PhySiViT : A Physics Simulation Vision Transformer

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PhySiViT HuggingFace

The Well Data Source

Introduction

Scientific simulations generate petabytes of complex, multi-channel, time-evolving data. Current machine learning models are narrow, domain-specific, and unable to generalize across physics types**.**

Vision transformers (ViTs) have revolutionized natural image understanding via models like CLIP and DINO, but **no equivalent foundation models exist for scientific spatiotemporal data**

Objective

To train a foundational image encoder model (PhySiViT) for scientific spatiotemporal data, enabling downstream tasks such as classification, temporal forecasting, and embedding visualization.

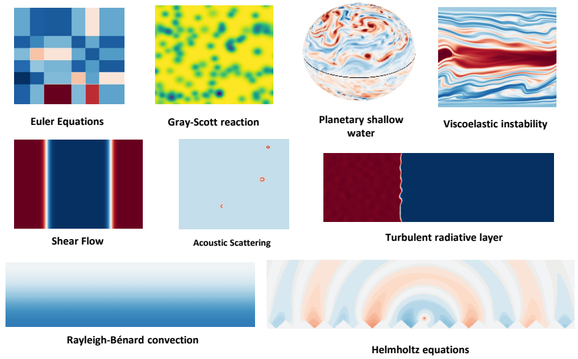


Figure 1: The following simulation classes were selected from **The Well**, which resulted in 7M 2D images to train the Vision Transformer.

2D simulations selected from "the Well" dataset are shown in **Figure 1.** For downstream task evaluation:

- Classification: logistic regression for domain labels (accuracy).
- Temporal forecasting: ridge regression for next timestep prediction (R^2/MSE).
- Embedding visualization: silhouette score for domain separation.

Methods

PhySiViT uses a standard Huge Vision Transformer architecture[2], summarized below. Custom augmentations, such as temporal splits and color schemes, were used on input data. physics

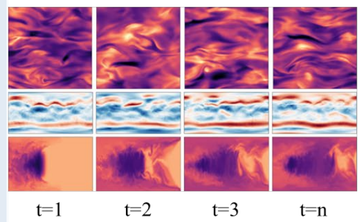


Image Preprocessing

Expand to Square

Random Color Scheme

Temporal Split

Train Valid

Model Architecture

32 Layers

1280 Hidden dim

16 Num Heads

Patch Size: 16 X 16

Evaluation

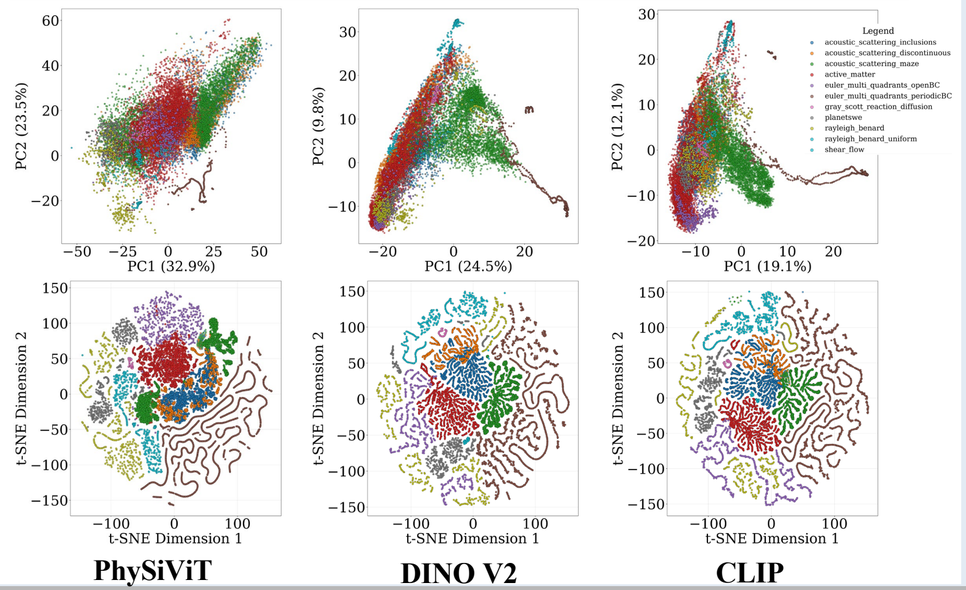
Domain Classification

Temporal Forecasting

Embedding Visualizations

Results

Model	Accuracy (↑)	R^2 (↑)	MSE (↓)	Silhouette (↑)
PhySiViT	0.98	**0.33**	**0.57**	**0.23**
DINOv2 Giant	**0.99**	0.23	0.62	0.20
CLIP-ViT Large	0.99	0.22	0.63	0.19



Training Considerations

Total Training Time on the Cerebras CS-3 (~7 Million Images)

Trained on one Cerebras CS-3 node with an effective batch size of 1470 for 78372 steps, which took 22.83 hours.

Training Speed Comparison (Single Device with 70,656 Images)

Compute Device	Total Time (hours)
AMD EPYC 7702P (CPU)	14.03
NVIDIA H100 80GB (GPU)	2.5
Cerebras CS-3	0.2

Conclusion & Future Work

PhySiViT is better at **physics-related tasks**, such as temporal prediction, and is comparable in general classification tasks, particularly silhouette scores represent ***clearer cluster of physical simulation domains in embedding space***.

Future Work:

- Hyperparameter tuning & data augmentation strategies.
- Comparative benchmarking on additional downstream tasks.
- Finetuning DINOv2 and CLIP & extending to DINOv3.
- Scaling PhySiViT to 3D volumetric scientific simulations.

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