Hodge Laplacian and biological applications

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Outline

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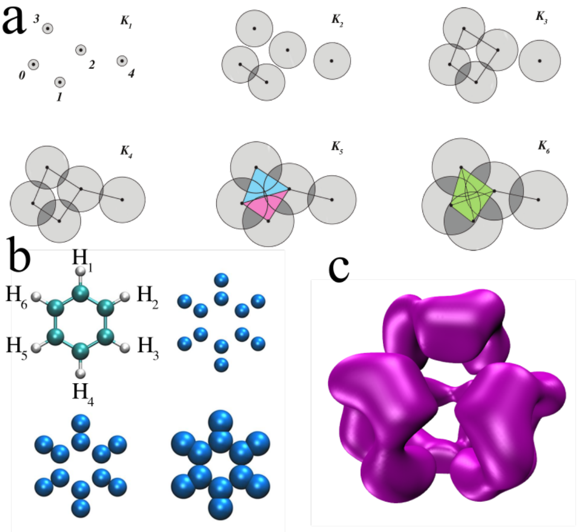
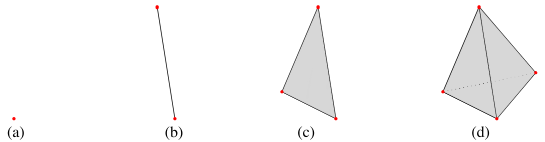
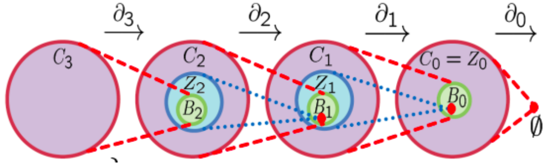


Figure 1: **a** illustration of filtration, **b** Benzene molecule and the filtration process, **c** EMD-1776, credits for **a** and **b** belongs to Rui Wang

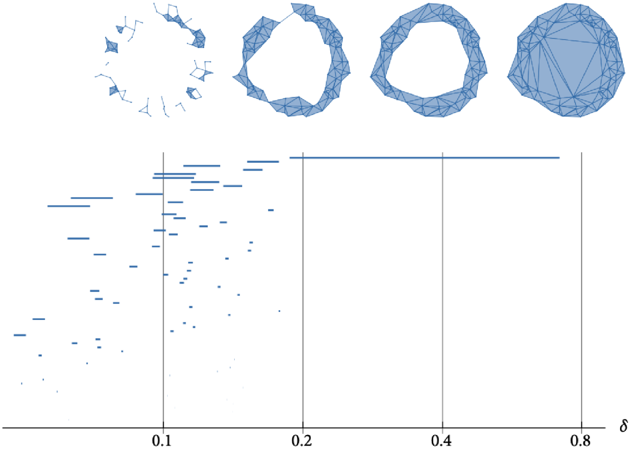
- Simplexes: (a) 0-simplex, (b) 1-simplex, (c) 2-simplex, (d) 3-simplex



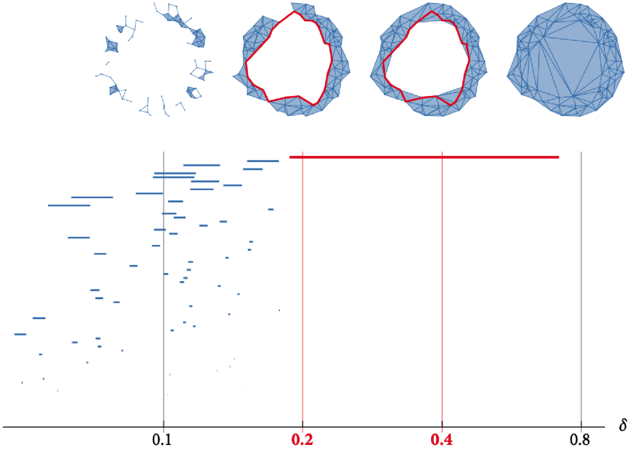
- k-chain: $K = \{\sum_j c_j \sigma_j^k\}$
- Chain group: $C_k(K, \mathbb{Z}_2)$
- Boundary operator: $\partial_k \sigma_k = \sum_{i=0}^{k} (-1)^i [v_0, \cdots, \hat{v}_i, \cdots, v_q]$
- Homology group: $H_k = \frac{Z_k}{B_k}$, $Z_k = \ker \partial_k$, $B_k = \mathrm{im}\ \partial_{k+1}$



