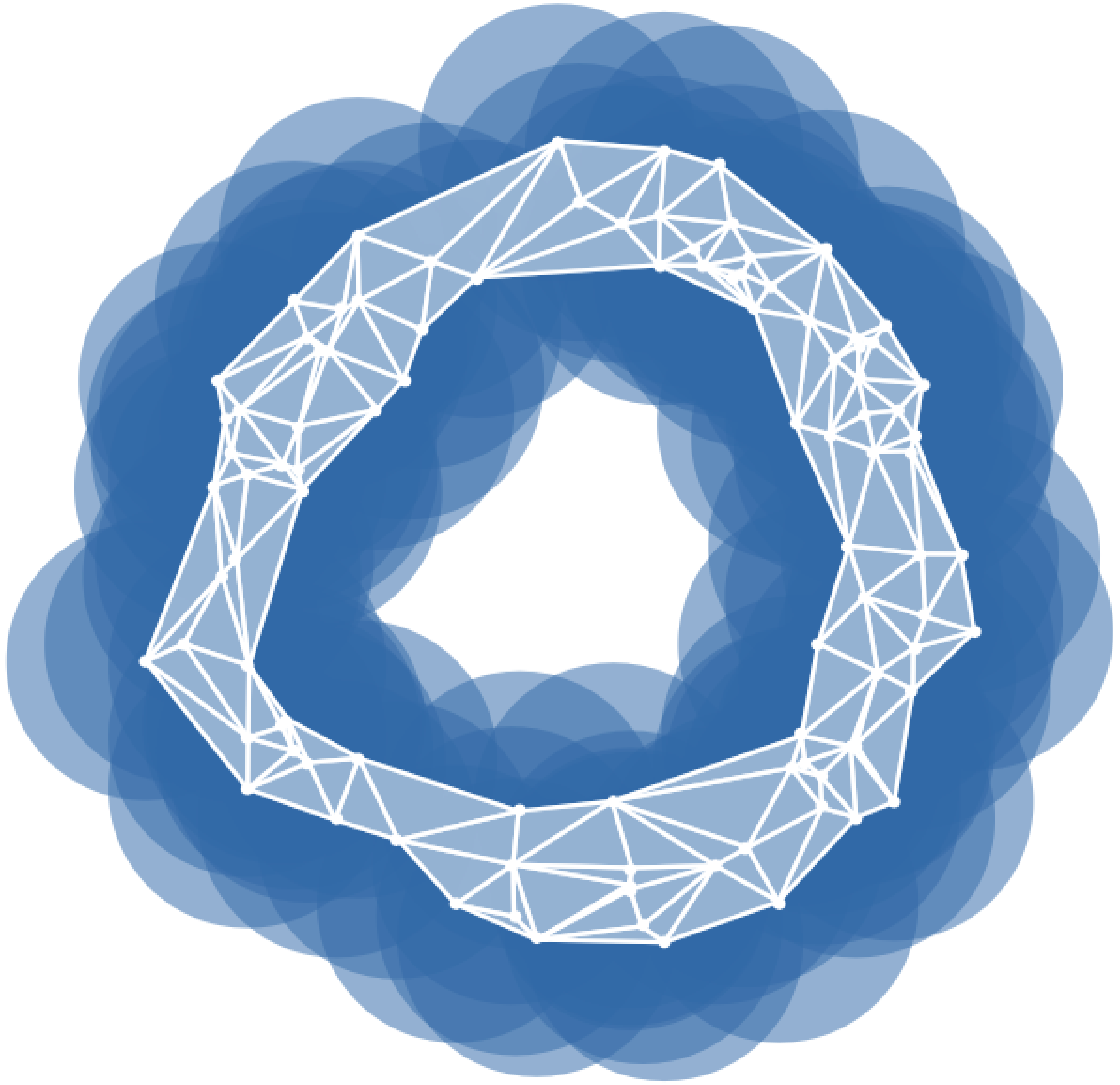


[Bauer 2019]

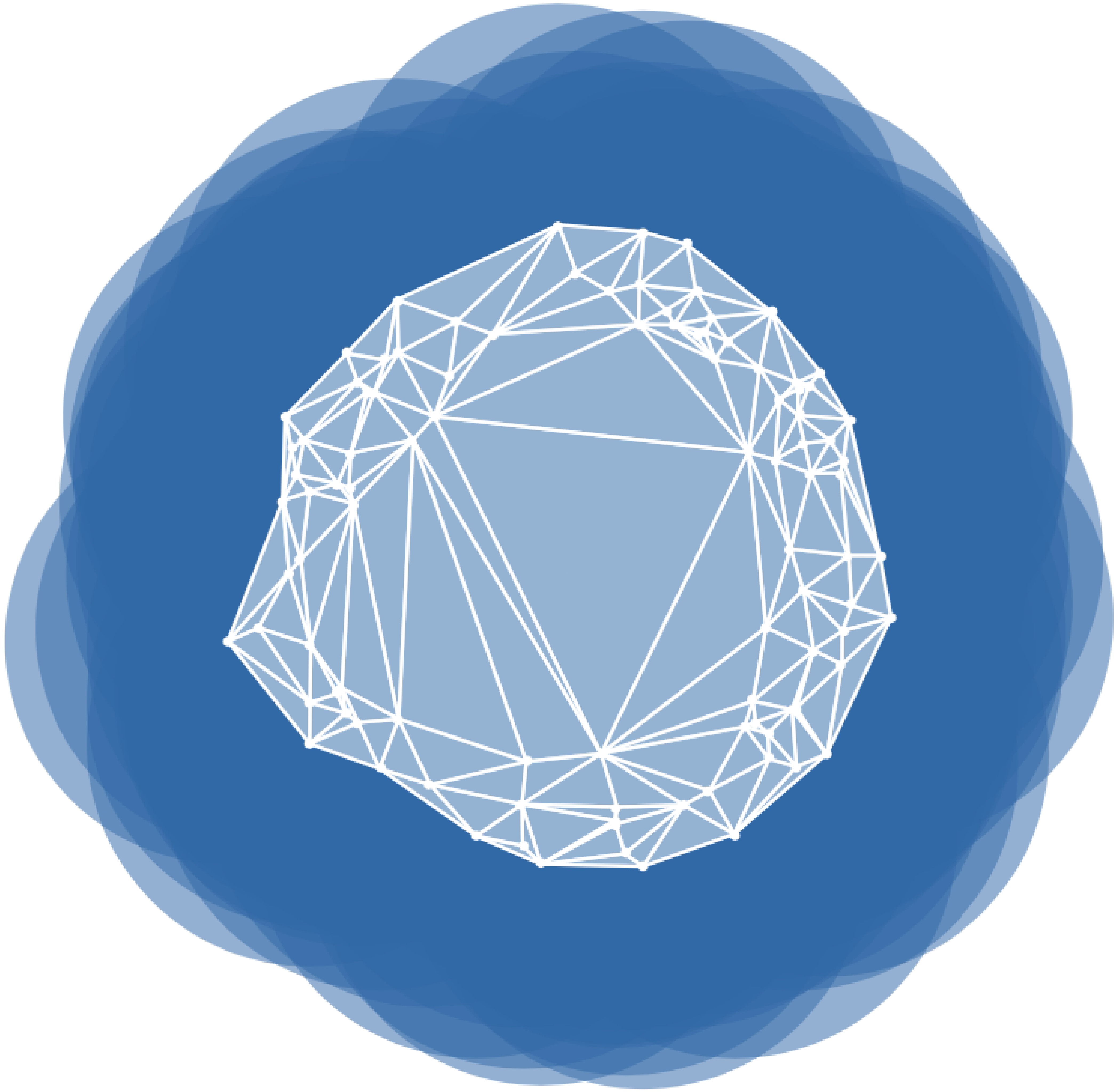


[Bauer 2019]

