# From Transolver to Transolver++ Enabling PDE Solving on Million-Scale Geometries

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# Solving PDEs

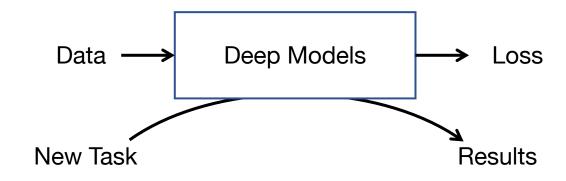
#### **Classic Numerical Methods**



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

**Huge computation costs** 

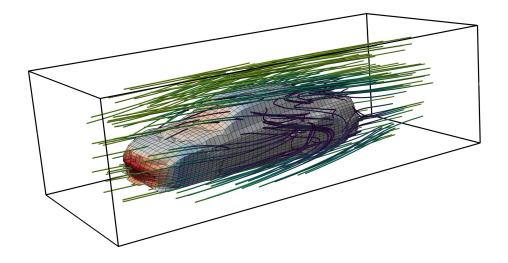
#### **Neural PDE Solver**



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

An efficient surrogate tool (In expectation)

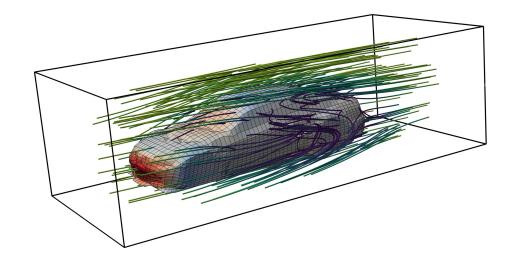
# Challenges in Practical Industrial Design



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



#### Transolver: A Fast Transformer Solver for PDEs on General Geometries

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Haixu Wu



Huakun Luo



Haowen Wang



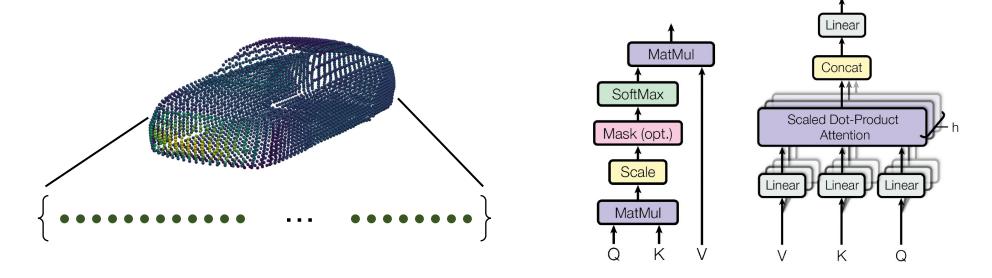
Jianmin Wang



Mingsheng Long



#### Transformer-based PDE Solvers

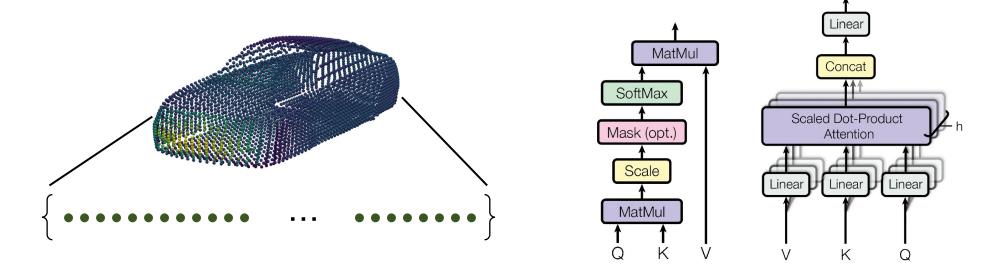


(1) Geometries as point sequences (2) Attention as Monte Carlo Integral

OFormer, Galerkin Transformer, GNOT, etc.

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

#### Transformer-based PDE Solvers



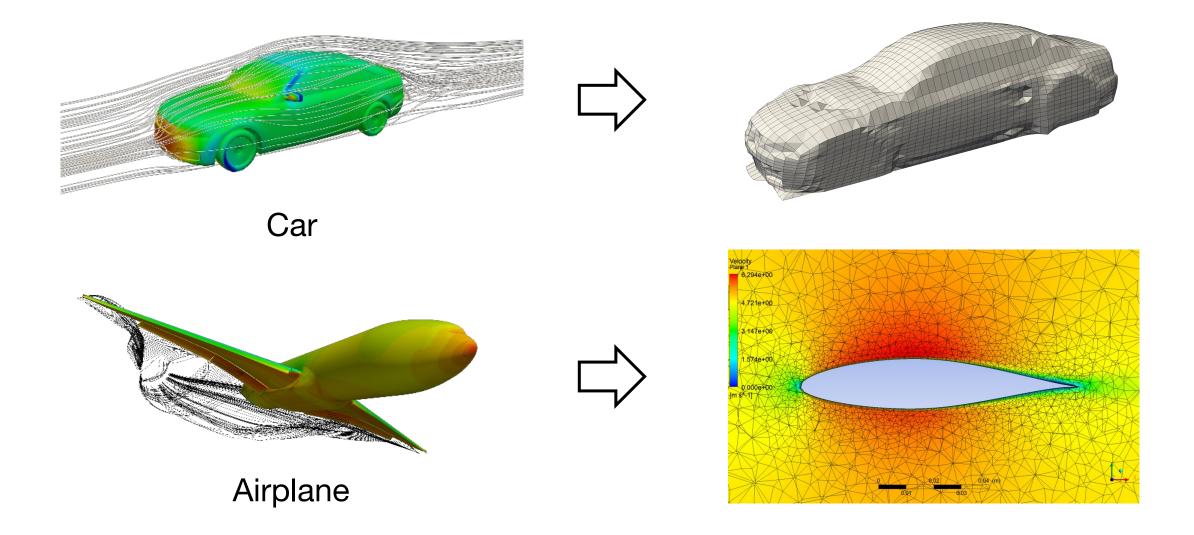
(1) Geometries as point sequences (2) Attention as Monte Carlo Integral

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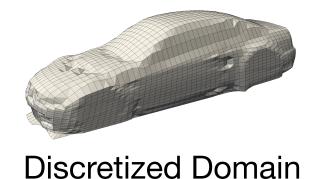
How to efficiently capture physical correlations underlying discretized meshes

