AI in the Sciences and Engineering HS 2025: Lecture 10

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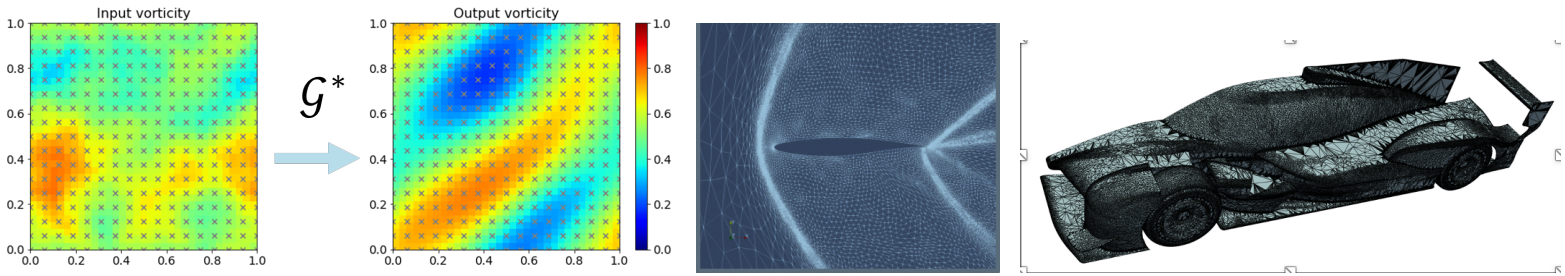
What we have learnt so far ?

- AIM: Learn PDEs using Deep Neural Networks
- Operator Learning: Learn the PDE Solution Operator from data.
- Examples: FNO, CNO, VIT, scOT etc.
- Very successful on PDEs on 2D Cartesian Domains !!
- Readily extended to time-dependent PDEs with all2all training.
- What are the caveats ?

Caveat II: PDEs on Arbitrary Domains

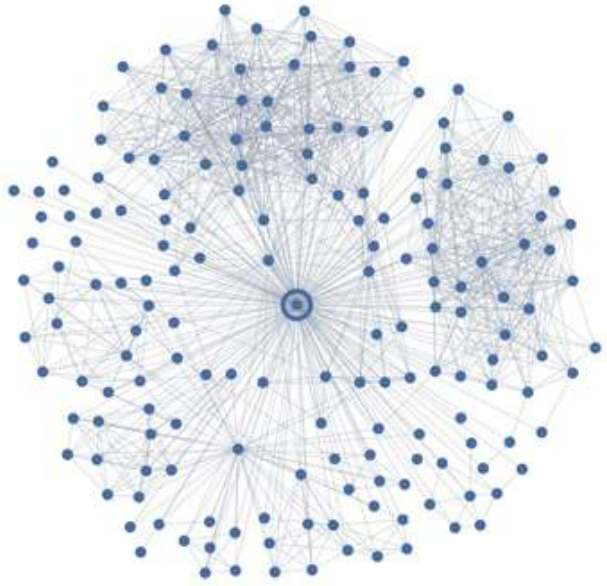


- Discussion so far has only focussed on Cartesian Domains
- Discretized with Uniform Grids.
- Most Real world PDEs are on Arbitrary Domains
- Discretized with Unstructured Grids or Point Clouds
- Need to handle such Data !!

Summary of Available Methods

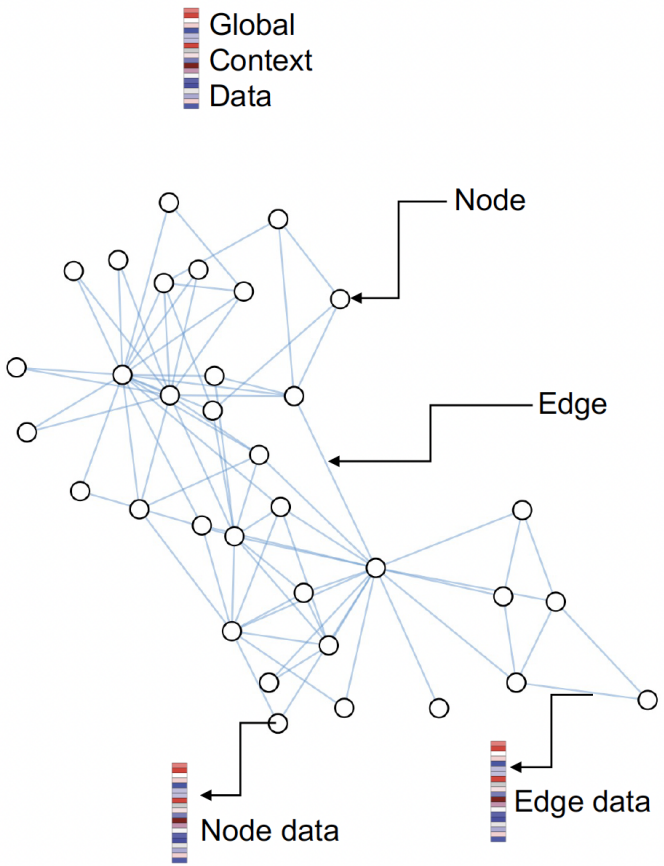
- Posing problem on Cartesian Domain through Masking.
- Direct Spectral Evaluations for FNO
  - DSE proposed in Lingsch, SM et. al., 2024
- Graph Neural Networks

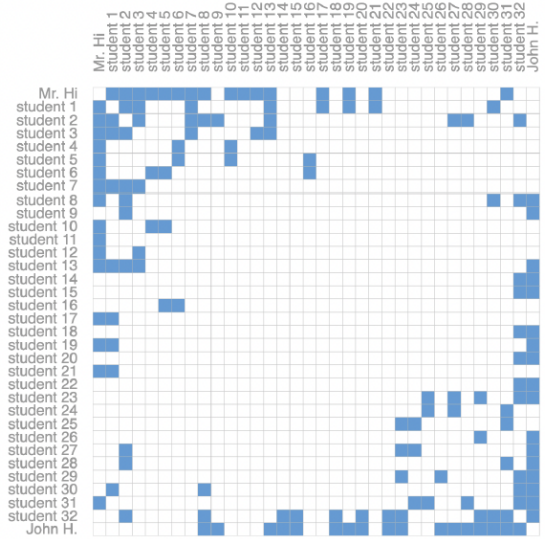
Learning Graph Structured data



- Input data on Graphs is ubiquitous:
  - Social networks, Recommender and Transport systems.
  - Chemistry and Biology (Molecules)
  - Mesh-based numerical simulations in Scientific computing

