



AQTIVATE

Automatic Differentiation and Machine Learning for Numerical Simulations

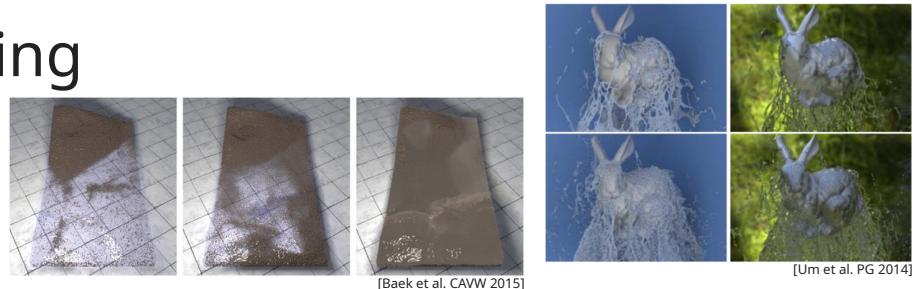
AQTIVATE ML Workshop

Kiwon Um



Personal background

- Computer science and engineering



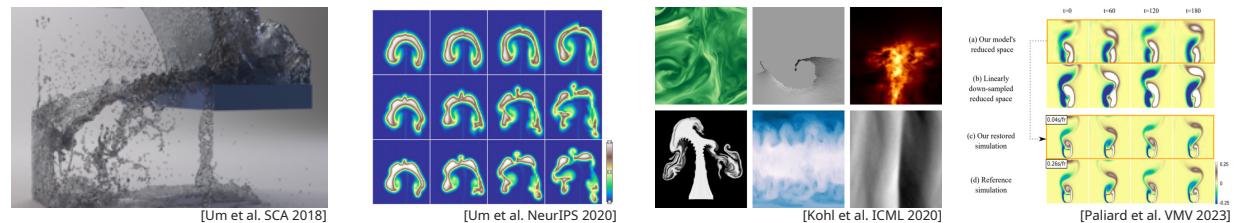
- Physics-based simulations, particularly for computer graphics



- Fluid simulations



- Soft-body simulations



- Deep learning

My research interests

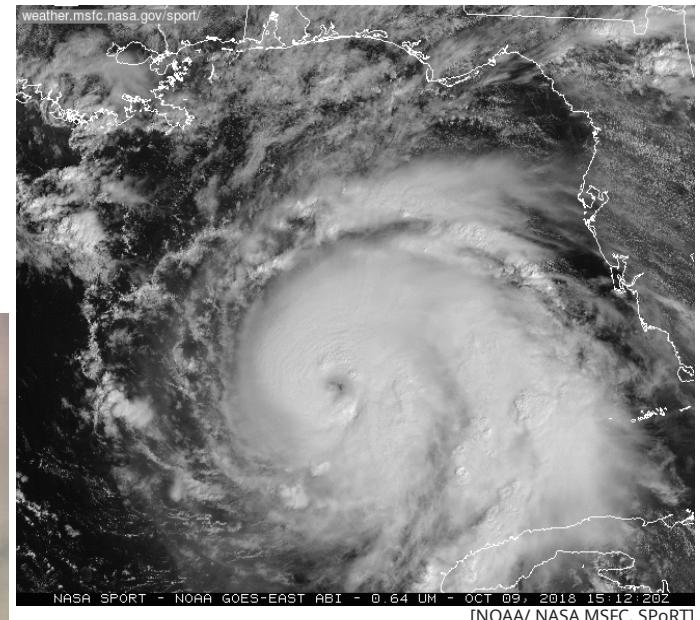
- Understanding natural phenomena and reproducing them
- Modeling the dynamics, e.g., using PDEs
- Solving PDEs - *numerical or learning-based or hybrid methods*



[Wikipedia]



[Wikipedia]



NASA SPoRT - NOAA GOES-EAST ABI - 0.64 UM - OCT 09, 2018 15:12:20Z
[NOAA/ NASA MSFC, SPoRT]

In this talk ...