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

# Solving PDEs: Discretization



#### A Foundational Idea of Transolver

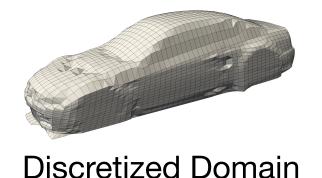


**Previous Work** 

Being "trapped" to superficial and unwieldy meshes

Difficulties in Complexity, Geometry, Physics

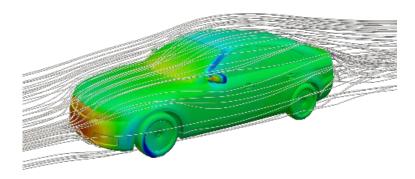
#### A Foundational Idea of Transolver



#### **Previous Work**

Being "trapped" to superficial and unwieldy meshes

Difficulties in Complexity, Geometry, Physics



**Physics Domain** 

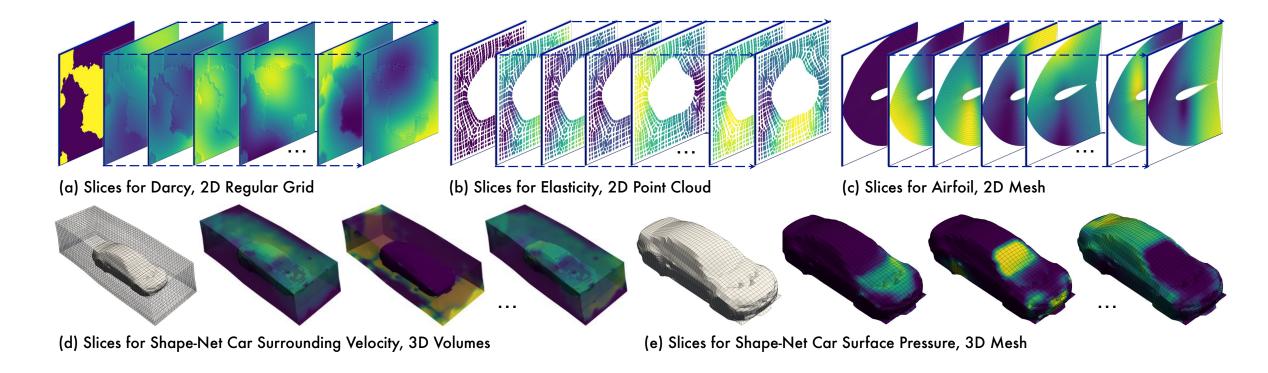
Transolver

Learning intrinsic physical states under

complex and large-scale geometrics

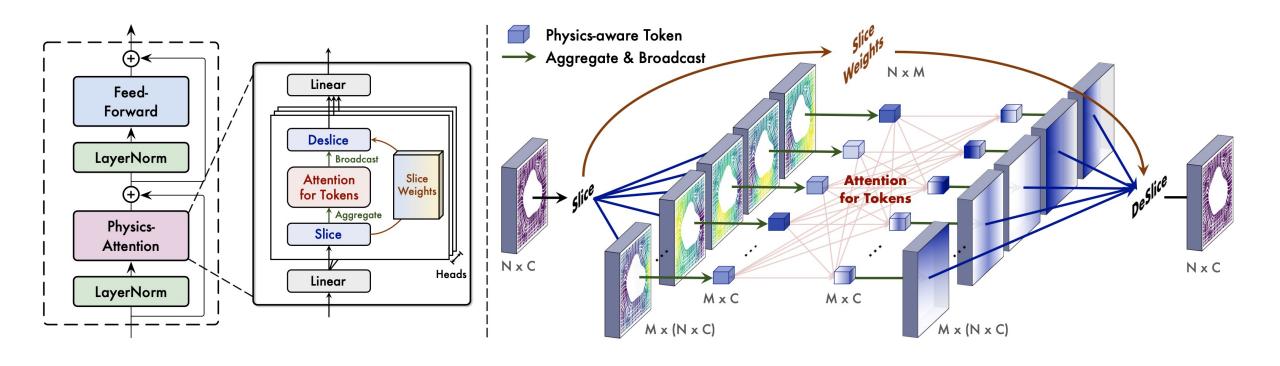
Better Complexity, Geometry, Physics Modeling

# Learning Physical States



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

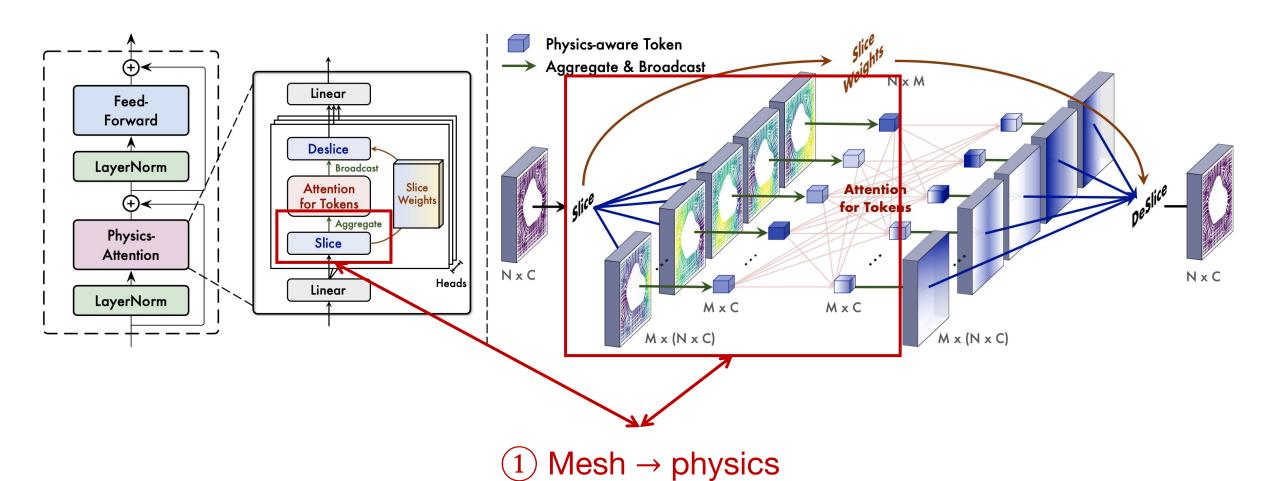
#### Overview of Transolver



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

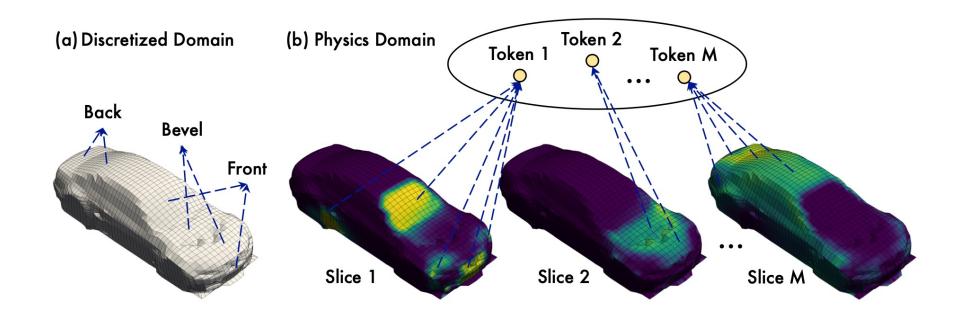
Mesh → physics ② Attention (Integral) ③ Physics → Mesh

#### Overview of Transolver



To obtain physics-aware tokens

# Mesh → physics



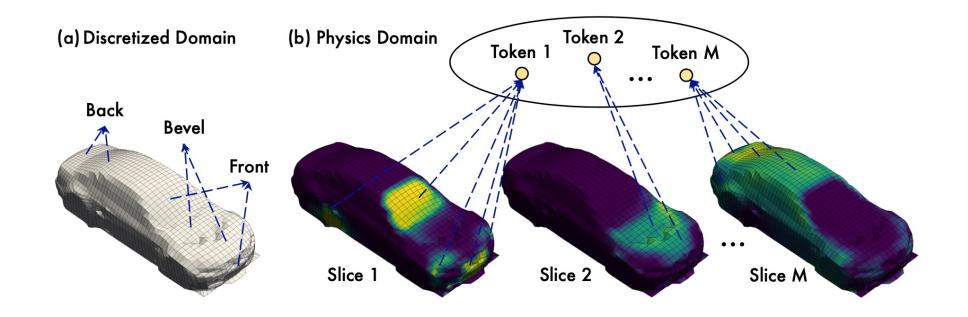
1. Assign each point to slices with weights learned from features

$$\{\mathbf{w}_i\}_{i=1}^N = \{\underbrace{\text{Softmax}}_{i=1} ( \text{Project}(\mathbf{x}_i) ) \}_{i=1}^N$$
$$\mathbf{s}_j = \{\mathbf{w}_{i,j}\mathbf{x}_i\}_{i=1}^N,$$

