Lecture 8: de Rham-Hodge Theory Based Modeling and Analysis

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Motivation and objective

Motivation:

To understand the structure, function, dynamics, and transport of biological macromolecules.

Objective:

To establish a unified paradigm to analyze the geometry, topology, flexibility and natural mode of macromolecules so to reveal their function, dynamics and transport.

Feasibility:

de Rham-Hodge theory bridges algebraic topology, differential geometry, partial differential equation, spectral geometry, and geometric algebra. Therefore, it has the potential.

de Rham-Hodge theory

- de Rham-hodge theory is a landmark of the 20th century's mathematics.
- It bridges algebraic topology, differential geometry, partial differential equation, spectral geometry, and geometric algebra.
- It has applications to quantum field theory, fluid dynamics, electrodynamics, computer science, etc.

Georges de Rham (September 10 1903 – October 9 1990), a Swiss mathematician, identified de Rham cohomology group as topological invariants.

Sir William Vallance Douglas Hodge (June 17 1903 – July 7 1975) discovered far-reaching topological relations between algebraic geometry and differential geometry—an area now called Hodge theory, having been a major influence on modern geometry.

Spectral geometry

Spectral geometry studies the relationship between manifold geometry and the spectra of differential operators (like Hodge Laplacian) defined on the manifold.

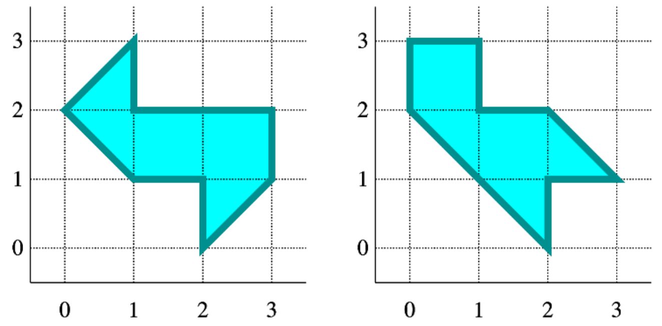
Hermann Weyl shew in 1911 that the asymptotic behavior of the eigenvalues for the Dirichlet boundary value problem of the Laplace operator on bounded domain in Euclidean space determines the volume of the domain.

Mark Kac (1966): Can one hear the shape of a drum?

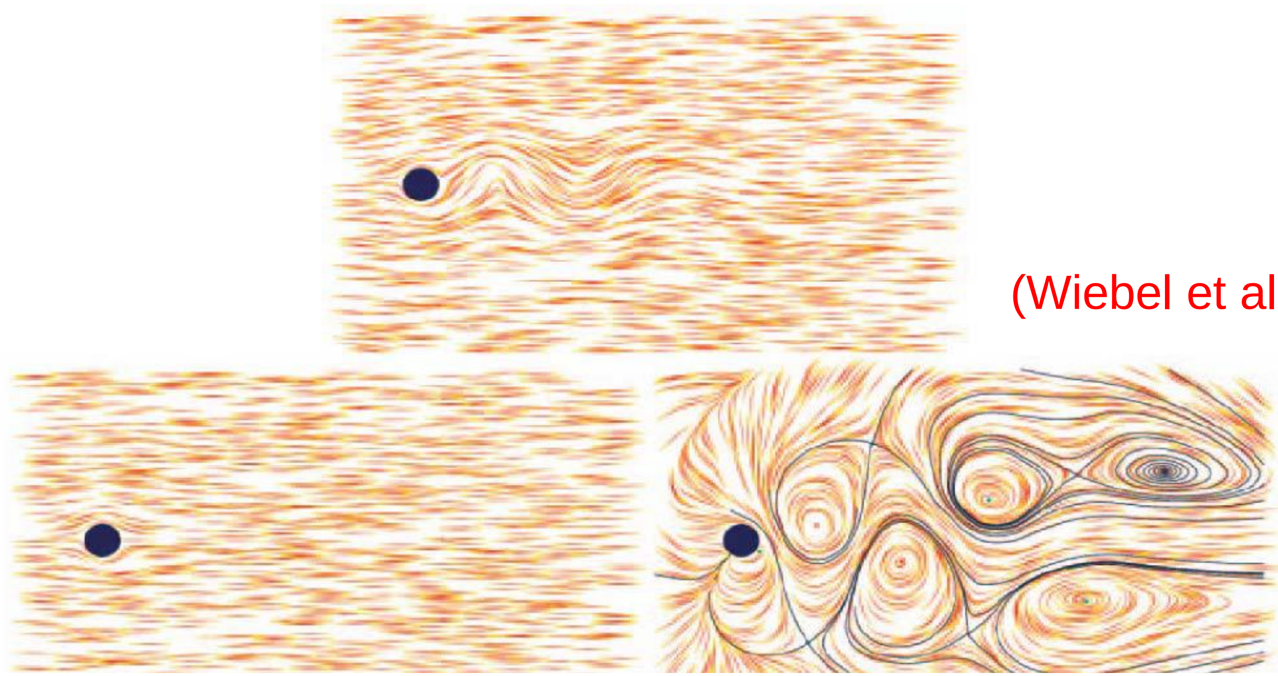
Gordon, Webb and Wolpert (1992): No in 2D, due to isospectra for isometry class of manifolds.

Question:

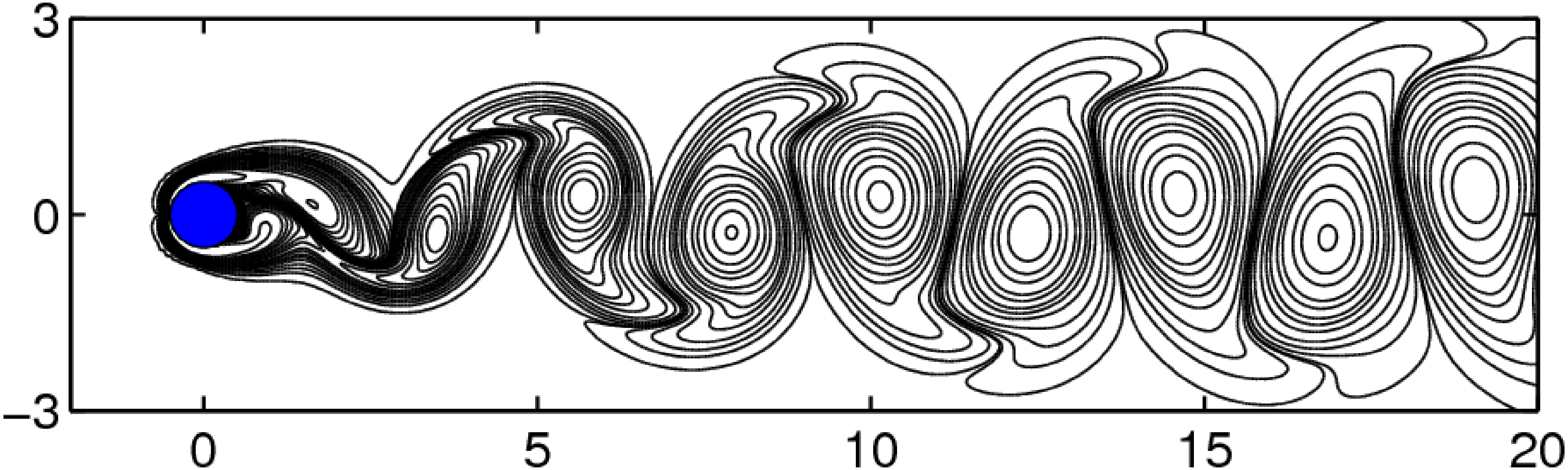
How much can one get from the spectra of a Hodge Laplacian defined on a given molecular structure and how to get more?



2D Hodge decomposition

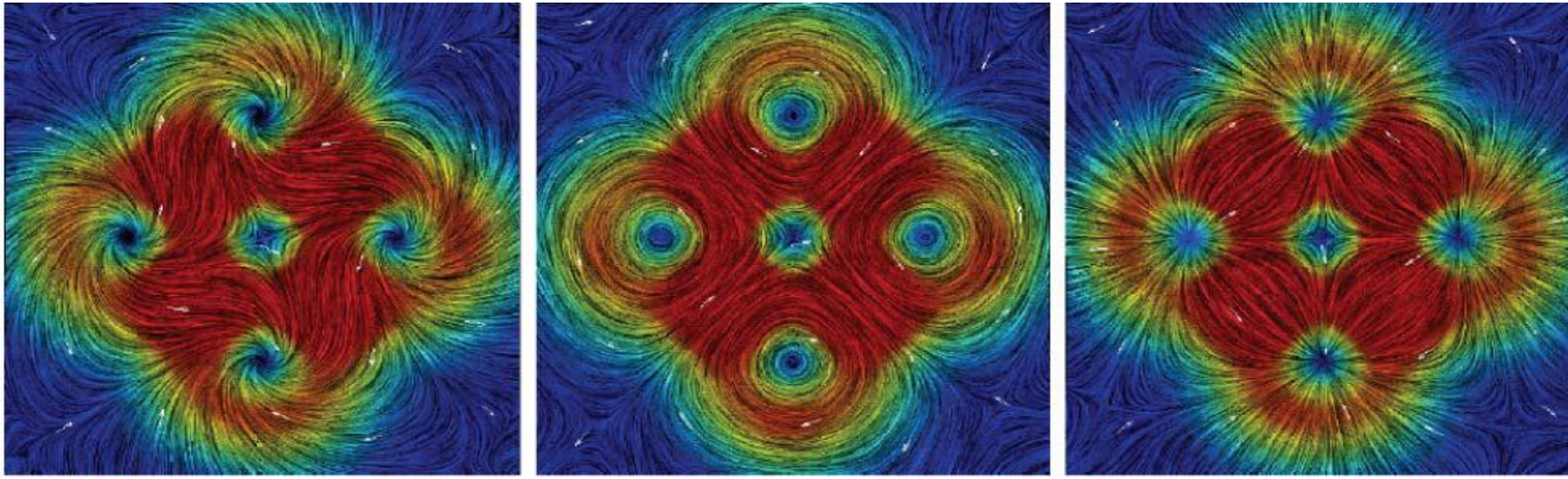


(Wiebel et al, Thesis, 2007)



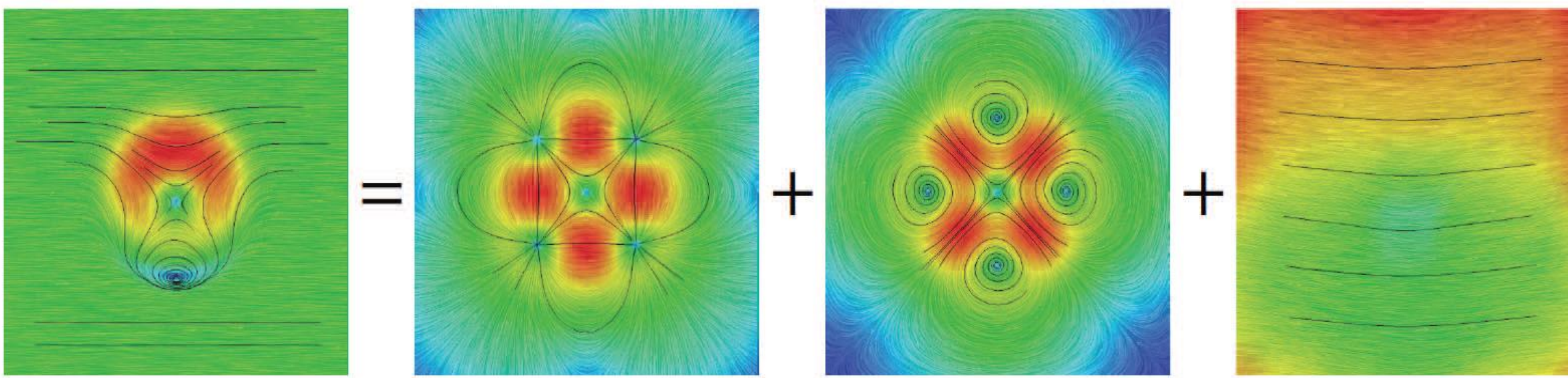
(YH Sun, YC Zhou and Wei, 2005)

Hodge decomposition of simulated fields in 2D



Original field divergence-free curl-free

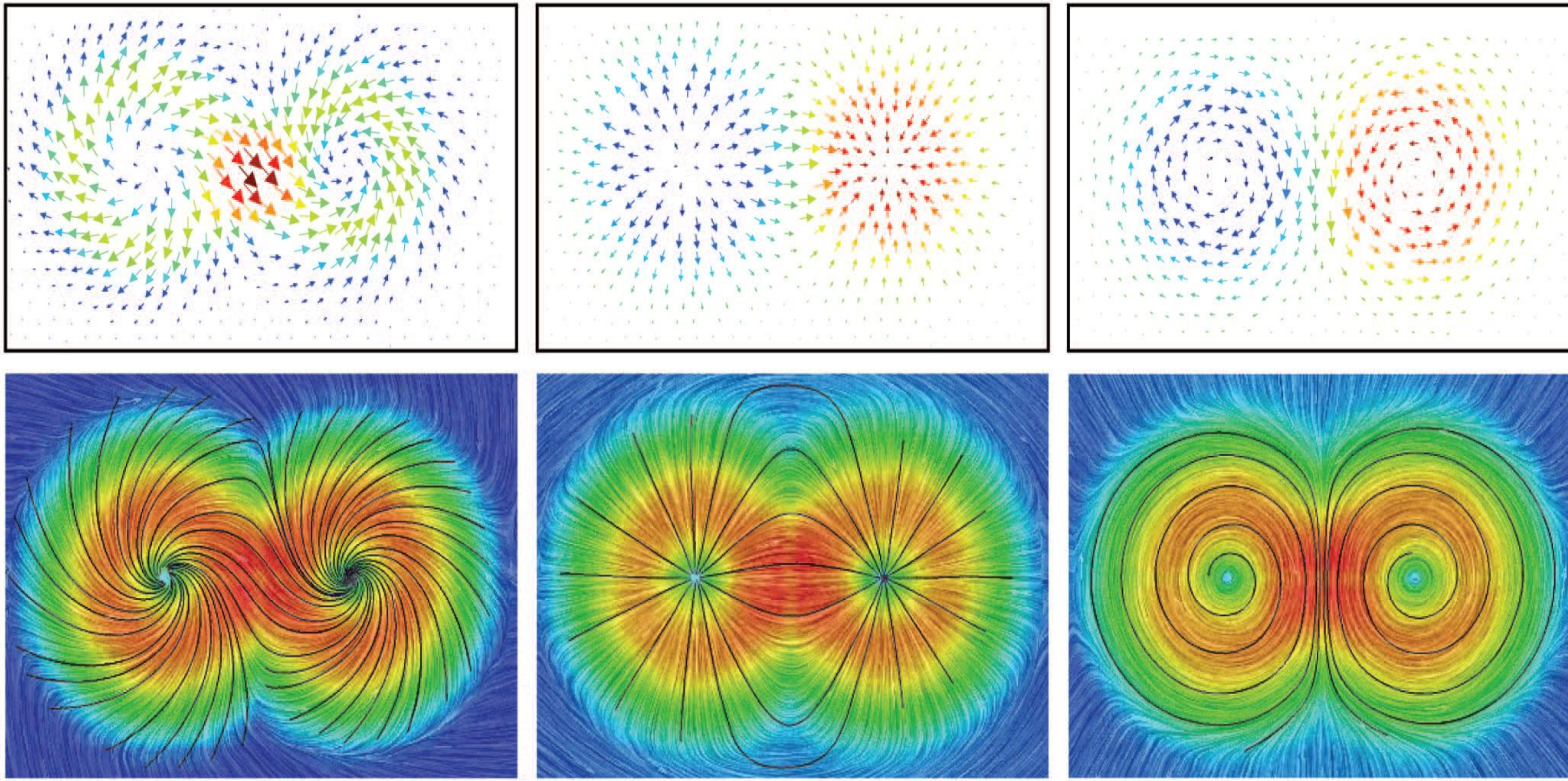
(Macedo and Castro, Technical Report 2010)