- Betti number: $\beta_k = \mathrm{Rank}(H_k)$



[Bauer 2019]



[Bauer 2019]

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3-dimensional volumes bounded by 2-manifolds in $\mathbb{R}^3$

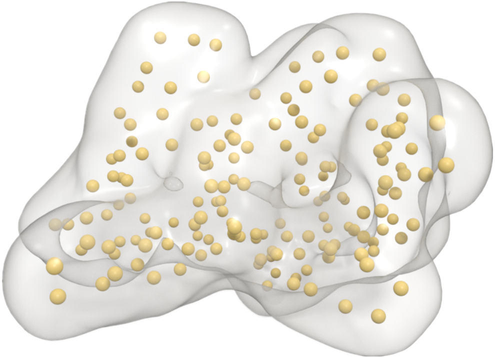


Figure 2: PDB: 3VZ9, C-alpha atoms (yellow spheres) are considered in this case. [7]

Every cohomology class has a differential form that vanishes under the Laplacian operator of the metric

Manifolds with boundary, (3-dimensional volumes bounded by 2-manifolds in $\mathbb{R}^3$)

- A differential k-form $\omega^k \in \Omega^k(M)$ is an antisymmetric covariant tensor of rank k on manifold M
- The *differential* operator (i.e., exterior derivative) d^k maps from a k-form on manifold to a $k+1$-form, $d^k : \Omega^k(M) \to \Omega^{k+1}(M)$
- The *Hodge k-star* $\star^k$ (aka Hodge dual) is linear map from a k-form to its dual form, $\star^k : \Omega^k(M) \to \Omega^{3-k}(M)$
- The *codifferential* operators $\delta^k : \Omega^k(M) \to \Omega^{k-1}(M)$, $\delta^k = (-1)^k \star^{4-k} d^{3-k} \star^k$, for $k = 1, 2, 3$

- The *de Rham-Laplace operator*, or *Hodge Laplacian*

$$\Delta^k \equiv d^{k-1}\delta^k + \delta^{k+1}d^k$$

- *de Rham complex*

$$0 \longrightarrow \Omega^0(M) \xrightarrow{d^0} \Omega^1(M) \xrightarrow{d^1} \Omega^2(M) \xrightarrow{d^2} \Omega^3(M) \xrightarrow{d^3} 0$$

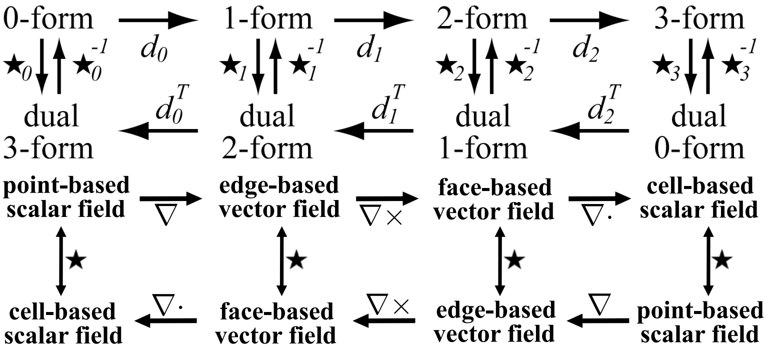
- *Bi-directional chain complex*

$$\Omega^0(M) \underset{\delta^1}{\overset{d^0}{\rightleftarrows}} \Omega^1(M) \underset{\delta^2}{\overset{d^1}{\rightleftarrows}} \Omega^2(M) \underset{\delta^3}{\overset{d^2}{\rightleftarrows}} \Omega^3(M)$$