# The Idea of Persistence

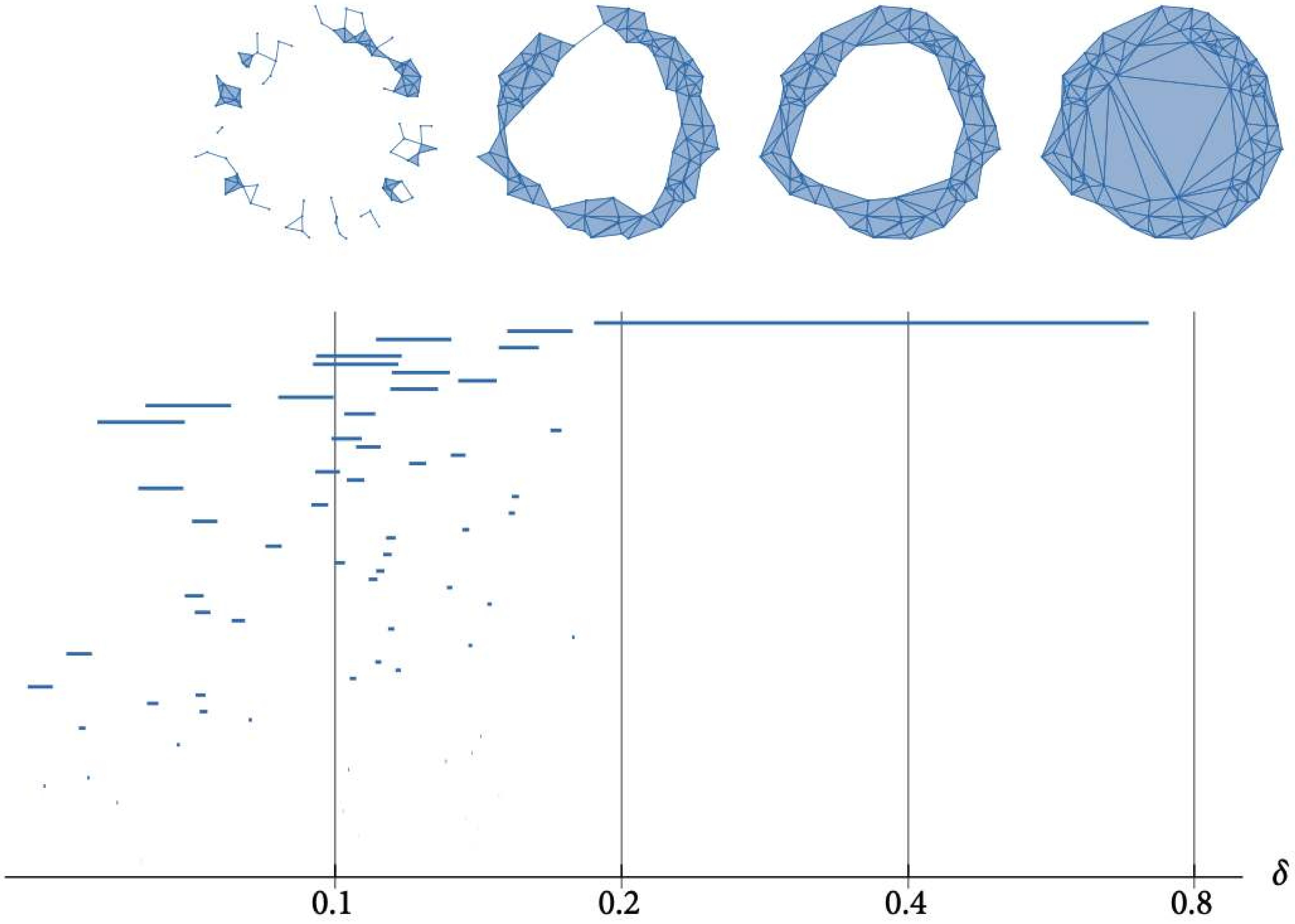


[Bauer 2019]



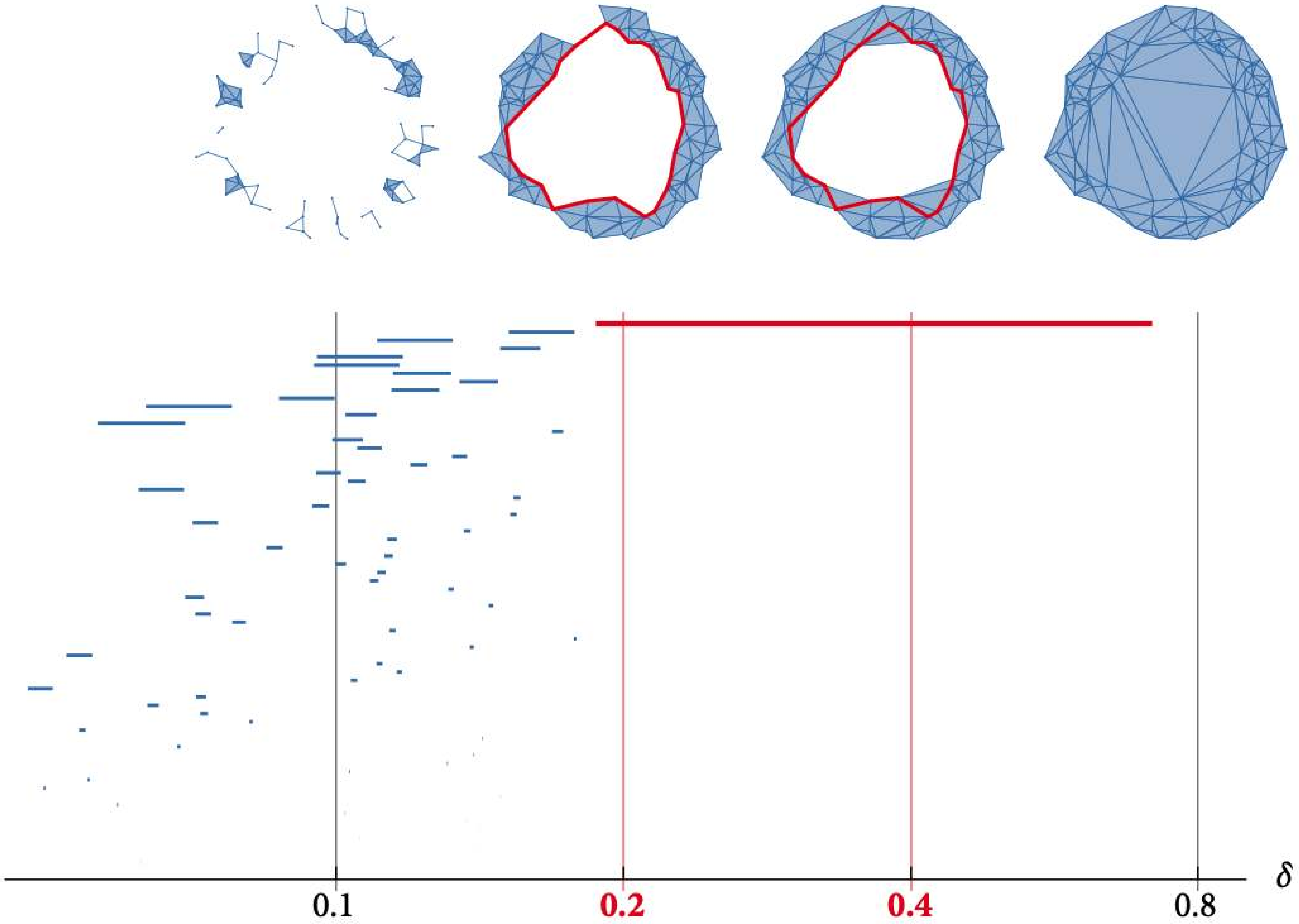
[Bauer 2019]