N Points to M Slices

Softmax for low-entropy slices

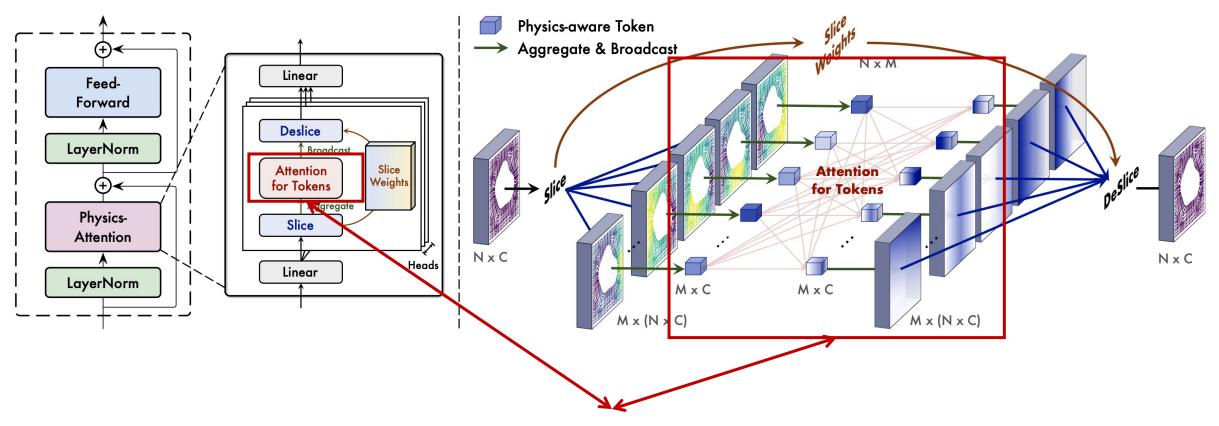
# Mesh → physics



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

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

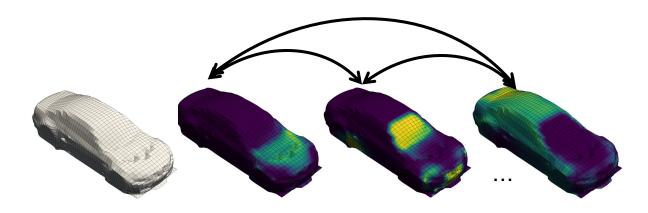
#### Overview of Transolver



2 Attention among physics tokens

Approximate Integral to solve PDEs

#### Attention among physics tokens

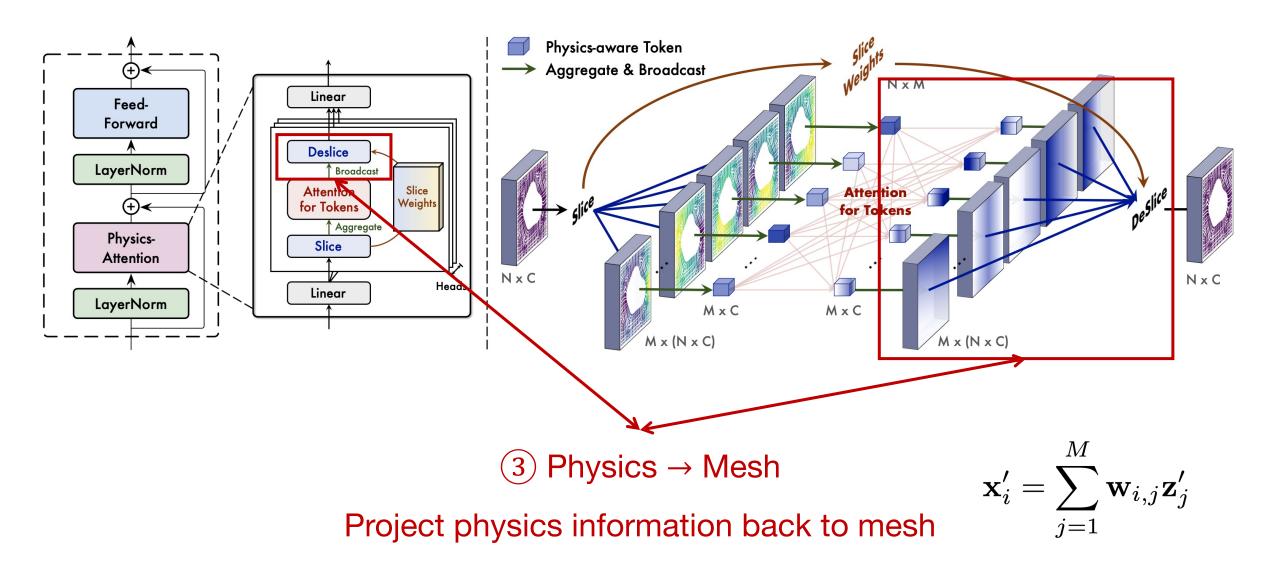


$$\mathbf{q}, \mathbf{k}, \mathbf{v} = \operatorname{Linear}(\mathbf{z}), \ \mathbf{z}' = \operatorname{Softmax}\left(\frac{\mathbf{q}\mathbf{k}^{\mathsf{T}}}{\sqrt{C}}\right)\mathbf{v}$$

Canonical attention among physics tokens

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

#### Overview of Transolver



# 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

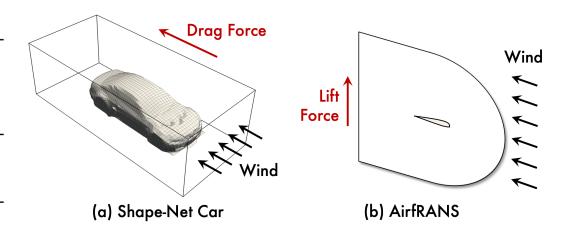
 $= \sum_{i=1}^{M} \mathbf{w}_{i,j} \sum_{t=1}^{M} \frac{\exp(\mathbf{q}_{j} \mathbf{k}_{t}^{\mathsf{T}} / \tau)}{\sum_{t=1}^{M} \exp(\mathbf{q}_{i} \mathbf{k}_{t}^{\mathsf{T}} / \tau)} \mathbf{v}_{t},$ 

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

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



Six standard benchmarks, two practical design tasks

More than 20 baselines

# Standard PDE-Solving Benchmarks

	POINT CLOUD	OUD STRUCTURED MESH			REGULAR GRID		
Model	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	0.0059	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	0.0017	0.0183	0.0168	0.1705	0.0124	
GNOT (HAO ET AL., 2023)	0.0086	0.0336	0.0076	0.0047	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

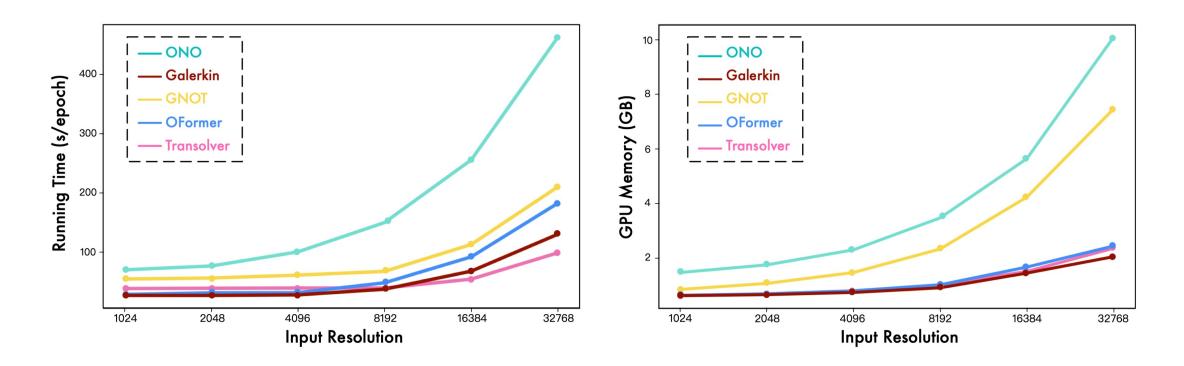
# Practical Design Tasks

	SHAPE-NET CAR				AIRFRANS			
MODEL*	Volume↓	Surf↓	$C_D\downarrow$	$ ho_D \uparrow$	Volume↓	Surf↓	$C_L\downarrow$	$ ho_L \uparrow$
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