- *de Rham cohomology* $H^k_{dR} = \ker d^k / \mathrm{im}\, d^{k-1}$, and $H^k_{dR} \cong \mathcal{H}^k_\Delta$,

$$\beta_k = \dim \mathcal{H}^k_{\Delta_t} = \dim \mathcal{H}^{3-k}_{\Delta_n}$$

Exterior calculus vs. traditional calculus



type	f^0	$\mathbf{v}^1$	$\mathbf{v}^2$	f^3
tangential	unrestricted	$\mathbf{v} \cdot \mathbf{n} = 0$	$\mathbf{v} \parallel \mathbf{n}$	$f\|_{\partial M} = 0$
normal	$f\|_{\partial M} = 0$	$\mathbf{v} \parallel \mathbf{n}$	$\mathbf{v} \cdot \mathbf{n} = 0$	unrestricted

- For tangential 0-forms or normal 3-forms,

$$\nabla_{\mathbf{n}} f|_{\partial M} = 0$$

- For tangential 1-forms or normal 2-forms,

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \nabla_{\mathbf{n}}(\mathbf{v} \cdot \mathbf{t}_1) + \kappa_1(\mathbf{v} \cdot \mathbf{t}_1) = 0, \quad \nabla_{\mathbf{n}}(\mathbf{v} \cdot \mathbf{t}_2) + \kappa_2(\mathbf{v} \cdot \mathbf{t}_2) = 0$$

- For tangential 2-forms or normal 1-forms,

$$\mathbf{v} \cdot \mathbf{t}_1 = 0, \quad \mathbf{v} \cdot \mathbf{t}_2 = 0, \quad \nabla_{\mathbf{n}}(\mathbf{v} \cdot \mathbf{n}) + 2H(\mathbf{v} \cdot \mathbf{n}) = 0$$

- For tangential 3-forms or normal 0-forms,

$$f|_{\partial M} = 0$$

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Manifold evolution

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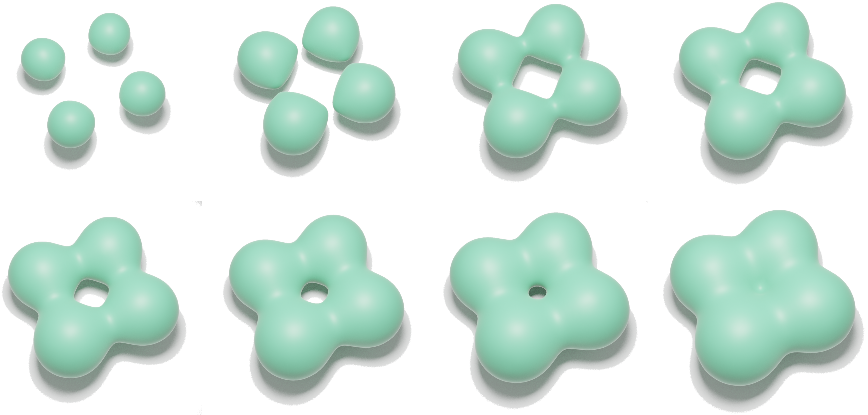
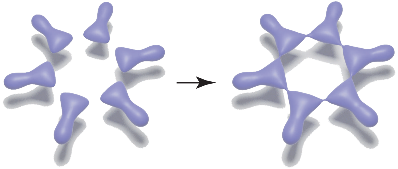
The inclusion map $\mathfrak{I}_{l,l+1} : M_l \hookrightarrow M_{l+1}$.

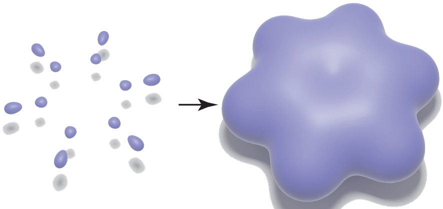
$$M_0 \xrightarrow{\mathfrak{I}_{0,1}} M_1 \xrightarrow{\mathfrak{I}_{1,2}} M_2 \xrightarrow{\mathfrak{I}_{2,3}} \cdots \xrightarrow{\mathfrak{I}_{n-1,n}} M_n \xrightarrow{\mathfrak{I}_{n,n+1}} M = M_{c_{\max}}.$$