# The Idea of Persistence




[Bauer 2019]

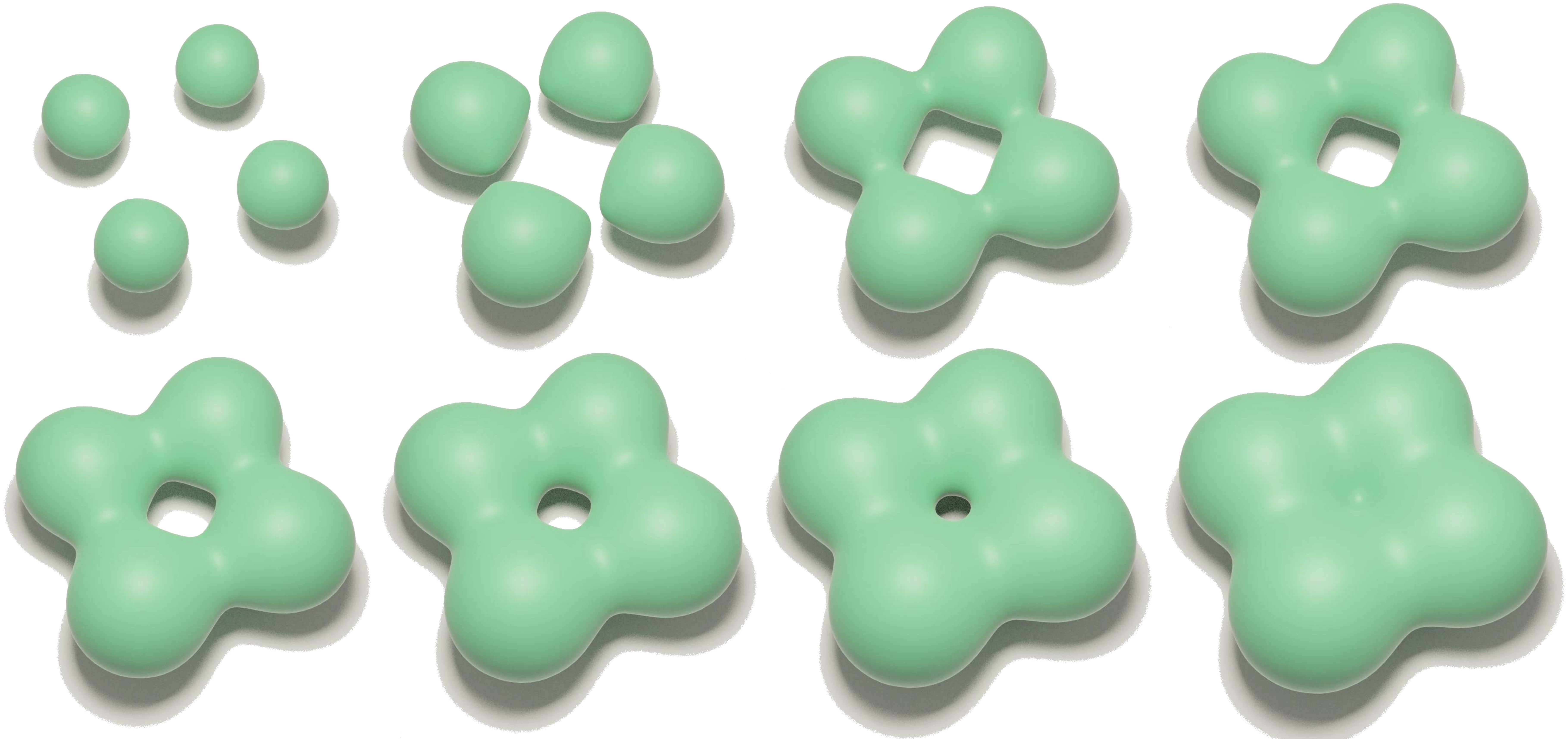
# The Idea of Persistence



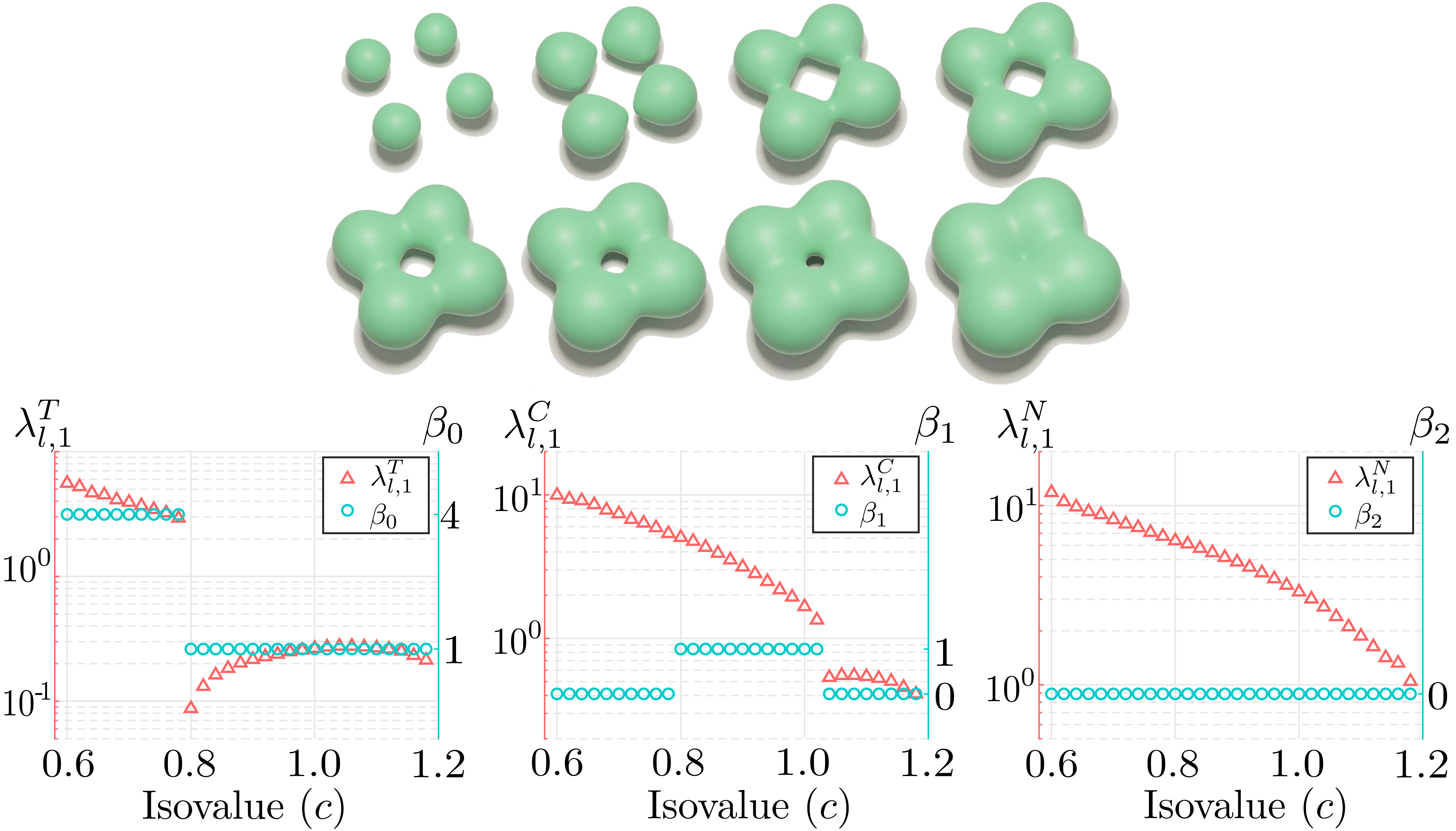