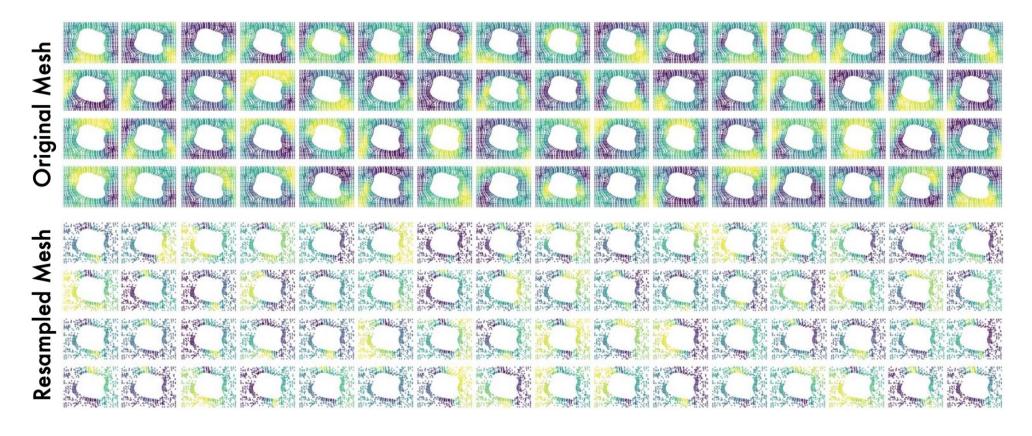
# Efficiency



Favorable efficiency and performance balance

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

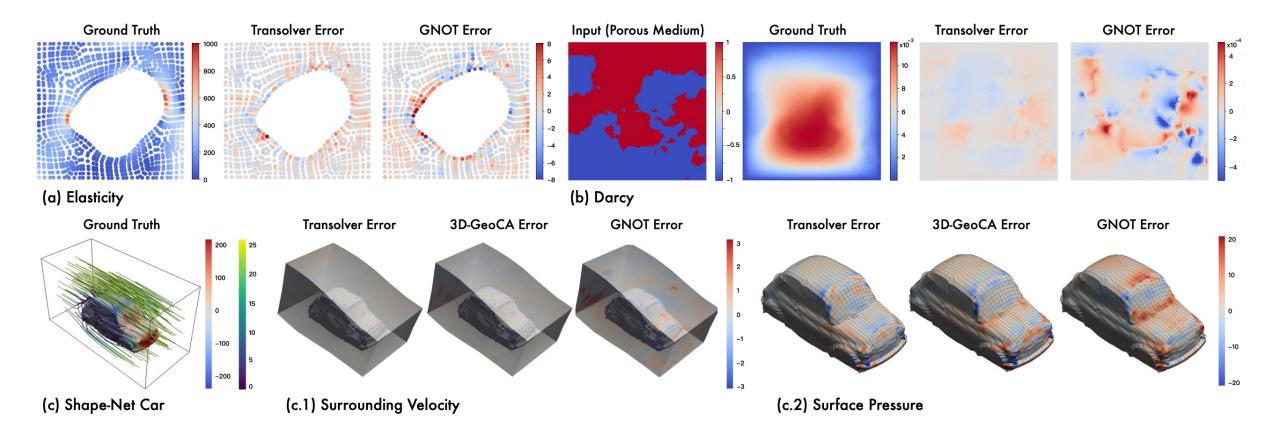
# Physics-Attention Visualization



Slice visualization on Elasticity

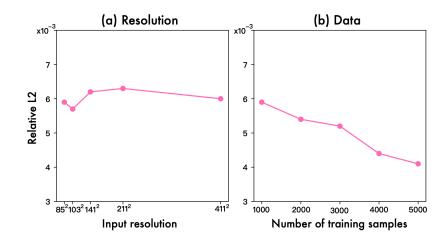
Transolver is mesh-free, precisely captures states even on broken meshes

#### Showcases

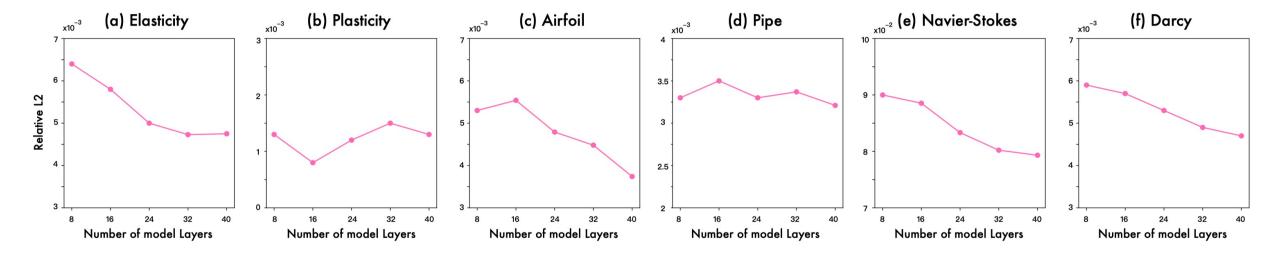


Transolver excels in solving multiphysics PDEs on hybrid geometrics

# 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

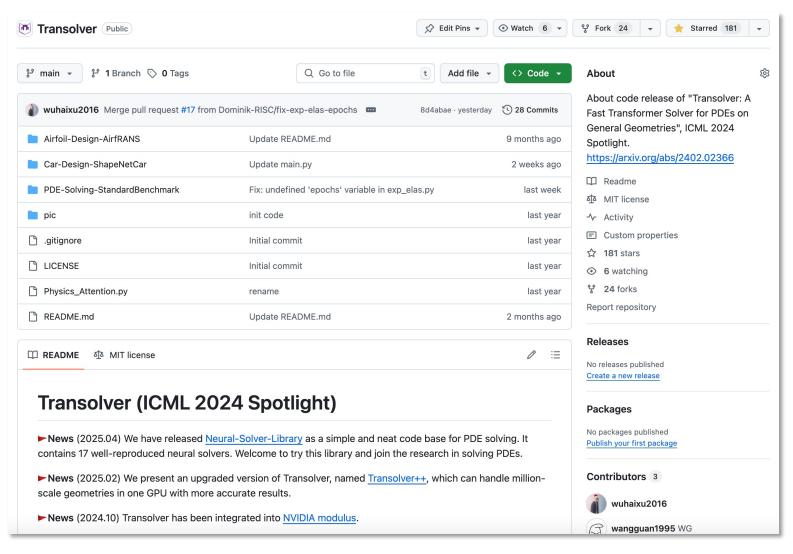


#### Pursuing PDE Foundation Models: Generalization

TRANSOLVER (OURS)	0.2996	0.9896	0.1500	0.9950	Flow direction
GINO (2023A)	$\overline{0.4180}$	0.9645	0.2583	0.9923	
GNOT (2023)	0.3268	0.9865	0.3497	0.9868	Angle of attack
GALERKIN (2021)	0.4615	$\overline{0.9826}$	0.3814	0.9821	
GNO (2020A)	0.4408	0.9878	0.3038	0.9884	
MeshGraphNet (2021)	1.7718	0.7631	0.6525	0.8927	
GRAPH U-NET (2019)	0.4664	0.9645		0.9816	Re > ~ 10 <sup>-5</sup>
PointNet $(2017)$	0.3836	0.9806	0.4425	0.9784	
GRAPHSAGE (2017)	0.4333	0.9707	0.2538	0.9894	
SIMPLE MLP	0.6205	0.9578	0.4128	0.9572	
Models	$\mid C_L \downarrow$	$ ho_L \uparrow$	$\mid C_L \downarrow$	$ ho_L \uparrow$	Re ~10 <sup>4</sup> - ~10 <sup>5</sup>
Model c	OOD R	EYNOLDS	OOD A	ANGLES	

