ICML | 2024

The Forty-first International Conference on Machine Learning

Transolver: A Fast Transformer Solver for PDEs on General Geometries

Haixu Wu [1] **Huakun Luo** [1] **Haowen Wang** [1] **Jianmin Wang** [1] **Mingsheng Long** [1]

Haixu Wu

Huakun Luo

Haowen Wang

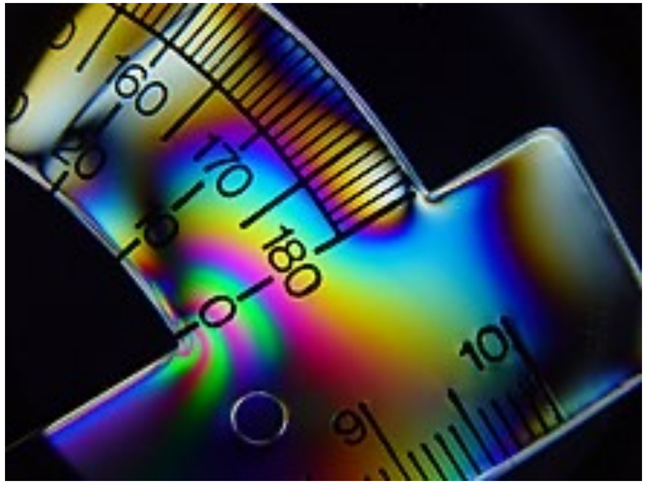
Jianmin Wang

Mingsheng Long

Real-world phenomena

Turbulence

Atmospheric circulation



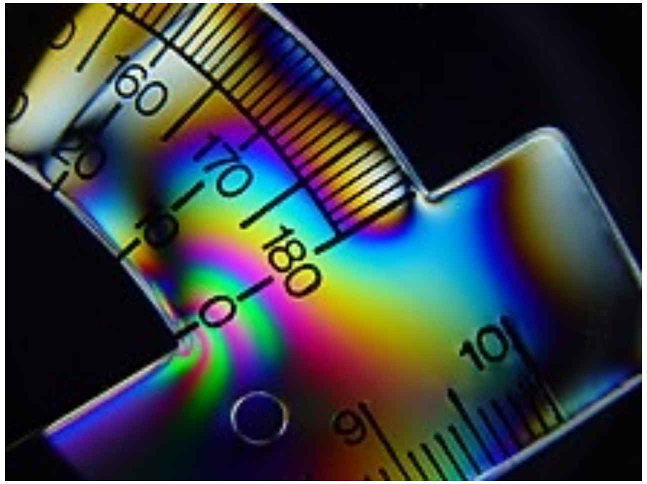
Stress

How to understand the world?

Real-world phenomena

Turbulence

Atmospheric circulation



Stress

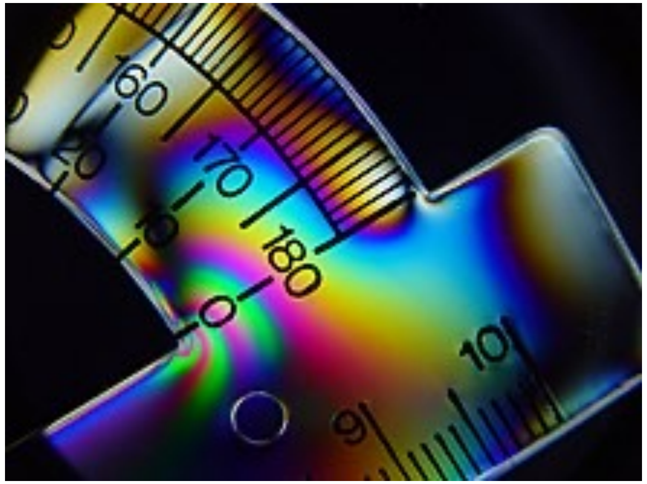
How to understand the world?

Images? Videos?

Real-world phenomena

Turbulence

Atmospheric circulation



Stress

Beyond appearances, these phenomena are governed by **scientific rules**.

Partial Differential Equations (PDEs)

- Fluid physics:

Navier-Stokes Equation
for fluid dynamics

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{U}) = 0$$

$$\frac{\partial \boldsymbol{U}}{\partial t} + \boldsymbol{U} \cdot \nabla \boldsymbol{U} = \boldsymbol{f} + \frac{1}{\rho} \nabla \cdot (\boldsymbol{T}_{ij} \boldsymbol{e}_i \boldsymbol{e}_j)$$

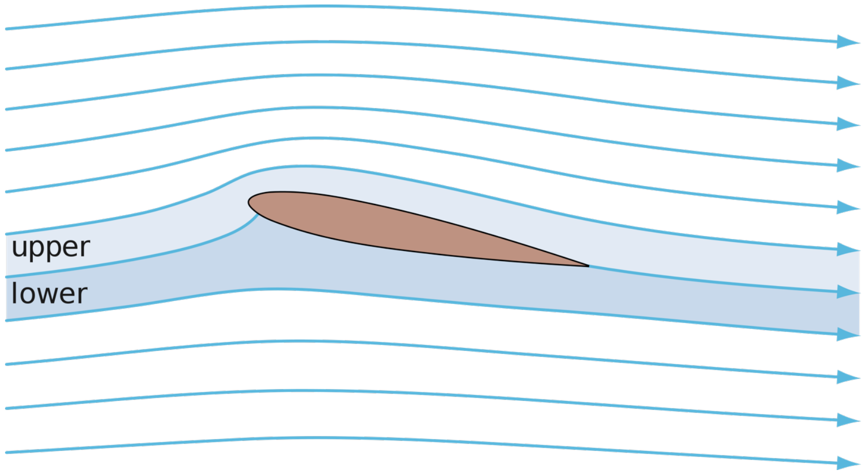
$$\frac{\partial (e + \frac{1}{2}\boldsymbol{U}^2)}{\partial t} + \boldsymbol{U} \cdot \nabla (e + \frac{1}{2}\boldsymbol{U}^2) = \boldsymbol{f} \cdot \boldsymbol{U} + \frac{1}{\rho} \nabla \cdot (\boldsymbol{U} \cdot \boldsymbol{T}_{ij} \boldsymbol{e}_i \boldsymbol{e}_j) + \frac{\lambda}{\rho} \Delta T$$

- Solid physics:

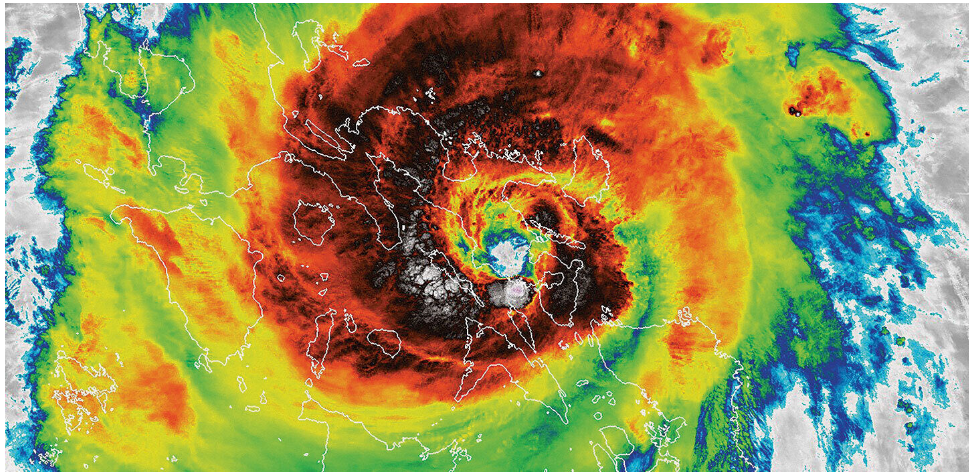
$$\rho^s \frac{\partial^2 \boldsymbol{u}}{\partial t^2} + \nabla \cdot \boldsymbol{\sigma} = 0$$

Inner stress
of solid materials

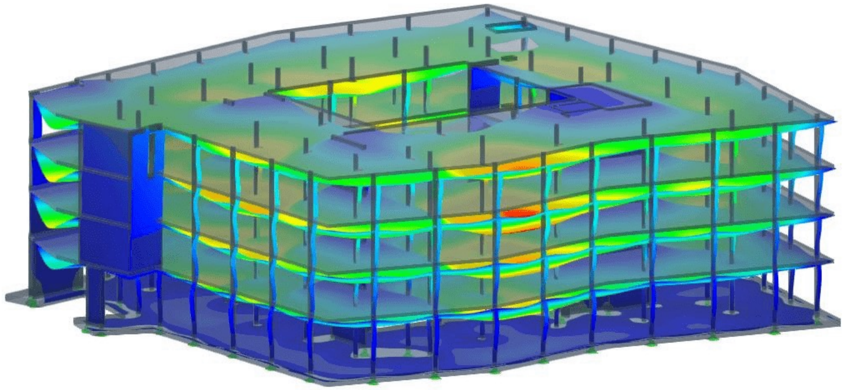
Wide Applications



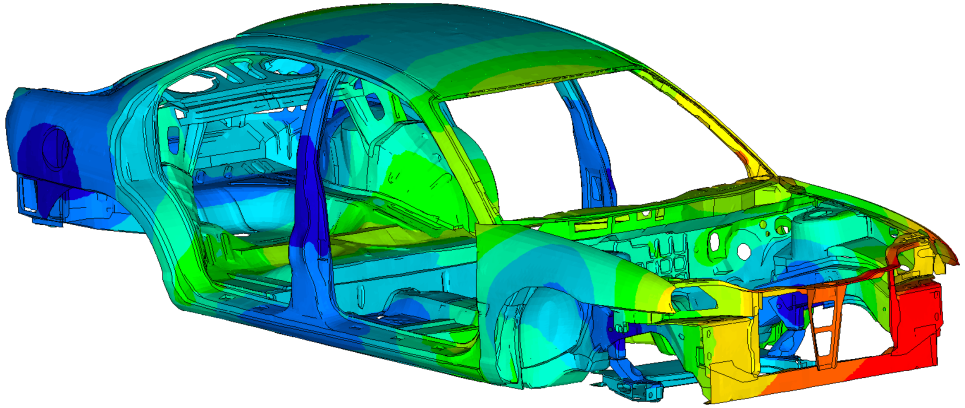
Airfoil design



Weather forecasting



Civil engineering



Vehicle manufacturing

Solving PDEs

Classic Numerical Methods

New Task → FEM or Spectral → Results

- Recalculation for every new sample
- Each round will take hours or even days for a precise simulation

Huge computation costs

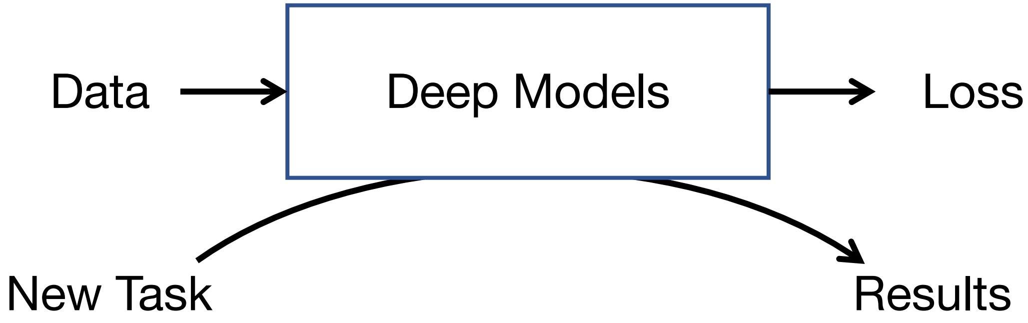
Solving PDEs

Classic Numerical Methods

- Recalculation for every new sample
- Each round will take hours or even days for a precise simulation