Original field curl-free divergence-free harmonic

(Petronetto et al. IEEE TVCG 2010)

Hodge decomposition of synthetic fields in 2D



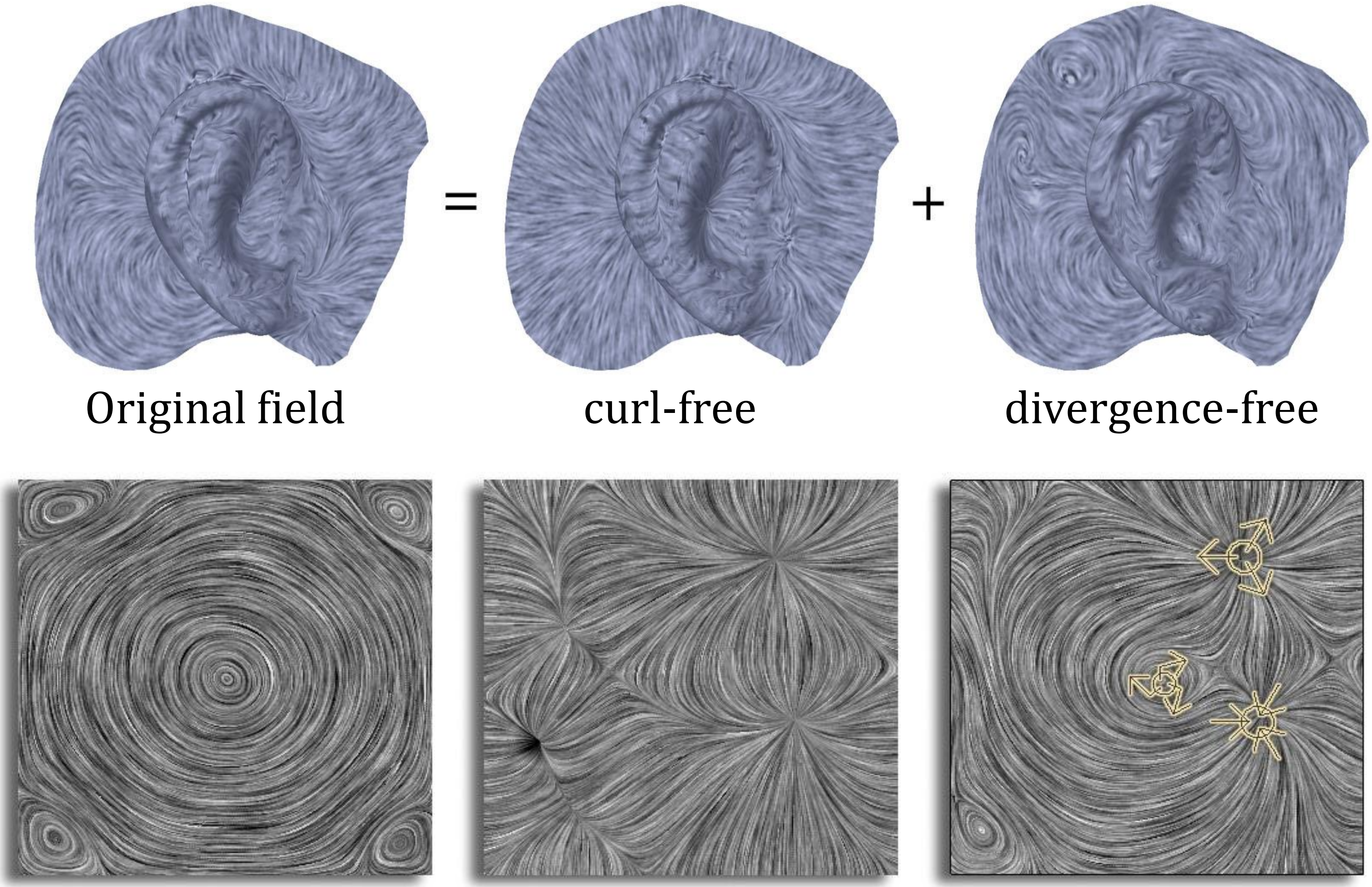
(a) Original field

(b) curl-free

(c) divergence-free

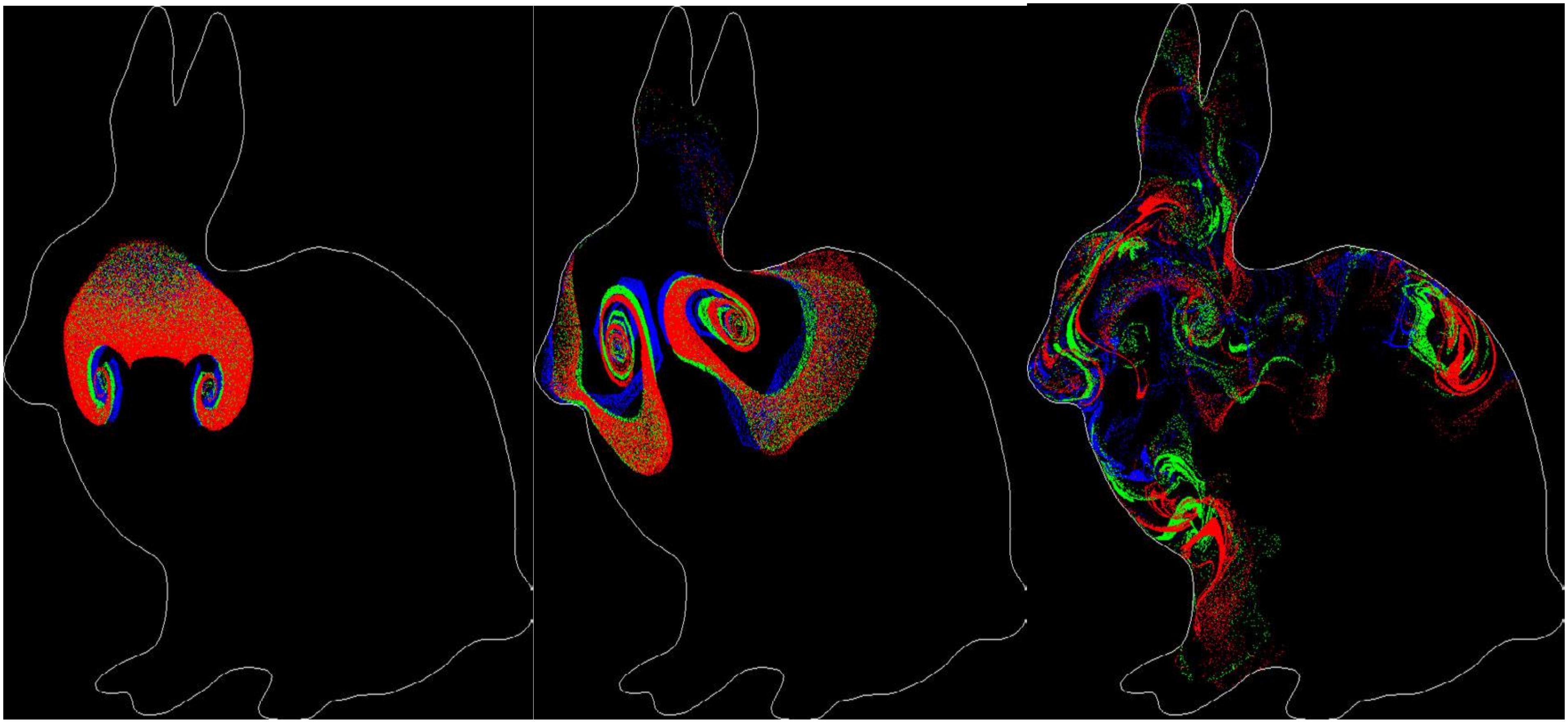
(Petronetto et al. IEEE TVCG 2010)

Hodge decomposition



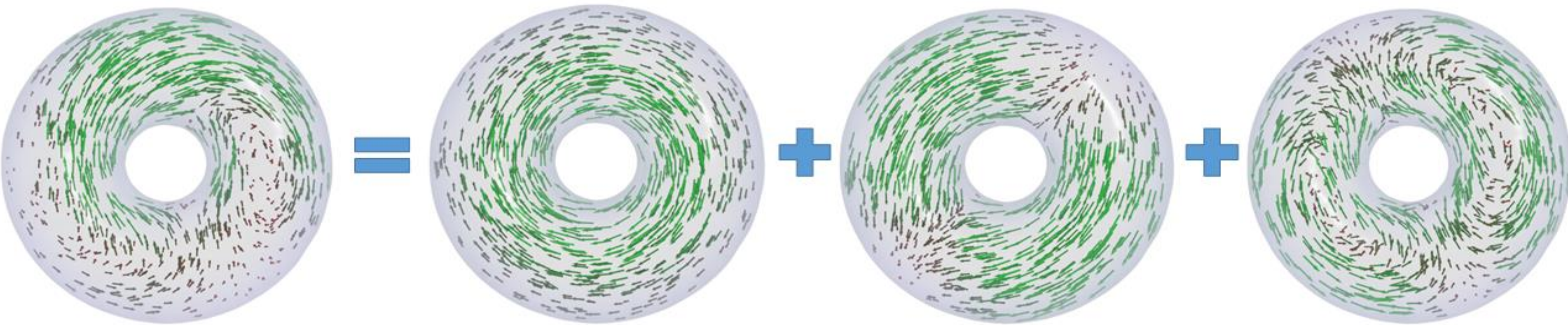
(Tong, Lombeyda, Hirani & Desbrun, ACM TG, 2003)

Hodge decomposition



(Beibei Liu, Mason, Hodgeson, Tong, & Desbrun, ACM DL, 2015)

3D Hodge decomposition

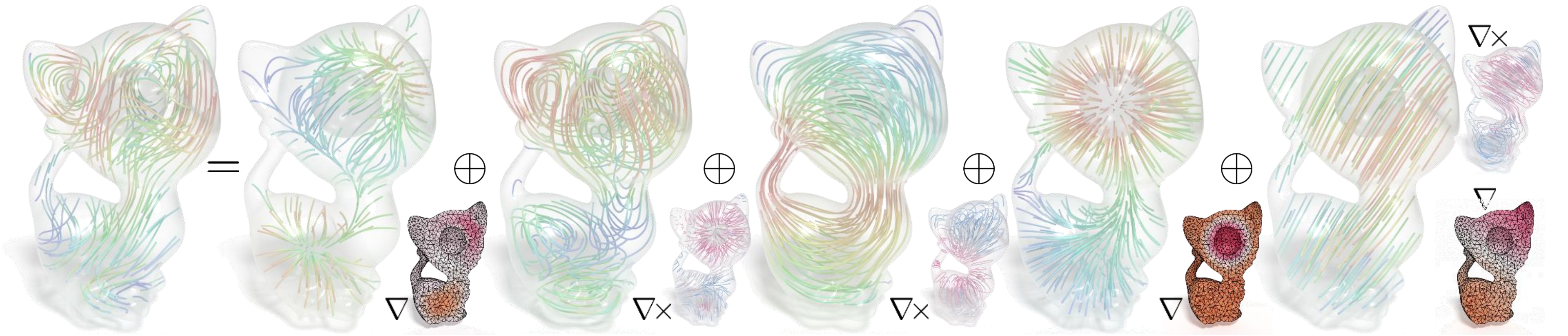


Vector field = harmonic + curl-free + divergent-free

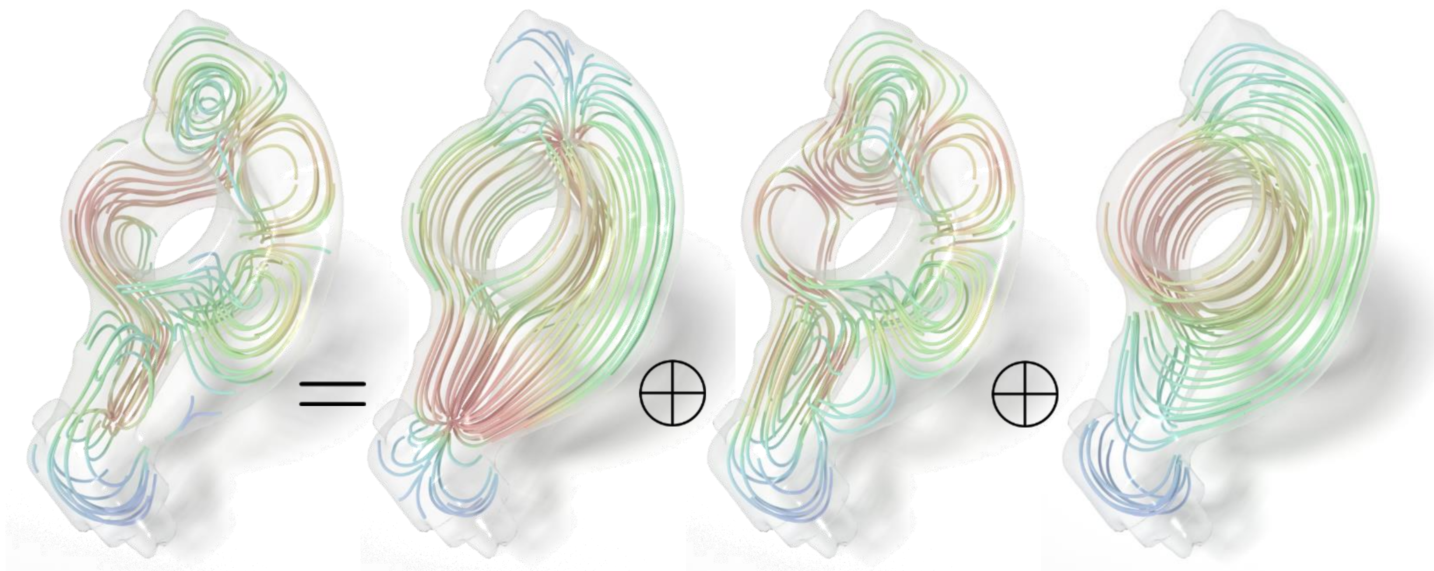
Vector field = curl-free + divergent-free + two harmonic terms

