Boundary-Value PDEs Meet Higher-Order Differential Topology-aware GNNs (Spotlight Paper)

哈爾濱工業大學（深圳） HARBIN INSTITUTE OF TECHNOLOGY, SHENZHEN

Yunfeng Liao, Yangxin Wu, Xiucheng Li

NEURAL INFORMATION PROCESSING SYSTEMS

Summary

- We design a differential topology-aware HOGNN(Higher-order Graph Neural Network), which naturally encodes and decodes PDE operators based on the principles of DEC (Discrete Exterior Calculus) and FEEC (Finite Element Exterior Calculus).
- Various physics-informed loss terms are derived under DEC-HOGNN, including the boundary condition ones, which can enable solving the boundary-value PDEs more effectively.
- The universal approximation property in solving Poisson problems (electrostatics and magnetostatics) is presented, and the performance excellence is demonstrated via empirical experiments.

Why Higher-order Graph?

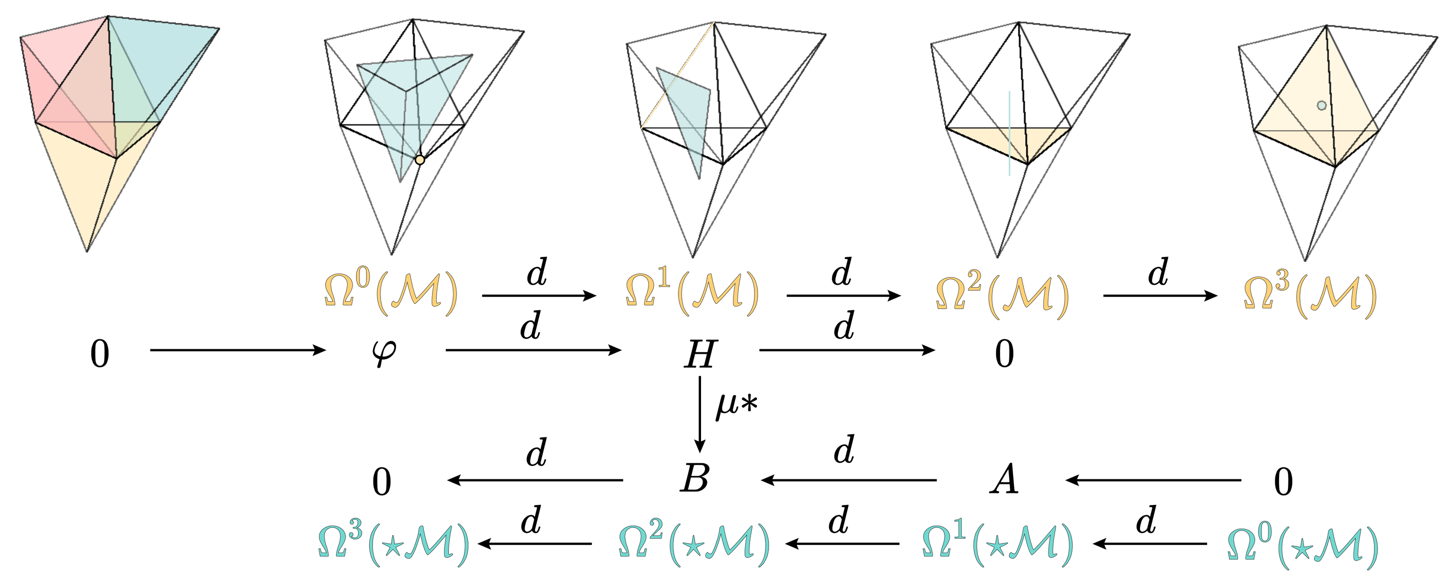
- Modern physics recognizes that **many vector fields are more naturally interpreted as differential forms on manifolds**. This is especially the case in electromagnetism, whose physics enjoys an elegant geometric structure dubbed Maxwell's House. The magnetostatics part of his *House* is shown below. **However, recent studies in PDE neural solvers have not yet fully realized the tight connection between higher-order graphs and this structure**.
- **Preliminary**. It is well known in magnetostatics, these scalar and vector fields (scalar potential φ, intensity $\mathbf{H}$, flux $\mathbf{B}$ and vector potential $\mathbf{A}$) have such relations:

$$\mathbf{H} = \nabla\varphi, \mathbf{B} = \nabla \times \mathbf{A}, \nabla \times \mathbf{H} = \mathbf{0}, \nabla \cdot \mathbf{B} = 0.$$

Surprisingly, these quantities can be incorporated into a unified geometric framework: the differential forms, or more exactly, the De Rham complex.

$$H = d\varphi, dH = 0, dA = B, dB = 0, B = \mu * dH.$$

- By identifying these k-forms as features k-dimensional elements(nodes, edges, faces and cells), solving PDEs is equivalent to looking for features on a hypergraph.