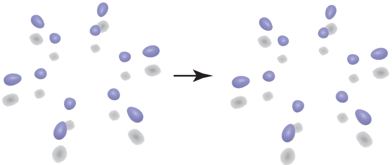
Persistence and progression



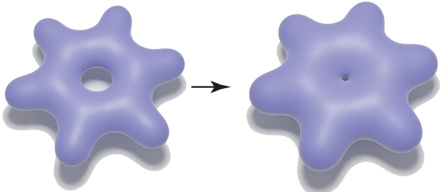
(a) Persistence



(b) Persistence and progression



(c) Identity map



(d) Progression

Figure 3: Persistence and progression on benzene.

Spectra representations

- $\{\lambda_{l,i}^T\}$, $\{\lambda_{l,i}^C\}$ and $\{\lambda_{l,i}^N\}$ give the eigenvalues of the T, C and N sets respectively.
- The multiplicities of the zero eigenvalues in $\lambda_{l,0}^T$, $\lambda_{l,0}^C$, and $\lambda_{l,0}^N$ are associated with Betti numbers β_0, β_1 and β_2, respectively.
- $\lambda_{l,1}^T$, $\lambda_{l,1}^C$, and $\lambda_{l,1}^N$ are the first non-zero eigenvalues

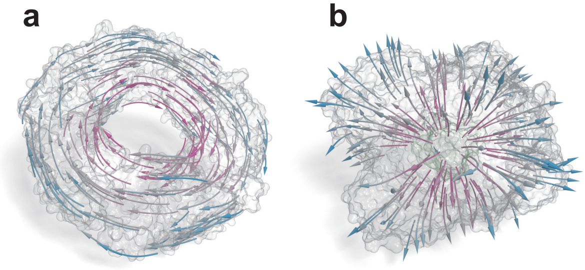
- Hodge decomposition

$$\Omega^k = d\Omega_n^{k-1} \oplus \delta\Omega_t^{k+1} \oplus \mathcal{H}^k,$$

- For any $\omega \in \Omega^k$, a sum of three k-forms from the three orthogonal subspaces,

$$\omega = d\alpha_n + \delta\beta_t + h,$$

where $\alpha_n \in \Omega_n^{k-1}$, $\beta_t \in \Omega_t^{k+1}$, and $h \in \mathcal{H}^k$



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Discrete exterior calculus (DEC) is applied for the discretization of exterior derivatives done by Desbrun [3]. There are other methods can do the similar tasks such as finite element exterior calculus by Arnold [1].

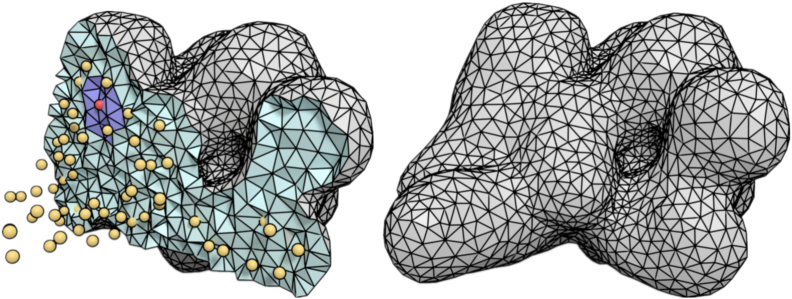

Figure 4: A 3-manifold embedded in 3D Euclidean space is tessellated into a 3D simplicial complex.

The boundary operator ∂ is defined as

$$\partial\sigma = \sum_{i=0}^{k}(-1)^i[v_0, v_1, ..., \hat{v}_i, ..., v_k],$$

where $\hat{v}_i$ means that the ith vertex is removed and an oriented k-simplex $\sigma = [v_0, v_1, ..., v_k]$.

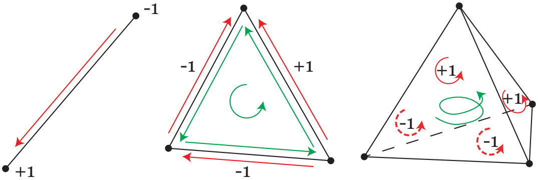

Figure 5: Pre-assigned orientation is colored in red. Induced orientation by ∂ is colored in green.