Basics on Graphs



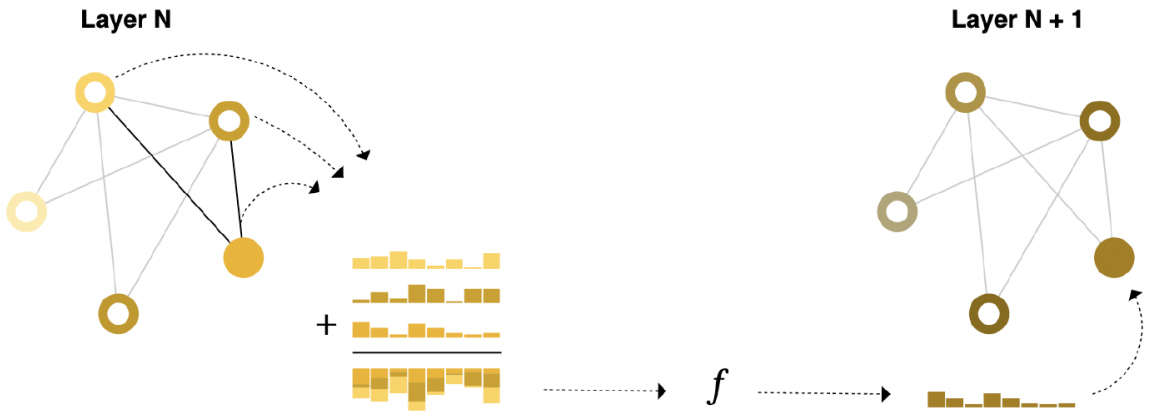


Adjacency matrix

What is a Graph Neural Network ?

- GNN is a composition of layers.
- Each layer updates Node + Edge features

Message Passing is the basis of all GNNs

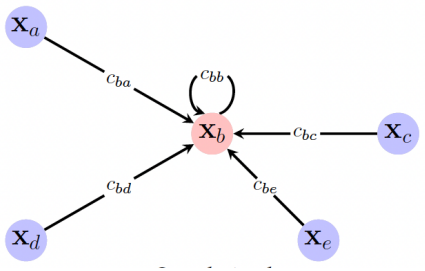


- Generic form of Message Passing:

$$h_i := f\left(v_i, \bigoplus_{j \in \mathcal{N}_i} \Psi(v_i, v_j)\right)$$

- f, Ψ are MLPs.
- $\bigoplus$ is an aggregation function

Ex I: Graph Convolutional Network (GCN)



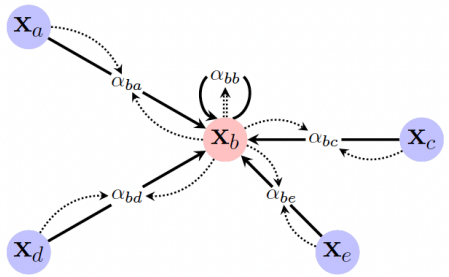
- Generic form of GCN:

$$\mathsf{h}_i := f\left(\mathsf{v}_i, \bigoplus_{j\in\mathcal{N}_i} c_{ij}\Psi(\mathsf{v}_j)\right)$$

- Specific example:

$$\mathsf{h}_i := g\left(\sum_{j\in\mathcal{N}_i\cup\{v_i\}} \frac{1}{\sqrt{\tilde{d}_i\tilde{d}_j}}\mathsf{W}\mathsf{v}_j\right), \quad \tilde{d}_i = 1 + \sum_j \mathsf{A}_{ij}$$

Ex II: Graph Attention Network (GAT)



- Generic form of GAT:

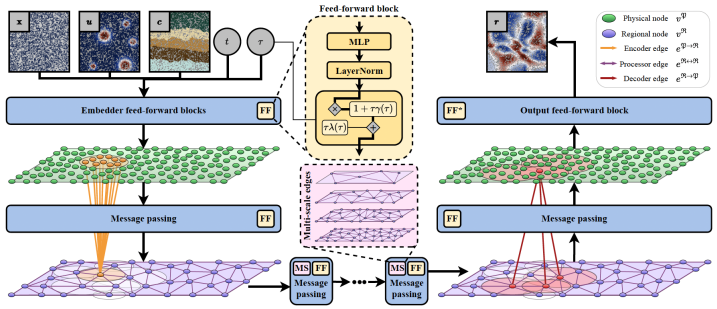
$$\mathsf{h}_i := f\left(\mathsf{v}_i, \bigoplus_{j\in\mathcal{N}_i} \alpha(v_i, v_j)\Psi(\mathsf{v}_j)\right)$$

- Specific example:

$$\mathsf{h}_i := g\left(\sum_{j\in\mathcal{N}_i\cup\{v_i\}} \alpha(v_i, v_j)\mathsf{W}\mathsf{v}_j\right),$$