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

# Open-Source Code









Code for Transolver in Modulus



Code for Transolver

Code Link: <a href="https://github.com/thuml/Transolver">https://github.com/thuml/Transolver</a>



#### Transolver++: An Accurate Neural Solver for PDEs on Million-Scale Geometries

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Haixu Wu



Hang Zhou



Lanxiang Xing



Yichen Di

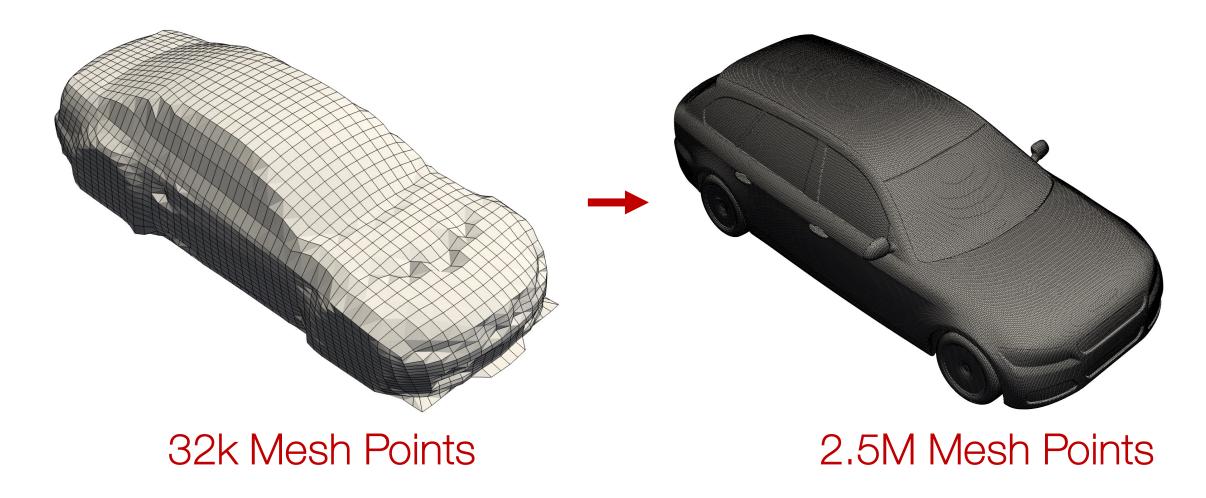


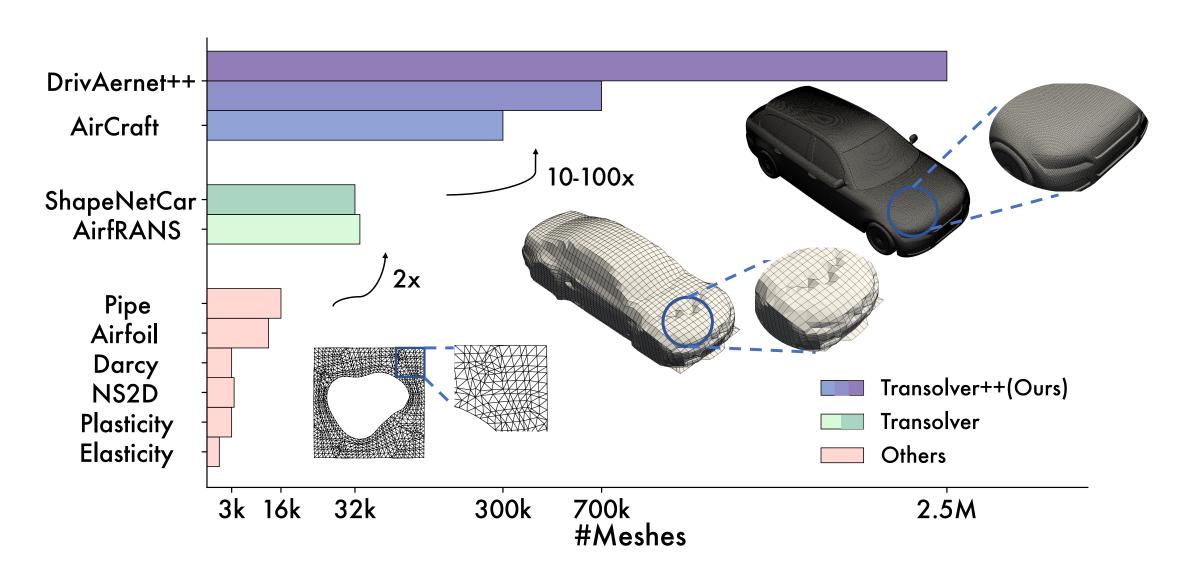
Jianmin Wang

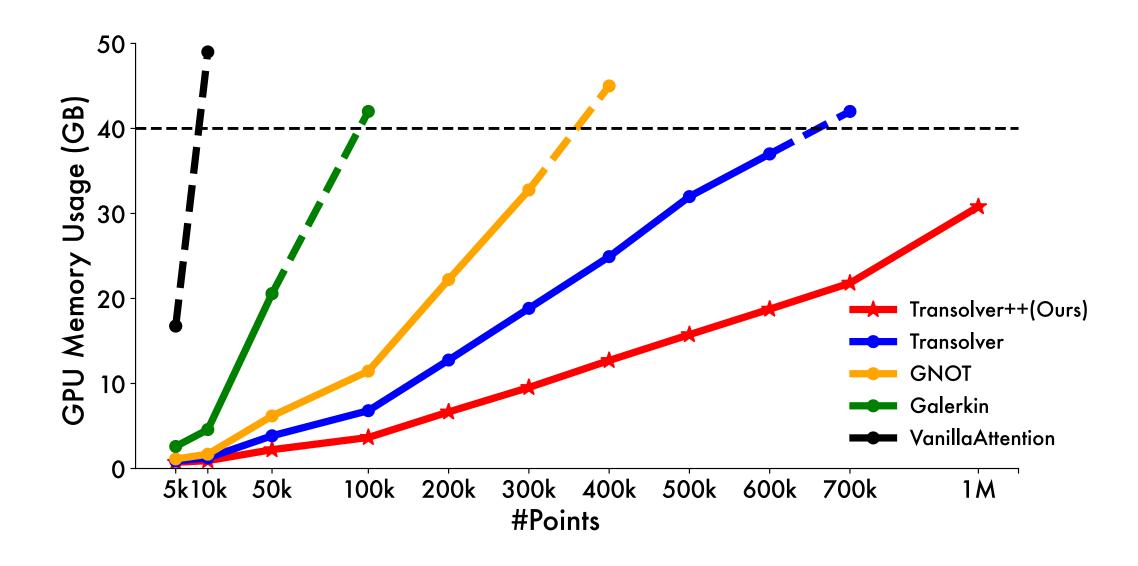


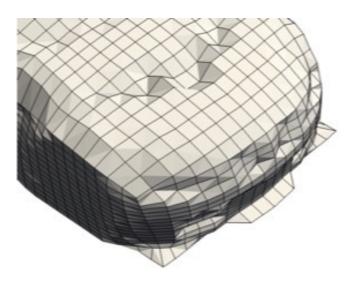
Mingsheng Long



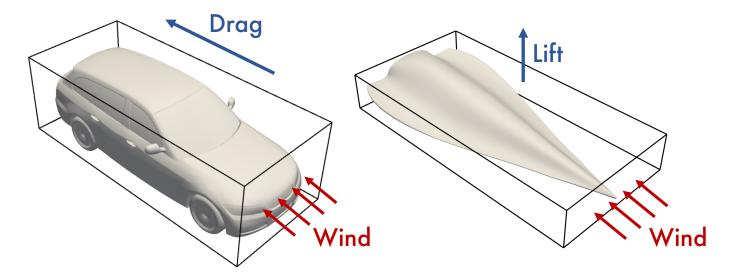








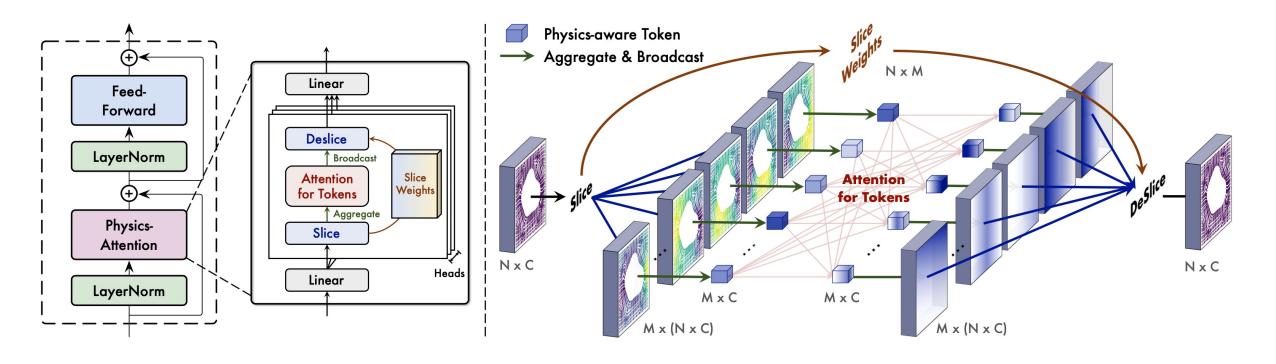




#### Large Geometrics In real-world applications

- 1. More complex geometrics with plenty of details
- 2. Deep models are expected to be Scalable
- 3. Models are expected to be more accurate

# Revisiting Transolver

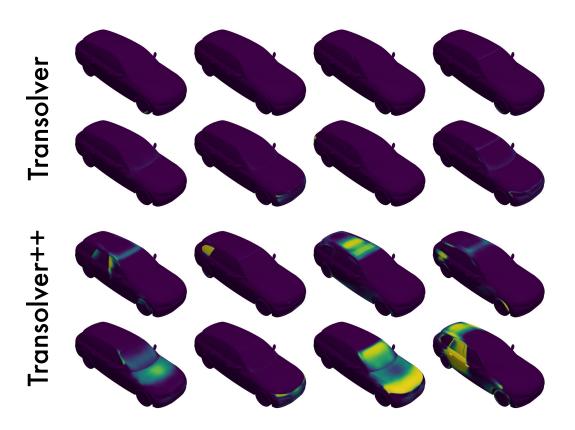


Transolver applies attention to learned physical states

Mesh → physics ② Physics-Attention ③ Physics → Mesh