Huge computation costs

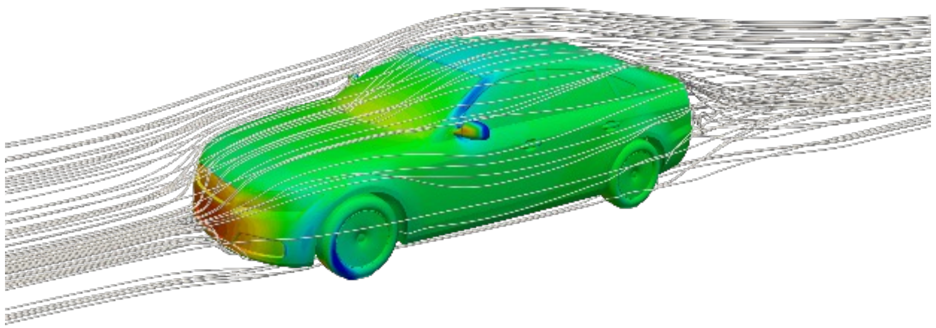
Neural PDE Solver



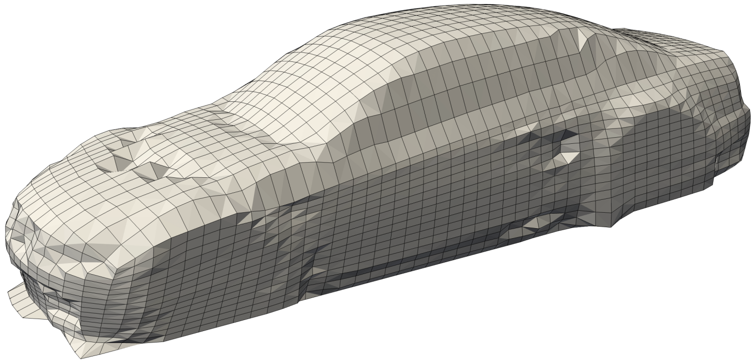
- Training once, inference a lot
- Each inference needs several seconds

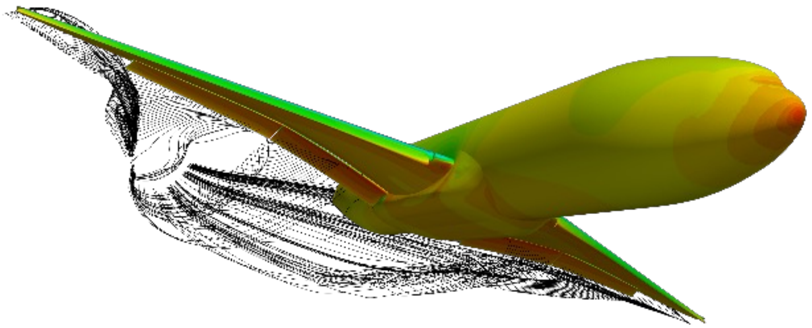
An efficient surrogate tool

Solving PDEs: Discretization

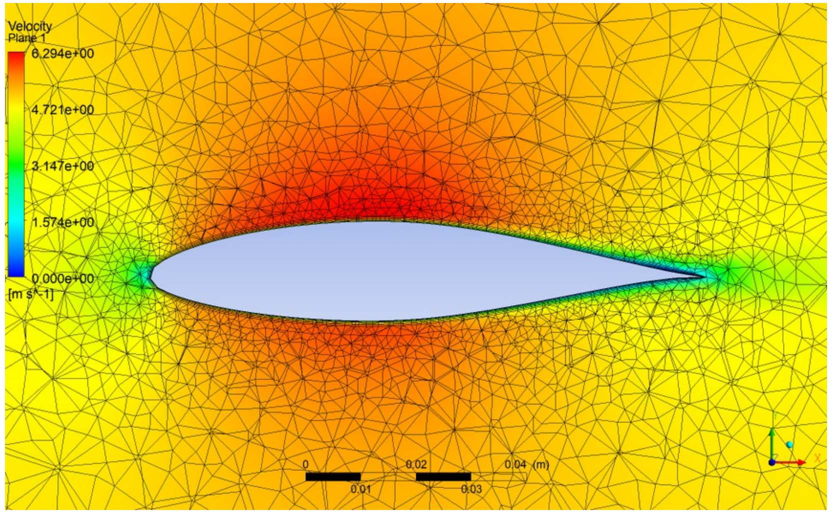


Car

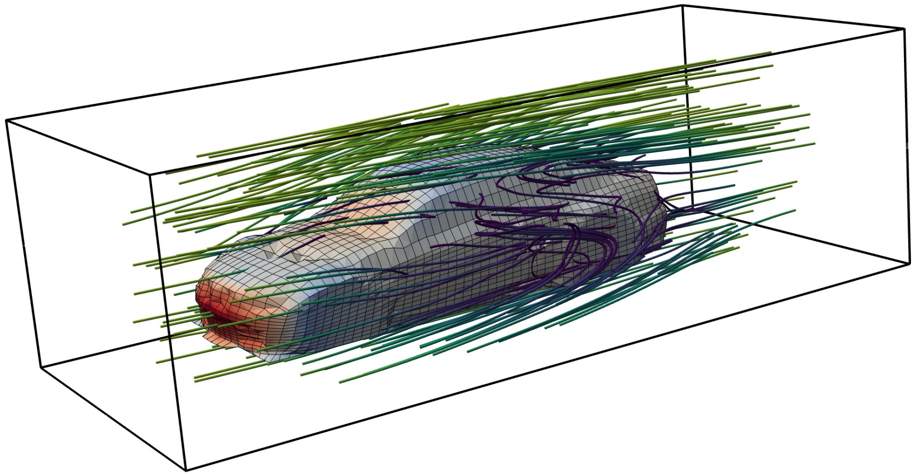




Airplane



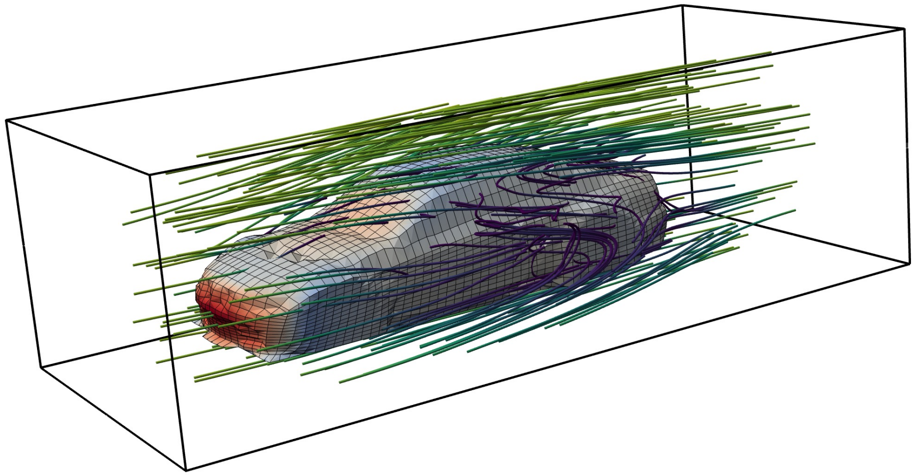
Challenges in Practical Industrial Design



Task: Estimate the drag coefficient of a given shape:

Surrounding Wind & Surface Pressure

Challenges in Practical Industrial Design

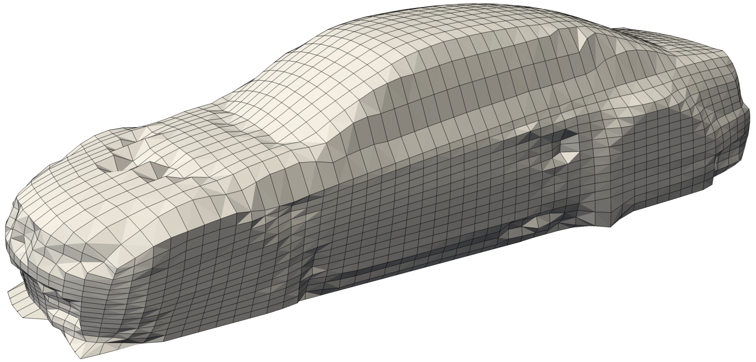


Task: Estimate the drag coefficient of a given shape:

Surrounding Wind & Surface Pressure

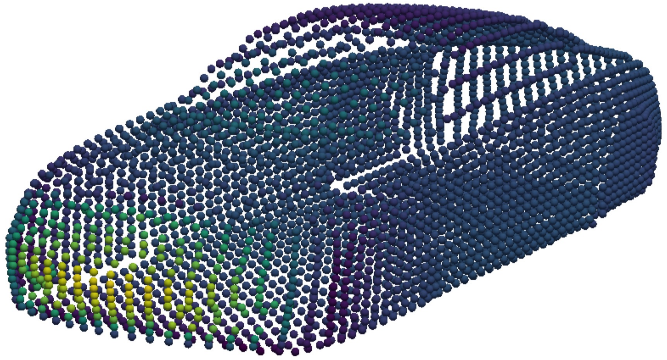
1. Large-scale meshes → **Huge computation cost**
2. Complex and unstructured geometrics → **Complex geometric learning**
3. Multiphysics interaction → **Intricate physical correlations**

Previous Work: Geometric Deep Learning



(1) Mesh

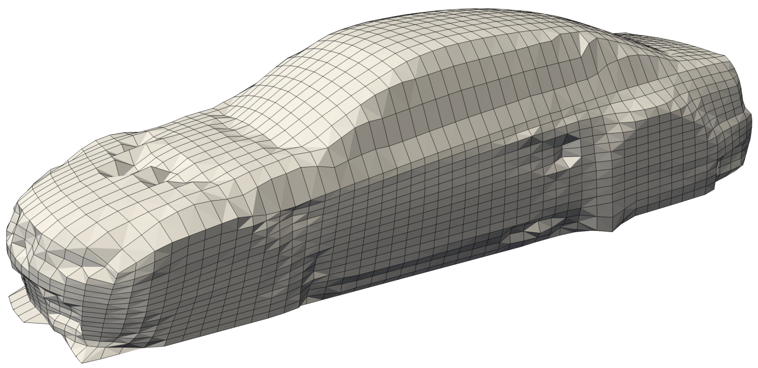
GraphSAGE, MeshGraphNet, etc

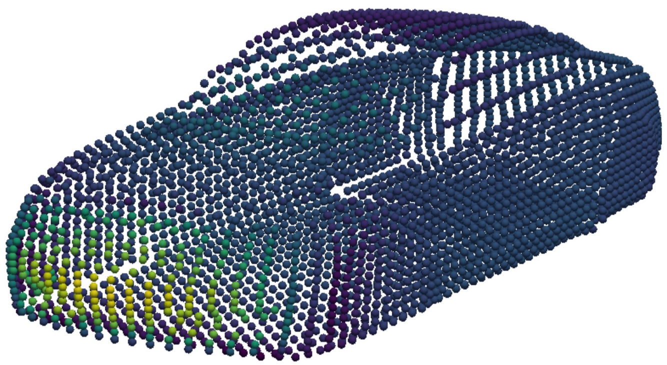


(2) Point Cloud

PointNet, Point Transformer, etc

Previous Work: Geometric Deep Learning





(1) Mesh

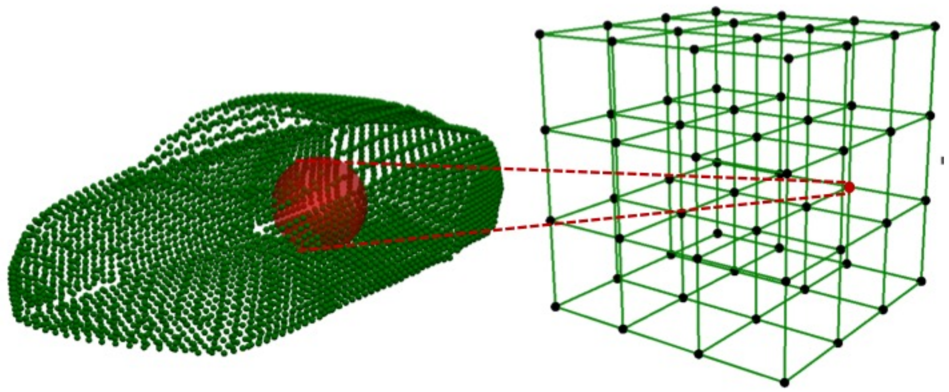
GraphSAGE, MeshGraphNet, etc

(2) Point Cloud

PointNet, Point Transformer, etc

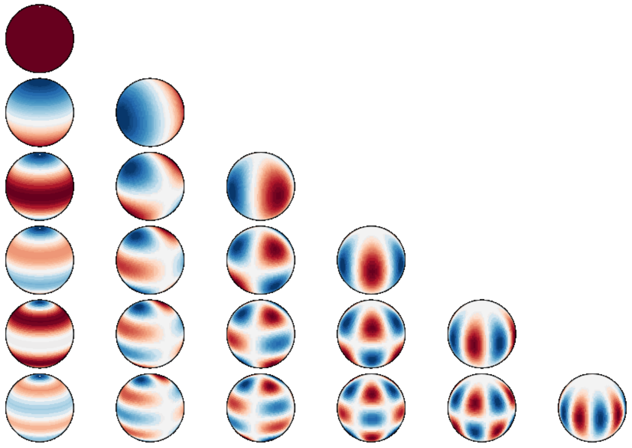
Excels in geometry modeling but fail in physics learning