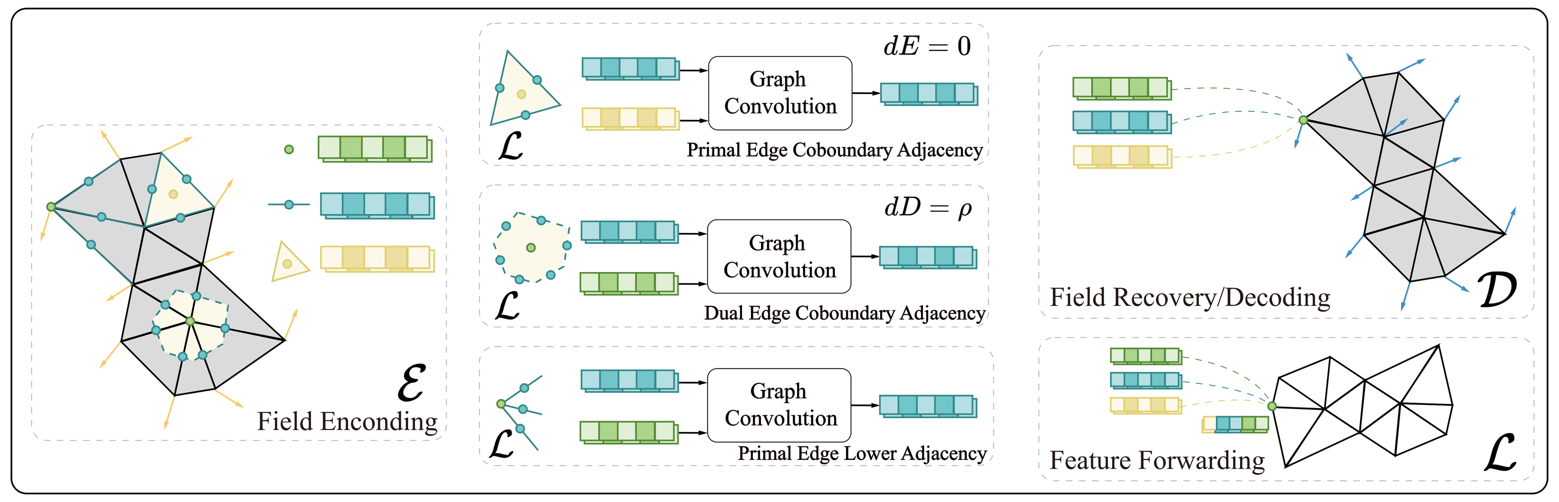
Birdview: Elegant Differential-form-version Physics-informed Loss

By Stokes theorem and identifying B as the features of faces, the divergence-free condition gives an elegant physics-informed loss:

$$dB = 0 \Leftrightarrow \nabla \cdot \mathbf{B} = 0 \Rightarrow \int_{\Omega} \nabla \cdot \mathbf{B} = \int_{\partial\Omega} \mathbf{B} \cdot \mathbf{n} = \sum_{\sigma_2 \in \partial\Omega} \int_{\sigma_2} \mathbf{B} \cdot \mathbf{n}_{\sigma_2} = \sum_{\sigma_2 \in \partial\Omega} \int_{\sigma_2} B = 0.$$

Message Passing on Hypergraph Coincides Stokes Theorem!

- Differential operators can be interpreted as simple linear combinations in DEC and FEEC thanks to Stokes theorem, aligning with the higher-order message passing framework. Once the PDEs are solved, we then translate the results into the vector field language for downstream analysis.