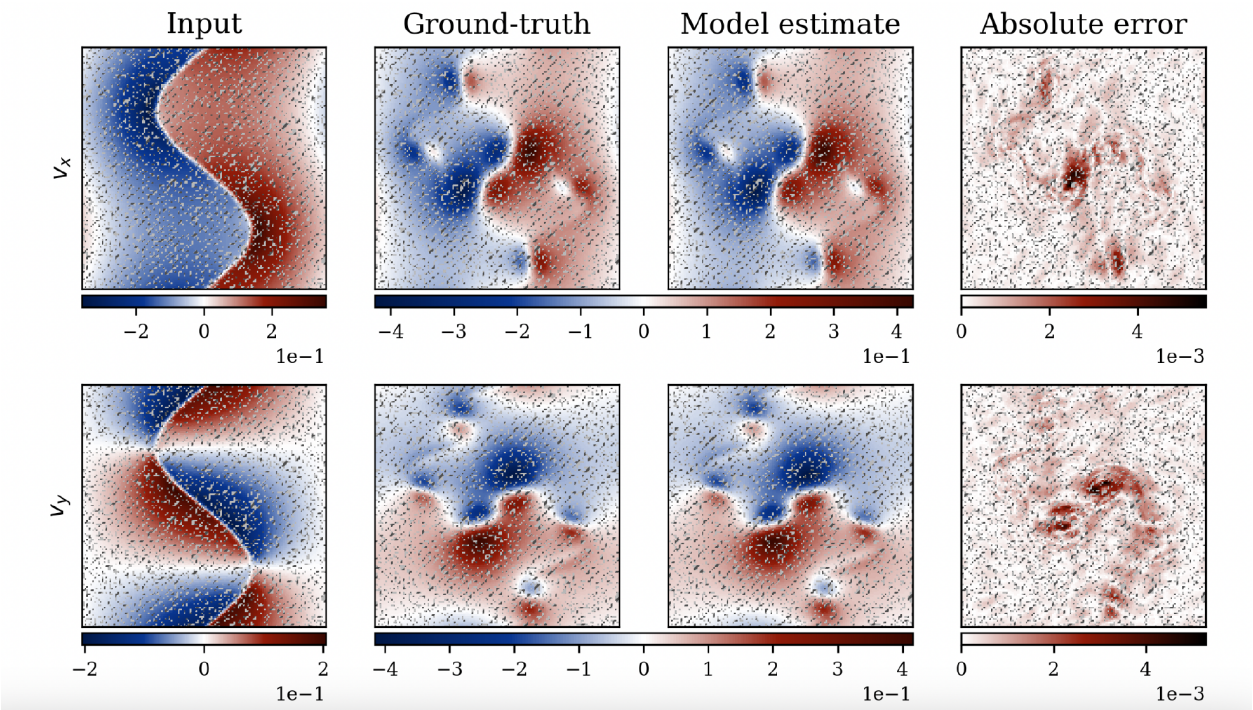
- α is a softmax based weight.

GNN for Operator Learning of PDEs ?



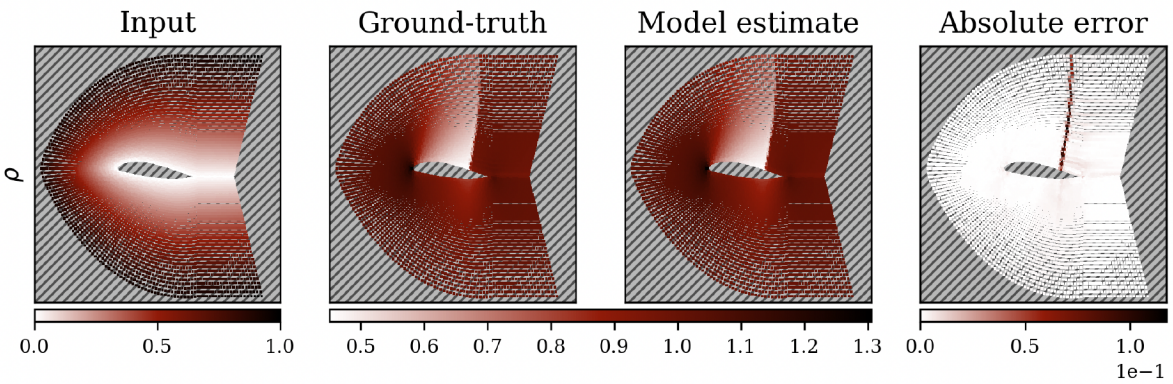
- RIGNO of Mousavi, SM, et. al., 2025
- Based on general MPNNs
- Multiple modifications to ensure:
  - Multiscale Information processing.
  - Temporal Continuity
  - Resolution Invariance

NS-SVS



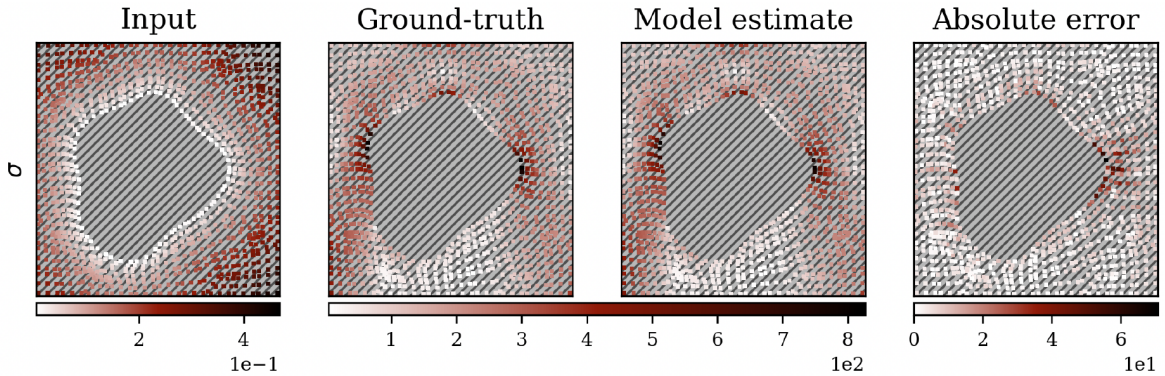
Model	FNO-DSE	GeoFNO	GINO	RIGNO
Errors (in %)	26.0	9.75	1.19	0.56

Flow Past Airfoills



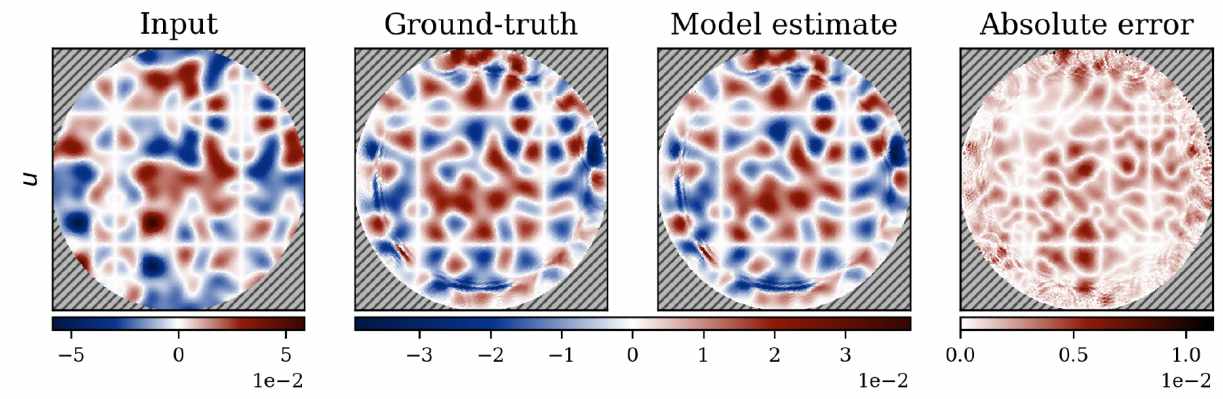
Model	FNO-DSE	GeoFNO	GINO	RIGNO
Errors (in %)	1.99	4.48	2.00	1.09