(Zhao, Desbrun, Wei, & Tong, 2019)

Five-Component Vector Field Decomposition



Original=curl-free+divergence-free+ 3 harmonic fields



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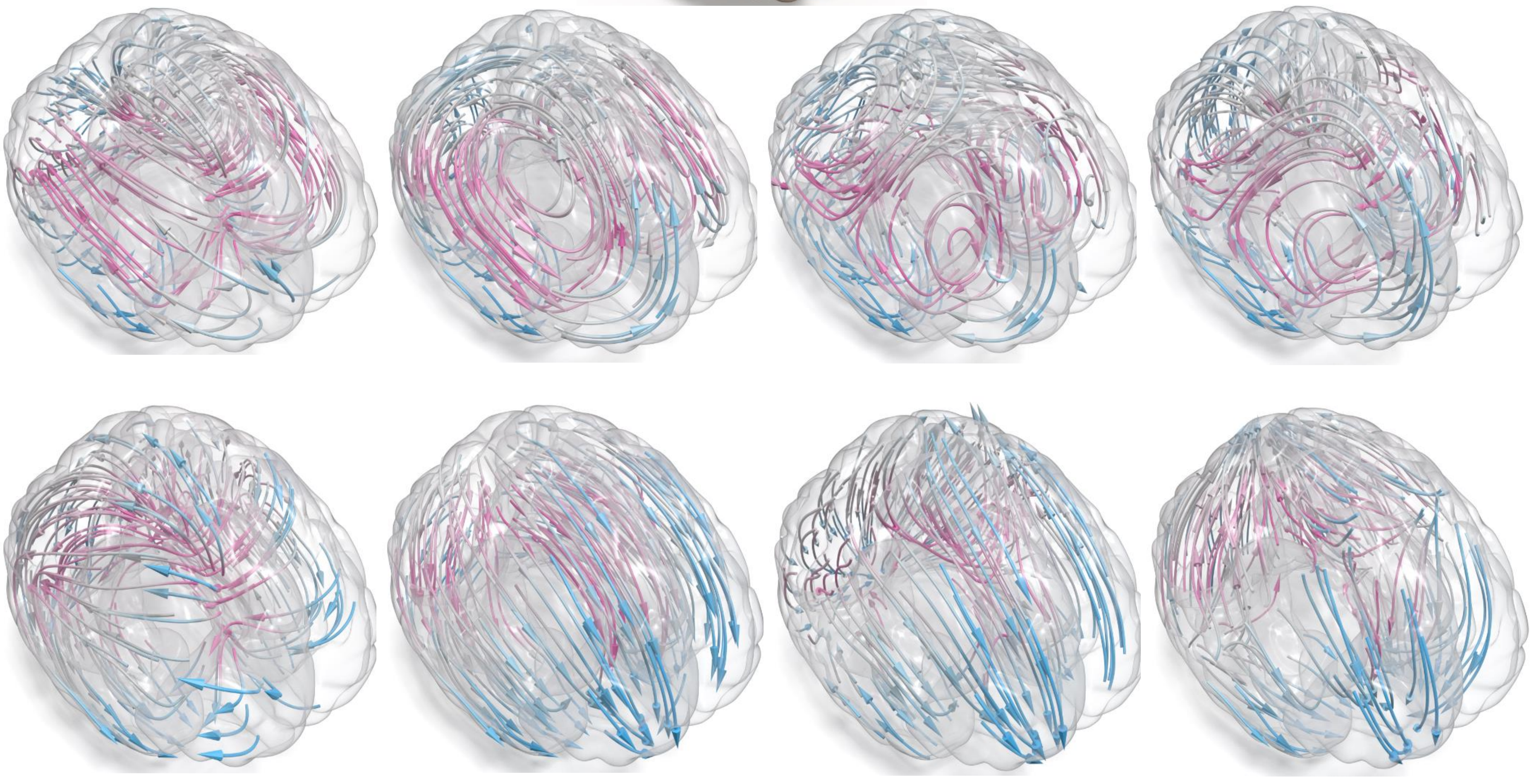
Tangential field = tangential gradient field+ tangential curl field + tangential harmonic field.

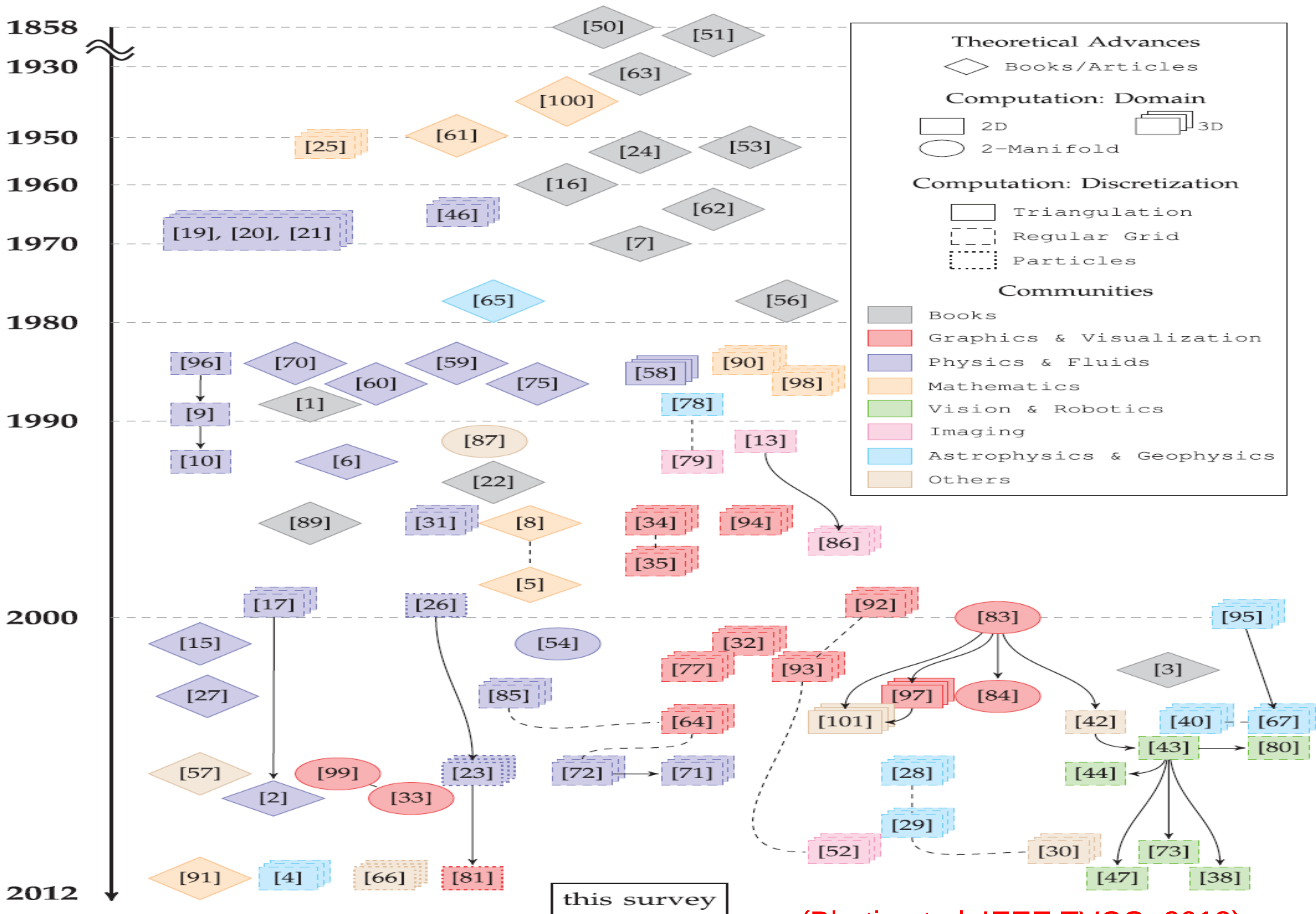
(RD Zhao, M Desbrun, GW Wei, YY Tong, 2019)

Eigenmodes of the vector Hodge-Laplacian operator

(Zhao, Desbrun, Wei, & Tong, 2019)



2013 Survey of Hodge decomposition

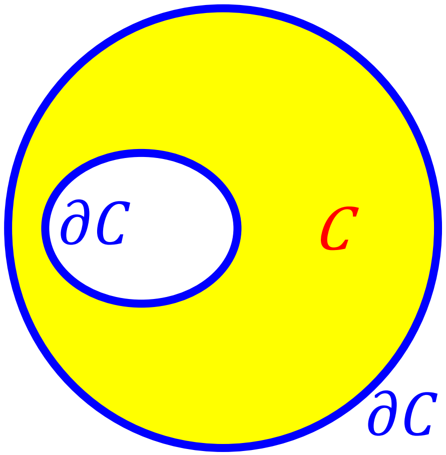


(Bhatia et al, IEEE TVCG, 2013)

Green's theorem and Stokes' theorem

Green's theorem in $\mathbb{R}^2$:

$$\oint_{\partial C} P dx + Q dy = \iint_C \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) dx dy$$



Two differential forms

1 − form: $\mathbf{A} = P dx + Q dy$

2 − form: $\mathrm{d}\mathbf{A} = \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right) dx dy$

Here d denotes the exterior divertive d: p-form to (p+1) form.

Stokes's theorem:

$$\oint_{\partial C} \mathbf{A} = \iint_C \mathrm{d}\mathbf{A}$$

Here C is the domain and is called a *chain* in topology. ∂C is the boundary and the boundary of a boundary vanishes: $\partial\partial C = 0$

Stokes theorem in $\mathbb{R}^3$: $\oint_\Gamma \boldsymbol{F} \cdot d\Gamma = \iint_S \nabla \times \boldsymbol{F} \cdot d\boldsymbol{S}$

Exterior derivatives and differential forms

More general, in $\mathbb{R}^3$

0 – form (scalar field, $\Omega^0(\mathbb{R}^3)$): $f = f(x,y,z)$

1 – form (gradient, $\Omega^1(\mathbb{R}^3)$): $\boldsymbol{\omega} = \mathrm{d}f = \dfrac{\partial f}{\partial x}dx + \dfrac{\partial f}{\partial y}dy + \dfrac{\partial f}{\partial z}dz$

2 – form (curl, $\Omega^2(\mathbb{R}^3)$): $\alpha = \mathrm{d}\boldsymbol{\omega}$

$$\mathrm{d}\boldsymbol{\omega} = \left(\frac{\partial R}{\partial y} - \frac{\partial Q}{\partial z}\right)dydz + \left(\frac{\partial P}{\partial z} - \frac{\partial R}{\partial x}\right)dzdx + \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y}\right)dxdy$$

$$\mathrm{d}\boldsymbol{\omega} = \det\begin{pmatrix} \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ P & Q & R \\ dydz & dzdx & dxdy \end{pmatrix}$$

Leibniz rule:

$\mathrm{d}\,(fg) = g\mathrm{d}f + f\mathrm{d}g$

`Chain' rule:

$\mathrm{d}\,f(g) = f'(g)\mathrm{d}g$

Boundary rule:

$\mathrm{dd}f = 0$ and $\mathrm{dd}\boldsymbol{\omega} = 0 \Rightarrow d^2 = 0$

3 – form (divergence, $\Omega^3(\mathbb{R}^3)$): $\beta = \mathrm{d}\alpha = \left(\dfrac{\partial A}{\partial x} + \dfrac{\partial B}{\partial y} + \dfrac{\partial D}{\partial z}\right)dxdydz$

de Rham-Hodge theory basics

A $p-$form β is called closed if its exterior derivative navishes

$$\mathrm{d}\beta = 0 \Rightarrow \text{conservation laws.}$$

A $p-$form β is called exact if it is an exterior derivative of some $(p-1)-$form: $\beta = \mathrm{d}\alpha, \;\Rightarrow\; \mathrm{d}\beta = \mathrm{dd}\alpha = 0.$

A cycle $C \in \mathcal{C}_p(M)$ is $p-$chain (or $p-$domain) such that $\partial C = 0.$

A boundary $C \in \mathcal{C}_p(M)$ is $p-$chain such that $C = \partial B.$ All boundaries are cycles: $\partial C = \partial\partial B = 0.$

A cocycle ω (i.e., closed form) is a cochain such that $\mathrm{d}\omega = 0.$

A coboundary ω (i.e., exact form) is cochain such that $\omega = \mathrm{d}\theta.$
All coboundaries are closed: $\mathrm{d}\omega = \mathrm{dd}\theta = 0.$

de Rham duality of forms (in geometry) and chains (in topology)

de Rham's period: $\Omega^p(M) \times \mathcal{C}_p(M) \to \mathbb{R}$:

$$\text{Period} := \int_C \omega := \langle C, \omega \rangle$$

Where $C \in \mathcal{C}_p(M)$ is a cycle and $\omega \in \Omega^p(M)$ is a cocycle.

Stokes theorem:

$$\int_{\partial C} \omega = \int_C d\omega \Leftrightarrow \langle \partial C, \omega \rangle = \langle C, d\omega \rangle$$

Where $C \in \mathcal{C}_p(M)$ is a cycle and $\omega \in \Omega^p(M)$ is a cocycle.

Main property of exterior differential:

$$0 = \langle \partial^2 C, \omega \rangle = \langle C, d^2 \omega \rangle = 0$$

de Rham chain and cochain complexes

de Rham's cochain complexes in

$$\mathbb{R}^1\colon\ 0 \to \Omega^0\ (\mathbb{R}^1) \underset{\text{der}}{\overset{\mathrm{d}}{\to}} \Omega^1(\mathbb{R}^1) \to 0$$

$$\mathbb{R}^2\colon\ 0 \to \Omega^0\ (\mathbb{R}^2) \underset{\text{grad}}{\overset{\mathrm{d}}{\to}} \Omega^1(\mathbb{R}^2) \underset{\text{rot}}{\overset{\mathrm{d}}{\to}} \Omega^2(\mathbb{R}^2) \to 0$$

$$\mathbb{R}^3\colon\ 0 \to \Omega^0\ (\mathbb{R}^3) \underset{\text{grad}}{\overset{\mathrm{d}}{\to}} \Omega^1(\mathbb{R}^3) \underset{\text{curl}}{\overset{\mathrm{d}}{\to}} \Omega^2(\mathbb{R}^3) \underset{\text{div}}{\overset{\mathrm{d}}{\to}} \Omega^3(\mathbb{R}^3) \to 0$$

$$\mathbb{R}^n\colon\ 0 \to \Omega^0\ (\mathbb{R}^n) \underset{\text{grad}}{\overset{\mathrm{d}}{\to}} \Omega^1(\mathbb{R}^n) \underset{\text{skew}}{\overset{\mathrm{d}}{\to}} \Omega^2(\mathbb{R}^n) \overset{\mathrm{d}}{\to} \cdots \overset{\mathrm{d}}{\to} \Omega^n(\mathbb{R}^n) \to 0$$

Vector calculus in $\mathbb{R}^3$:

$$\text{curl} \cdot \text{grad} = 0 \quad \text{and} \quad \text{div} \cdot \text{curl} = 0$$

de Rham's chain complexes in $\mathbb{R}^3$ as a duality:

$$0 \to \mathcal{C}_3(\mathbb{R}^3) \overset{\partial}{\to} \mathcal{C}_2(\mathbb{R}^3) \overset{\partial}{\to} \mathcal{C}_1(\mathbb{R}^3) \overset{\partial}{\to} \mathcal{C}_0(\mathbb{R}^3) \to 0$$

de Rham cohomology and homology

The pth de Rham's cohomology of a mnifold M :

$$H^p(M) := \frac{Z^p(M)}{B^p(M)} = \frac{\mathrm{Ker}\left(\mathrm{d}\colon \Omega^p(M) \to \Omega^{p+1}(M)\right)}{\mathrm{Im}\left(\mathrm{d}\colon \Omega^{p-1}(M) \to \Omega^p(M)\right)}$$

Where : $B^p(M) \subset Z^p(M) \subset \Omega^p(M)$

$Z^p(M)$: subspace of all closed $p-$ forms.