[Bauer 2019]

# The Idea of Persistence

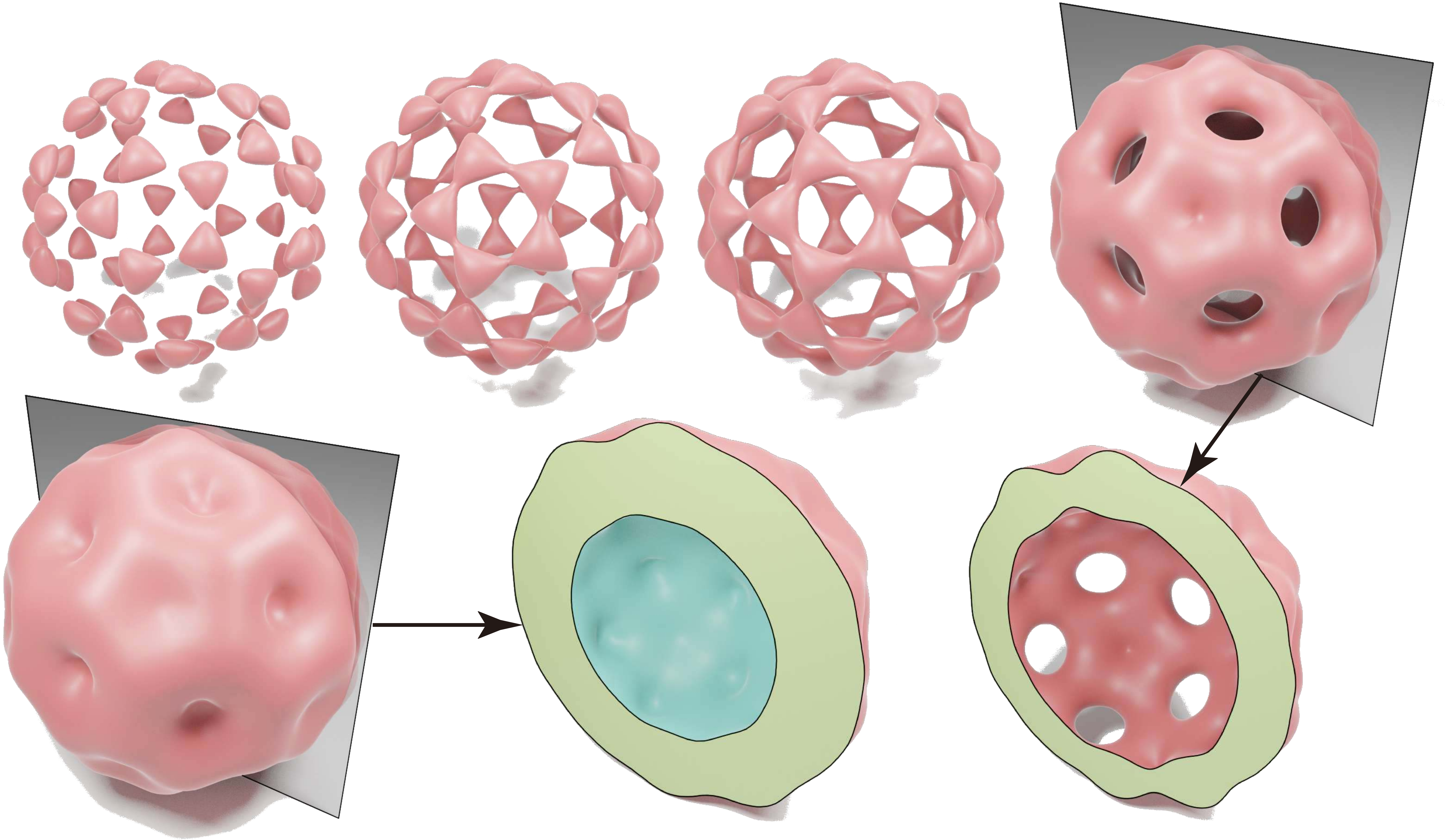
- Topology information is captured.
- Geometry information is lost.