Plasticity



Model	FNO-DSE	GeoFNO	GINO	RIGNO
Errors (in %)	4.81	5.53	4.38	4.31

Waves in a Circle

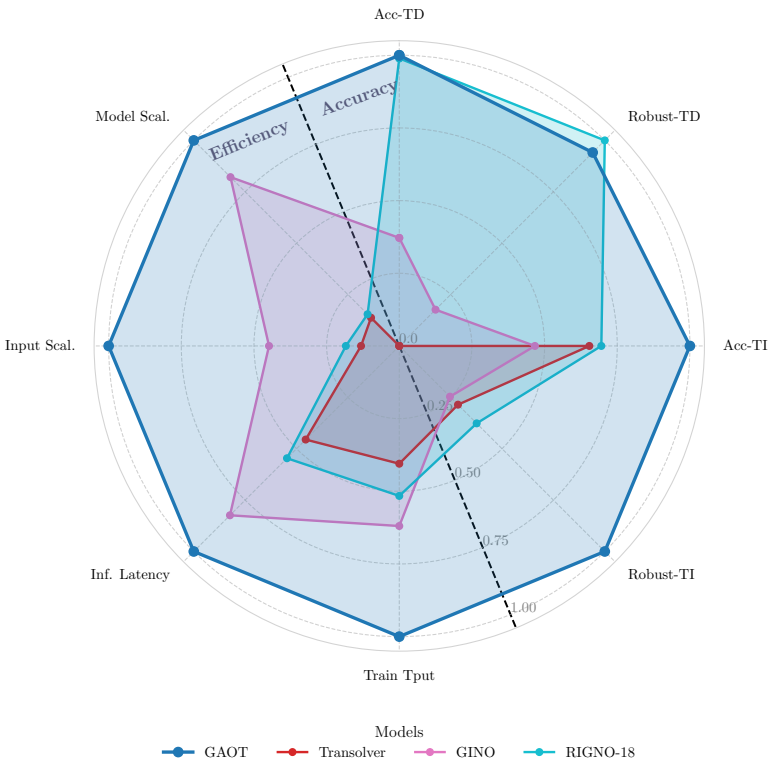


Model	FNO-DSE	GeoFNO	GINO	RIGNO
Errors (in %)	5.52	13.1	5.82	5.35

RIGNO is very accurate

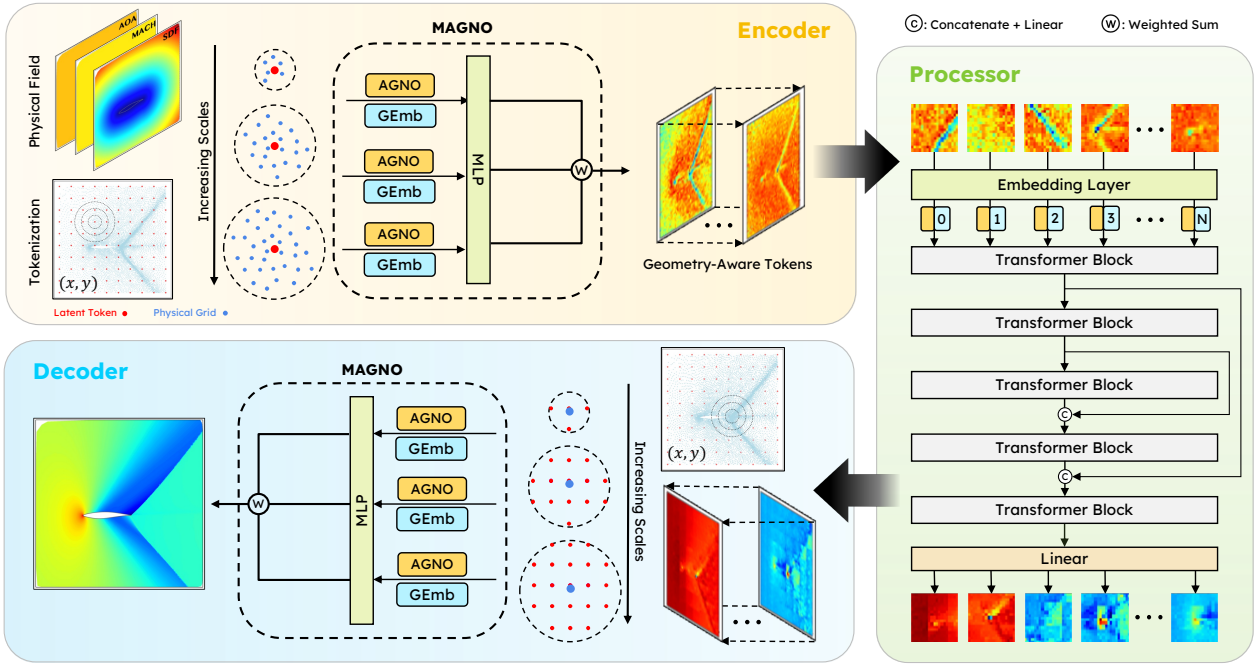
Dataset	Median relative L^1 error [%]				
(unstructured)	**RIGNO-18**	**RIGNO-12**	**GeoFNO**	**FNO DSE**	**GINO**
Heat-L-Sines	**0.04**	**0.05**	0.15	0.53	0.19
Wave-C-Sines	**5.35**	6.25	13.1	**5.52**	5.82
NS-Gauss	**2.29**	**3.80**	41.1	38.4	13.1
NS-PwC	**1.58**	**2.03**	26.0	56.7	5.85
NS-SL	**1.28**	**1.91**	24.3	29.6	4.48
NS-SVS	**0.56**	**0.73**	9.75	26.0	1.19
CE-Gauss	**6.90**	**7.44**	42.1	30.8	25.1
CE-RP	**3.98**	**4.92**	18.4	27.7	12.3
ACE	**0.01**	**0.01**	1.09	1.29	3.33
Wave-Layer	**6.77**	**9.01**	11.1	28.3	19.2
AF	**1.00**	**1.09**	4.48	1.99	2.00
Elasticity	**4.31**	4.63	5.53	4.81	**4.38**
(uniform grid)	**RIGNO-18**	**RIGNO-12**	**CNO**	**scOT**	**FNO**
NS-Gauss	**2.74**	3.78	10.9	**2.92**	14.24
NS-PwC	**1.12**	**1.82**	5.03	7.11	11.24
NS-SL	**1.13**	**1.82**	2.12	2.49	2.08
NS-SVS	**0.56**	0.75	**0.70**	0.99	6.21
CE-Gauss	**5.47**	**7.56**	22.0	9.44	28.69
CE-RP	**3.49**	**4.43**	18.4	9.74	31.19
ACE	**0.01**	**0.01**	0.28	0.21	0.60
Wave-Layer	**6.75**	8.97	**8.28**	13.44	28.01