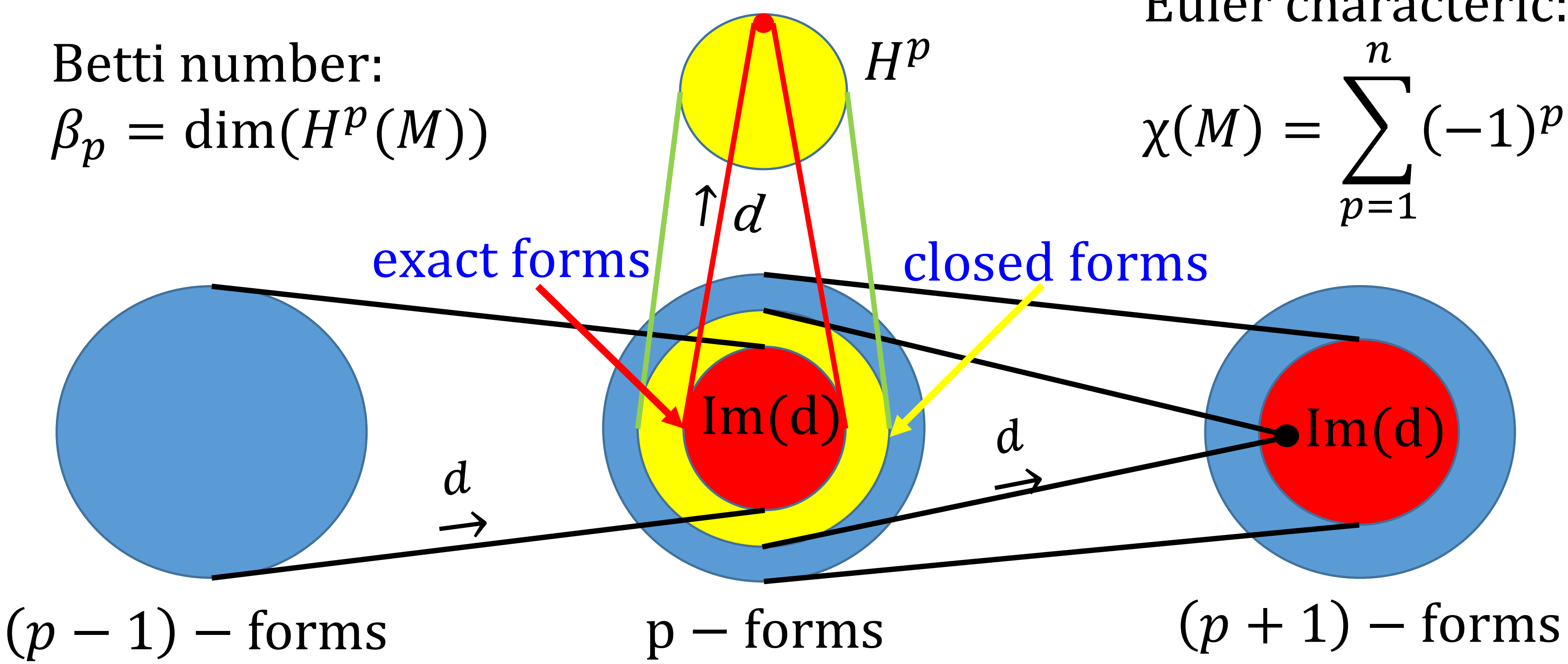
$B^p(M)$: subspace of all exact $p-$ forms.

Euler characteristic:

$$\chi(M) = \sum_{p=1}^{n} (-1)^p \beta_p$$

Betti number:

$$\beta_p = \dim(H^p(M))$$



Hodge star operator

Hodege star operator $\star$ on an $n-$ manifold M: $\Omega^p(M) \to \Omega^{n-p}(M)$:

$$\alpha \wedge \star\beta = \beta \wedge \star\alpha = \langle \alpha, \beta \rangle \mu \quad \text{for } \alpha, \beta \in \Omega^p(M),$$

$$\star\star\alpha = (-1)^{p(n-p)}\alpha,$$
$$\star(c_1\alpha + c_2\beta) = c_1(\star\alpha) + c_2(\star\beta),$$
$$\alpha \wedge \star\alpha = 0 \Longrightarrow \alpha \equiv 0.$$

The volume form μ:

$$\mu = \mathrm{vol} = \star(1) = \sqrt{\det(g_{ij})}\, dx^1 \wedge \cdots \wedge dx^n,$$

where $g = (g_{ij})$ is the Riemannian metric.

In Euclidean $\mathbb{R}^3$, $1-$form is related to $2-$form by $\star$:

$$\star dx = dy \wedge dz, \quad \star dy = dz \wedge dx, \quad \star dz = dx \wedge dy.$$

Hodge inner product

For $\alpha, \beta \in \Omega^p\ (M)$, Hodge L^2-inner product:

$$(\alpha, \beta) := \int_M \langle \alpha, \beta \rangle \star (1) = \int_M \alpha \ \wedge \star \beta,$$

$$(\alpha, \alpha) \geq 0,$$
$$(\alpha, \alpha) = \|\alpha\| = 0 \quad \text{iff } \alpha = 0$$

Hodge codifferential operator

Hodge dual to $\mathrm{d}: \Omega^p(M) \rightarrow \Omega^{p+1}(M)$ is $\delta\colon\ \Omega^p(M) \rightarrow \Omega^{p-1}(M)$:

$$\delta = (-1)^{n(p+1)+1} \star \mathrm{d} \star \quad \Longrightarrow \quad \mathrm{d} = (-1)^{np} \star \delta \star$$

Hodge codifferential δ is a generalization of divergence and satisfies:

$$\delta\delta = \delta^2 = 0 \quad \Leftrightarrow \quad \mathrm{dd} = \mathrm{d}^2 = 0;$$
$$\delta \star = (-1)^{p+1} \star \mathrm{d}; \quad \star\, \delta = (-1)^p \star \mathrm{d};$$
$$d\delta \star = \star\, \delta \mathrm{d}; \quad \star\, d\delta = \delta d \star.$$

Hodge Laplacian operator

Hodge Laplacian Δ: $\Omega^p(M) \to \Omega^p(M)$, a harmonic generalization of the Laplace-Beltrami operator:

$$\Delta = \delta\mathrm{d} + \mathrm{d}\delta = (\mathrm{d} + \delta)^2$$

Properties:

$$\delta\Delta = \Delta\delta = \delta\mathrm{d}\delta; \quad \mathrm{d}\Delta = \Delta\mathrm{d} = \mathrm{d}\delta\mathrm{d}; \quad \star\Delta = \Delta\star$$

For $\alpha \in \Omega^p(M)$, it is harmonic iff

$$\Delta\alpha = 0 \Leftrightarrow (\mathrm{d}\alpha = 0, \delta\alpha = 0)$$

Hodge adjoints and self-adjoints

For $\alpha \in \Omega^p(M)$ and $\beta \in \Omega^{p+1}(M)$,

$(\mathrm{d}\alpha, \beta) = (\alpha, \delta\beta)$ and $(\delta\alpha, \beta) = (\alpha, \mathrm{d}\beta)$

Recap

(Essentially, four operators and two inner products)

de Rham's cochain complexes and Hodge duals in $\mathbb{R}^3$:

$$
\begin{tikzcd}
\Omega^0(\mathbb{R}^3) \arrow[r, "\mathrm{d}", "\mathrm{grad}"'] \arrow[d, "\star"] & \Omega^1(\mathbb{R}^3) \arrow[r, "\mathrm{d}", "\mathrm{curl}"'] \arrow[d, "\star"] & \Omega^2(\mathbb{R}^3) \arrow[r, "\mathrm{d}", "\mathrm{div}"'] \arrow[d, "\star"] & \Omega^3(\mathbb{R}^3) \arrow[d, "\star"] \\
\Omega^3(\mathbb{R}^3) \arrow[r, "\delta"] & \Omega^2(\mathbb{R}^3) \arrow[r, "\delta"] & \Omega^1(\mathbb{R}^3) \arrow[r, "\delta"] & \Omega^0(\mathbb{R}^3)
\end{tikzcd}
$$

de Rham's chain complexes in $\mathbb{R}^3$ as a duality:

$$0 \to \mathcal{C}_3(\mathbb{R}^3) \xrightarrow{\partial} \mathcal{C}_2(\mathbb{R}^3) \xrightarrow{\partial} \mathcal{C}_1(\mathbb{R}^3) \xrightarrow{\partial} \mathcal{C}_0(\mathbb{R}^3) \to 0$$

de Rham's period:

$$\langle \partial C, \omega \rangle = \langle C, d\omega \rangle$$

Hodge $L^2 -$ inner product:

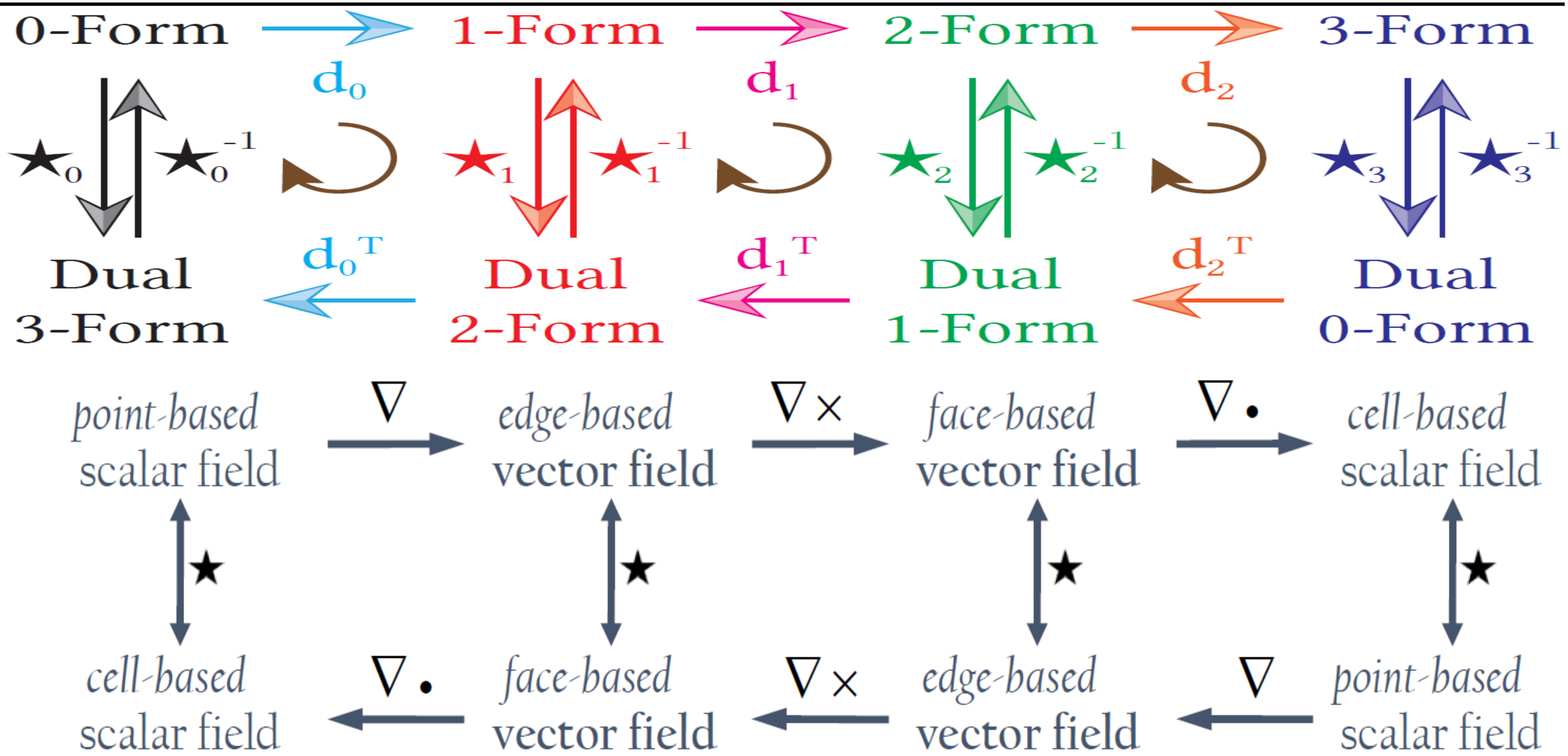
$$(\mathrm{d}\alpha, \beta) = (\alpha, \delta\beta) \;\text{ and }\; (\delta\alpha, \beta) = (\alpha, \mathrm{d}\beta)$$

Hodge decomposition theorem

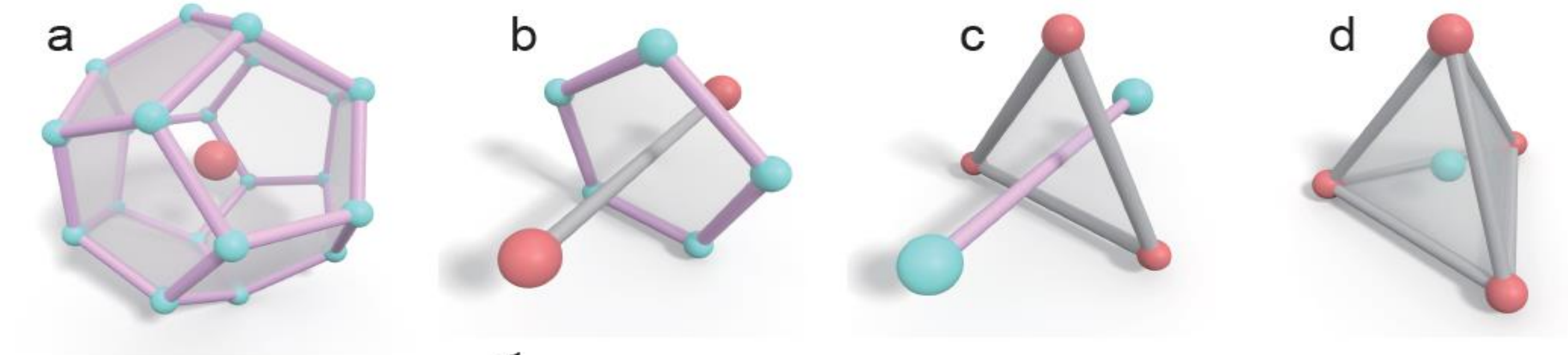
For $\alpha \in \Omega^{p-1}(M)$, $\beta \in \Omega^{p+1}(M)$, and $\gamma \in \Omega^{p}(M)$,