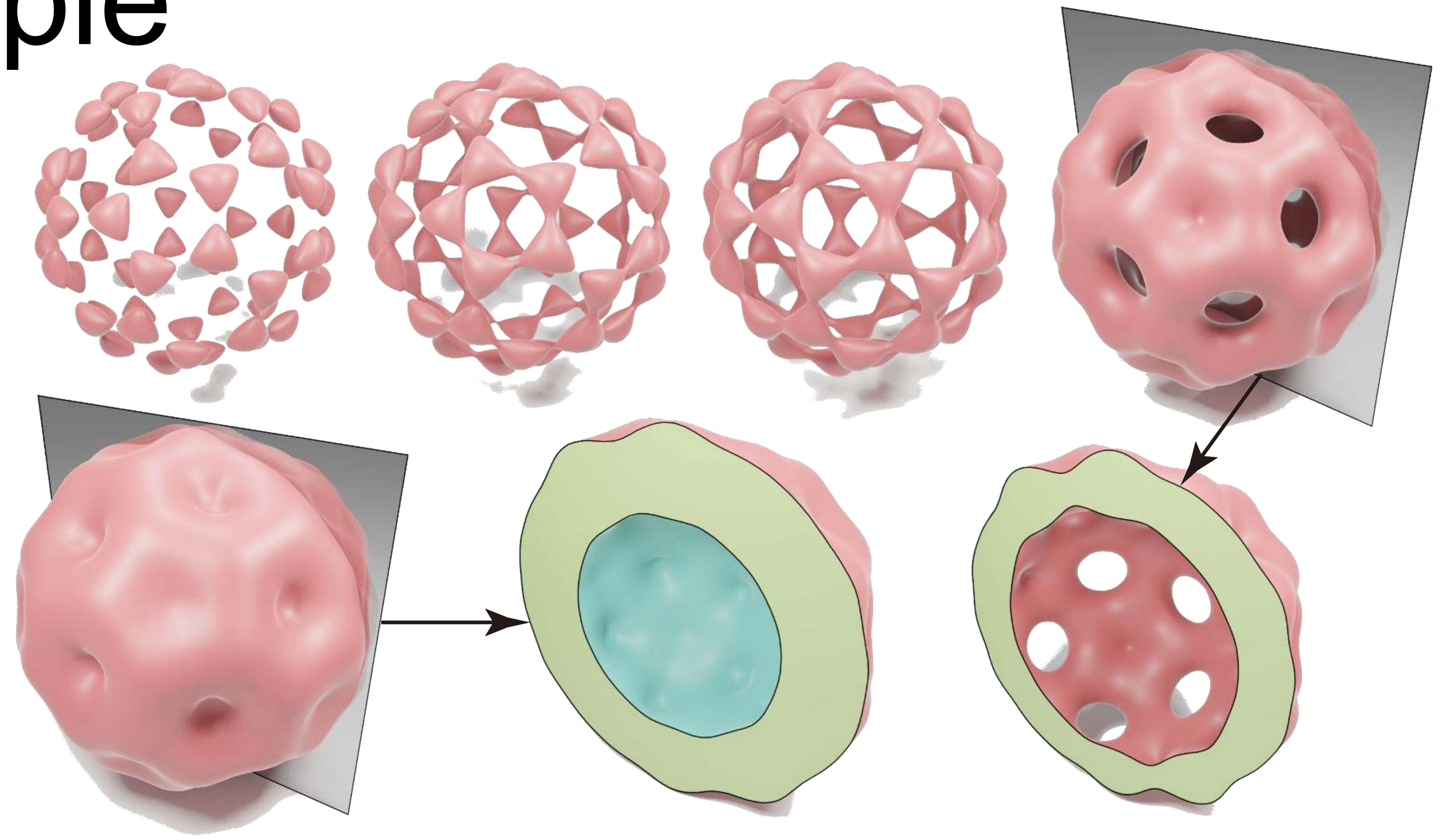
# Capture Geometry Information

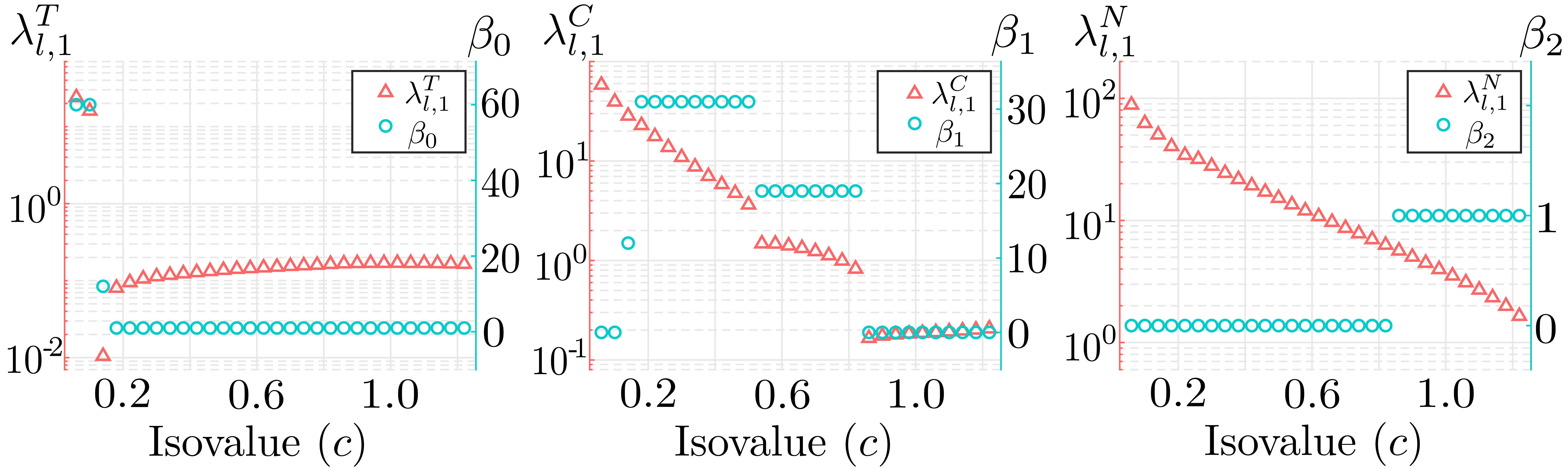


# Another Example

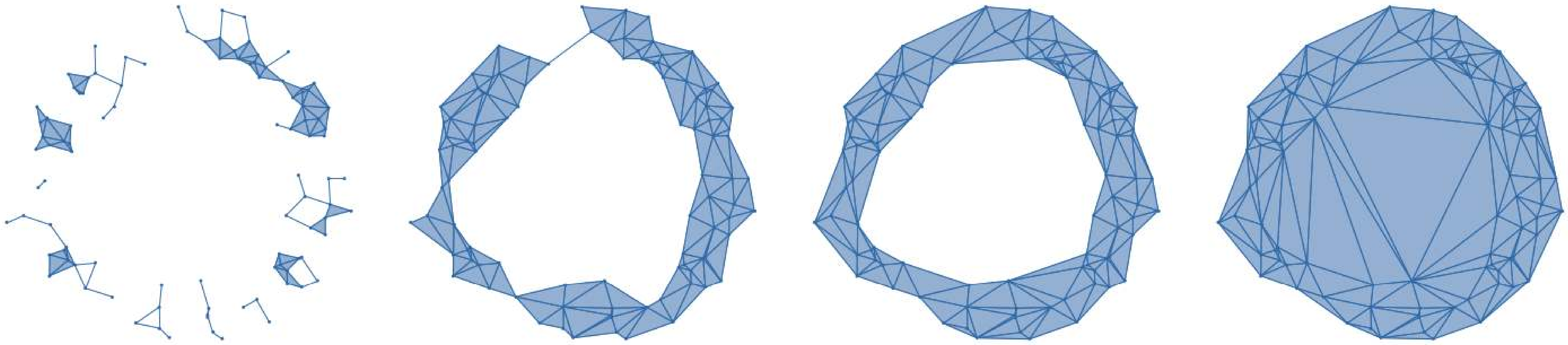


# Another Example





# Theory - Persistent Homology

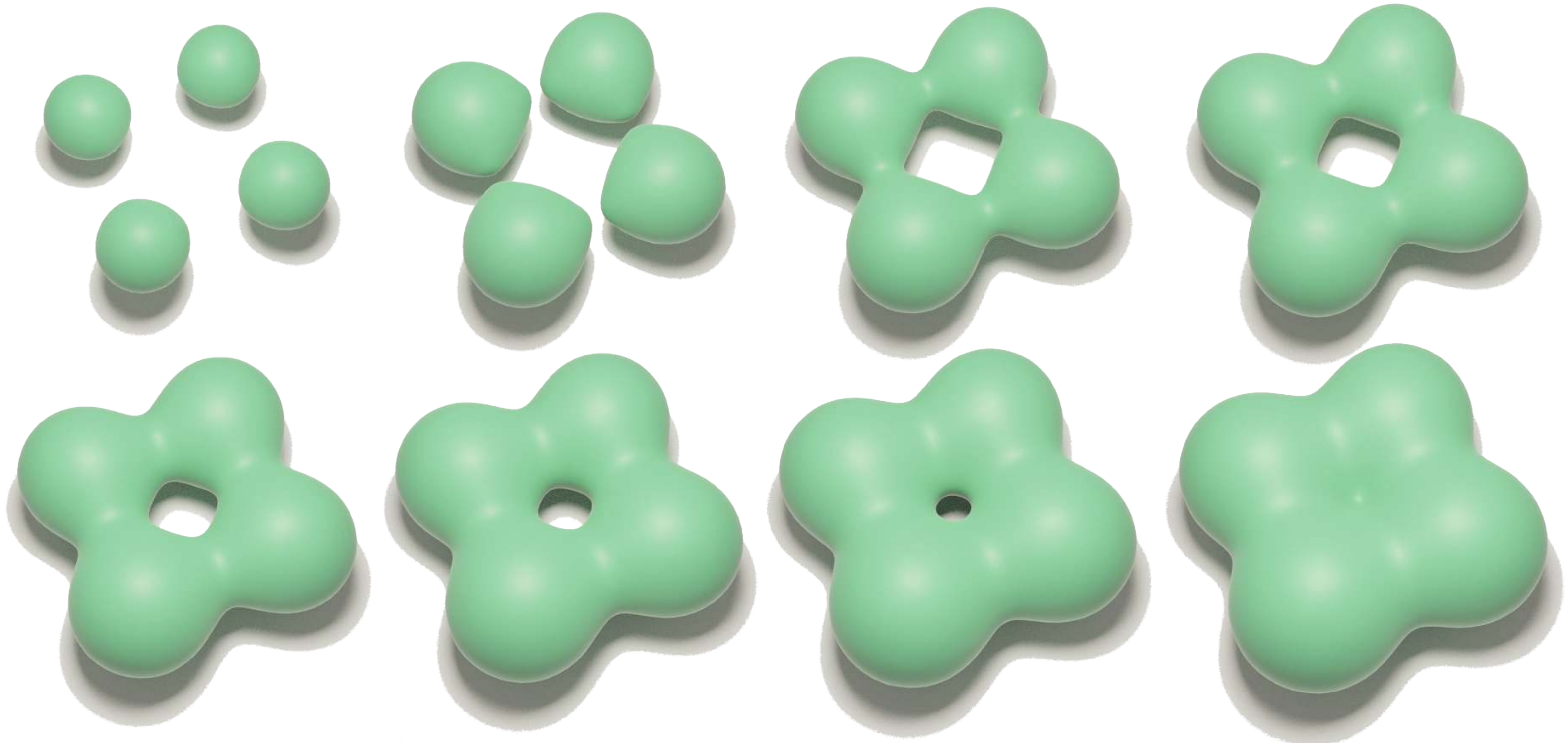