What is the Issue then ?



- But not Efficient (more than 2d of training) !!
- Due to Repeated Sparse Memory Access

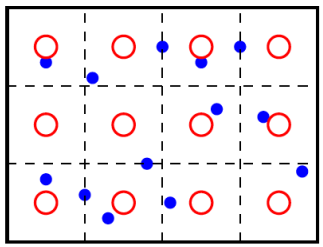
Solution ?: Use Graphs + Transformers



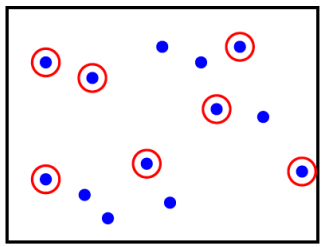
- Geometry Aware Operator Transformer: Wen, SM et. al, 2025

On GAOT

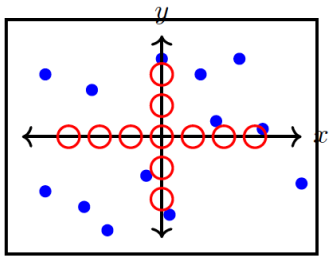
- Based on the Encode-Process-Decode Strategy.
- Encoder: Input Point Cloud $\mapsto$ Latent Grid
- Different choices of Latent Grid:



(a) Strategy I



(b) Strategy II



(c) Strategy III

GAOT Encoder

- Given input field a, Encoder outputs w_e at any Latent point y

$$w_e(y) = \sum_{y=1}^{n_y} \alpha_k K(y, x_k, a(x_k))\varphi(a(x_k)), \quad |y - x_k| \leq r$$

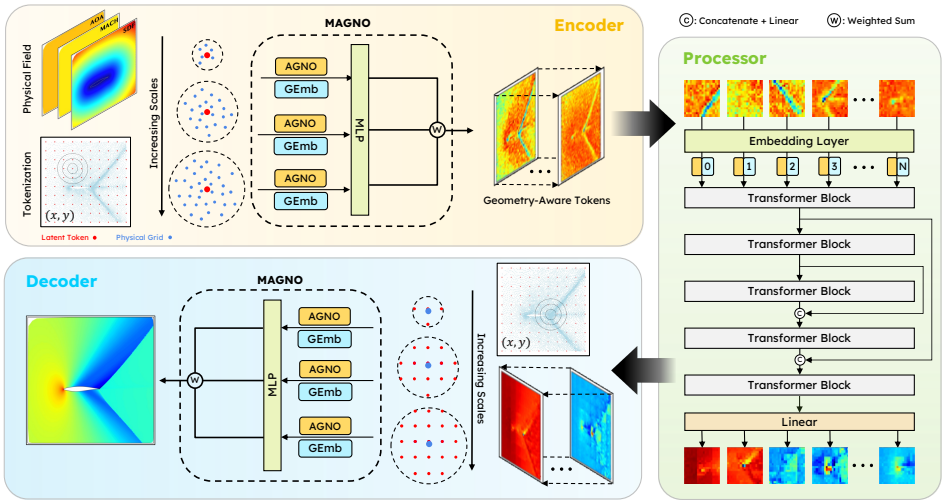
- MLPs: K, φ
- Quadrature weights α chosen by Attention:

$$\alpha_k = \frac{\exp(e_k)}{\sum_{k'=1} n_y exp(e_{k'})}, \quad e_k = \frac{\langle W_q y, W_k x_k \rangle}{\sqrt{d}}$$

- We use Multiscale Aggregation over m scales:

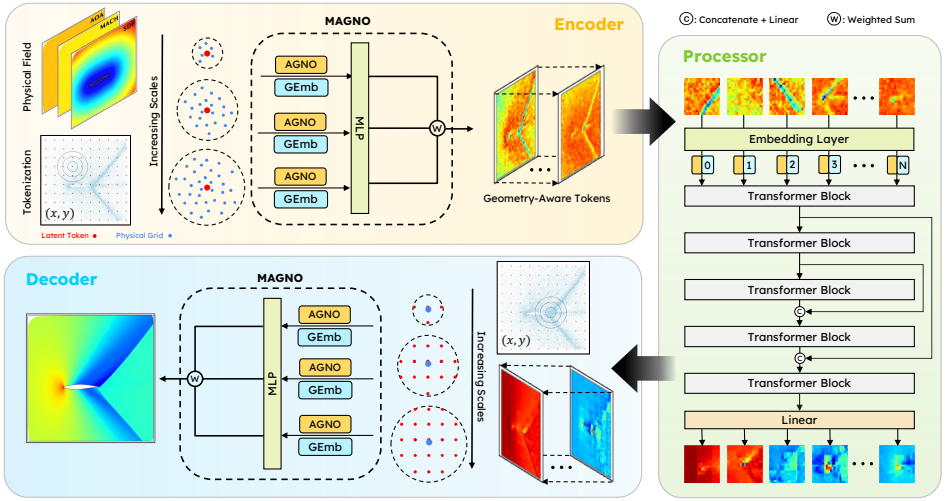
$$w_e^m(y) = \sum_{y=1}^{n_y^m} \alpha_k^m K^m(y, x_k, a(x_k))\varphi^m(a(x_k)), \quad |y - x_k| \leq r_m$$

What about the Geometry ?