Previous Work: Geometry-General Neural Operators



(1) GNN as Operators

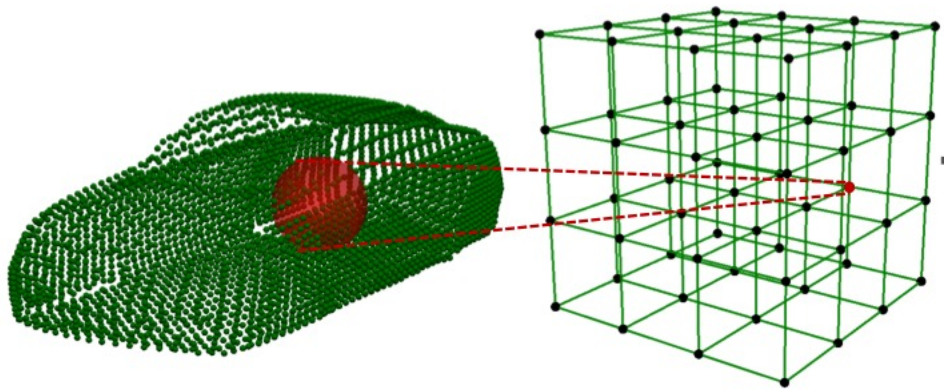
GNO, GINO, etc



(2) FNO-Variants

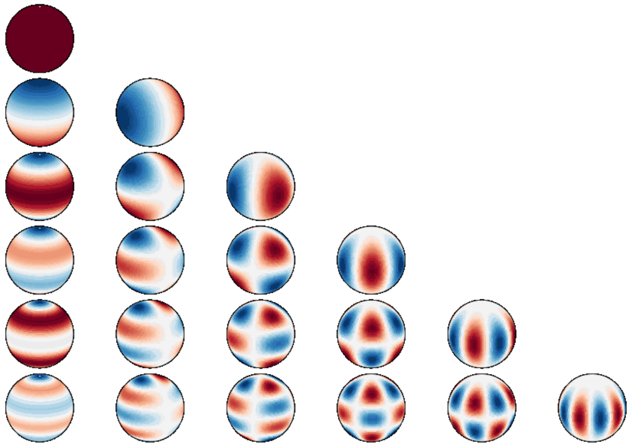
geoFNO, SFNO, etc

Previous Work: Geometry-General Neural Operators



(1) GNN as Operators

GNO, GINO, etc

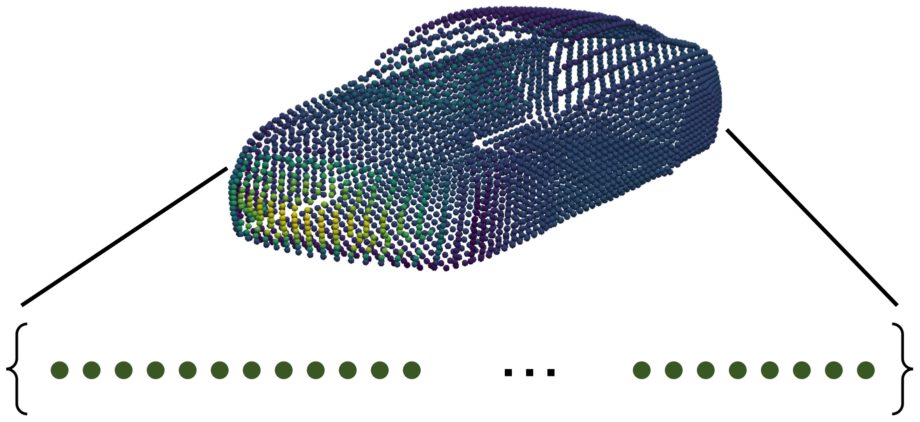


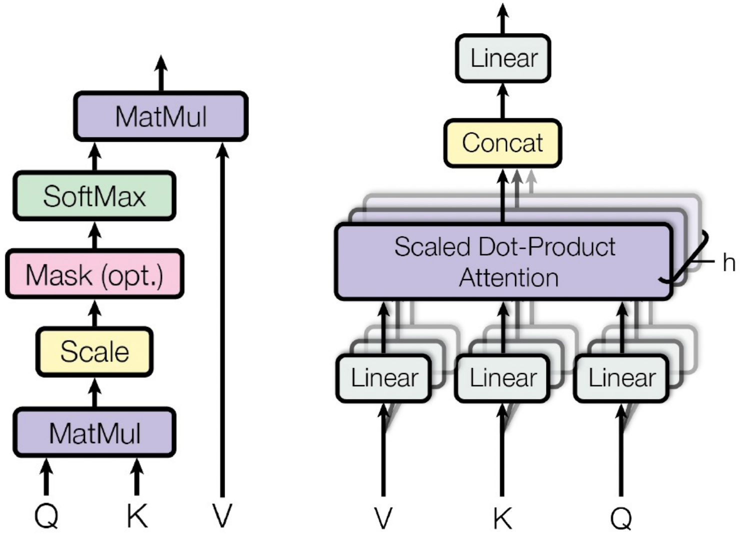
(2) FNO-Variants

geoFNO, SFNO, etc

Only focus on local physics or limited to periodic boundary

Transformer-based PDE Solvers



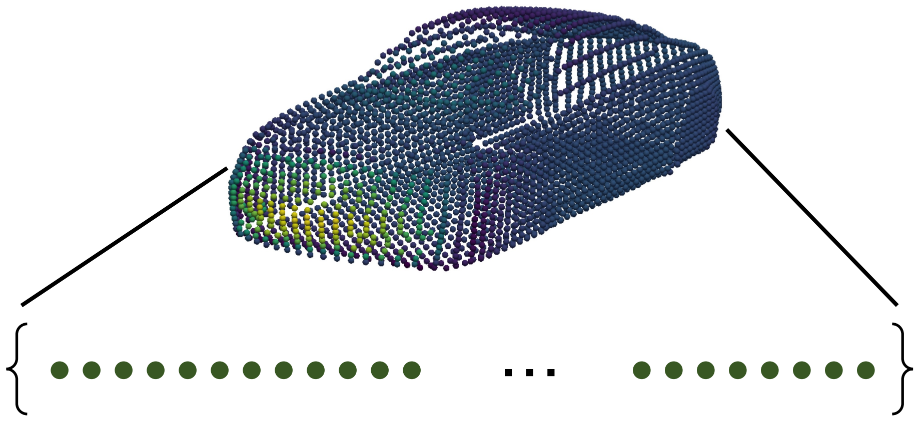


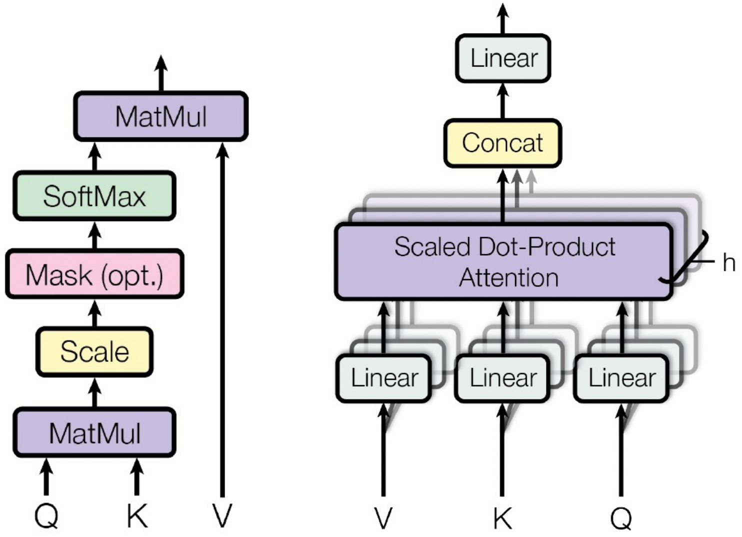
(1) Geometries as point sequences (2) Attention as Monte Carlo Integral

OFormer, Galerkin Transformer, etc

1. **Quadratic complexity**
2. **Hard to capture physical correlations among massive points**

Transformer-based PDE Solvers





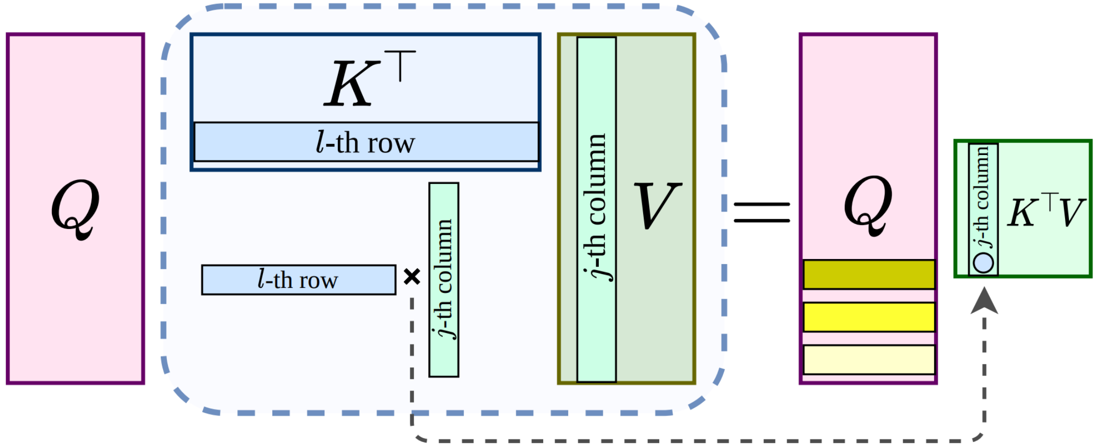
(1) Geometries as point sequences (2) Attention as Monte Carlo Integral

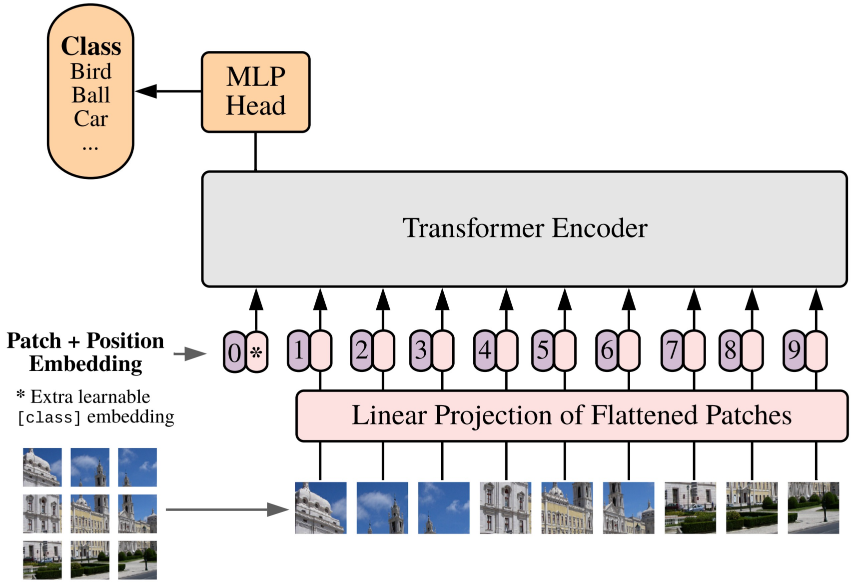
OFormer, Galerkin Transformer, etc

How to efficiently capture physical correlations underlying discretized meshes

is the key to "transform" Transformers into practical PDE solvers

Related Work





(1) Linear Transformers

1. Less informative attention

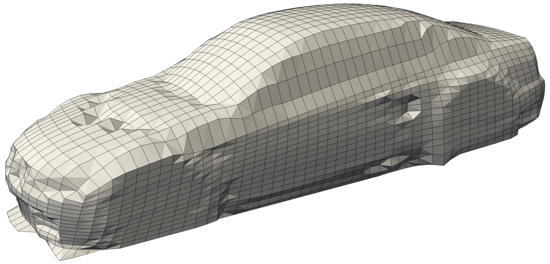
2. Individual points is insufficient for physics learning