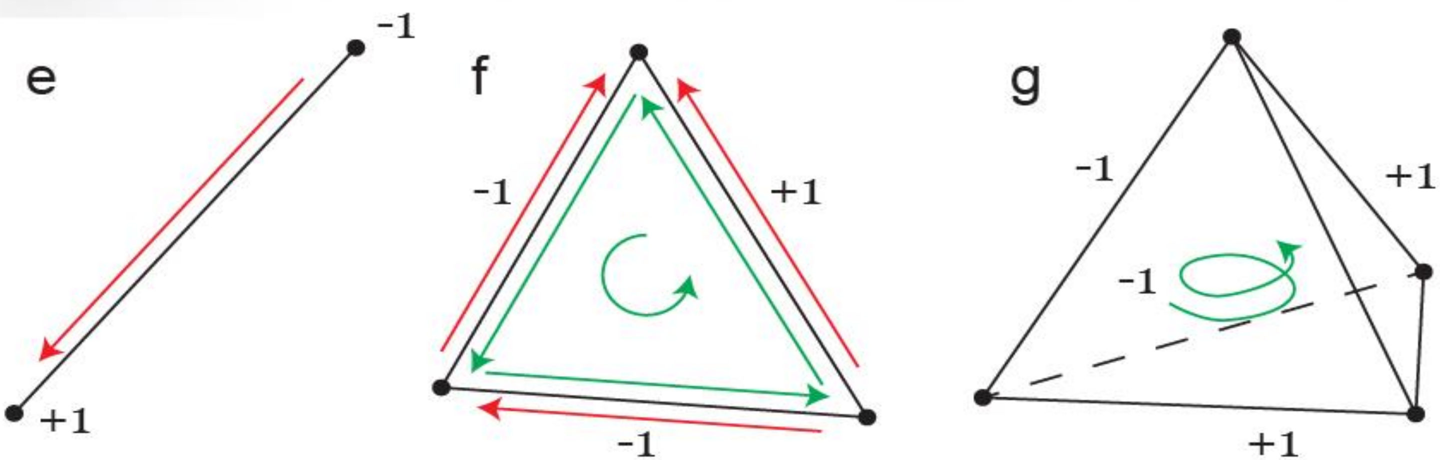
$$\omega = d\alpha + \delta\beta + \gamma$$

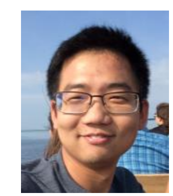
ω	$d\alpha$	$\delta\beta$	γ
any form	exact	co-exact	harmonic
	curl-free	divergence-free	



Discrete exterior calculus







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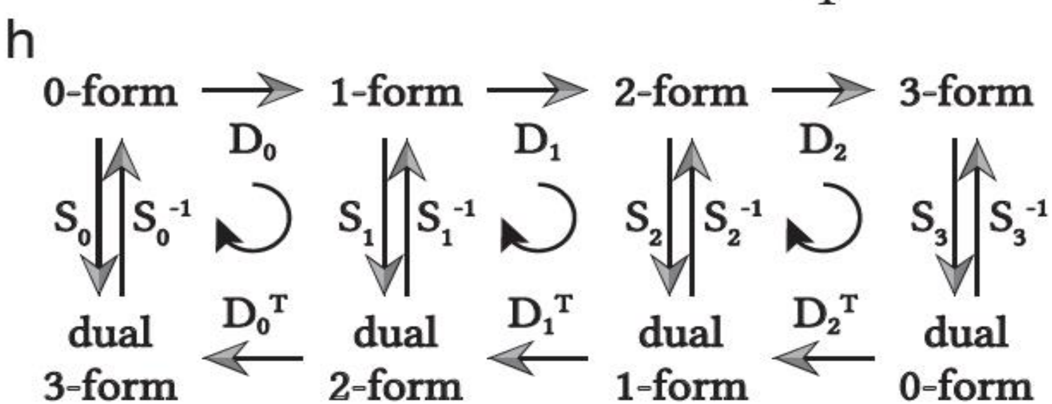

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$$L_0 = D_0^T S_1 D_0$$

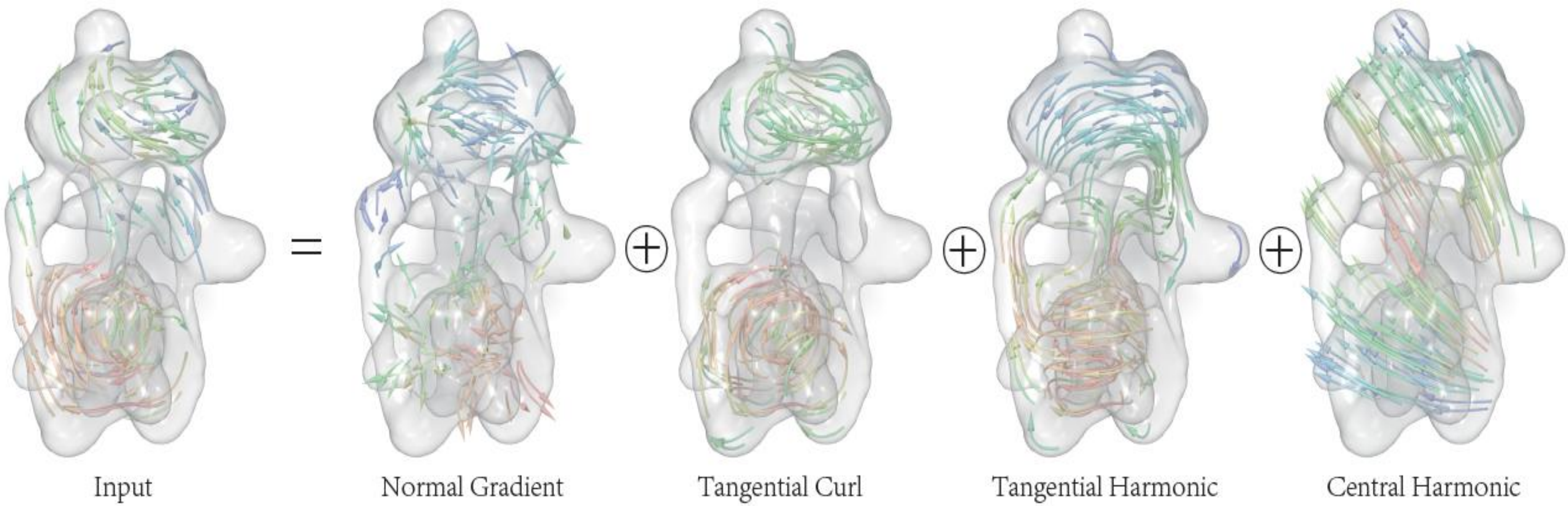
$$L_1 = D_1^T S_2 D_1 + S_1 D_0 S_0^{-1} D_0^T S_1$$

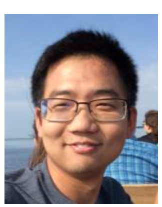
$$L_2 = D_2^T S_3 D_2 + S_2 D_1 S_1^{-1} D_1^T S_2$$

$$L_3 = S_3 D_2 S_2^{-1} D_2^T S_3$$

(Zhao, Wang, Tong & Wei, 2019)

Hodge decomposition of a synthetized cryo-EM vector field (EMD 1590)





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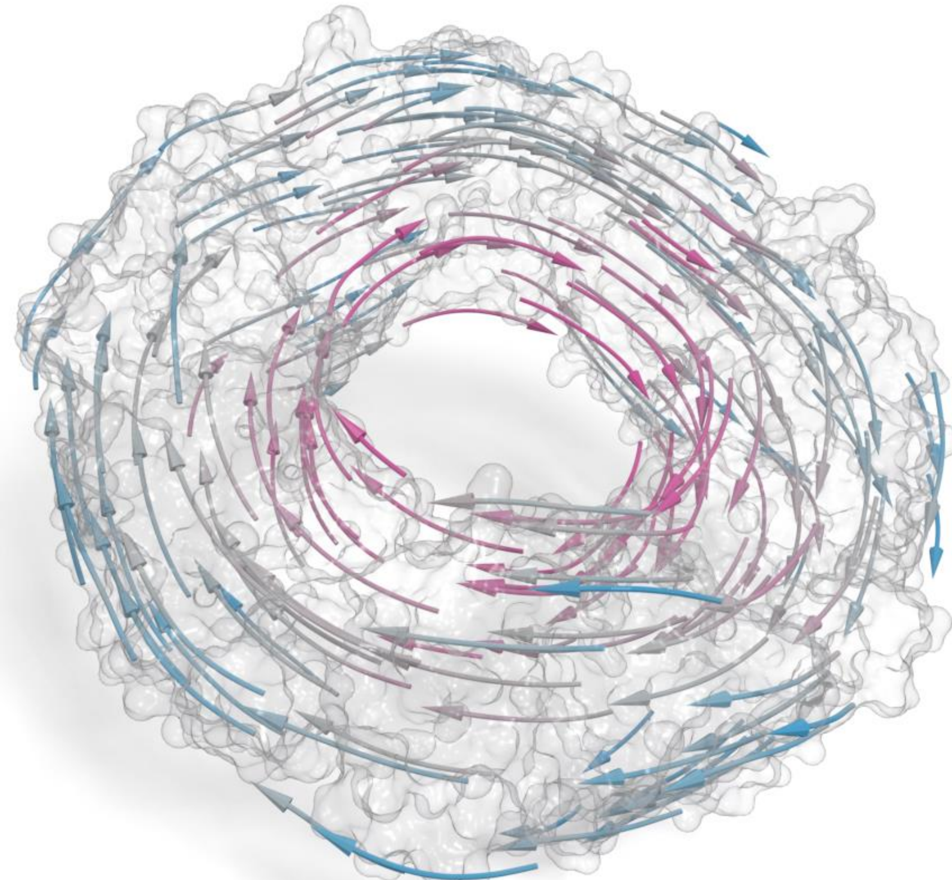
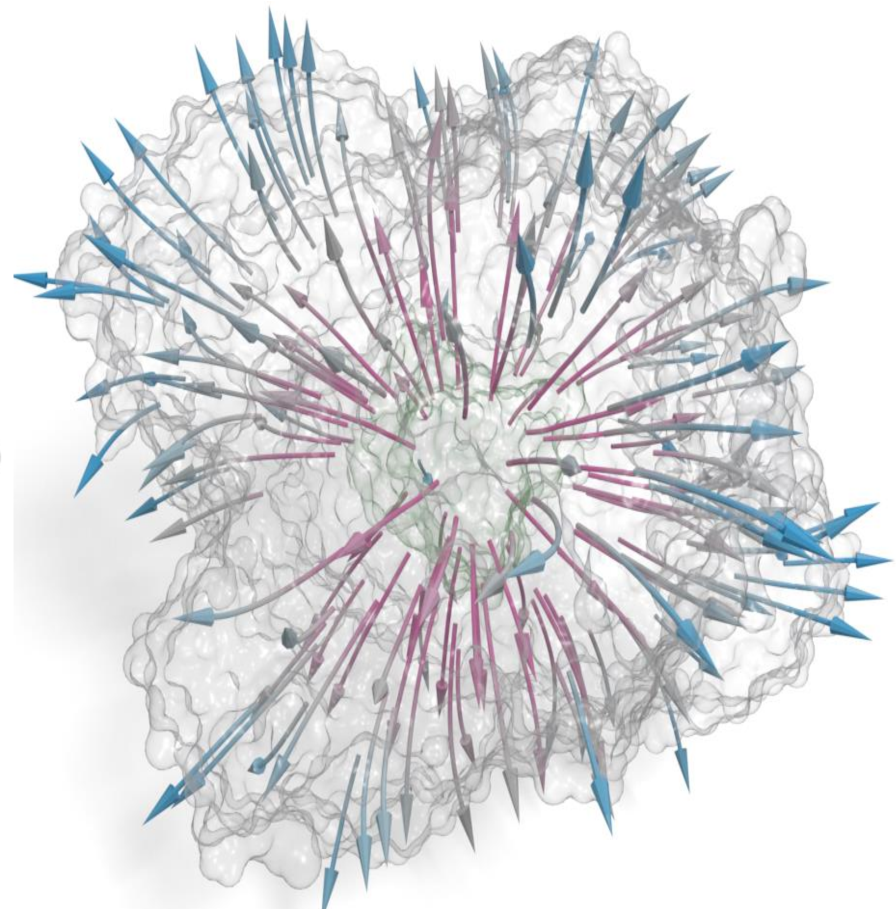
(Zhao, Wang, Tong & Wei, 2019)

Eigen fields of the null space of Laplace-de Rham operators indicating the topology



Tangential boundary



Normal boundary

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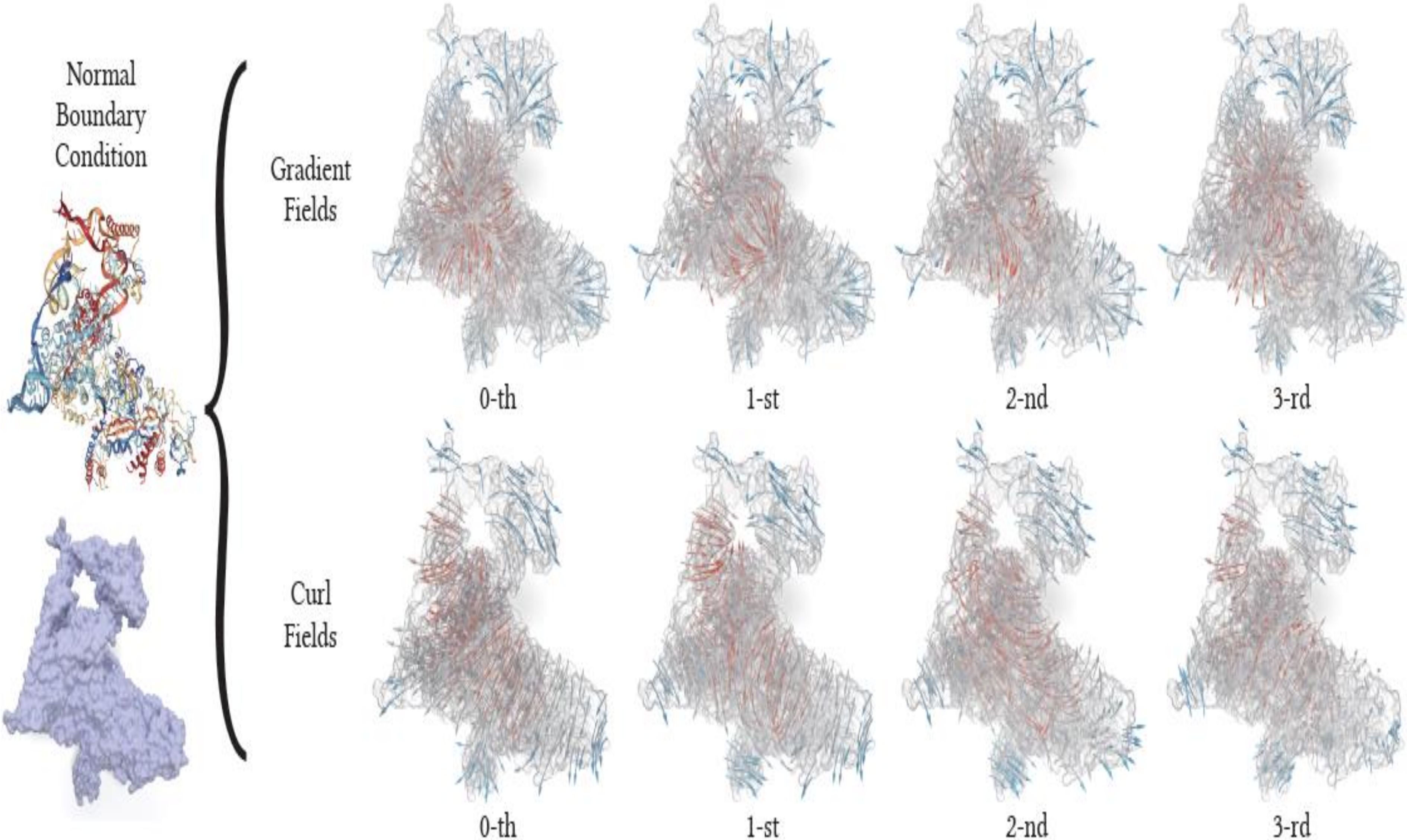
(Zhao, Wang, Tong & Wei, 2019)