- Geometric Information is conveyed through:
- Point coordinates
- Signed Distance functions (SDFs)
- Local Statistical Embeddings $g_m(y)$ based on,
  - Number of Neighbors,
  - Average Distance + its Variance
  - Local Anistropy through PCs of the distance covariance matrix

MAGNO Encoder

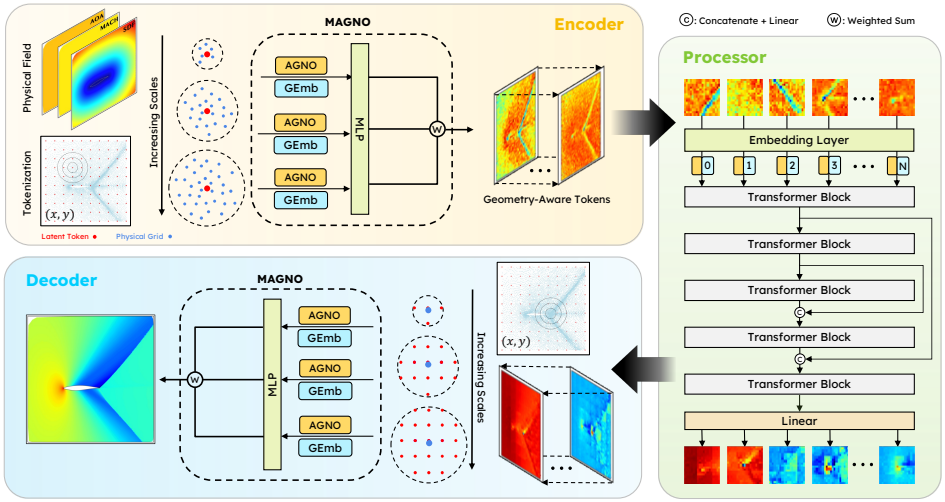


- Final form of the Encoder:

$$w_e(y) = \sum_{m=1}^{M} \beta_k^m \widehat{w}^m(y), \quad \beta_m(y) = \frac{\exp(\Psi_m(y))}{\sum_{m'=1}^{M} exp(\Psi_{m'}(y))}$$

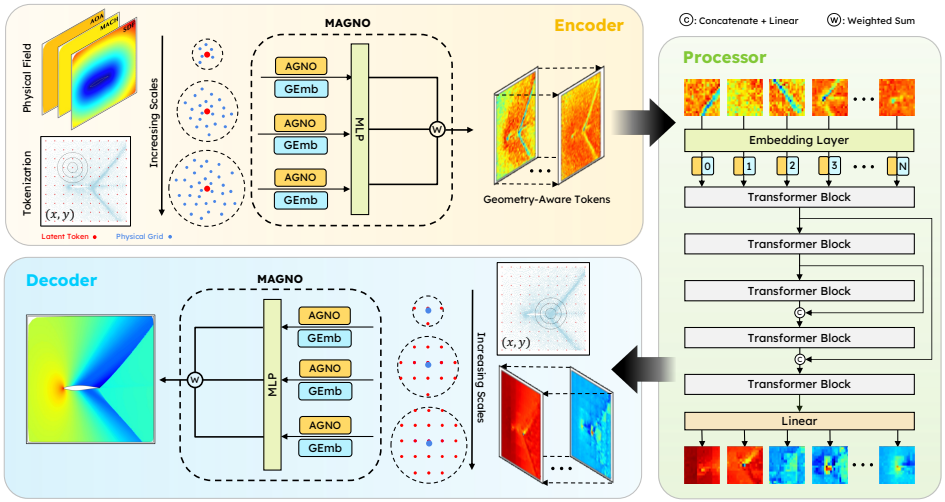
- Provide a set of Geometry Aware Tokens

GOAT Processor



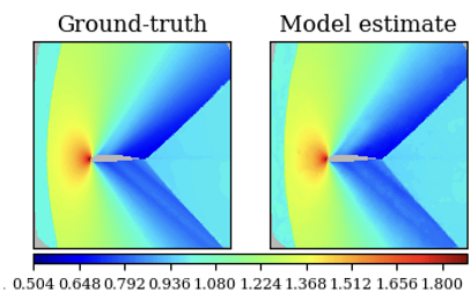
- Use of ViT or SWIN for Cartesian Latent Grids.
- Allows for Patching
- Standard seq2seq Transformers for Unstructured Latent Grids.

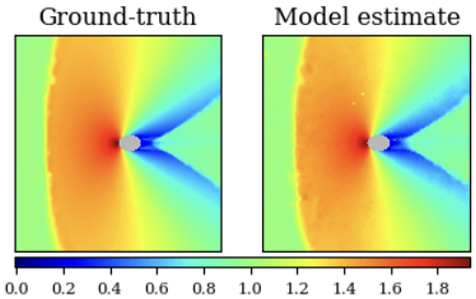
GOAT Decoder

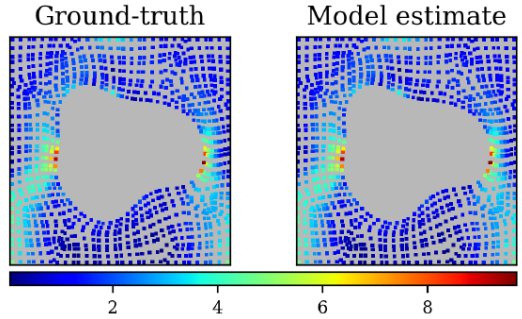


- MAGNO Decoder
- Allows evaluation of output at any query point $y \in D$
- ensures Neural Field Property.
- GINO:
  - Single scale GNO encoder + decoder
  - FNO processor.