Automatic differentiation

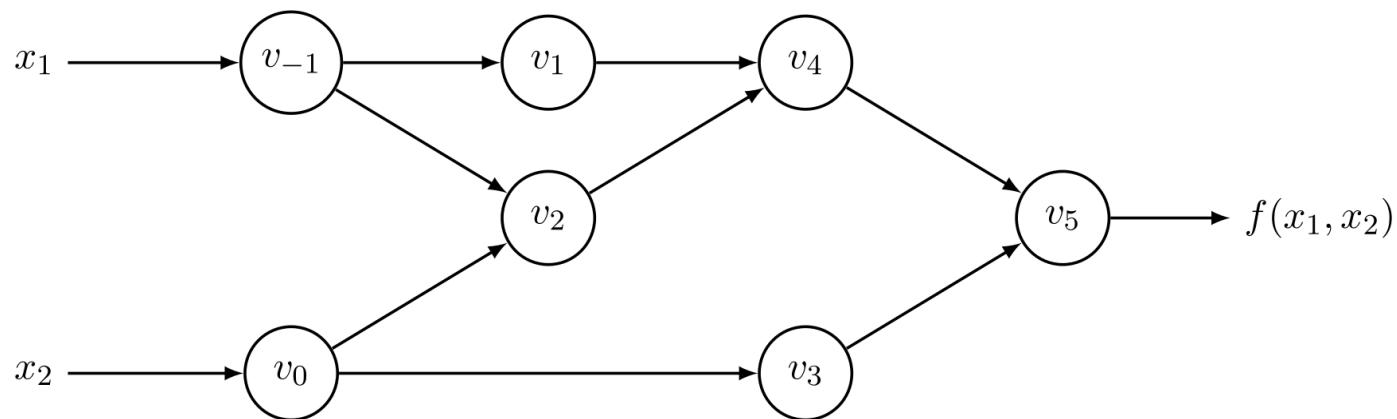
- A technical term
 - Refer to a specific family of techniques
 - Compute derivatives through the accumulation of values
 - Execute code to generate numerical **derivative evaluations** rather than **derivative expressions**
- Shortly, "*Autodiff*"
- Also called "*Algorithmic differentiation*"
- Versus
 - Manual differentiation
 - Numerical differentiation
 - Symbolic differentiation
- ... a nice survey
 - [2018, Baydin et al., Automatic differentiation in machine learning: a survey]

Forward mode

- An example function:

$$f(x_1, x_2) = \ln(x_1) + x_1 x_2 - \sin(x_2) = y$$

- Want to evaluate \dot{y} for **a given input**, e.g., $(x_1 = 2, x_2 = 5)$
- Computational graph
 - Trace of elementary operations

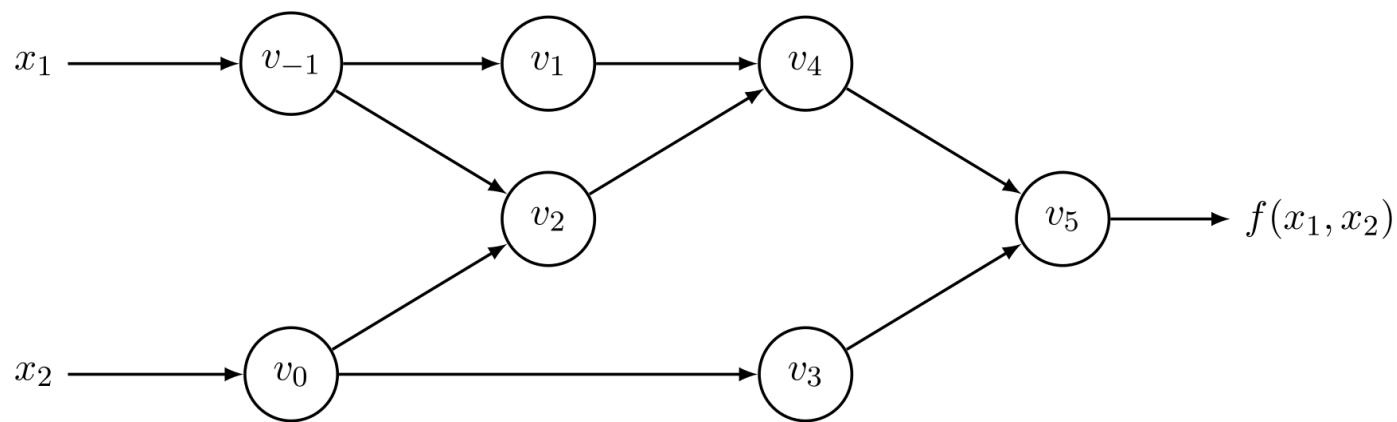


Forward mode (cont'd)