#### Challenges within Transolver

#### 1. Homogeneous physical states



(b) Slice Weights Visualization

#### 2. Efficiency Bottleneck

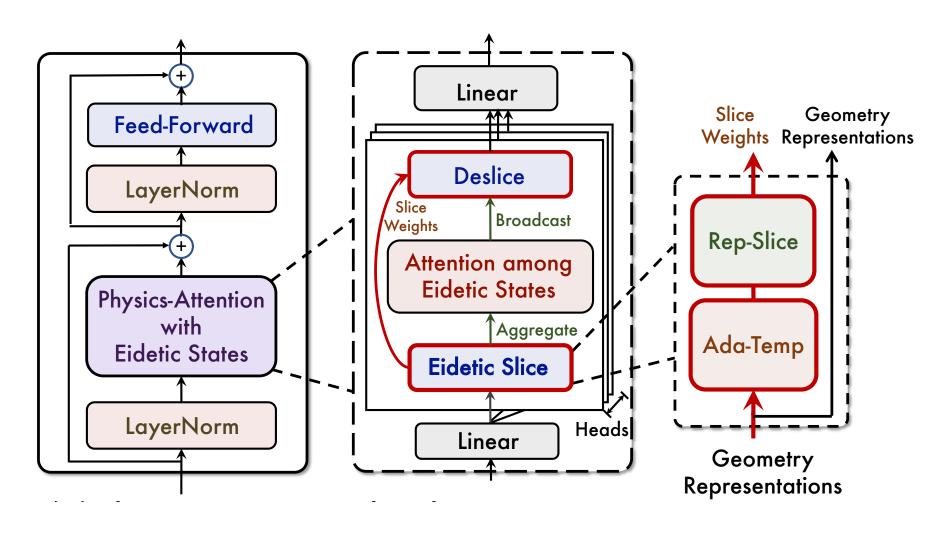
Slice weights:  $\mathbf{w} = \operatorname{Softmax} \left( \operatorname{Linear}(\mathbf{x}) / \tau_0 \right)$ 

Physical states: 
$$\{\mathbf{s}_j\}_{j=1}^M = \left\{\frac{\sum_{i=1}^N \mathbf{w}_{ij} \mathbf{x}_i}{\sum_{i=1}^N \mathbf{w}_{ij}}\right\}_{j=1}^M$$

- Even a single intermediate representation of one million mesh points will consume 2GB GPU memory
- Previous upper bound of geometry scale is 600k on one single GPU supported by Transolver

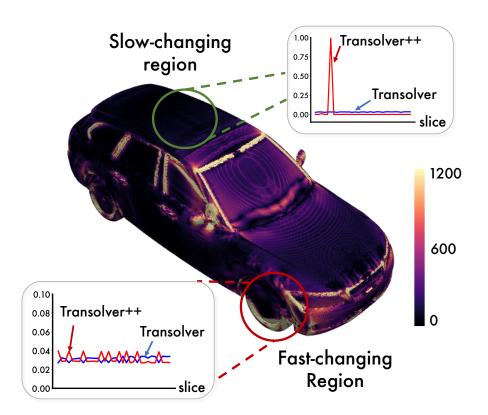
# Solutions to challenges – Physics-Attention with Eidetic States

#### Architectural Design



# Solutions to challenges – Physics-Attention with Eidetic States

#### Local Adaptive Mechanism



Ada-Temp: 
$$\tau = \{\tau_i\}_{i=1}^N = \{\tau_0 + \text{Linear}(\mathbf{x}_i)\}_{i=1}^N$$
,

- Utilize the local properties of each mesh point
- Learns the uncertainty of each points
- Adaptively change the temperature of each point