GAOT is very flexible wrt Domain Geometry





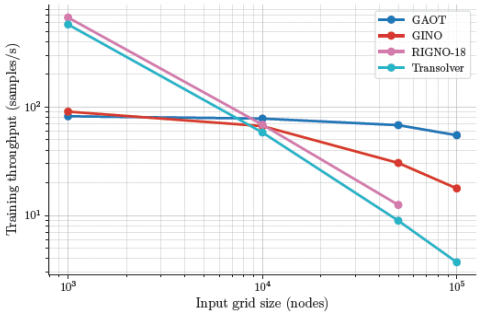


GAOT is vey accurate and robust

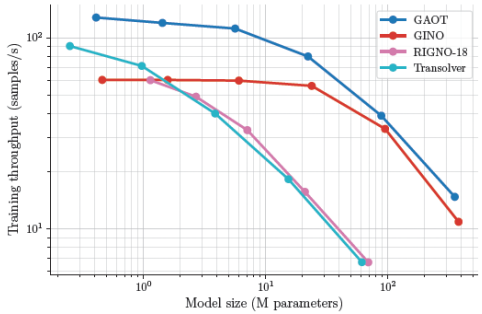
Dataset	Median relative L^1 error [%]					
Time-Independent	**GAOT**	**RIGNO-18**	**Transolver**	**GNOT**	**UPT**	**GINO**
Poisson-C-Sines	**3.10**	**6.83**	77.3	100	100	20.0
Poisson-Gauss	**0.83**	2.26	**2.02**	88.9	48.4	7.57
Elasticity	**1.34**	**4.31**	4.92	10.4	12.6	4.38
NACA0012	**6.81**	**5.30**	8.69	6.89	16.1	9.01
NACA2412	**6.66**	**6.72**	8.51	8.82	17.9	9.39
RAE2822	6.61	**5.06**	**4.82**	7.15	16.1	8.61
Bluff-Body	**2.25**	5.76	**1.78**	44.2	5.81	3.49
Time-Dependent	**GAOT**	**RIGNO-18**	**GeoFNO**	**FNO DSE**	**UPT**	**GINO**
NS-Gauss	**2.91**	**2.29**	41.1	38.4	92.5	13.1
NS-PwC	**1.50**	**1.58**	26.0	56.7	100	5.85
NS-SL	**1.21**	**1.28**	13.7	22.6	51.5	4.48
NS-SVS	**0.46**	**0.56**	9.75	26.0	4.2	1.19
CE-Gauss	**6.40**	**6.90**	42.1	30.8	64.2	25.1
CE-RP	**5.97**	**3.98**	18.4	27.7	26.8	12.3
Wave-Layer	**5.78**	**6.77**	11.1	28.3	19.6	19.2
Wave-C-Sines	**4.65**	**5.35**	13.1	5.52	12.7	5.82

GAOT is also very Efficient

- In terms of
- Training Throughput
- Inference Latency
- wrt Model Size + Input Size.
- This is due to Efficient Implementation

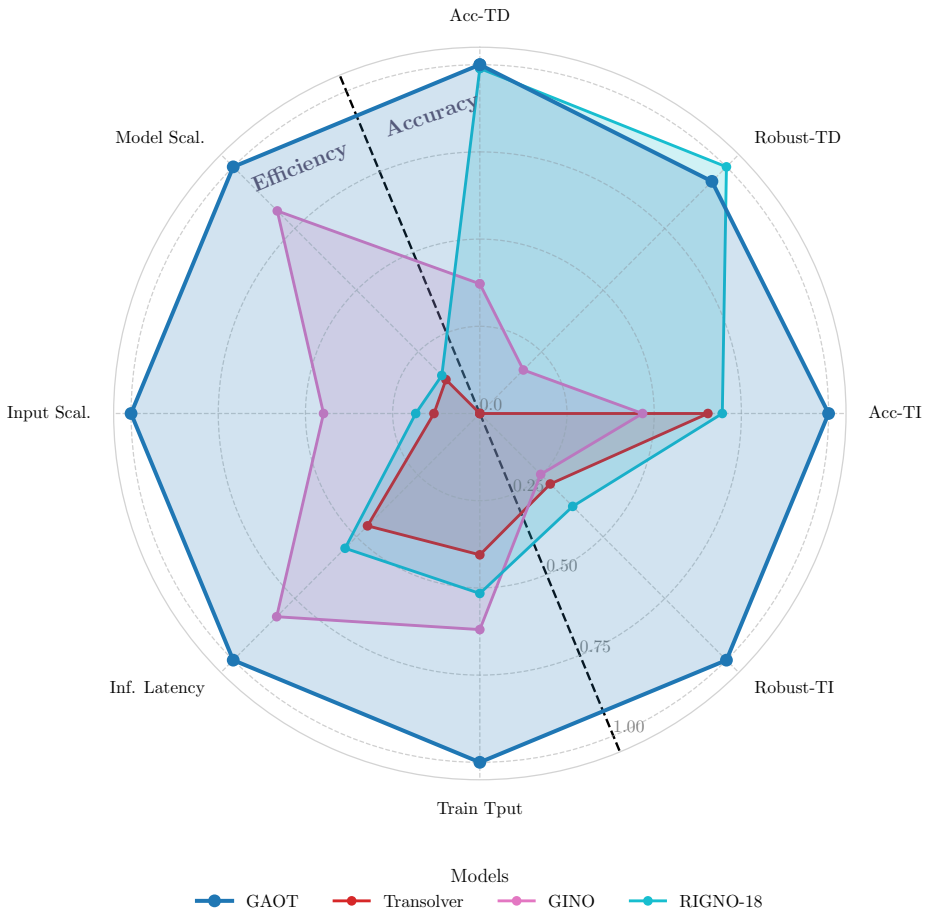


(a) Grid vs. Throughput



(b) Model vs. Throughput

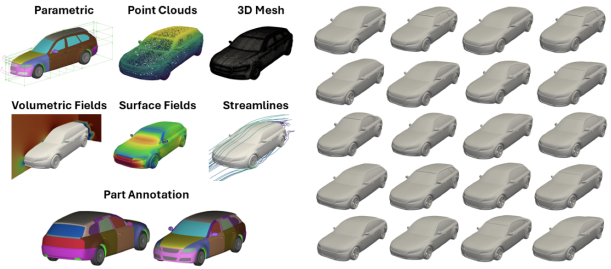
GAOT combines best of both Worlds



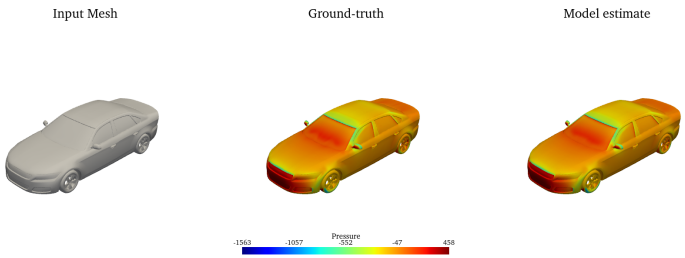
- We can scale it to 3d Industrial Scale datasets.