- Forward primal and tangent (derivative) traces for $\partial y / \partial x_1$

v_{-1}	$= x_1$	$= 2$	
v_0	$= x_2$	$= 5$	
v_1	$= \ln(v_{-1})$	$= \ln(2)$	$= 0.693$
v_2	$= v_{-1} \times v_0$	$= 2 \times 5$	$= 10$
v_3	$= \sin(v_0)$	$= \sin(5)$	$= -0.959$
v_4	$= v_1 + v_2$	$= 0.693 + 10$	$= 10.693$
v_5	$= v_4 - v_3$	$= 10.693 + 0.959$	$= 11.652$
y	$= v_5$	$= 11.652$	

\dot{v}_{-1}	$= \dot{x}_1$	$= 1$	
\dot{v}_0	$= \dot{x}_2$	$= 0$	
\dot{v}_1	$= \dot{v}_{-1}/v_{-1}$	$= 1/2$	$= 0.5$
\dot{v}_2	$= \dot{v}_{-1} \times v_0 + v_{-1} \times \dot{v}_0$	$= 1 \times 5 + 0 \times 2$	$= 5$
\dot{v}_3	$= \dot{v}_0 \times \cos v_0$	$= 0 \times \cos(5)$	$= 0$
\dot{v}_4	$= \dot{v}_1 + \dot{v}_2$	$= 0.5 + 5$	$= 5.5$
\dot{v}_5	$= \dot{v}_4 - \dot{v}_3$	$= 5.5 - 0$	$= 5.5$
\dot{y}	$= \dot{v}_5$	$= 5.5$	



Forward mode (cont'd)

- Simple to evaluate
- Can be generalized to computing the Jacobian of a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$
 - Require n evaluations for each independent variable x_i
- In general, when $n < m$,
 - Very efficient to evaluate the derivative
- Unfortunately, however,
 - It's the other way around for machine learning.
 - I.e., we need to evaluate the derivative *with respect to* a lot of trainable parameters.

Reverse mode

- Also called *adjoint* or *cotangent linear* mode
- Trace the **sensitivity** of an output y_j with respect to changes in intermediate variables v_i

$$\bar{v}_i = \frac{\partial y_j}{\partial v_i}$$

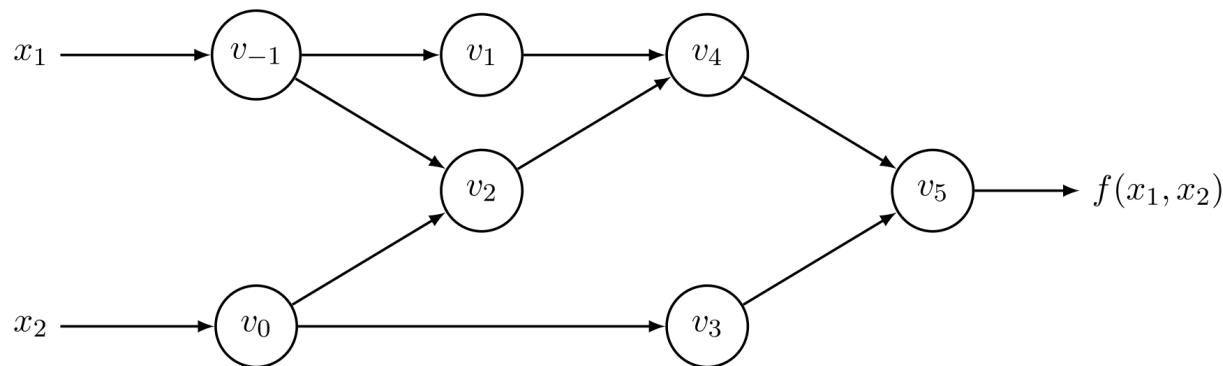
- Two-phase process
 - The 1st phase: forward
 - Populating intermediate variables v_i and recording the dependencies
 - The 2nd phase: reverse
 - Propagating adjoints \bar{v}_i from the outputs to the inputs
- A generalized *backpropagation* algorithm
 - Remind that ML practice principally involves the gradient of a scalar-valued objective with respect to a large number of parameters.