$$\varnothing = K_0 \to K_1 \to \ldots \to K_n = K$$

Inclusion Map: $K_i \hookrightarrow K_{i+1}$

$\Rightarrow$ Homomorphism: $f_p^{i,i+1} : H_p(K_i) \to H_p(K_{i+1})$

# Theory - Our Extension



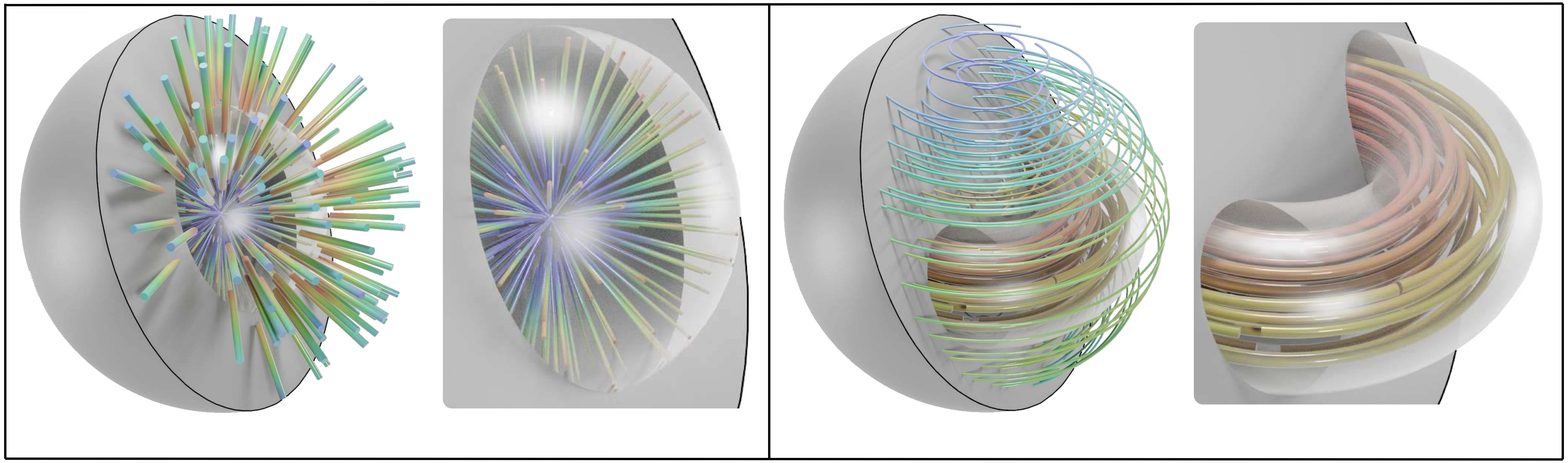
$$\emptyset = K_0 \to K_1 \to \ldots \to K_n = K$$