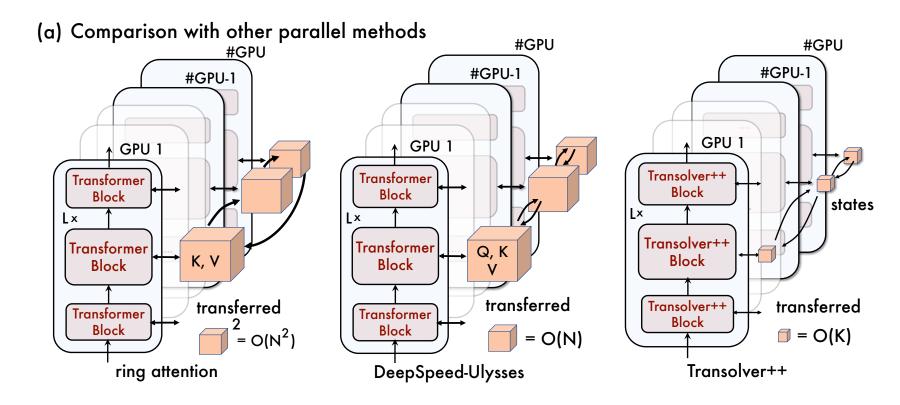
Slice reparameterization

Rep-Slice(
$$\mathbf{x}, \tau$$
) = Softmax  $\left(\frac{\text{Linear}(\mathbf{x}) - \log(-\log \epsilon)}{\tau}\right)$ , (4)

# Solutions to challenges – Parallel Transolver++

#### Parallel Formulation

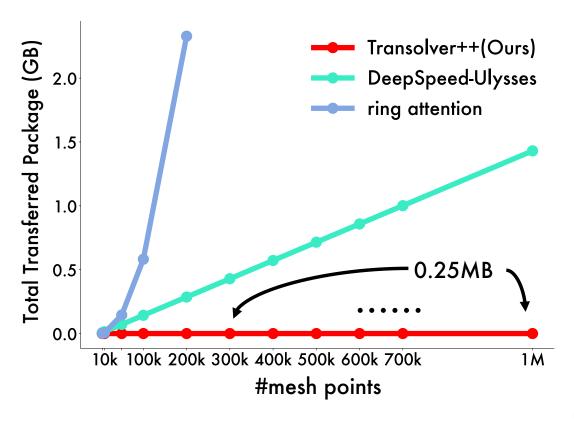
$$\mathbf{s}_{j} = \frac{\sum_{i=1}^{N_{1}} \mathbf{w}_{ij}^{(1)} \mathbf{x}_{i}^{(1)} \oplus \cdots \oplus \sum_{i=1}^{N_{\#\text{gpu}}} \mathbf{w}_{ij}^{(\#\text{gpu})} \mathbf{x}_{i}^{(\#\text{gpu})}}{\sum_{i=1}^{N_{1}} \mathbf{w}_{ij}^{(1)} \oplus \cdots \oplus \sum_{i=1}^{N_{\#\text{gpu}}} \mathbf{w}_{ij}^{(\#\text{gpu})}}$$



# Solutions to challenges – Parallel Transolver++

#### Overhead Analysis

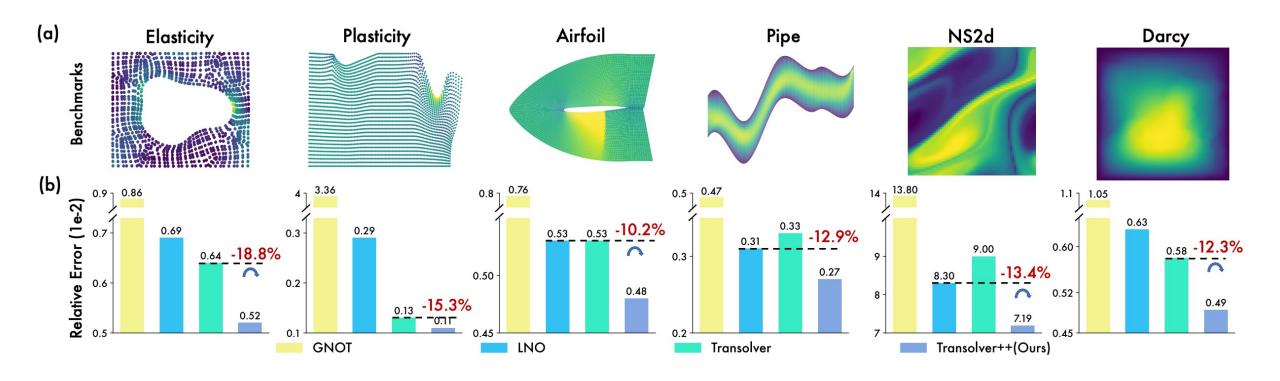
#### (b) Scalability of Transferred Package



#### Further SpeedUp

```
Algorithm 1 Parallel Physics-Attention with Eidetic States
    Input: Input features \mathbf{x}^{(k)} \in \mathbb{R}^{N_k \times C} on the k-th GPU.
    Output: Updated output features \mathbf{x}'^{(k)} \in \mathbb{R}^{N_k \times C}.
    // drop f to save 50% memory.
    Compute \mathbf{f}^{(k)}, \mathbf{x}^{(k)} \leftarrow \text{Project}(\mathbf{x}^{(k)})
    Compute \tau^{(k)} \leftarrow \tau_0 + \text{Ada-Temp}(\mathbf{x}^{(k)})
    Compute weights \mathbf{w}^{(k)} \leftarrow \text{Rep-Slice}(\mathbf{x}^{(k)}, \tau^{(k)})
    Compute weights norm \mathbf{w}_{\text{norm}}^{(k)} \leftarrow \sum_{i=1}^{N_k} \mathbf{w}_i^{(k)}
    Reduce slice norm \mathbf{w}_{\text{norm}} \leftarrow \text{AllReduce}(\mathbf{w}_{\text{norm}}^{(k)}) \mathcal{O}(M)
    Compute eidetic states \mathbf{s}^{(k)} \leftarrow \mathbf{w}^{(k)\mathsf{T}}\mathbf{x}^{(k)}\mathbf{s}^{(k)}
    Reduce eidetic states s \leftarrow AllReduce(s^{(k)})
                                                                                        \mathcal{O}(MC)
    Update eidetic states s' \leftarrow Attention(s)
    Deslice back to \mathbf{x}'^{(k)} \leftarrow \text{Deslice}(\mathbf{s}', \mathbf{w}^{(k)})
    Return \mathbf{x}'^{(k)}
```

# Standard PDE-Solving Benchmarks



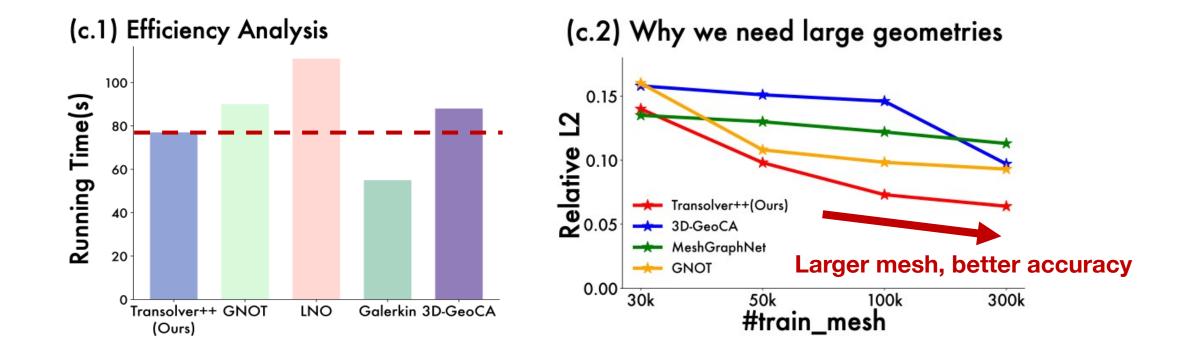
Transolver++ achieves averaged 13% error reduction than previous methods.