Reverse mode (cont'd)

- Forward primal trace and reverse adjoint (derivative) trace

$$\begin{array}{lll}
 v_{-1} &= x_1 &= 2 \\
 v_0 &= x_2 &= 5 \\
 \hline
 v_1 &= \ln(v_{-1}) &= \ln(2) = 0.693 \\
 v_2 &= v_{-1} \times v_0 &= 2 \times 5 = 10 \\
 v_3 &= \sin(v_0) &= \sin(5) = -0.959 \\
 v_4 &= v_1 + v_2 &= 0.693 + 10 = 10.693 \\
 v_5 &= v_4 - v_3 &= 10.693 + 0.959 = 11.652 \\
 \hline
 y &= v_5 &= 11.652
 \end{array}$$

$$\begin{array}{llll}
 \bar{x}_1 &= \bar{v}_{-1,1} + \bar{v}_{-1,2} &= 0.5 + 5 &= 5.5 \\
 \bar{x}_2 &= \bar{v}_{0,2} + \bar{v}_{0,3} &= 2 - 0.284 &= 1.716 \\
 \hline
 \bar{v}_{-1,1} &= \bar{v}_{1,4} \frac{\partial v_1}{\partial v_{-1}} = \bar{v}_{1,4}/v_{-1} &= 1/2 &= 0.5 \\
 \bar{v}_{0,2} &= \bar{v}_{2,4} \frac{\partial v_2}{\partial v_0} = \bar{v}_{2,4} \times v_{-1} &= 1 \times 2 &= 2 \\
 \bar{v}_{-1,2} &= \bar{v}_{2,4} \frac{\partial v_2}{\partial v_{-1}} = \bar{v}_{2,4} \times v_0 &= 1 \times 5 &= 5 \\
 \bar{v}_{0,3} &= \bar{v}_{3,5} \frac{\partial v_3}{\partial v_0} = \bar{v}_{3,5} \times \cos(v_0) &= -1 \times 0.284 &= -0.284 \\
 \bar{v}_{2,4} &= \bar{v}_{4,5} \frac{\partial v_4}{\partial v_2} = \bar{v}_{4,5} \times 1 &= 1 \times 1 &= 1 \\
 \bar{v}_{1,4} &= \bar{v}_{4,5} \frac{\partial v_4}{\partial v_1} = \bar{v}_{4,5} \times 1 &= 1 \times 1 &= 1 \\
 \bar{v}_{3,5} &= \bar{v}_{5,y} \frac{\partial v_5}{\partial v_3} = \bar{v}_{5,y} \times (-1) &= 1 \times -1 &= -1 \\
 \bar{v}_{4,5} &= \bar{v}_{5,y} \frac{\partial v_5}{\partial v_4} = \bar{v}_{5,y} \times 1 &= 1 \times 1 &= 1 \\
 \hline
 \bar{v}_{5,y} &= \bar{y} &= 1
 \end{array}$$



Automatic differentiation in TensorFlow

- Perform the **reverse mode** differentiation
- *Gradient tapes*: TensorFlow API for automatic differentiation
 - `tf.GradientTape`
 - Record relevant operations executed inside this context onto a "tape"
 - `GradientTape.gradient(target, sources)`
 - Calculate the gradient

```
x = tf.Variable(3.0)
with tf.GradientTape() as tape:
    y = x**2
```

```
dy_dx = tape.gradient(y, x)
dy_dx.numpy()
```

```
6.0
```

- The "best" material for the details
 - <https://www.tensorflow.org/guide/autodiff>

Gradients w.r.t. a model in TensorFlow

- In most cases
 - We want to calculate gradients with respect to a model's trainable variables.
 - *Why?*
 - Update the model's parameters: **Backpropagation!**

```
layer = tf.keras.layers.Dense(2, activation='relu') # 2 outputs
x = tf.constant([[1., 2., 3.]])                  # 1 x 3 inputs

with tf.GradientTape() as tape:
    # Forward pass
    y = layer(x)                      # x:[1x3] . w:[3x2] + b:[1x2] = y:[1x2]
    loss = tf.reduce_mean(y**2)

# Calculate gradients with respect to every trainable variable
grad = tape.gradient(loss, layer.trainable_variables)

for var, g in zip(layer.trainable_variables, grad):
    print(f'{var.name}, shape: {g.shape}')
```

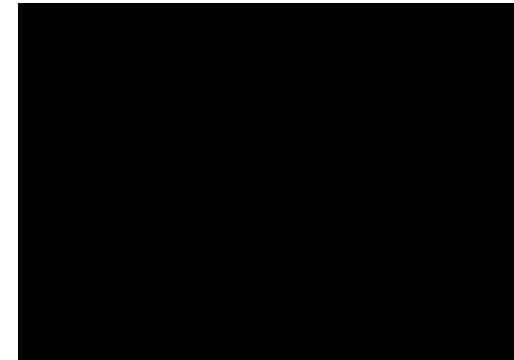
```
dense/kernel:0, shape: (3, 2)
dense/bias:0, shape: (2, )
```

What can we do with this?