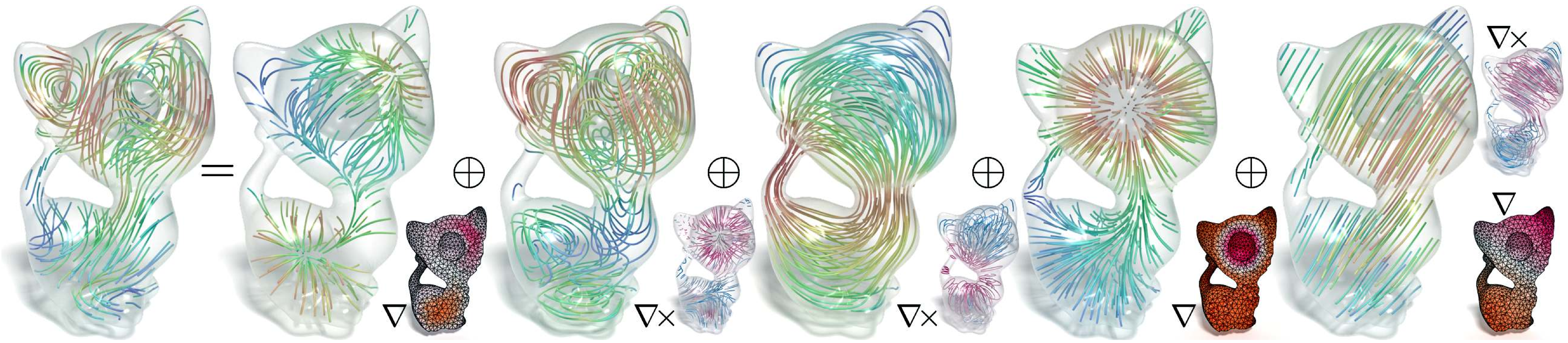
Inclusion Map: $K_i \hookrightarrow K_{i+1}$