The discrete Hodge star matrices S_k is just converting primal forms and dual forms by the following equation

$$\frac{1}{|\sigma_k|}\int_{\sigma_k}\omega = \frac{1}{|*\sigma_k|}\int_{*\sigma_k}\star\omega.$$

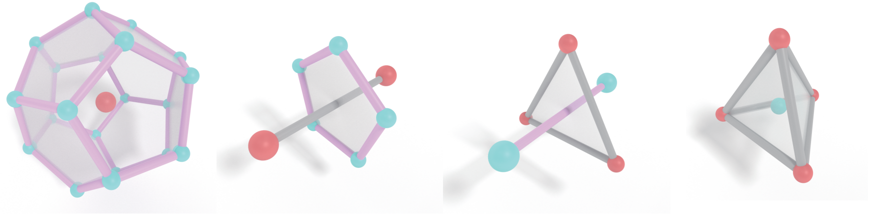

Figure 6: Illustration of the dual and primal elements of the tetrahedral mesh.

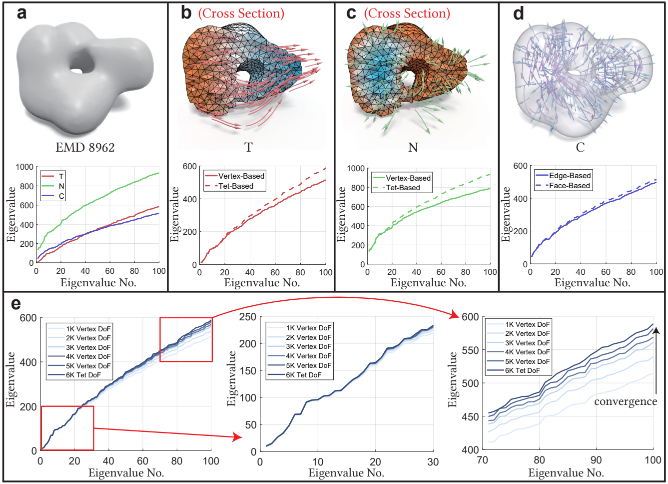

Figure 7: This figure shows the properties of 3 spectral groups, namely, tangential gradient eigenfields (T), normal gradient eigenfields (N),and curl eigenfields (C), for EMD 8962.

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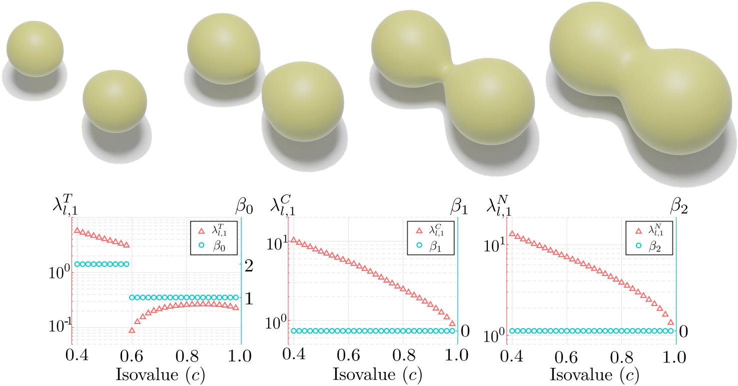

Figure 8: Eigenvalues and Betti numbers vs isovalue (c) of the two-body system with $\eta = 1.19$ and $\max(\rho) \approx 1.0$.