# Industrial Applications

MODEL	DrivAernet++ Full		DrivAernet++ Surf			AIRCRAFT		
1/10222	VOLUME ↓	Surf↓	$C_D\downarrow$	$R_L^2 \uparrow$	Surf↓	$C_L\downarrow$	$R_L^2\uparrow$	Surf↓
GRAPHSAGE (2017) POINTNET (2017) GRAPH U-NET* (2019)	0.328 0.285 0.241	0.284 0.478 0.260	0.282 0.301 0.272	0.859 0.831 0.876	0.294 0.237 0.193	0.040 0.095 0.063	0.988 0.982 0.953	0.109 0.169 0.161
MESHGRAPHNET* (2021)	0.529	0.422	0.260	0.870	0.209	0.038	0.993	0.113
GNO* (2020A) GALERKIN* (2021) GEO-FNO* (2022) GINO (2023A) GNOT* (2023) LNO* (2024) 3D-GEOCA* (2024) TRANSOLVER* (2024)	0.510 0.234 0.718 0.586 0.174 0.180 0.389 0.173	0.664 0.274 0.892 0.638 0.171 0.203 0.224 <u>0.167</u>	0.252 0.267 0.288 0.323 0.158 0.208 0.205 <u>0.061</u>	0.882 0.792 0.831 0.725 0.901 0.855 0.883 <u>0.931</u>	0.196 0.235 0.291 0.220 0.167 0.195 0.175 <u>0.145</u>	0.031 0.069 0.243 0.047 0.033 0.091 <u>0.022</u> 0.037	0.991 0.879 0.903 0.983 0.991 0.992 0.993 0.994	0.129 0.118 0.395 0.133 0.093 0.137 0.097 0.092
TRANSOLVER++ (OURS) RELATIVE PROMOTION	<b>0.154</b> 11.0%	<b>0.146</b> 12.6%	<b>0.036</b> 41.0%	0.997 -	<b>0.110</b> 24.1%	<b>0.014</b> 36.3%	0.999 -	<b>0.064</b> 30.4%

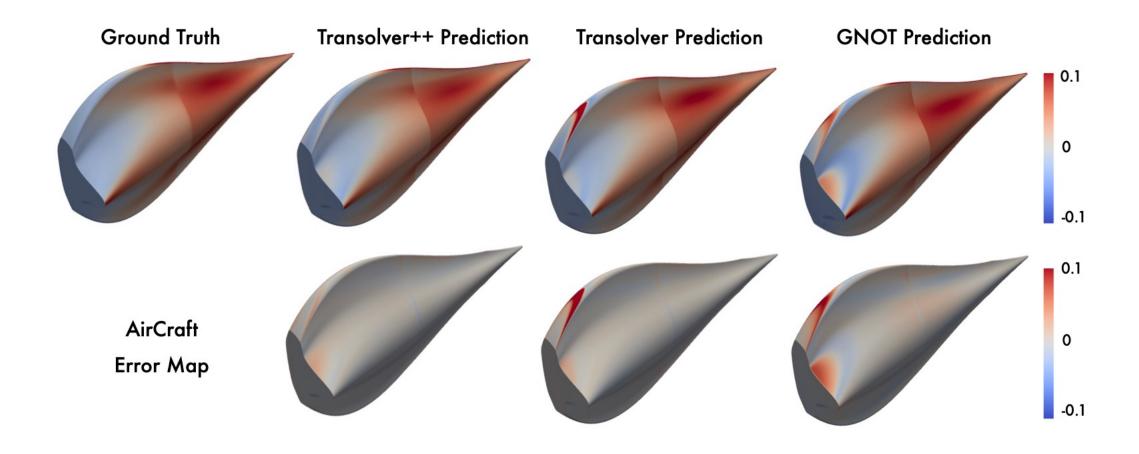
Transolver++ achieves over 20% error reduction.

# Efficiency and Scalability

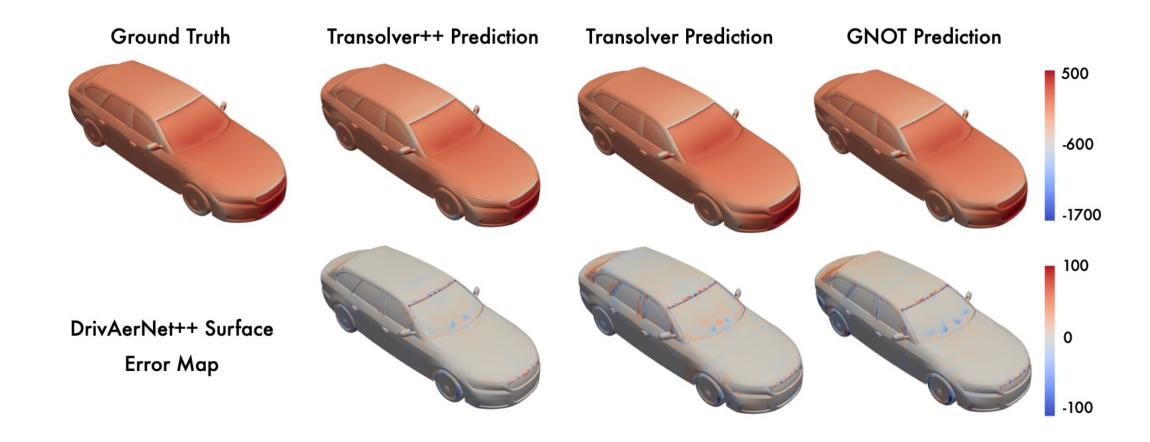


Transolver++ strikes a favorable balance between performance and efficiency.

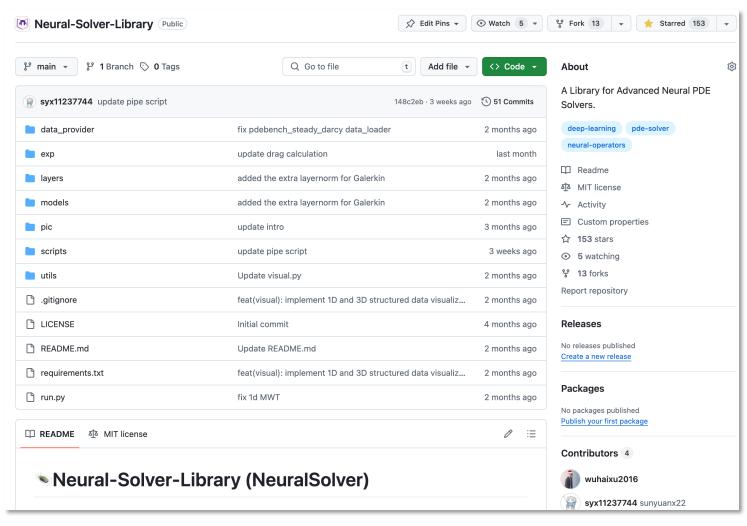
#### Showcases



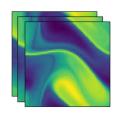
#### Showcases

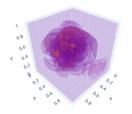


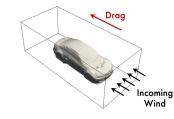
# Neural-Solver-Library



- √ 17 different PDE solvers
- ✓ 6 standard benchmarks, PDEBench
  and design tasks







Task 1: Standard

Task 2: PDEBench

Task 3: ShapeNet Car

# Welcome to join us and add a new feature to this Library!



Code for NeuralSolver

Code Link: <a href="https://github.com/thuml/Neural-Solver-Library">https://github.com/thuml/Neural-Solver-Library</a>

# Acknowledgement







Mingsheng Long







长按关注, 获取最新资讯



Hang Zhou



Yuezhou Ma



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Yuanxu Sun



Huikun Weng



Haowen Wang