Vector Hodge Laplacian eigenvectors

(Zhao, Wang, Tong & Wei, 2019)



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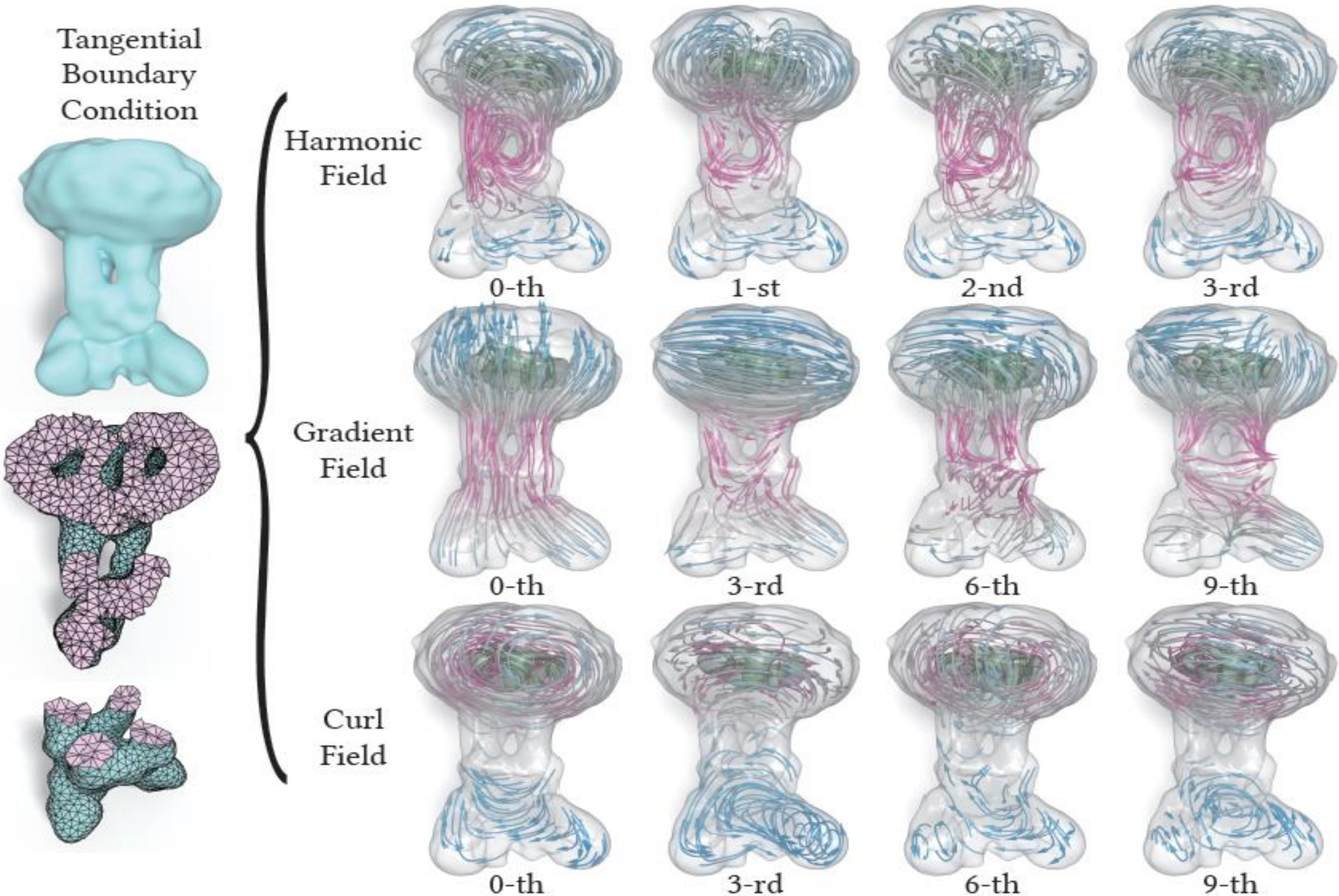
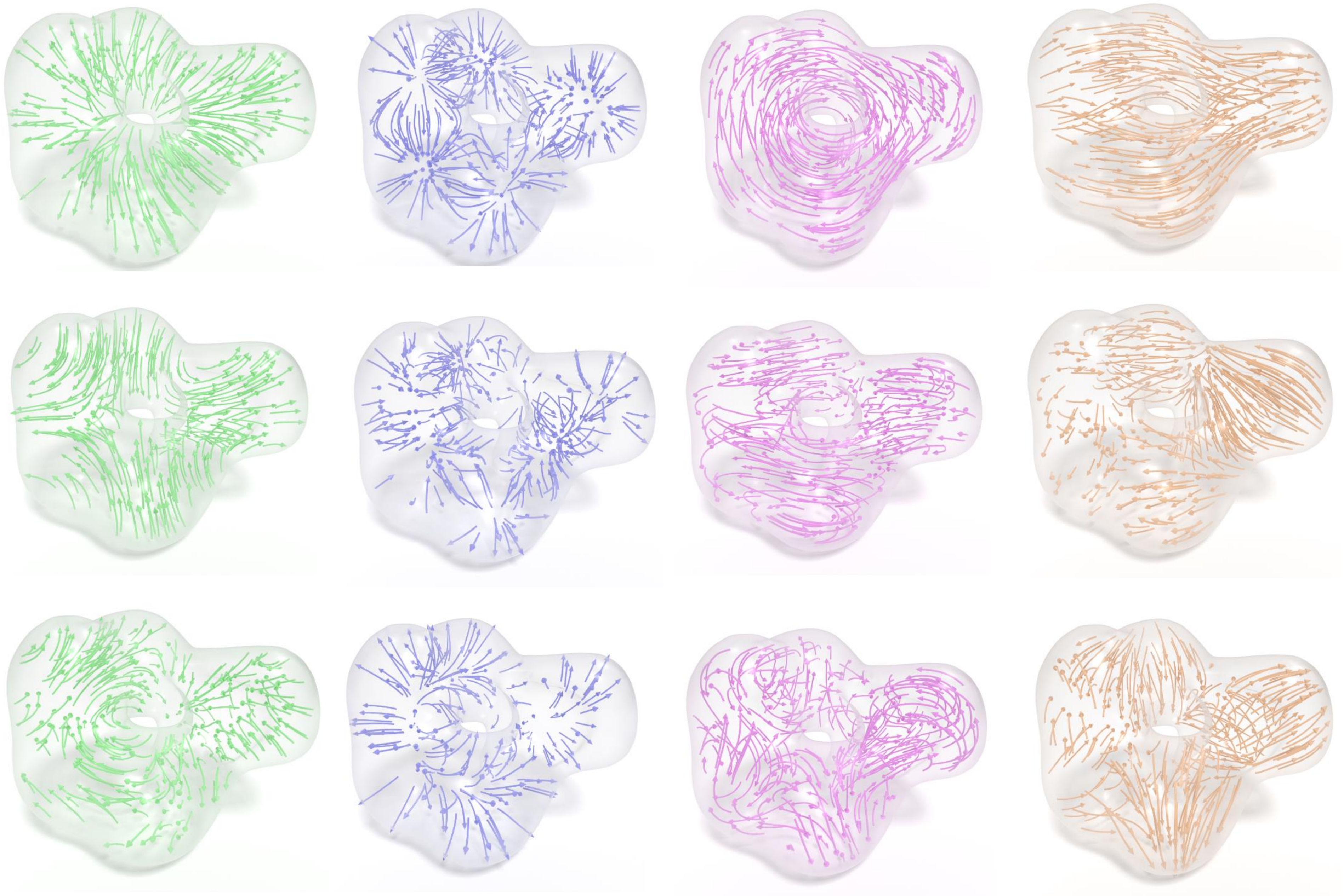
Vector Hodge Laplacian eigenvectors

(Zhao, Wang, Tong & Wei, 2019)

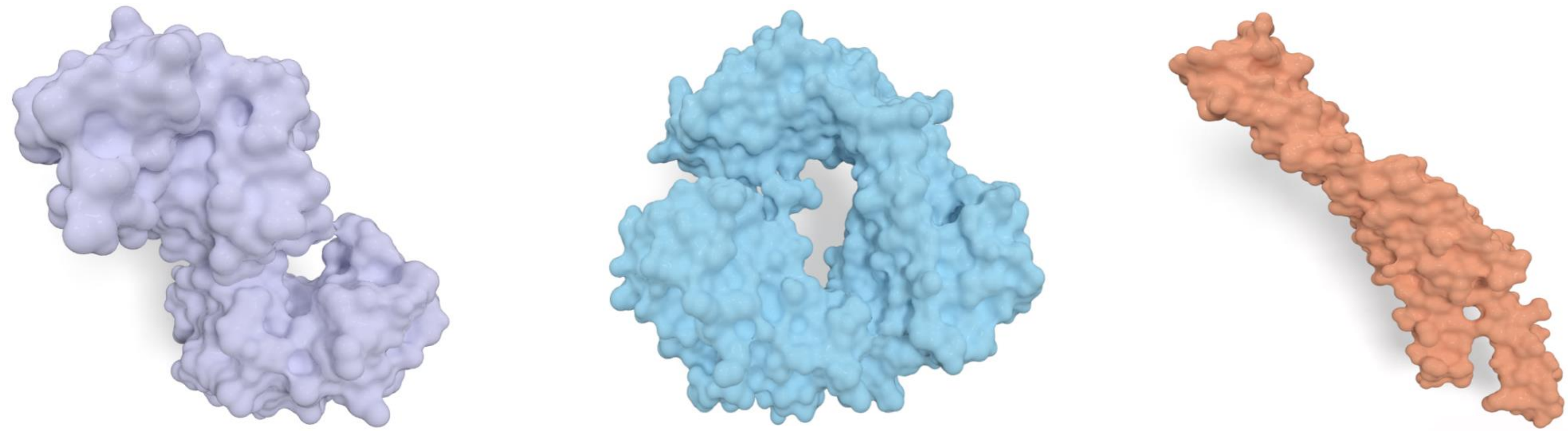


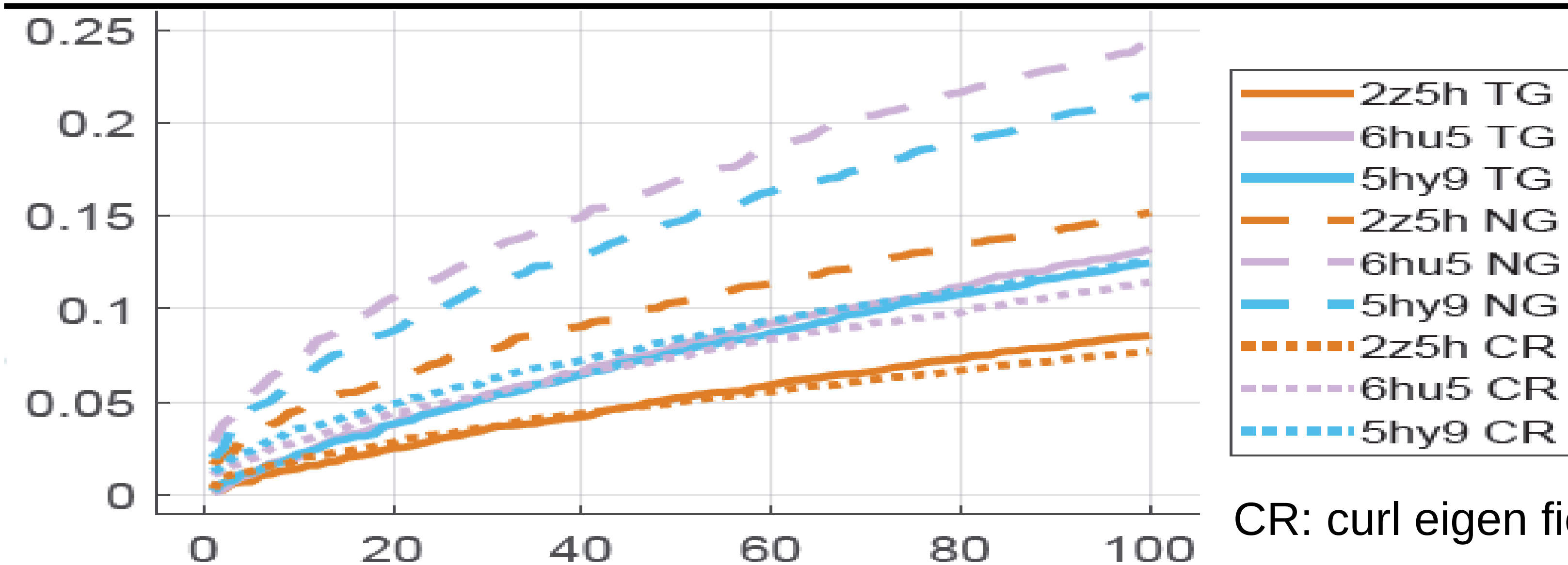
Vector Hodge-Laplacian Eigen modes



Vector Hodge Laplacian Eigenvalue distributions

(Zhao, Wang, Tong & Wei, 2019)





CR: curl eigen fields

TG: tangential gradient eigen fields; NG: normal gradient eigen fields.