(2) Vision Transformer

Augment features with patch ✓

Not applicable to irregular meshes

A foundational Idea of Transolver



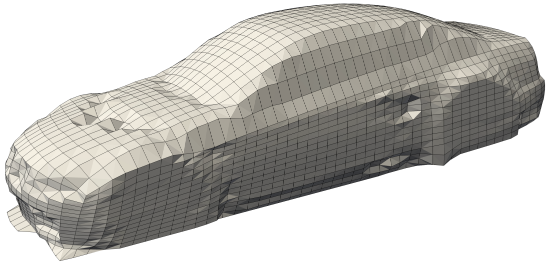
Discretized Domain

Previous Work

Being “trapped” to superficial and unwieldy meshes

Difficulties in Complexity, Geometry, Physics

A foundational Idea of Transolver

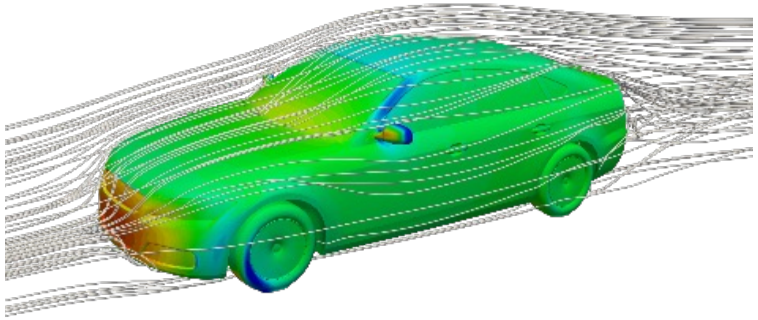


Discretized Domain

Previous Work

Being "trapped" to superficial and unwieldy meshes

Difficulties in Complexity, Geometry, Physics



Physics Domain

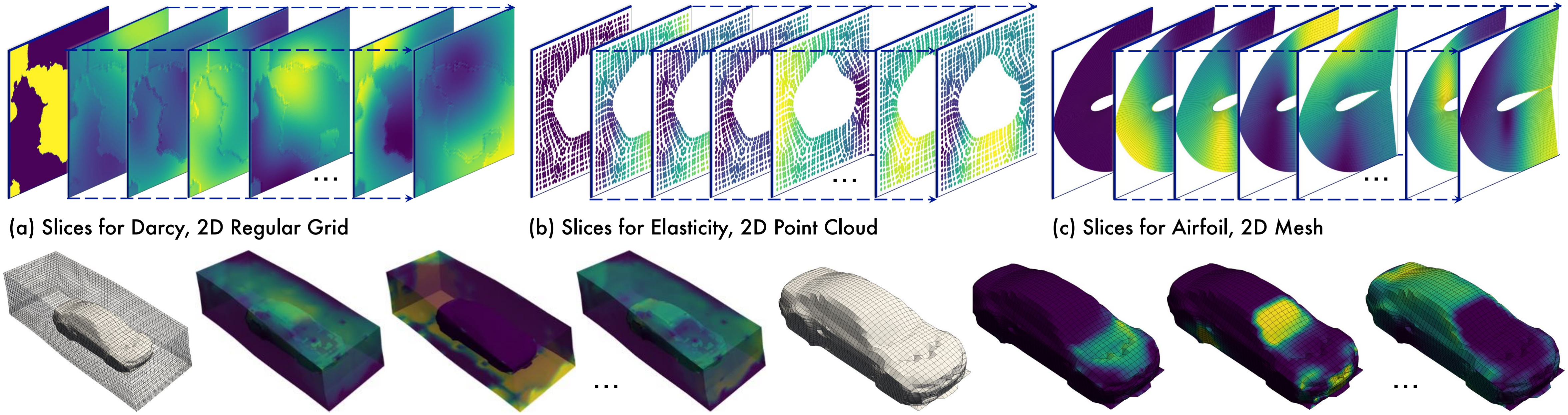
Transolver

Learning **intrinsic physical states** under

complex and large-scale geometrics

Better Complexity, Geometry, Physics Modeling

Learning Physical States

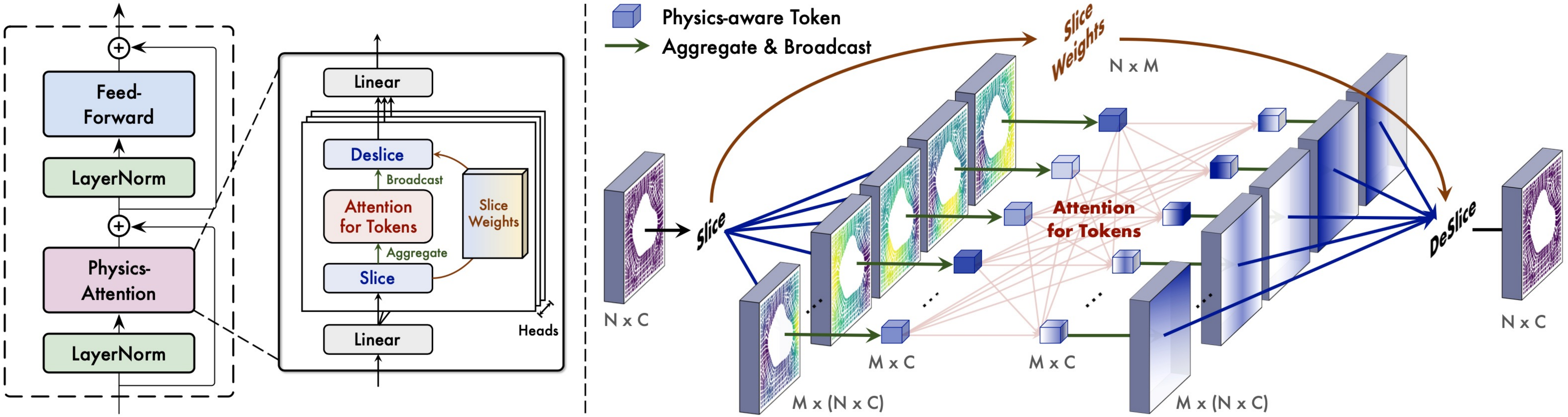


(a) Slices for Darcy, 2D Regular Grid (b) Slices for Elasticity, 2D Point Cloud (c) Slices for Airfoil, 2D Mesh

(d) Slices for Shape-Net Car Surrounding Velocity, 3D Volumes (e) Slices for Shape-Net Car Surface Pressure, 3D Mesh

Mesh points under **similar physical states** will be ascribed to the same **slice** and then encoded into a physics-aware token.