The DrivaerNet++ Benchmark

- Flow past Cars Dataset (8K Car Shapes with 0.5M nodes)



- GAOT: SOTA for Surface Pressure, Shear Stress

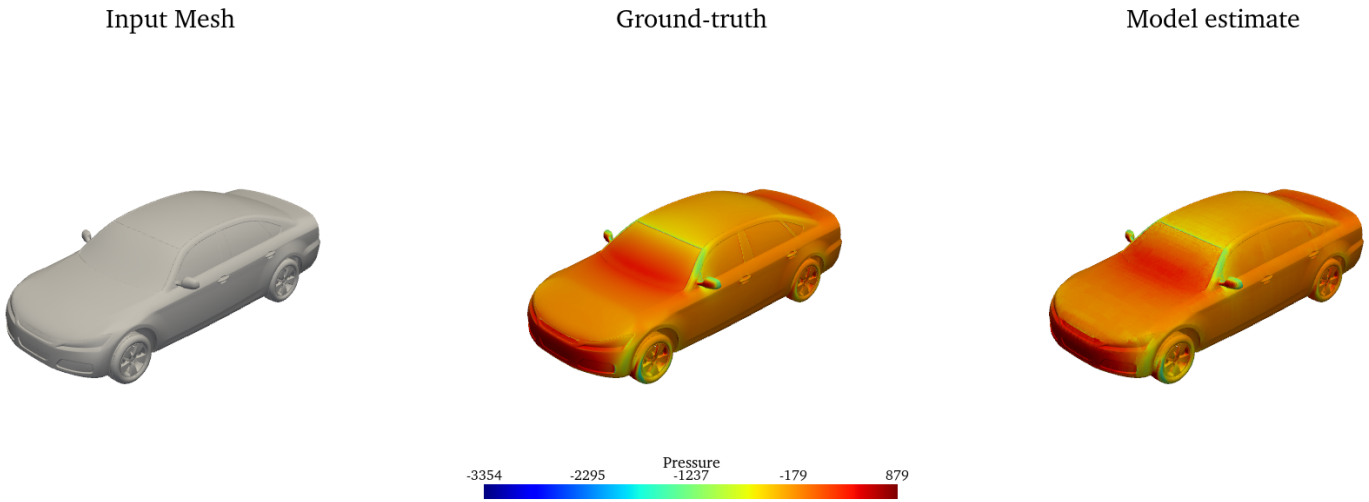


Model	GAOT	FigConvNet	TripNet	RegDGCNN
L^1 Pressure Err.	0.110	0.122	0.125	0.161
L^1 Shear Err.	0.156	0.222	0.215	0.364

- CFD: 375 Node hours vs. GAOT: 0.36 seconds !!!

The DrivaerML Benchmark

- HR-LES simulations of flow past 500 cars.
- More accurate than RANS for Drivearnet++.
- 9 M surface nodes handled accurately by GAOT !!

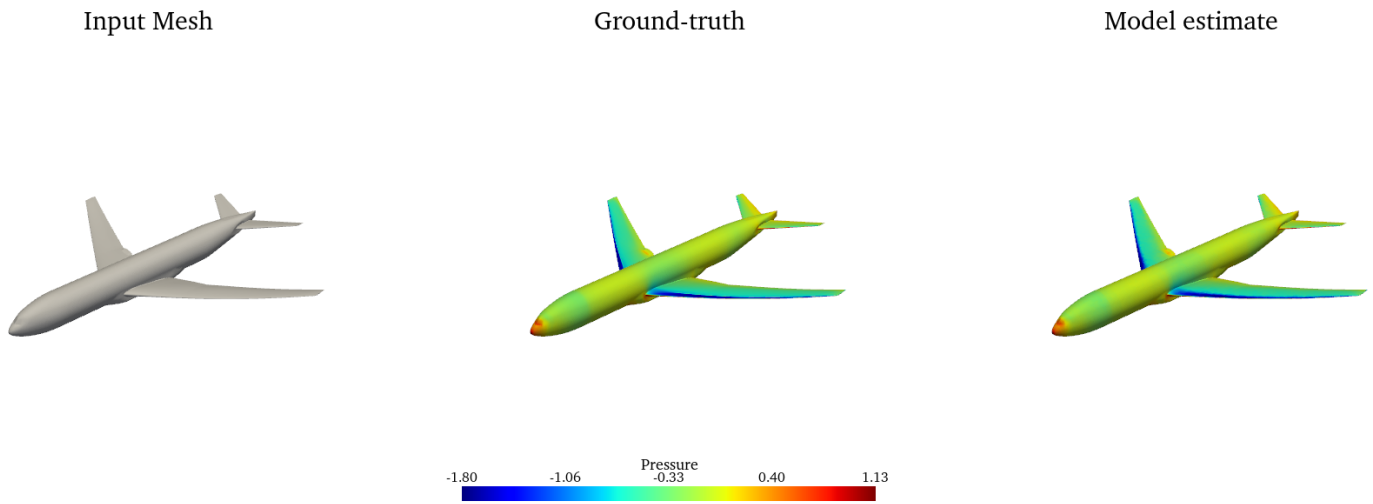


Model	GAOT	GINO
L^1 Pressure Err.	0.123	0.152
L^1 Shear Err.	0.216	0.273

- CFD: 61K Node hours vs. GAOT: 14 seconds !!!

Flow Past an entire Aircraft

- AIAA's NASA CRM Benchmark.
- GAOT predicts Surface Pressure+Skin Friction accurately !!



Model	GAOT	GINO
L^1 Pressure Err.	0.160	0.174
L^1 Skin Friction Err.	0.223	0.242