- **Example**. The integral version of $dD = \rho$ is $\int_{\mathcal{M}} \rho = \int_{\mathcal{M}} dD = \int_{\partial\mathcal{M}} D$. The left-most term is about the feature of some cells while the rightmost is about those of some faces. This is simply a special case of the message aggregation in higher-order GNNs, i.e., the message aggregation according to the lower-adjacency.

Any Higher-order GNN can Get Involved

- Any network attempting to excavate higher-order element features on the structure of cell complex can take part. For instance, all higher-order GNNs based on generalized message passing fall into this category.

$$\mathbf{h}'_c = \varphi\left(\mathbf{h}_c, \mathbf{m}_c^{\mathcal{B}}, \mathbf{m}_c^{\mathcal{C}}, \mathbf{m}_c^{\mathcal{N}_\downarrow}, \mathbf{m}_c^{\mathcal{N}_\uparrow}\right), \quad c \in \mathcal{M}, \tag{1}$$

$$\mathbf{m}_c^{\mathcal{B}} = \text{Aggregate}_{d \in \mathcal{B}(c)}\, \varphi_{\mathcal{B}}(\mathbf{h}_c, \mathbf{h}_d), \tag{2}$$

$$\mathbf{m}_c^{\mathcal{C}} = \text{Aggregate}_{d \in \mathcal{C}(c)}\, \varphi_{\mathcal{C}}(\mathbf{h}_c, \mathbf{h}_d), \tag{3}$$

$$\mathbf{m}_c^{\mathcal{N}_\uparrow} = \text{Aggregate}_{d \in \mathcal{N}_\uparrow(c),\ \delta \in \mathcal{C}(c) \cap \mathcal{C}(d)}\, \varphi_{\mathcal{N}_\uparrow}(\mathbf{h}_c, \mathbf{h}_d, \mathbf{h}_\delta), \tag{4}$$

$$\mathbf{m}_c^{\mathcal{N}_\downarrow} = \text{Aggregate}_{d \in \mathcal{N}_\downarrow(c),\ \delta \in \mathcal{B}(c) \cap \mathcal{B}(d)}\, \varphi_{\mathcal{N}_\downarrow}(\mathbf{h}_c, \mathbf{h}_d, \mathbf{h}_\delta). \tag{5}$$

- **Example**. Higher-order GCN, GAT and Graph Transformer:

Table: Possible implementations for co-boundary/lower adjacency layers.

Layer	Co-boundary and lower adjacencies
Convolution	$\mathbf{h}_c'^{(k)} = \sigma\left(\lvert\mathcal{N}_\downarrow(c)\rvert^{-\frac{1}{2}} \sum_{(d,\delta)\in\mathcal{N}_\downarrow(c)} \left(L^{(k)}\mathbf{h}^{(k)}\Theta^{(k)}\right)_d + \left(L^{(k+1)}\mathbf{h}^{(k+1)}\Theta^{(k+1)}\right)_\delta\right)$
	$\mathbf{h}_c'^{(k)} = \sigma\left(\lvert\mathcal{C}(c)\rvert^{-\frac{1}{2}} \sum_{d\in\mathcal{C}(c)} \left(\tilde{L}^{(k)}\mathbf{h}^{(k)}\Theta^{(k)}\right)_d\right)$
Attention	$\mathbf{h}'_c = \sigma(W_C\mathbf{h}_c + \sum_{(d,\delta)\in\mathcal{N}_\downarrow(c)} \text{softmax}_{\mathcal{N}_\downarrow(c)}(\alpha_{d\delta})W_N\mathbf{h}_{c,d,\delta}), \alpha_{d\delta} = W_A\mathbf{h}_{c,d,\delta}$
	$\mathbf{h}'_c = \sigma(W_C\mathbf{h}_c + \sum_{d\in\mathcal{C}(c)} \text{softmax}_{\mathcal{C}(c)}(\alpha_d)W_N\mathbf{h}_{c,d}), \alpha_d = W_A\mathbf{h}_{c,d}$
Transformer	$\mathbf{h}'_c = \sigma(W_C\mathbf{h}_c + \sum_{(d,\delta)\in\mathcal{N}_\downarrow(c)} \text{softmax}_{\mathcal{N}_\downarrow(c)}(\lvert\mathcal{N}_\downarrow(c)\rvert^{-\frac{1}{2}}\mathbf{q}_c^\top\mathbf{k}_d)W_N\mathbf{h}_d)$
	$\mathbf{h}'_c = \sigma(W_C\mathbf{h}_c + \sum_{d\in\mathcal{C}(c)} \text{softmax}_{\mathcal{C}(c)}(\lvert\mathcal{C}(c)\rvert^{-\frac{1}{2}}\mathbf{q}_c^\top\mathbf{k}_d)W_N\mathbf{h}_d)$