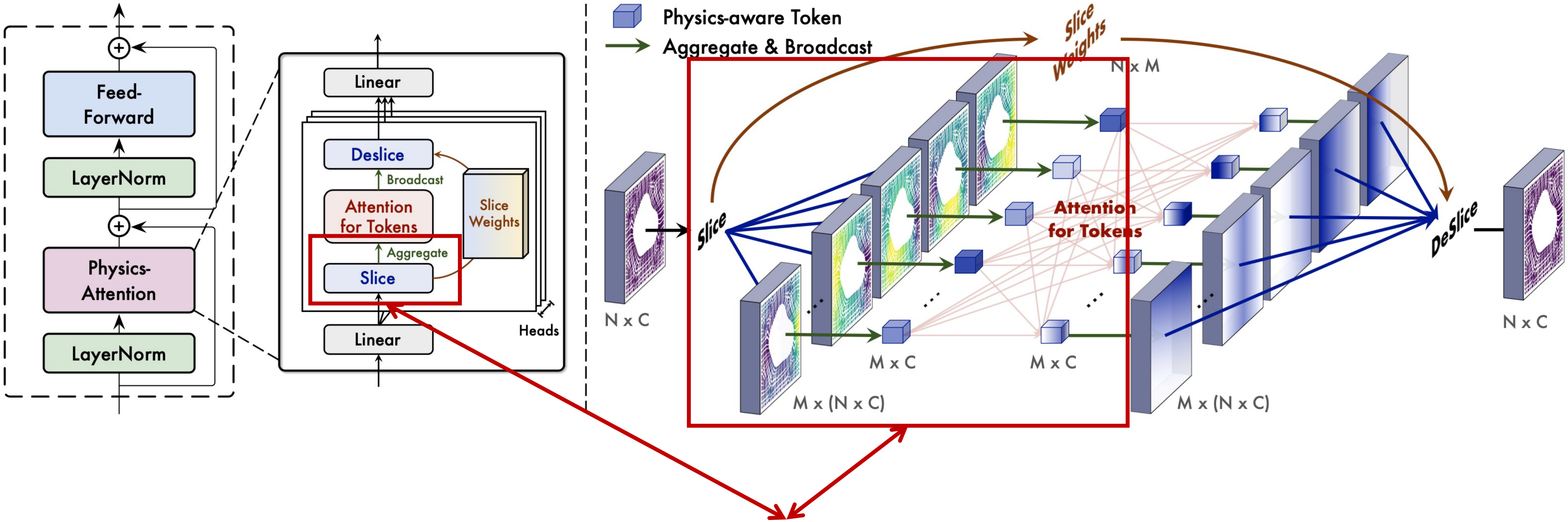
Overview of Transolver



Transolver applies attention to learned physical states **(Physics-Attention)**

① Mesh → physics ② Attention (Integral) ③ Physics → Mesh

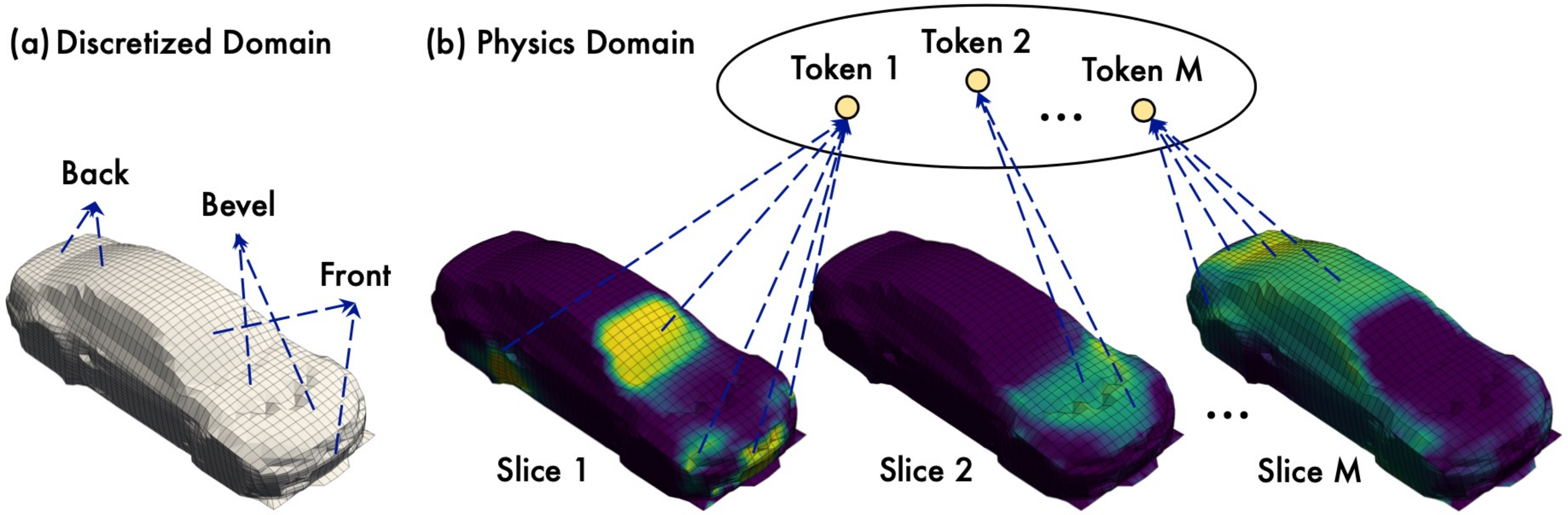
Overview of Transolver



① Mesh → physics

To obtain physics-aware tokens

Mesh → physics



1. Assign each point to slices with weights learned from features

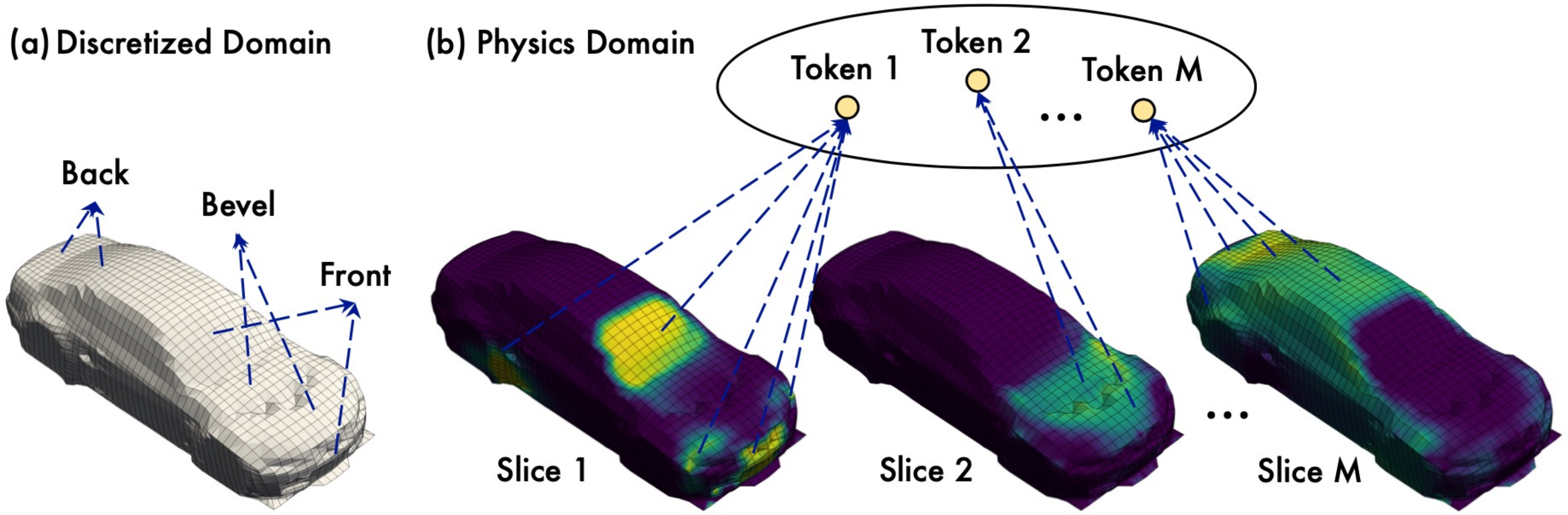
$$\{\mathbf{w}_i\}_{i=1}^{N} = \{\underline{\mathrm{Softmax}\,(}\,\mathrm{Project}\,(\mathbf{x}_i)\,)\,\}_{i=1}^{N}$$

$$\mathbf{s}_j = \{\mathbf{w}_{i,j}\mathbf{x}_i\}_{i=1}^{N}\,,$$

***N* Points to *M* Slices**

Softmax for low-entropy slices

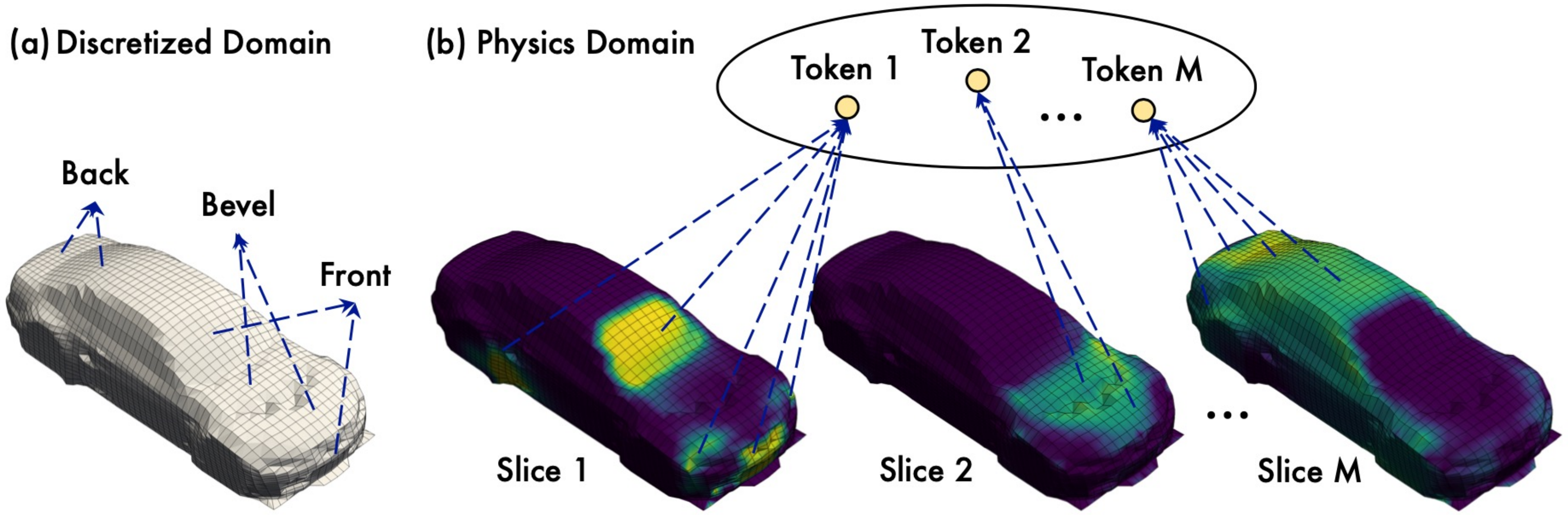
Mesh → physics



1. Assign each point to slices 2. Aggregate slices for physics-aware tokens

$$\mathbf{z}_j = \frac{\sum_{i=1}^{N} \mathbf{s}_{j,i}}{\sum_{i=1}^{N} \mathbf{w}_{i,j}} = \frac{\sum_{i=1}^{N} \mathbf{w}_{i,j}\mathbf{x}_i}{\sum_{i=1}^{N} \mathbf{w}_{i,j}}$$

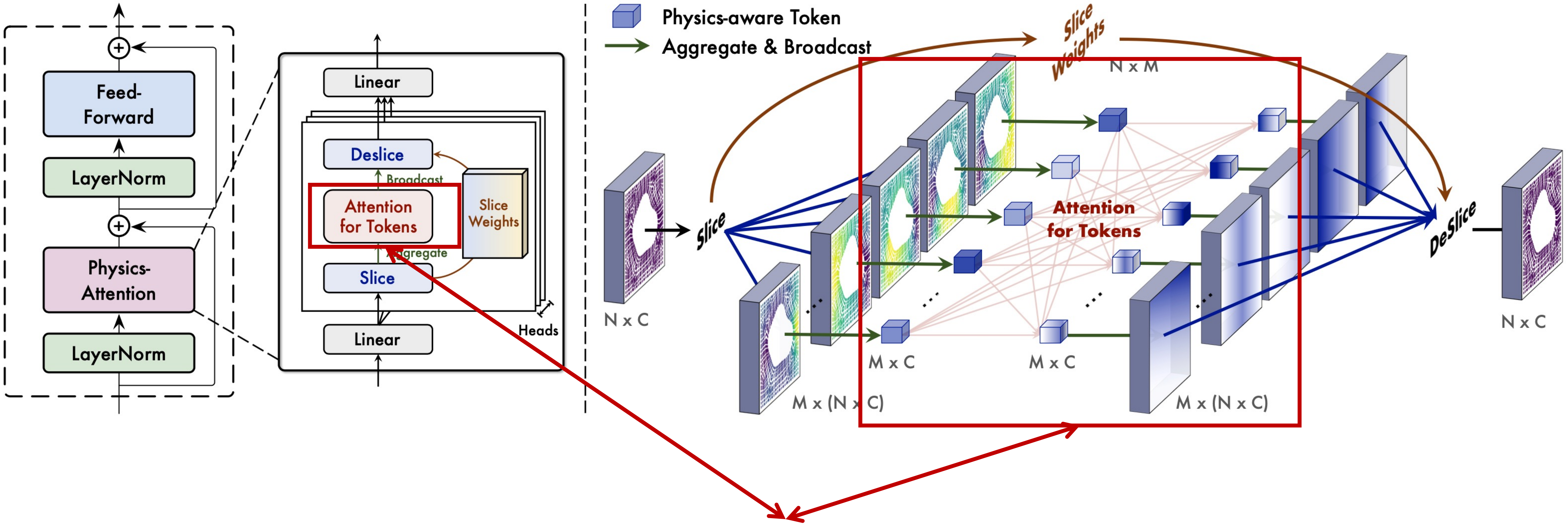
Mesh → physics



1. Why slices can learn physically internal-consistent information
2. Learning slice is different from splitting computation area

   Ascribe physically similar but spatially distant points to the same slice

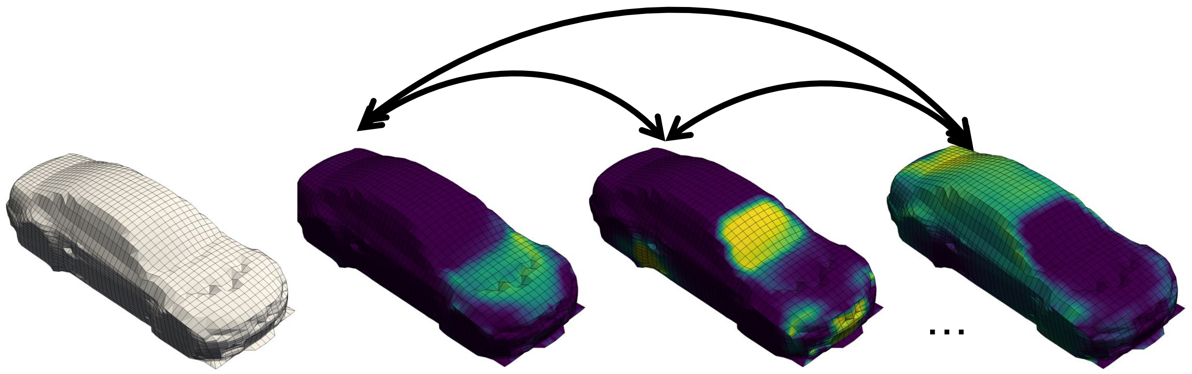
Overview of Transolver



② Attention among physics tokens

Approximate Integral to solve PDEs

Attention among physics tokens

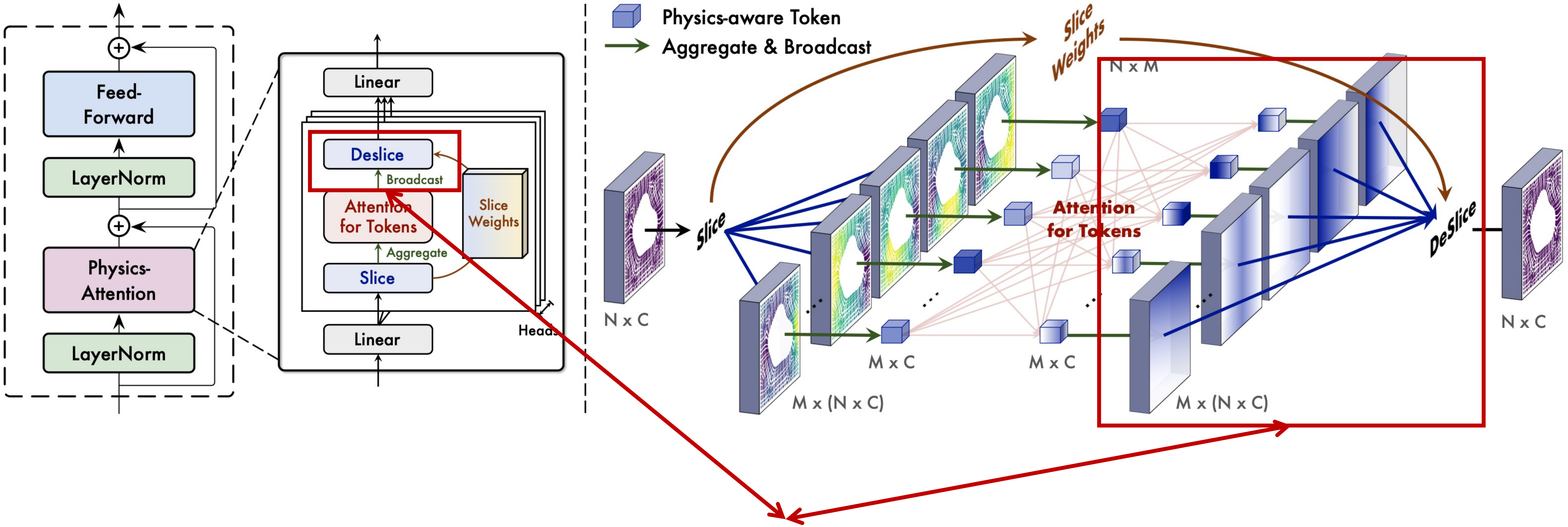


$$\mathbf{q}, \mathbf{k}, \mathbf{v} = \mathrm{Linear}(\underline{\mathbf{z}}), \quad \mathbf{z}' = \mathrm{Softmax}\left(\frac{\mathbf{q}\mathbf{k}^{\mathsf{T}}}{\sqrt{C}}\right)\mathbf{v}$$