Hodge-Laplacian protein B factor prediction

Using the eigenvalues λ_j^k and eigenmodes $\omega_j^k(\boldsymbol{r})$ of the k-form Laplace-de Rham operator (tested for 364 proteins):

$$\mathrm{B}_{k,i}^{\mathrm{dRH}} = a\sum_j \frac{1}{\lambda_j^k}\left[\omega_j^k(\boldsymbol{r})\left(\omega_j^k(\boldsymbol{r}')\right)^T\right]_{\boldsymbol{r}=\boldsymbol{r}_i,\boldsymbol{r}'=\boldsymbol{r}_i}$$

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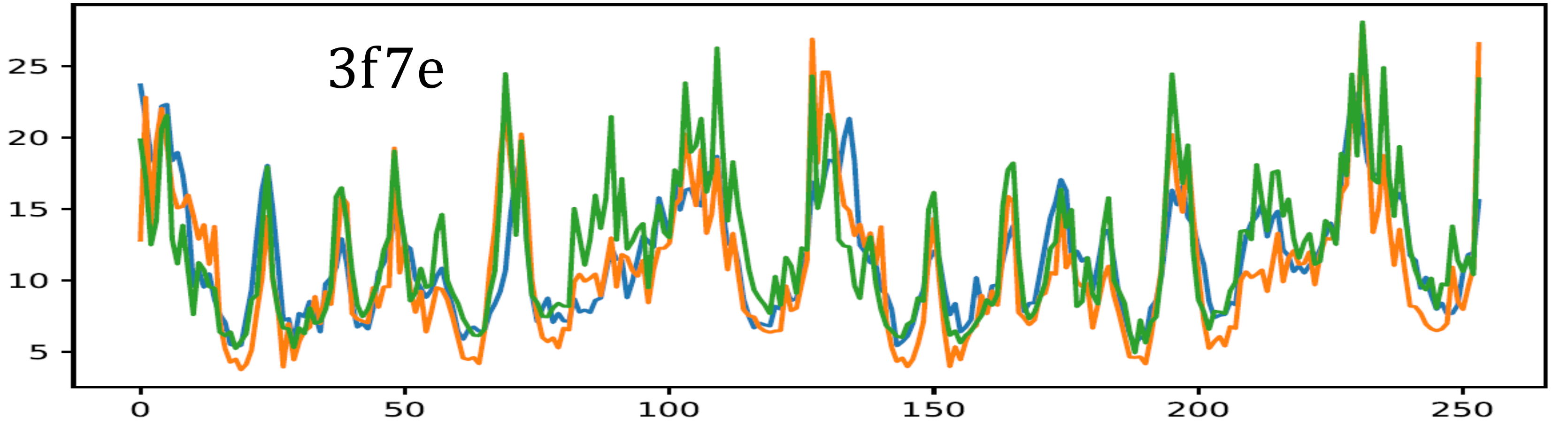
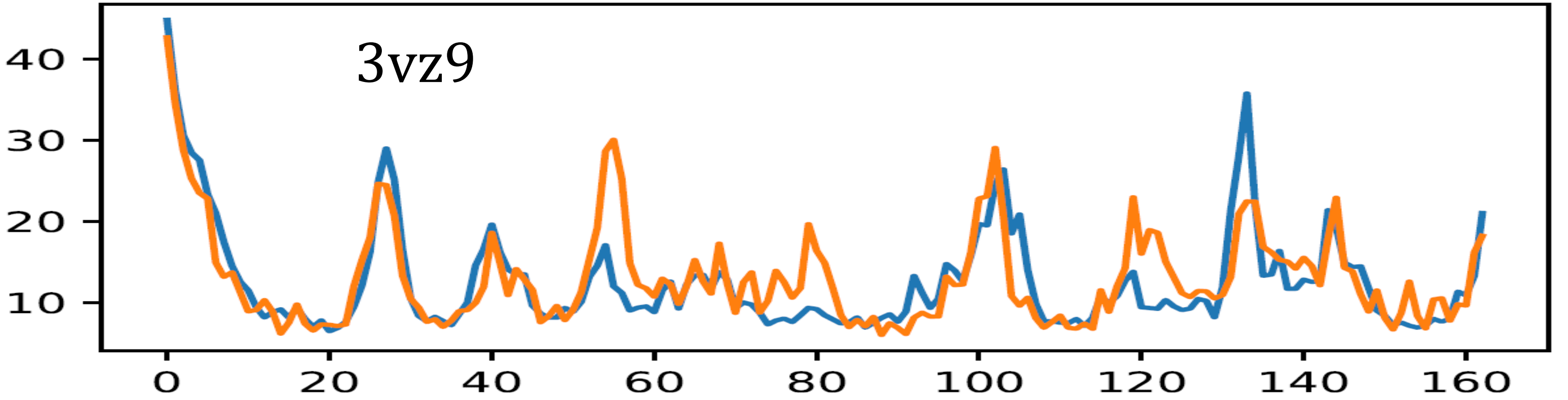
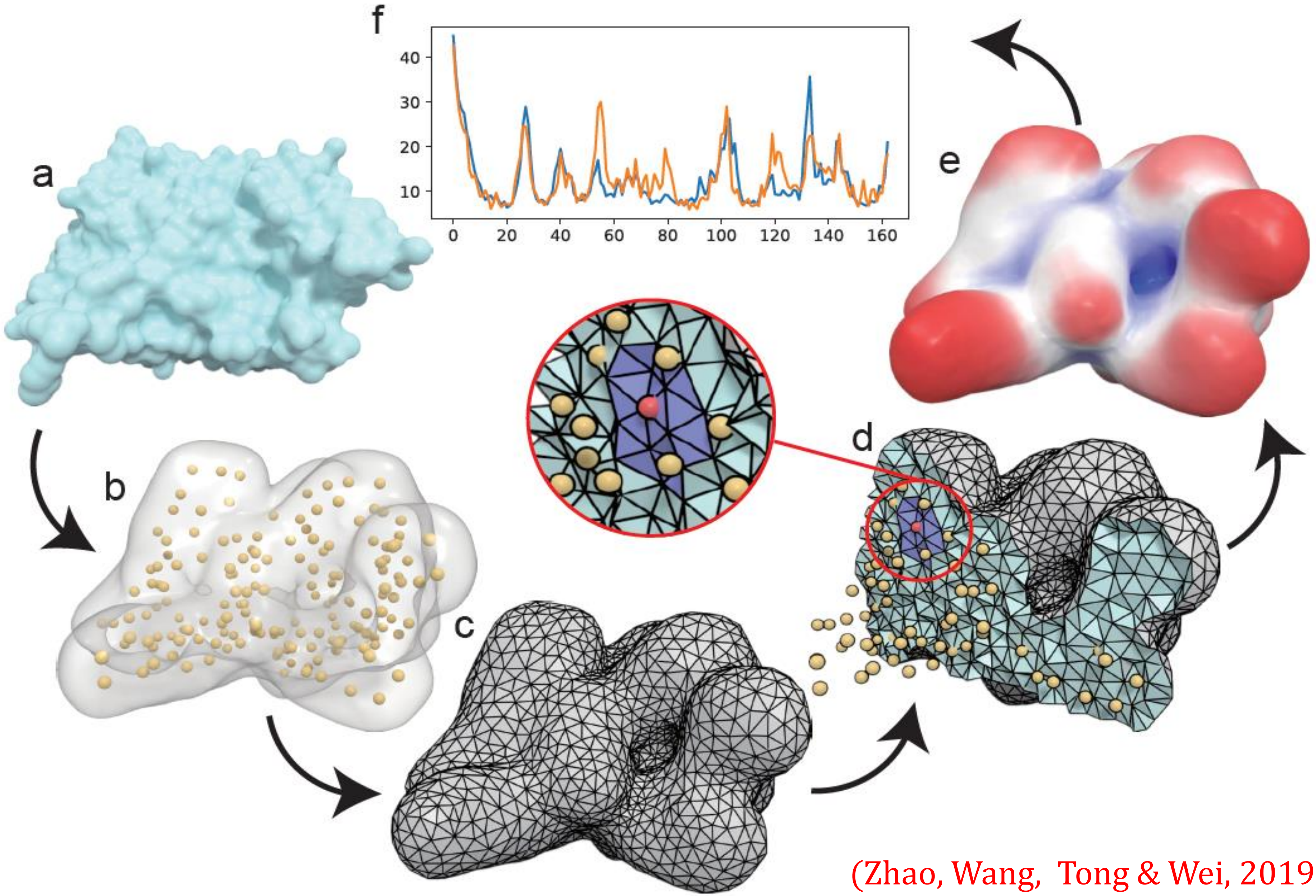




Numerical procedure for Protein B factor prediction



(Zhao, Wang, Tong & Wei, 2019)

Natural modes of EMD 1258

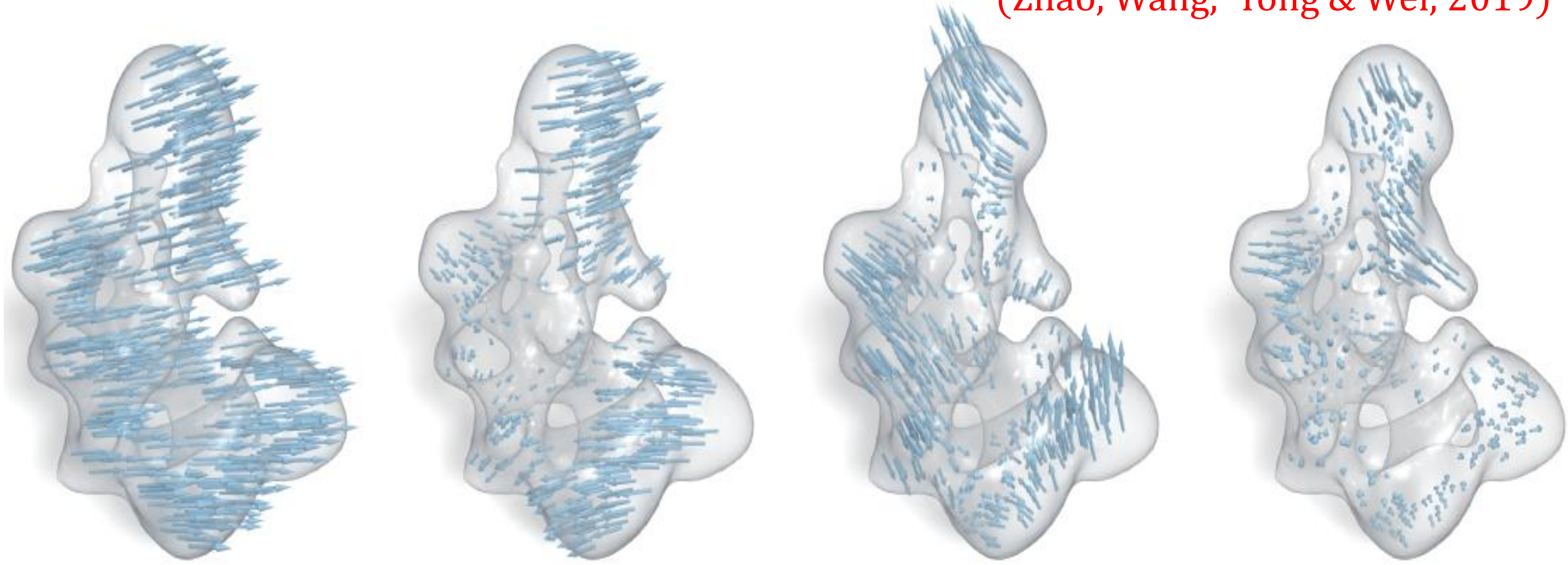
Natural modes are obtained by diagonalizing the canonically defined 1-form Laplace-de Rham operator equipped with a boundary constraint from a Helfrich-type curvature potential (1-form Laplace-de Rham-Helfrich operator):

$$E_\mu = d_0 \star_0^{-1} d_0^T \star_1 + \star_1^{-1} d_1^T \star_2 d_1 + G^T Q G$$

where $Q = \frac{\partial^2}{\partial X^2}\left(\mu \int_{\partial M} (H - H_0)^2 dA\right)$

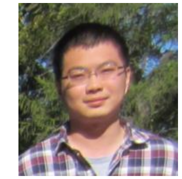
Rundong Zhao

(Zhao, Wang, Tong & Wei, 2019)

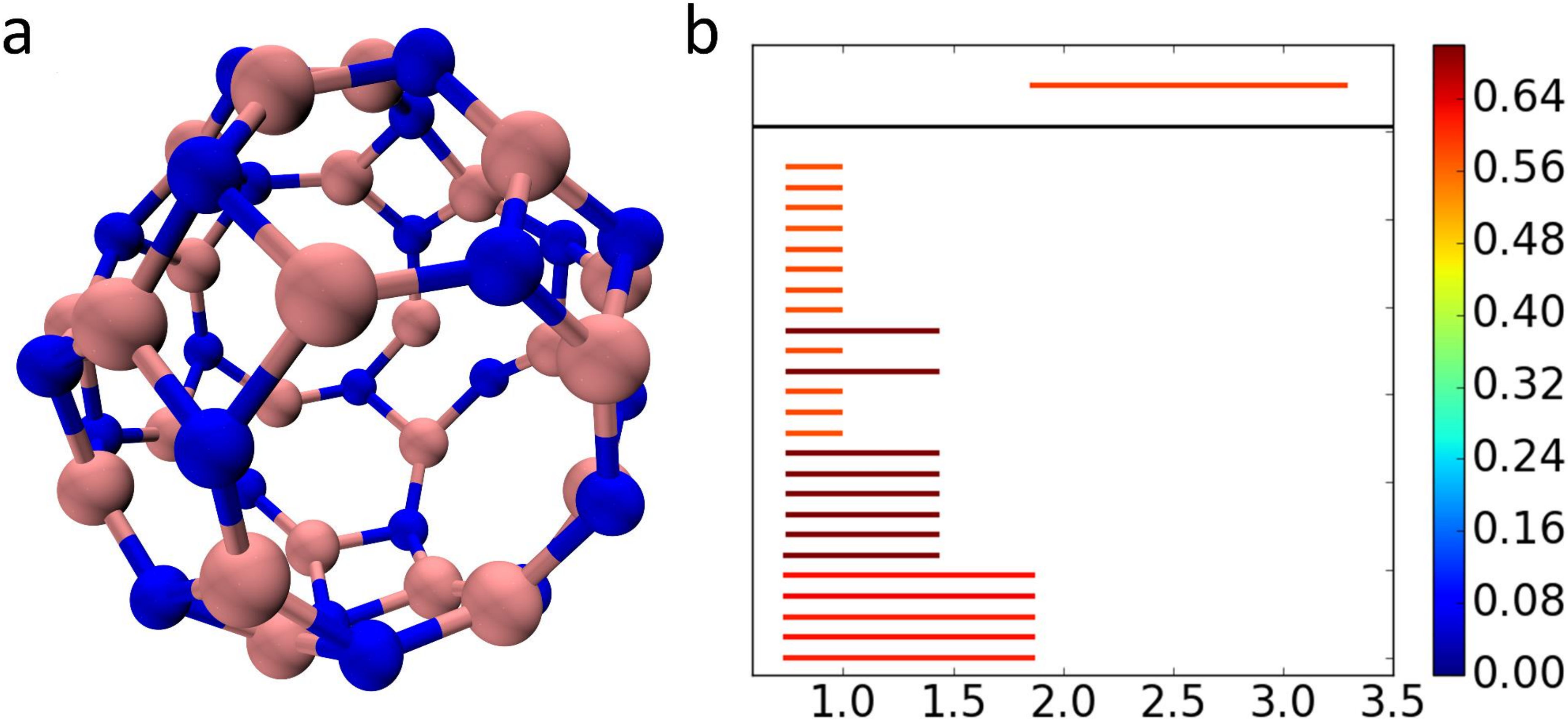


Persistent de Rham cohomology

To embed both geometric and non-geometric information, i.e., multi-element information, into unified topological descriptions.