Walk on the Dual Manifold

Since forms in a PDE can be defined on both $\mathcal{M}$ and $\star\mathcal{M}$, we also propose a higher-order MPNN on the dual manifold $\star\mathcal{M}$ for dual forms by the fact:

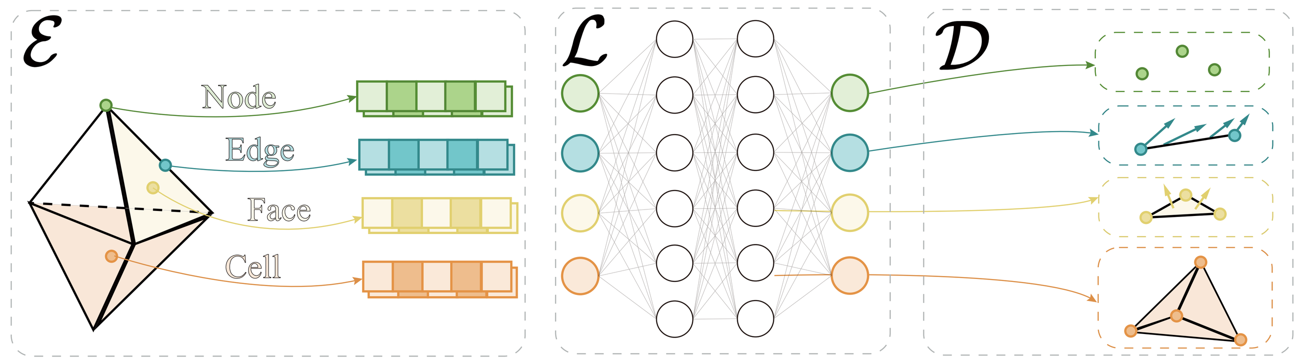
$$\mathcal{B}(\star c) = \{\star d : d \in \mathcal{C}(c)\}, \quad \mathcal{C}(\star c) = \{\star d : d \in \mathcal{B}(c)\},$$
$$\mathcal{N}_\uparrow(\star c) = \{\star d : d \in \mathcal{N}_\downarrow(c)\}, \quad \mathcal{N}_\downarrow(\star c) = \{\star d : d \in \mathcal{N}_\uparrow(c)\}.$$

This is more than a trick to fully leverage the topological structure: it has an exact physics interpretation in electromagnetism, that is, the Constitution Law:

$$B = \mu * H, D = \varepsilon * E.$$

Claims

- **Non-cycle Integrated Dual Form Estimation**: It will not be too hard to implement learning on the dual manifold.
- **Proper Encoder-Decoder**: Converting fields into forms will not lose much information.



- **Universal Approximation**: It can serve as a qualified neural operator.

Numerical Results

- **On Higher-Order Interactions**. Different types of interactions can contribute variably to the performance of DEC-HOGNN. Empirically, only those aligning with the underlying physics are efficient. P / D in the table below indicates that interactions on the primal / dual manifold are considered.

Table: Test loss and performance drop of different variants against the entire models.

Interactions								
Lower adjacency	PD	P	D	None	PD	PD	PD	None
Co-boundary	PD	PD	PD	PD	D	P	None	None
Test loss (mean square error)	0.652	0.676	0.678	0.719	0.954	0.959	1.244	2.077
Performance drop (%)	0.00	3.81	4.12	10.34	46.35	47.23	90.98	218.87

- **On Performance Degeneration due to Mesh Quality and Different Topological Characteristics**. The left panel reflects that dropping edges from a triangularized mesh is followed by mesh degeneration. Also, minor degeneration would not affect the performance violently and thus these negative effects are tolerable. The right panel shows the performance excellence over datasets with **different topology**, named after *(Connected Component Amount, Hole Amount)*.