Canonical attention among physics tokens

1. Complexity: $\mathcal{O}(N^2C) \rightarrow \mathcal{O}(M^2C)$
2. Capture interactions among physics states
3. Theorem: Attention as learnable integral operator

Overview of Transolver



③ Physics → Mesh

Project physics information back to mesh

$$\mathbf{x}'_i = \sum_{j=1}^{M} \mathbf{w}_{i,j}\mathbf{z}'_j$$

Theoretical Understanding of Transolver

1. Corollary of *Attention is a learnable integral*

Since attention mechanism is applied to tokens encoded from slices, **the step 2 (attention part of Transolver) is a learnable integral for the physics domain**

Is Physics-Attention still an input domain integral?

$$\mathcal{G}(\boldsymbol{u})(\mathbf{g}^*) = \int_{\Omega} \kappa(\mathbf{g}^*, \boldsymbol{\xi})\boldsymbol{u}(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}$$

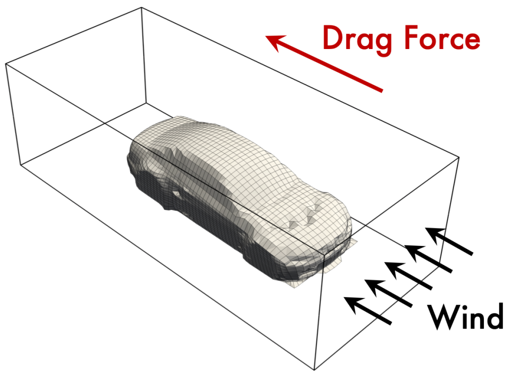
Theoretical Understanding of Transolver

$$
\begin{aligned}
\mathcal{G}(\boldsymbol{u})(\mathbf{g}) &= \int_{\Omega} \kappa(\mathbf{g},\boldsymbol{\xi})\boldsymbol{u}(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \\
&= \int_{\Omega_\mathrm{s}} \kappa_{\mathrm{ms}}\left(\mathbf{g},\boldsymbol{\xi}_\mathrm{s}\right)\boldsymbol{u}_\mathrm{s}\left(\boldsymbol{\xi}_\mathrm{s}\right)\mathrm{d}\boldsymbol{g}^{-1}(\boldsymbol{\xi}_\mathrm{s}) && (\kappa_{\mathrm{ms}}(\cdot,\cdot):\Omega\times\Omega_\mathrm{s}\to\mathbb{R}^{C\times C}\text{ is a kernel function}) \\
&= \int_{\Omega_\mathrm{s}} \kappa_{\mathrm{ms}}\left(\mathbf{g},\boldsymbol{\xi}_\mathrm{s}\right)\boldsymbol{u}_\mathrm{s}\left(\boldsymbol{\xi}_\mathrm{s}\right)|\det(\nabla_{\boldsymbol{\xi}_\mathrm{s}}\boldsymbol{g}^{-1}(\boldsymbol{\xi}_\mathrm{s}))|\mathrm{d}\boldsymbol{\xi}_\mathrm{s} \\
&= \int_{\Omega_\mathrm{s}} \left(\frac{\int_{\Omega_\mathrm{s}} w_{\mathbf{g},\boldsymbol{\xi}'_\mathrm{s}}\kappa_{\mathrm{ss}}\left(\boldsymbol{\xi}'_\mathrm{s},\boldsymbol{\xi}_\mathrm{s}\right)\mathrm{d}\boldsymbol{\xi}'_\mathrm{s}}{\int_{\Omega_\mathrm{s}} w_{\mathbf{g},\boldsymbol{\xi}'_\mathrm{s}}\mathrm{d}\boldsymbol{\xi}'_\mathrm{s}}\right)\boldsymbol{u}_\mathrm{s}\left(\boldsymbol{\xi}_\mathrm{s}\right)|\det(\nabla_{\boldsymbol{\xi}_\mathrm{s}}\boldsymbol{g}^{-1}(\boldsymbol{\xi}_\mathrm{s}))|\mathrm{d}\boldsymbol{\xi}_\mathrm{s} && (\kappa_{\mathrm{ms}}\text{ is a linear combination of }\kappa_{\mathrm{ss}}\text{ with weights }w_{*,*}) \\
&= \int_{\Omega_\mathrm{s}} \underbrace{w_{\mathbf{g},\boldsymbol{\xi}'_\mathrm{s}}}_{\text{DeSlice}}\int_{\Omega_\mathrm{s}} \underbrace{\kappa_{\mathrm{ss}}\left(\boldsymbol{\xi}'_\mathrm{s},\boldsymbol{\xi}_\mathrm{s}\right)}_{\text{Attention among slice tokens}}\underbrace{\boldsymbol{u}_\mathrm{s}\left(\boldsymbol{\xi}_\mathrm{s}\right)}_{\text{Slice token}}|\det(\nabla_{\boldsymbol{\xi}_\mathrm{s}}\boldsymbol{g}^{-1}(\boldsymbol{\xi}_\mathrm{s}))|\mathrm{d}\boldsymbol{\xi}_\mathrm{s}\mathrm{d}\boldsymbol{\xi}'_\mathrm{s} && \left(\text{Suppose that }\int_{\Omega_\mathrm{s}} w_{\mathbf{g},\boldsymbol{\xi}'_\mathrm{s}}\mathrm{d}\boldsymbol{\xi}'_\mathrm{s}=1\right) \\
&\approx \underbrace{\sum_{j=1}^{M}\mathbf{w}_{i,j}}_{\text{Eq. (4)}}\underbrace{\sum_{t=1}^{M}\frac{\exp\left(\left(\mathbf{W}_\mathbf{q}\boldsymbol{u}_\mathrm{s}(\boldsymbol{\xi}_{\mathrm{s},j})\right)\left(\mathbf{W}_\mathbf{k}\boldsymbol{u}_\mathrm{s}(\boldsymbol{\xi}_{\mathrm{s},t})\right)^\mathsf{T}/\tau\right)}{\sum_{p=1}^{M}\exp\left(\left(\mathbf{W}_\mathbf{q}\boldsymbol{u}_\mathrm{s}(\boldsymbol{\xi}_{\mathrm{s},j})\right)\left(\mathbf{W}_\mathbf{k}\boldsymbol{u}_\mathrm{s}(\boldsymbol{\xi}_{\mathrm{s},p})\right)^\mathsf{T}/\tau\right)}\mathbf{W}_\mathbf{v}}_{\text{Eq. (3)}}\underbrace{\left(\frac{\sum_{p=1}^{N}\mathbf{w}_{p,t}\boldsymbol{u}(\mathbf{g}_p)}{\sum_{p=1}^{N}\mathbf{w}_{p,t}}\right)}_{\text{Eq. (2)}} && (\text{Lemma A.1}) \\
&= \sum_{j=1}^{M}\mathbf{w}_{i,j}\sum_{t=1}^{M}\frac{\exp(\mathbf{q}_j\mathbf{k}_t^\mathsf{T}/\tau)}{\sum_{p=1}^{M}\exp(\mathbf{q}_j\mathbf{k}_p^\mathsf{T}/\tau)}\mathbf{v}_t,
\end{aligned}
$$

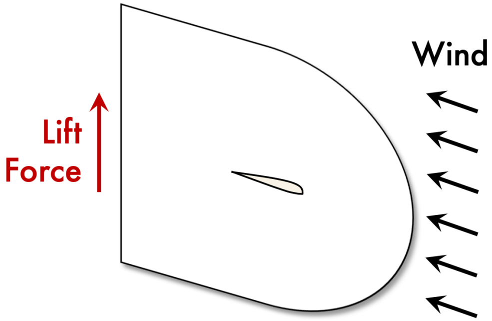
All the designs in Transolver can be directly derived.

Experiments

GEOMETRY	BENCHMARKS	#DIM	#MESH
POINT CLOUD	ELASTICITY	2D	972
STRUCTURED MESH	PLASTICITY AIRFOIL PIPE	2D+TIME 2D 2D	3,131 11,271 16,641
REGULAR GRID	NAVIER–STOKES DARCY	2D+TIME 2D	4,096 7,225
UNSTRUCTURED MESH	SHAPE-NET CAR AIRFRANS	3D 2D	32,186 32,000



(a) Shape-Net Car



(b) AirfRANS

Six standard benchmarks, two practical design tasks

More than 20 baselines

Standard PDE-Solving Benchmarks

Model	Point Cloud	Structured Mesh			Regular Grid	
	Elasticity	Plasticity	Airfoil	Pipe	Navier–Stokes	Darcy
FNO (Li et al., 2021)	/	/	/	/	0.1556	0.0108
WMT (Gupta et al., 2021)	0.0359	0.0076	0.0075	0.0077	0.1541	0.0082
U-FNO (Wen et al., 2022)	0.0239	0.0039	0.0269	0.0056	0.2231	0.0183
geo-FNO (Li et al., 2022)	0.0229	0.0074	0.0138	0.0067	0.1556	0.0108
U-NO (Rahman et al., 2023)	0.0258	0.0034	0.0078	0.0100	0.1713	0.0113
F-FNO (Tran et al., 2023)	0.0263	0.0047	0.0078	0.0070	0.2322	0.0077
LSM (Wu et al., 2023)	0.0218	0.0025	<u>0.0059</u>	0.0050	0.1535	<u>0.0065</u>
Galerkin (Cao, 2021)	0.0240	0.0120	0.0118	0.0098	0.1401	0.0084
HT-Net (Liu et al., 2022)	/	0.0333	0.0065	0.0059	0.1847	0.0079
OFormer (Li et al., 2023c)	0.0183	<u>0.0017</u>	0.0183	0.0168	0.1705	0.0124
GNOT (Hao et al., 2023)	<u>0.0086</u>	0.0336	0.0076	<u>0.0047</u>	0.1380	0.0105
FactFormer (Li et al., 2023d)	/	0.0312	0.0071	0.0060	0.1214	0.0109
ONO (Xiao et al., 2024)	0.0118	0.0048	0.0061	0.0052	<u>0.1195</u>	0.0076
Transolver (Ours)	**0.0064**	**0.0012**	**0.0053**	**0.0033**	**0.0900**	**0.0057**
Relative Promotion	25.6%	29.4%	10.2%	29.7%	24.7%	12.3%