$\Rightarrow$ Homomorphism: $f^p_{i,i+1} : H^p(K_i) \to H^p(K_{i+1})$

# Differential Form Extension

Homomorphism: $f^p_{i,i+1} : H^p(K_i) \to H^p(K_{i+1})$



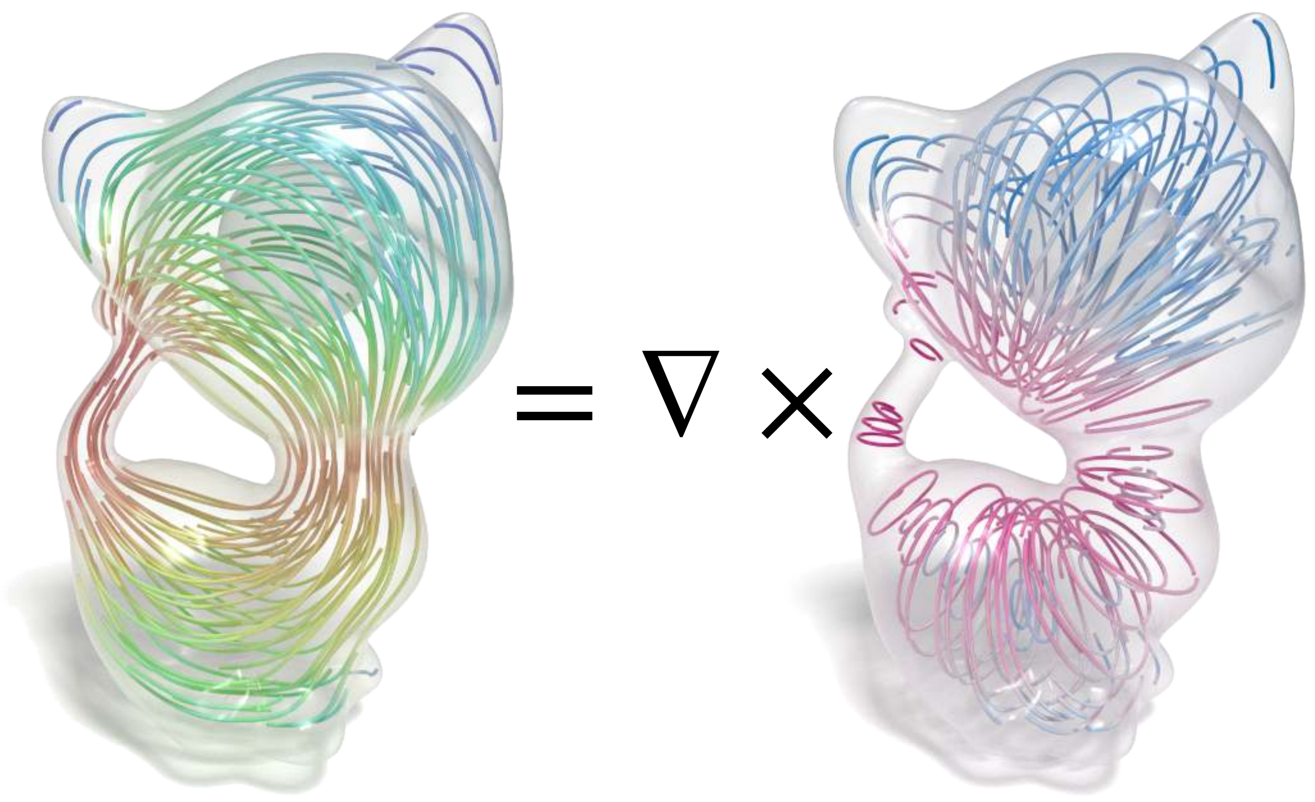



# Section V: Summary

# Summary

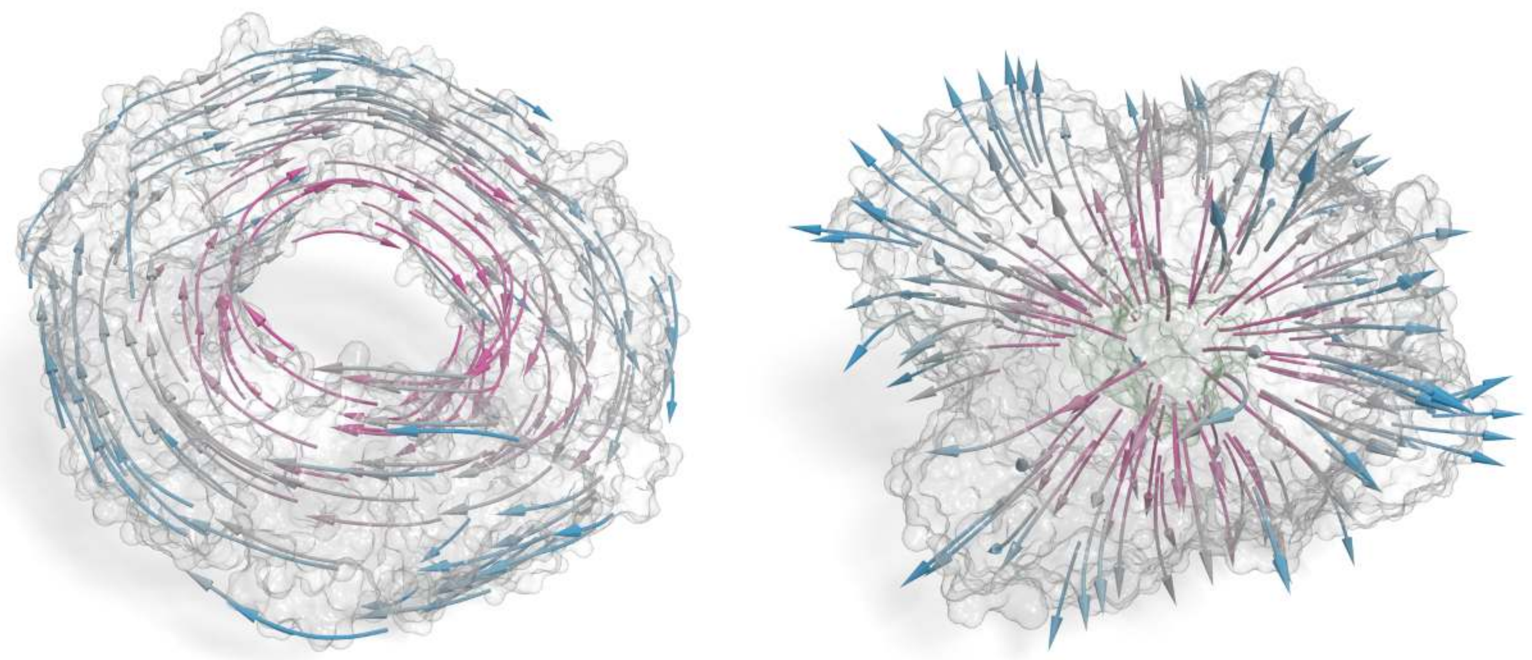
## Discrete Theory

- Boundary Condition
- Arbitrary Topology
- Efficient
- Accurate
- Versatile



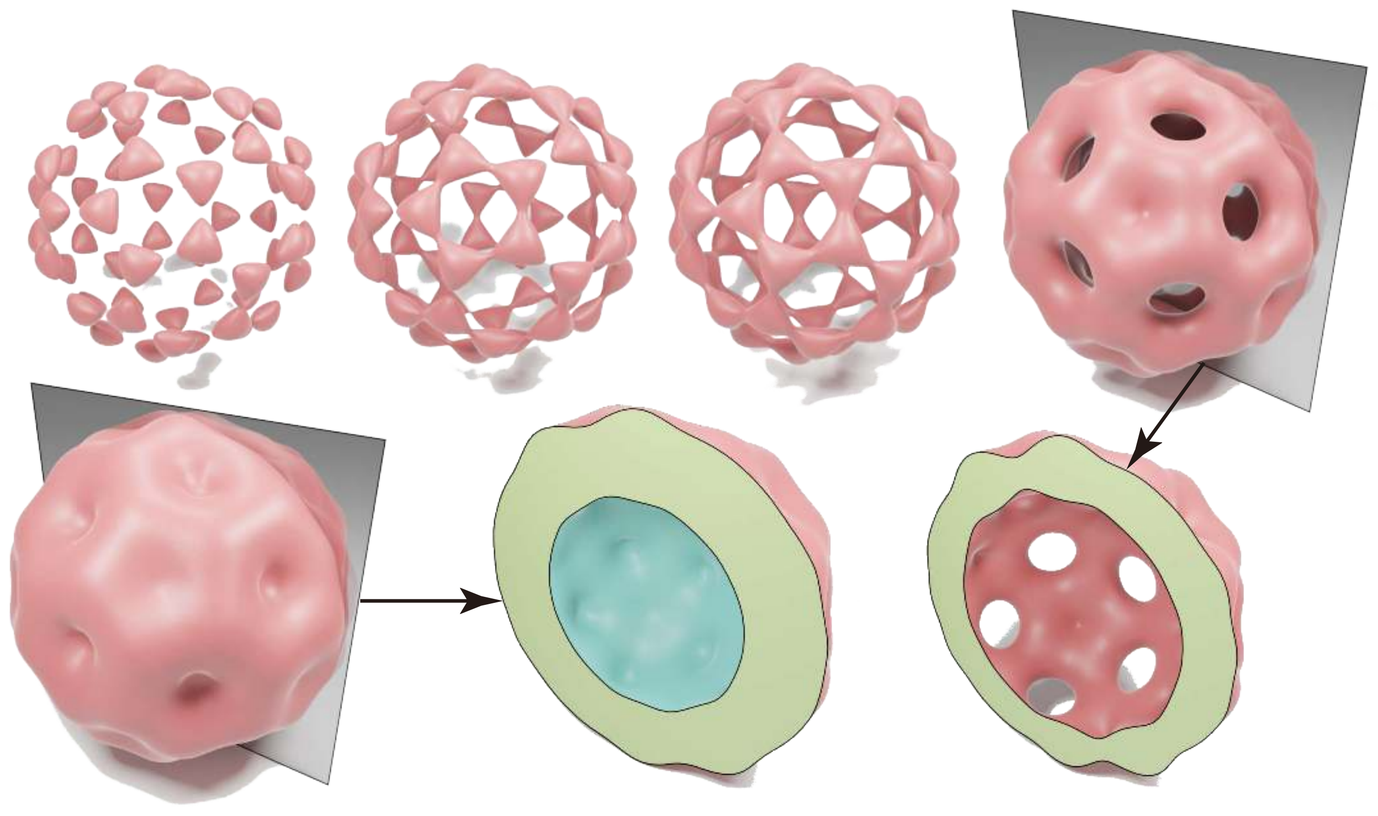

## Spectral Analysis

- Group the spectra into 3 sets
- A direct application on shape analysis



## Evolutionary Analysis

- Bring the idea of persistence homology
- Providing additional information with geometric progression



# Reference

[1] R. Zhao, M. Desburn, G. W. Wei, and Y. Tong, 3D hodge decompositions of edge- and face-based vector fields, *ACM Transactions on Graphics* 38 (6), 1-13, 2019

[2] R. Zhao, M. Wang, J. Chen, Y. Tong, and G. W. Wei, The de Rham-Hodge analysis and modeling of biomolecules, *Bulletin of Mathematical Biology* 82 (8), 1-38, 2020

[3] J. Chen, R. Zhao, Y. Tong, and G. W. Wei, Evolutionary de Rham-Hodge method, *DCDS-B* 25, 2020

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# Thank you!