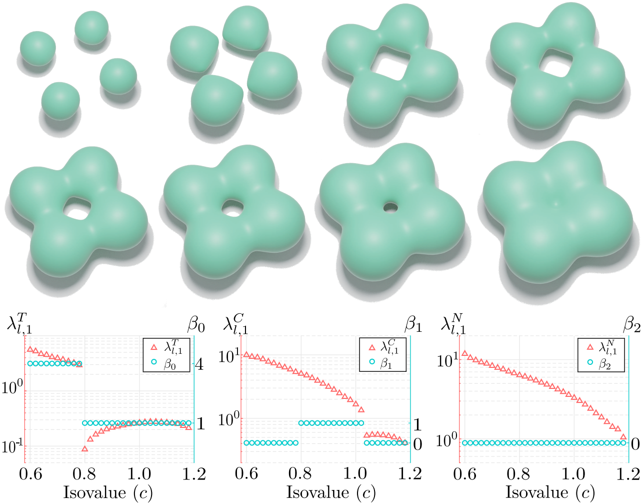

Figure 9: Eigenvalues and Betti numbers vs isovalue (c) of the four-body system with $\eta = 1.19$ and $\max(\rho) \approx 1.2$.

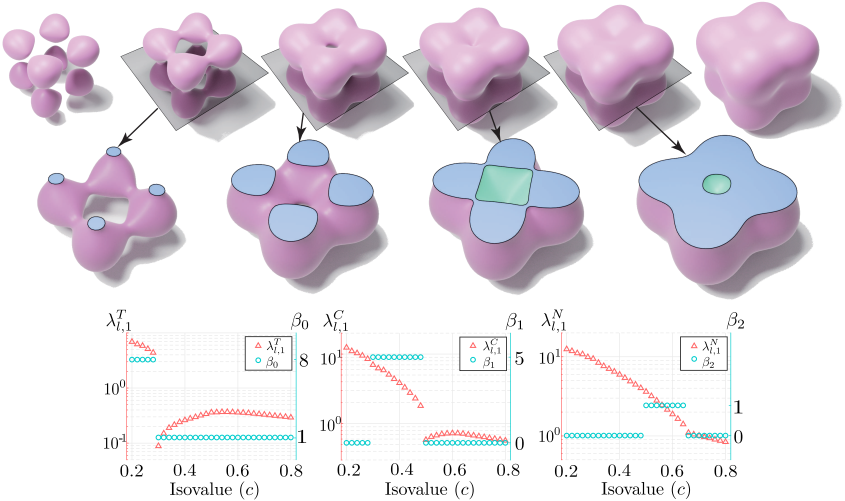

Figure 10: Eigenvalues and Betti numbers vs isovalue (c) of the eight-body system with $\eta = 1.53$ and $\max(\rho) \approx 1.1$.

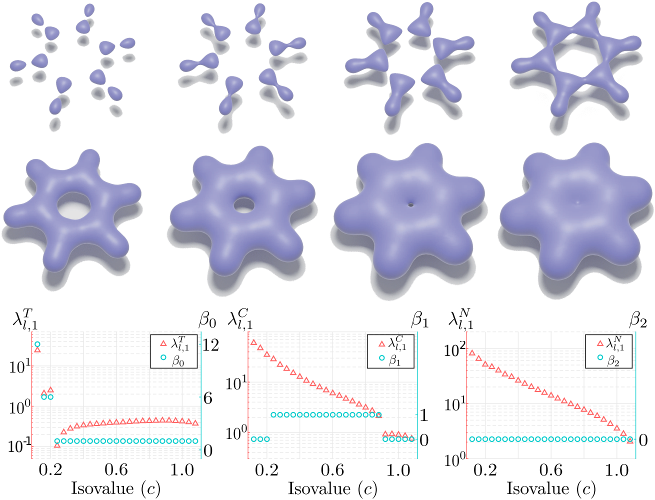

Figure 11: Manifold evolution of benzene with $\eta = 0.45 \times r_{\text{vdw}}$.

Conclusion

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- Three unique sets of singular spectra associated with the tangential gradient eigen field (T), the curl eigen field (C), and the tangential divergent eigen field (N).
- The multiplicities of the zero eigenvalues corresponding to the T, C, and N sets of spectra are exactly the persistent Betti-0 (β_0), Betti-1 (β_1), and Betti-2 (β_2) numbers one would obtain from persistent homology.
- The first non-zero eigenvalues, i.e., Fiedler values, of the T, C, and N sets of evolutionary spectra unveil both the persistence for topological features and the geometric progression for the shape analysis.

Thank you!

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