Transolver achieves 22% error reduction over the second-best model

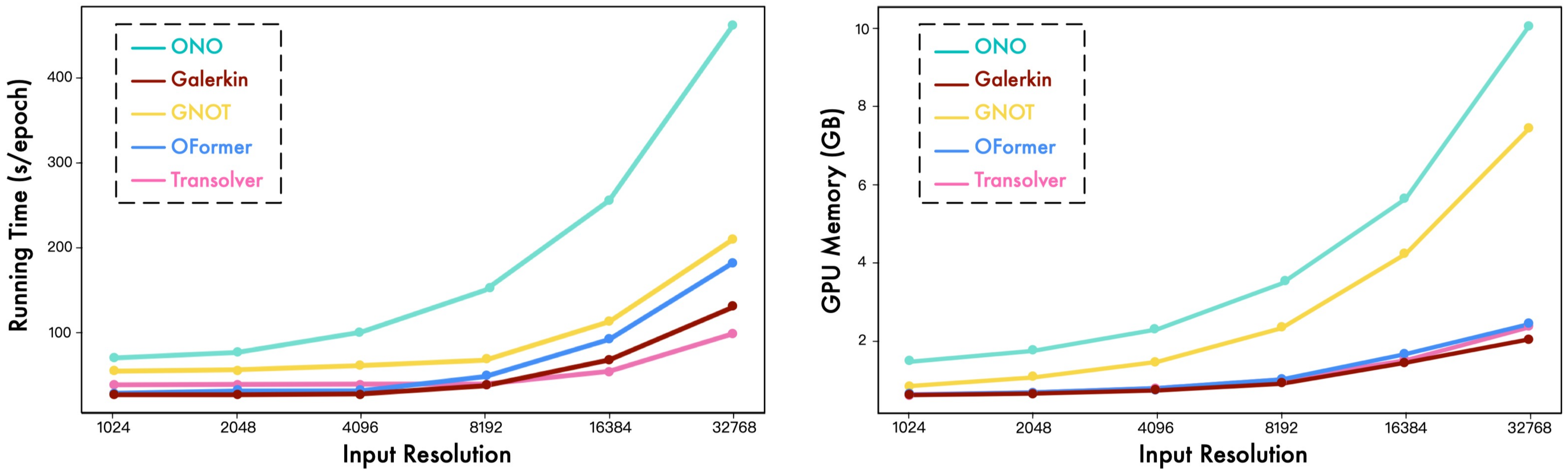
Practical Design Tasks

Model*	Shape-Net Car				AirfRANS			
	Volume ↓	Surf ↓	C_D ↓	ρ_D ↑	Volume ↓	Surf ↓	C_L ↓	ρ_L ↑
Simple MLP	0.0512	0.1304	0.0307	0.9496	0.0081	0.0200	0.2108	0.9932
GraphSAGE (Hamilton et al., 2017)	0.0461	0.1050	0.0270	0.9695	0.0087	0.0184	0.1476	0.9964
PointNet (Qi et al., 2017)	0.0494	0.1104	0.0298	0.9583	0.0253	0.0996	0.1973	0.9919
Graph U-Net (Gao & Ji, 2019)	0.0471	0.1102	0.0226	0.9725	0.0076	0.0144	0.1677	0.9949
MeshGraphNet (Pfaff et al., 2021)	0.0354	0.0781	0.0168	0.9840	0.0214	0.0387	0.2252	0.9945
GNO (Li et al., 2020a)	0.0383	0.0815	0.0172	0.9834	0.0269	0.0405	0.2016	0.9938
Galerkin (Cao, 2021)	0.0339	0.0878	0.0179	0.9764	0.0074	0.0159	0.2336	0.9951
geo-FNO (Li et al., 2022)	0.1670	0.2378	0.0664	0.8280	0.0361	0.0301	0.6161	0.9257
GNOT (Hao et al., 2023)	0.0329	0.0798	0.0178	0.9833	0.0049	0.0152	0.1992	0.9942
GINO (Li et al., 2023a)	0.0386	0.0810	0.0184	0.9826	0.0297	0.0482	0.1821	0.9958
3D-GeoCA (Deng et al., 2024)	0.0319	0.0779	0.0159	0.9842	/	/	/	/
Transolver (Ours)	**0.0207**	**0.0745**	**0.0103**	**0.9935**	**0.0037**	**0.0142**	**0.1030**	**0.9978**

Design-oriented metrics: Drag/lift coefficients and their Spearman's correlation

Transolver performs best in both physics and design-oriented metrics

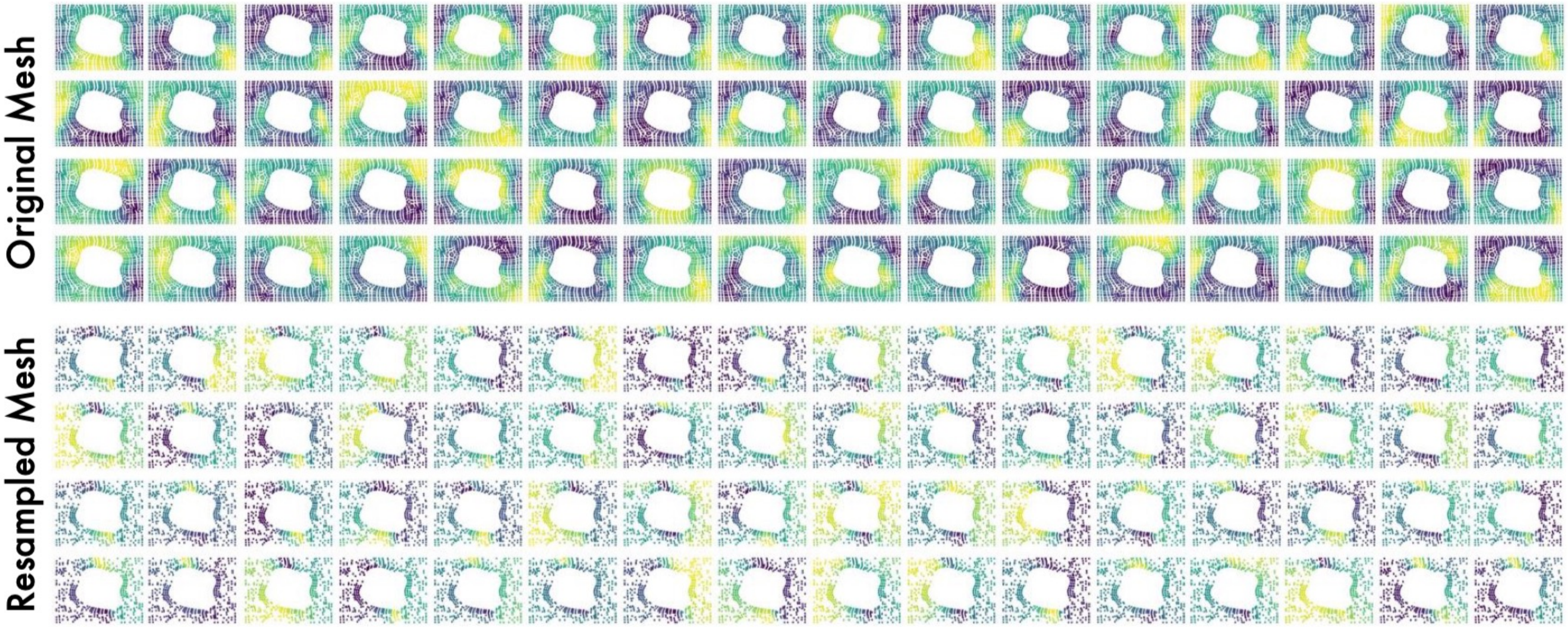
Efficiency



Favorable efficiency and performance balance

Transolver is faster than linear Transformers in large-scale meshes.

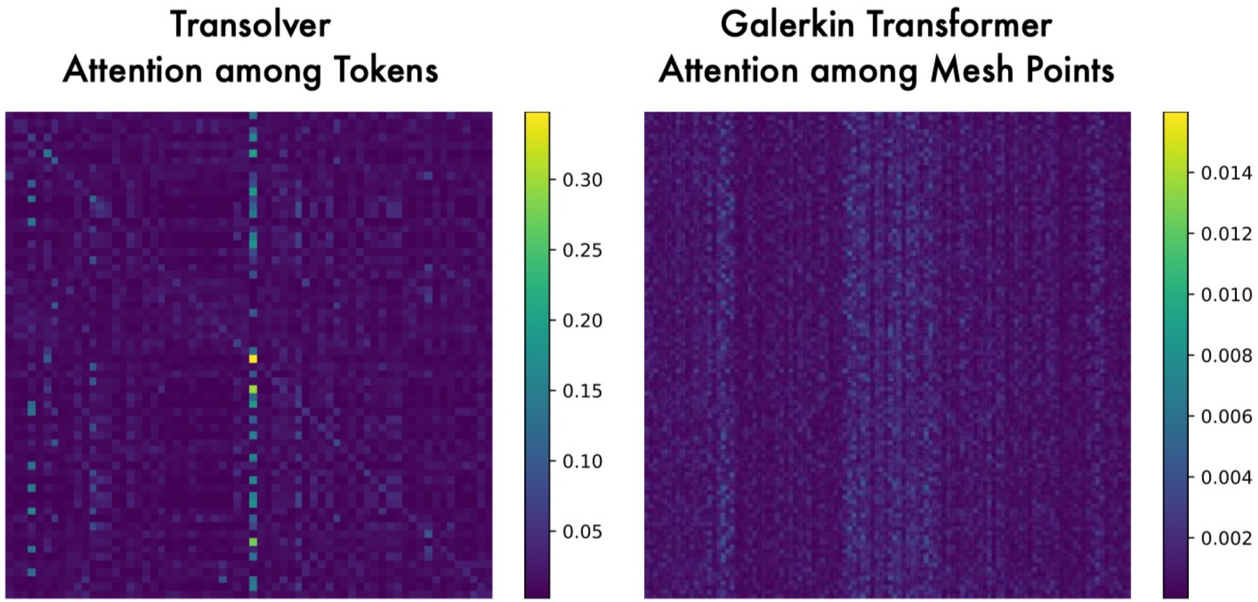
Physics-Attention Visualization



Slice visualization on Elasticity

Transolver is mesh-free, precisely captures states **even on broken meshes**

Physics-Attention Visualization

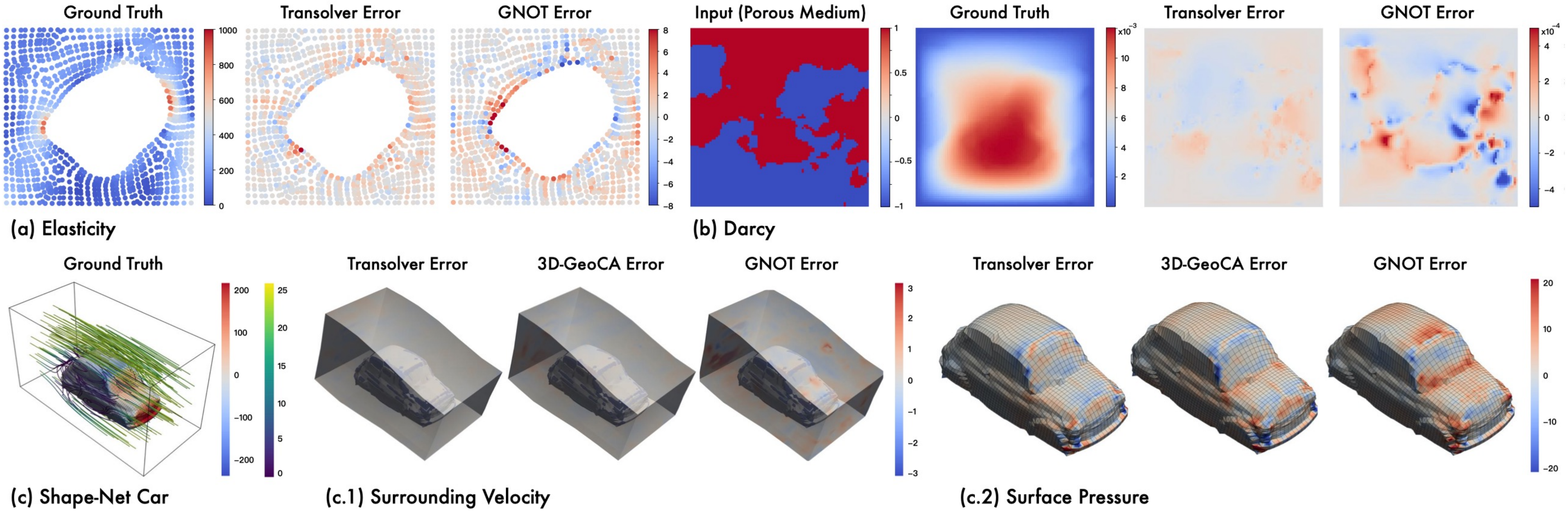


Kullback–Leibler (KL) divergence between attention weights and uniform distribution

BENCHMARKS	GALERKIN (CAO, 2021)	TRANSOLVER (OURS)
ELASTICITY (972 MESH POINTS)	0.3803	**1.7795**
DARCY (7,225 MESH POINTS)	0.2739	**1.8274**