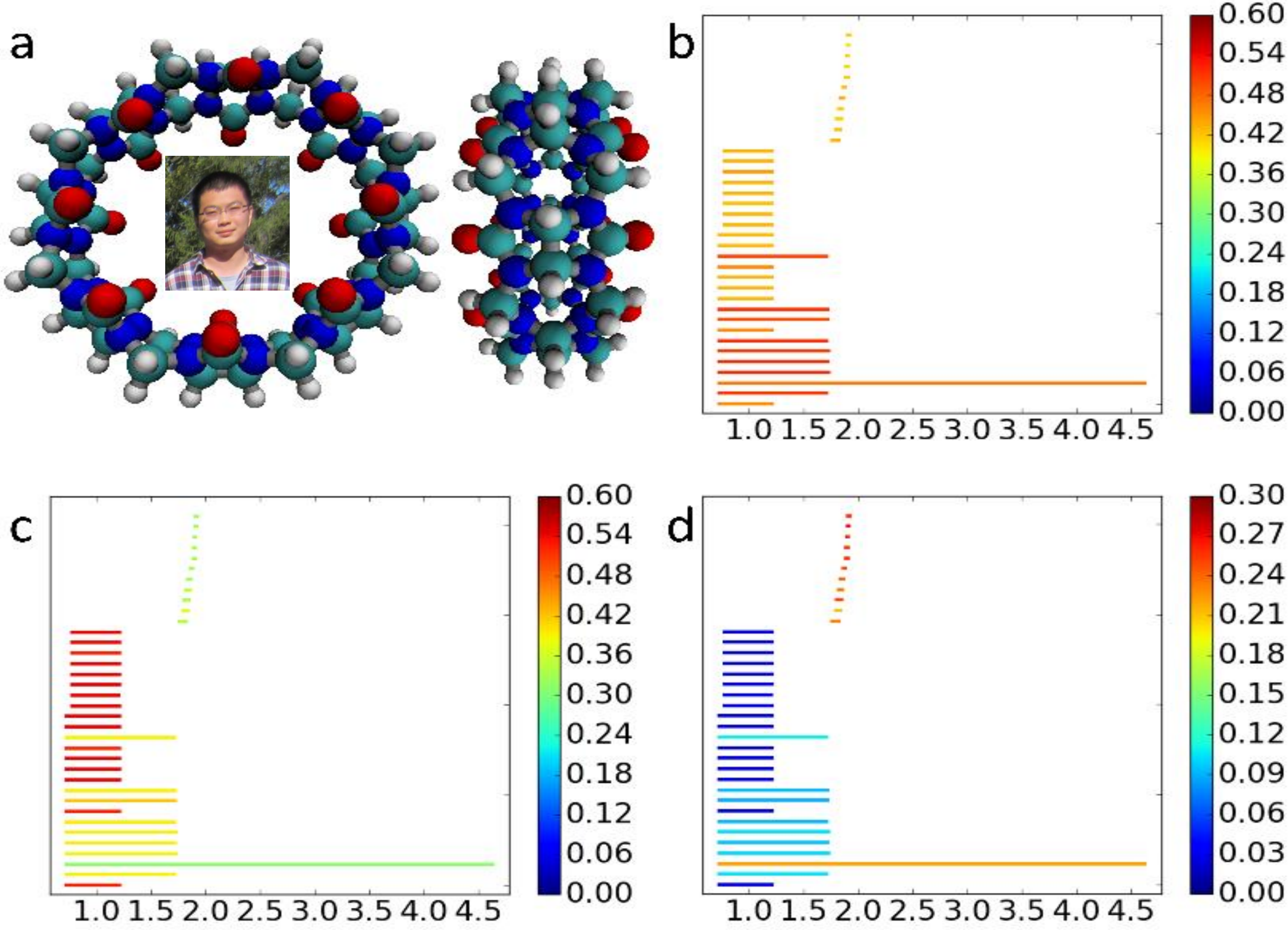


Zixuan Cang

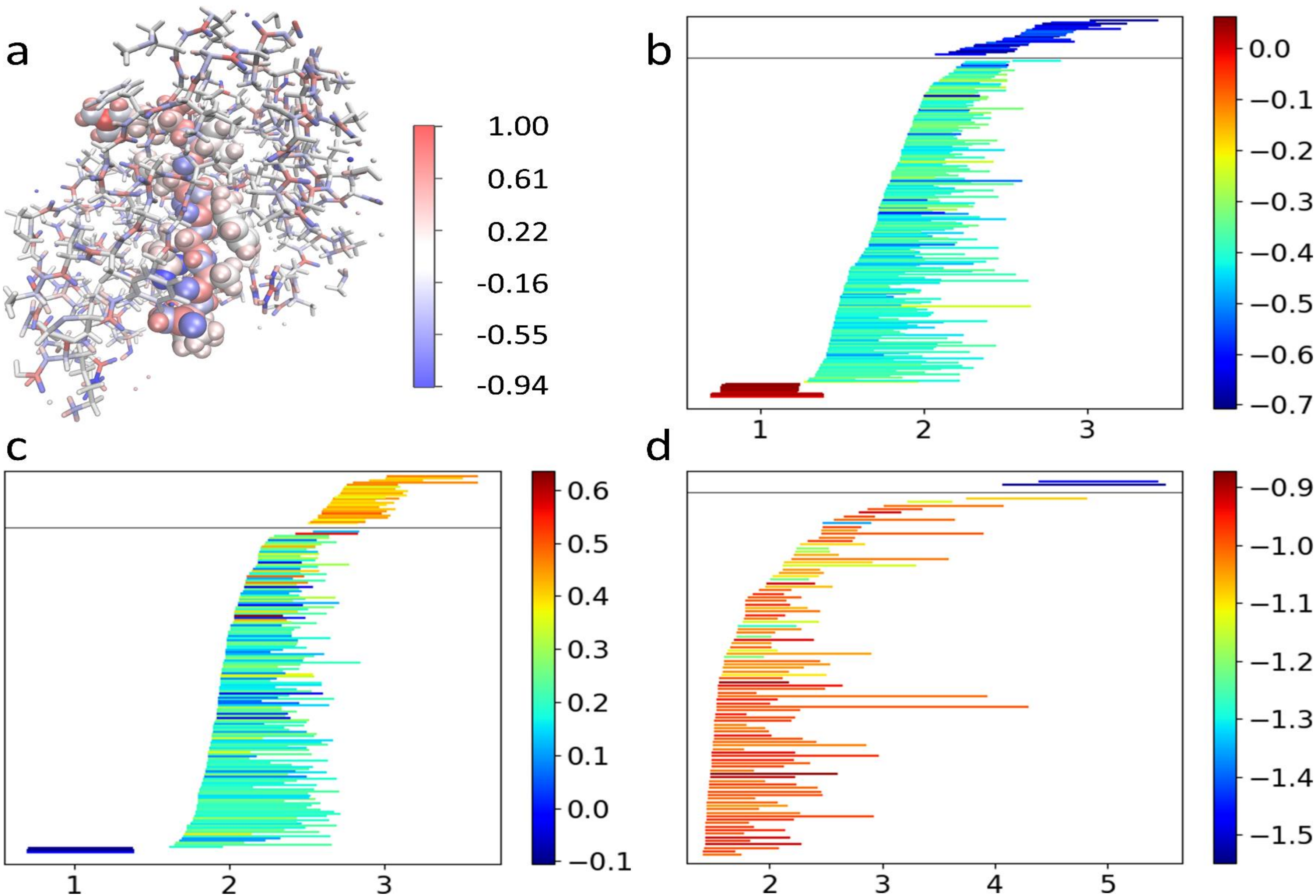


(Cang & Wei, 2018)

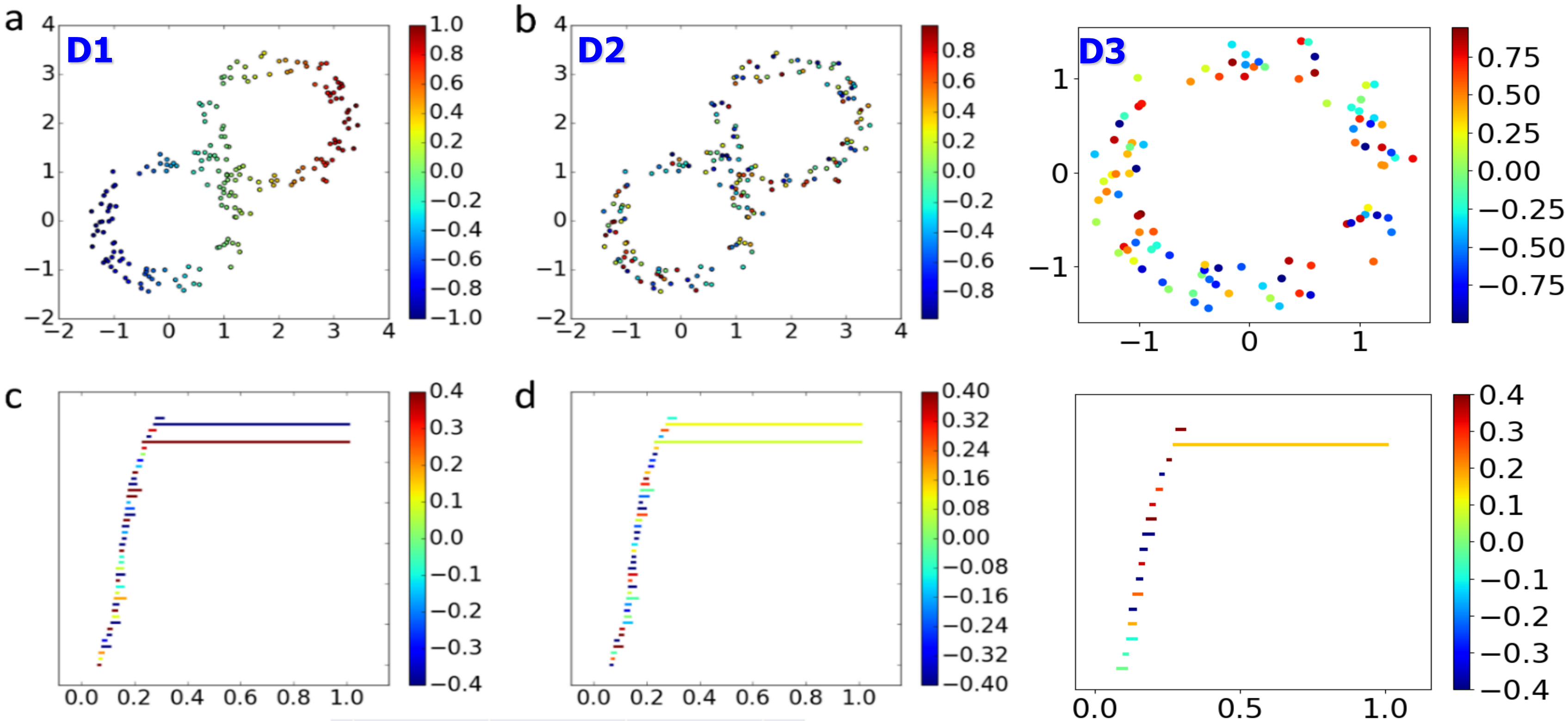
Persistent de Rham cohomology (Cang & Wei, 2018)

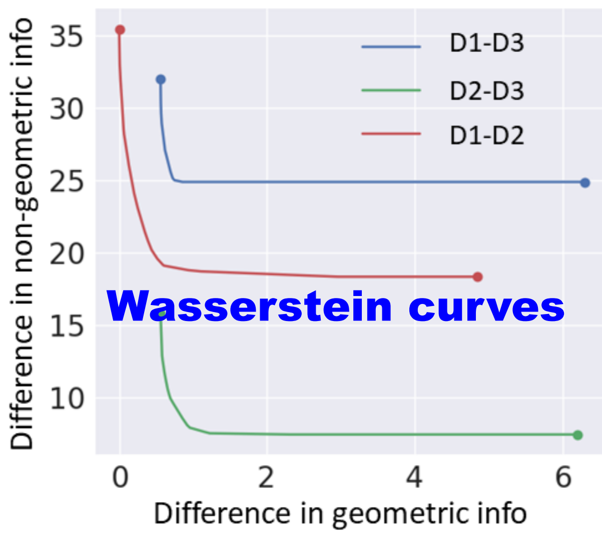


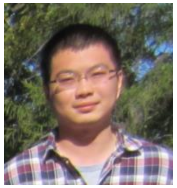
Persistent de Rham cohomology



Persistent de Rham cohomology







Zixuan Cang

(Cang & Wei, 2018)

Pearson correlation of protein-ligand binding affinity using persistent homology (PH) and cohomology (PC)

PDBbind	v2007	v2013	v2015	v2016
Dim 0 PH	0.802 (1.47))	0.754 (1.56)	0.745 (1.56)	0.824 (1.32)
Dim 0 PC	0.796 (1.50)	0.768 (1.53)	0.763 (1.53)	0.833 (1.31)
Dim 1&2 PH	0.726 (1.65)	0.706 (1.67)	0.718 (1.62)	0.767 (1.46)
Dim 1&2 PC	0.738 (1.64)	0.734 (1.60)	0.737 (1.59)	0.778 (1.44)

Root mean squared errors are in parentheses

(Cang & Wei, 2018)

Further topics and future directions

- Element specific Hodge-Laplacian spectral analysis of biomolecular interactions.
- Hodge decomposition of molecular interaction forces.
- Hodge-Laplacian spectral analysis of molecular dynamics and asymptotic configuration.
- Cohomology modeling of atomic interactions and enzymatic processes.
- Geometric algebra analysis of biomolecules.
- Persistent de-Rham-Hodge theory for biomolecules.
- Spectral sequence modeling of biomolecules.
- Vector Hodge-Laplacian operator analysis of biomolecular reactivity, signaling pathway, etc.
- Vector Hodge-Laplacian operator modeling of cryo-EM data.
- Vector Hodge-Laplacian operator modeling of protein structural stability, anisotropic motion and entropy.
- Chern-Simons theory for DNA/RNA knots
- Application of characteristic classes and characteristic numbers to biomolecular analysis.


thank you