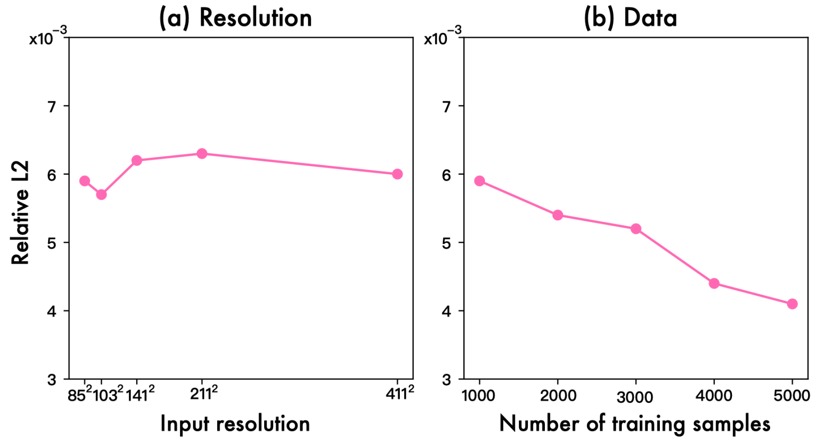
Physics-Attention can learn **more informative physical correlations**

Showcases

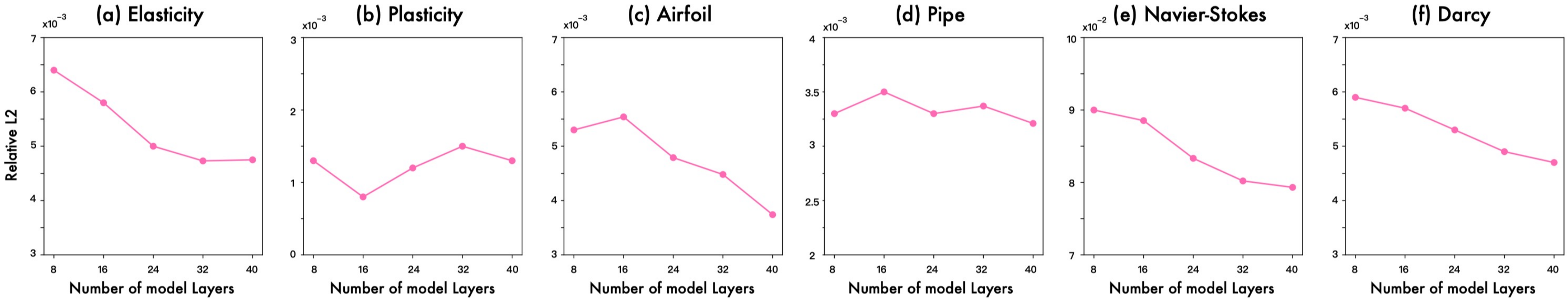


Transolver excels in solving **multiphysics PDEs on hybrid geometrics**

Pursuing PDE Foundation Models: **Scalability**

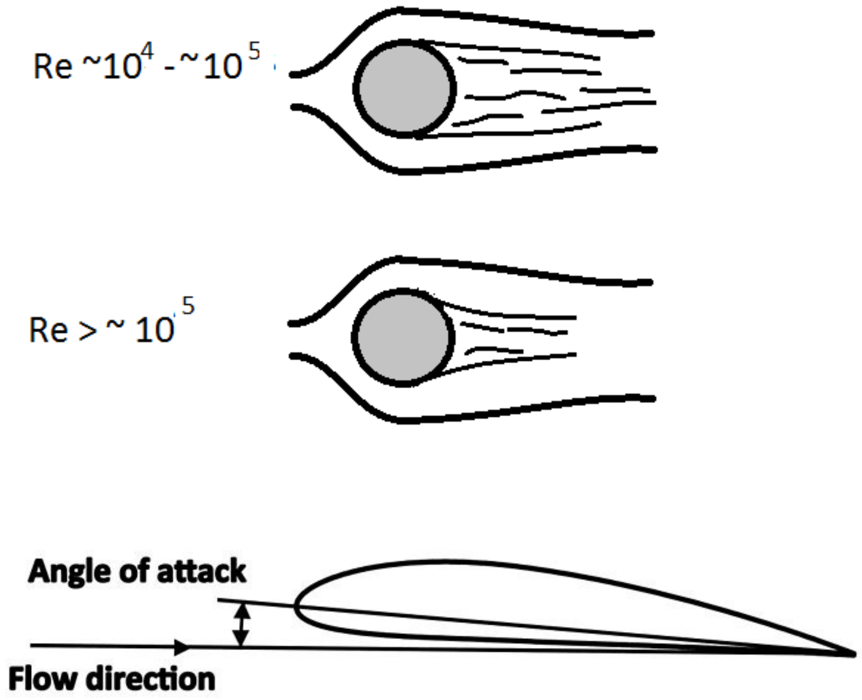


1. **Resolution:** Consistent performance at varied scales
2. **Data:** Benefiting from larger training data
3. **Parameter:** Benefiting from more parameters



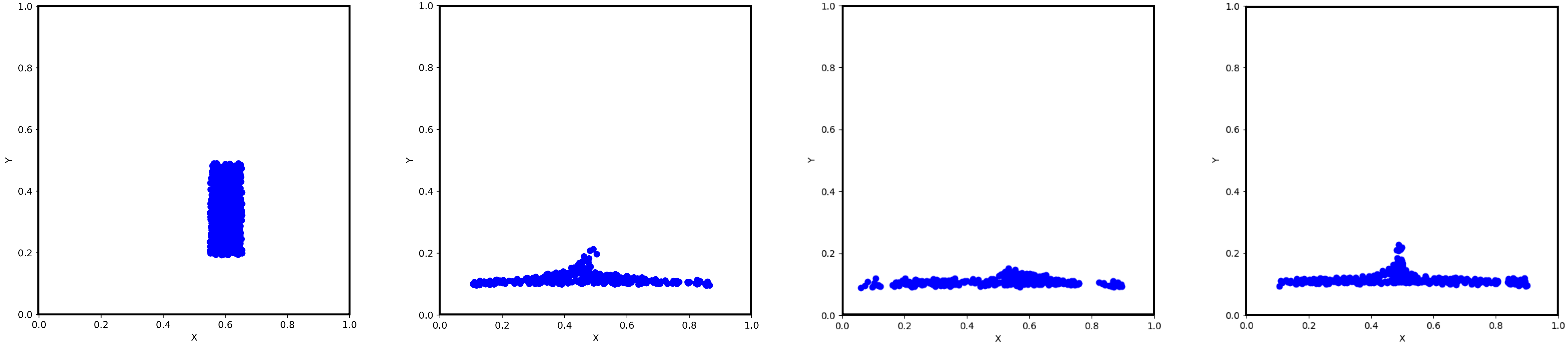
Pursuing PDE Foundation Models: **Generalization**

MODELS	OOD REYNOLDS $C_L \downarrow$	OOD REYNOLDS $\rho_L \uparrow$	OOD ANGLES $C_L \downarrow$	OOD ANGLES $\rho_L \uparrow$
SIMPLE MLP	0.6205	0.9578	0.4128	0.9572
GRAPHSAGE (2017)	0.4333	0.9707	0.2538	0.9894
POINTNET (2017)	0.3836	0.9806	0.4425	0.9784
GRAPH U-NET (2019)	0.4664	0.9645	0.3756	0.9816
MESHGRAPHNET (2021)	1.7718	0.7631	0.6525	0.8927
GNO (2020A)	0.4408	0.9878	0.3038	0.9884
GALERKIN (2021)	0.4615	0.9826	0.3814	0.9821
GNOT (2023)	0.3268	0.9865	0.3497	0.9868
GINO (2023A)	0.4180	0.9645	0.2583	0.9923
TRANSOLVER (OURS)	**0.2996**	**0.9896**	**0.1500**	**0.9950**



Transolver still performs best (**Spearman's correlation ~ 99%**) in OOD settings

Pursuing PDE Foundation Models: **Versatile**



Initial State | Ground Truth (400th step) | GNN | GNN + Transolver

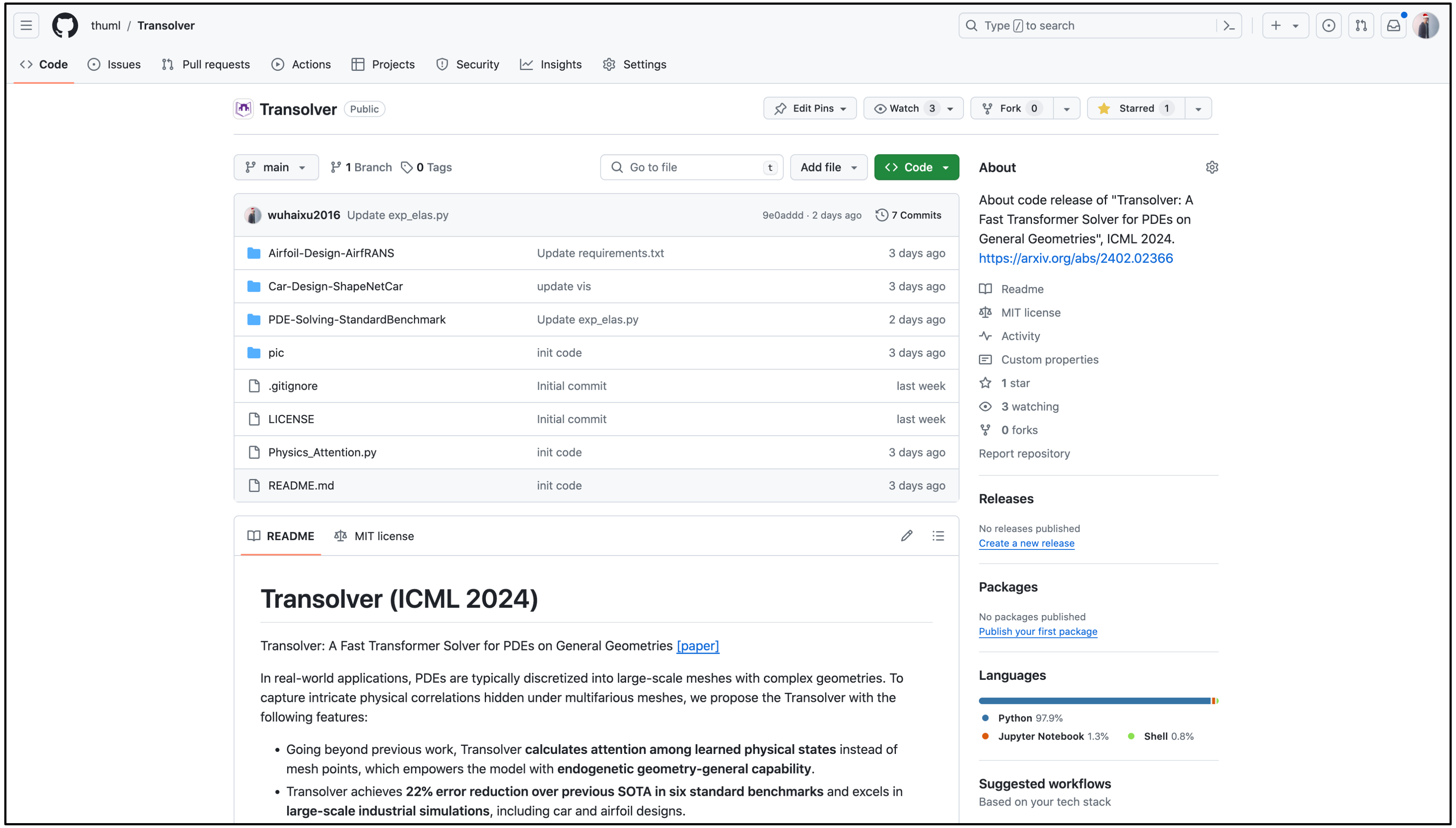
MODEL	MSE ↓
GNN (SANCHEZ-GONZALEZ ET AL., 2020)	0.0182
GNN + TRANSOLVER (OURS)	**0.0069**
RELATIVE PROMOTION	62.1%

Transolver can also be extended to

Lagrangian Settings

(Ever-changing geometrics)

Open Source



Code is available at https://github.com/thuml/Transolver

Thank You!

wuhx23@mails.tsinghua.edu.cn

长按关注，获取最新资讯