Numerical simulations

- Numerical methods → errors
 - Discrete simulation of PDEs
 - Higher-order methods: preferable but difficult in practice
 - As numerical solutions are integrated over time, error often grows exponentially.

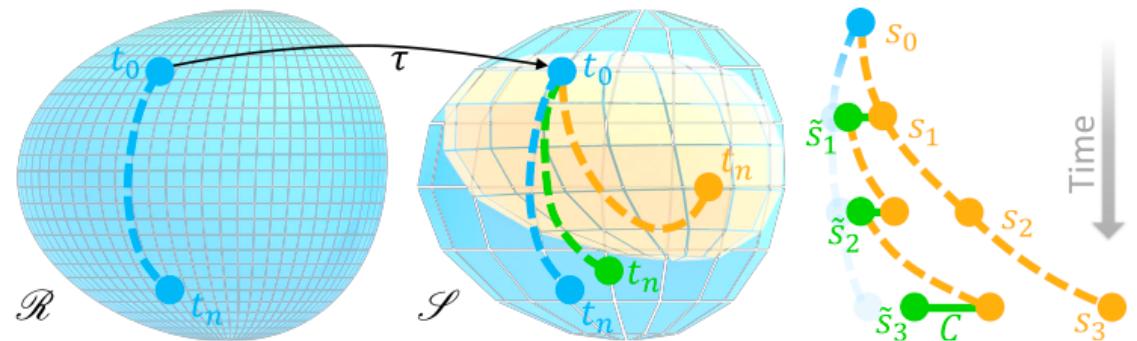
- Our target:
 - A discretized PDE solver \mathcal{P} solving for discrete time steps Δt using a regular grid



- Each subsequent step depends on any number of previous steps.
 - E.g., $\mathbf{u}(\mathbf{x}, t + \Delta t) = \mathcal{P}(\mathbf{u}(\mathbf{x}, t), \mathbf{u}(\mathbf{x}, t - \Delta t), \mathbf{u}(\mathbf{x}, t - 2\Delta t), \dots)$
 - $\mathbf{x} \in \Omega \subset \mathbb{R}^d$
 - $t \in \mathbb{R}^+$

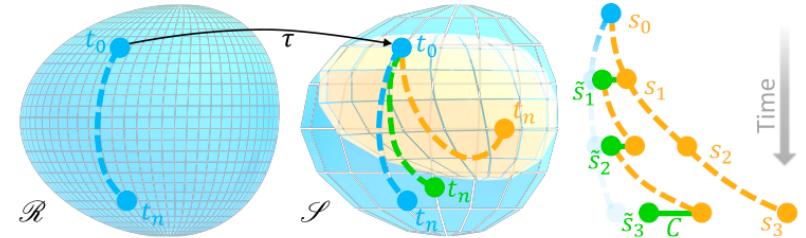
Different numerical solvers

- Two different solvers of the same PDE
 - \mathcal{P}_R : **accurate** solver
 - Solutions $\mathbf{r} \in \mathcal{R}$ from *reference* manifold
 - \mathcal{P}_S : **efficient** solver
 - Approximated solutions $\mathbf{s} \in \mathcal{S}$ from *source* manifold
- Reference sequence: $\{\mathbf{r}_t, \mathbf{r}_{t+\Delta t}, \dots, \mathbf{r}_{t+k\Delta t}\}$
- Source sequence: $\{\mathbf{s}_t, \mathbf{s}_{t+\Delta t}, \dots, \mathbf{s}_{t+k\Delta t}\}$
- Mapping operator \mathcal{T}
 - Transform a phase space point from one solution manifold to a suitable point in the other manifold
 - E.g., $\mathbf{s} = \mathcal{T}\mathbf{r}$



Problem statement

- Evaluating \mathcal{P}_R for \mathcal{R}
 - $\mathbf{r}_{t+\Delta t} = \mathcal{P}_R(\mathbf{r}_t)$
 - ... $\mathbf{r}_{t+k\Delta t}$... simply \mathbf{r}_{t+k}
- Different numerical approximations: $\mathcal{T}\mathbf{r}_{t+1} \neq \mathcal{P}_S(\mathcal{T}\mathbf{r}_t)$
- Deviations, l^2 -norm: $\mathcal{L}(\mathbf{s}_t, \mathcal{T}\mathbf{r}_t) = \|\mathbf{s}_t - \mathcal{T}\mathbf{r}_t\|_2$
- Goal: find a correction operator $\mathcal{C}(\mathbf{s})$
 - $\mathcal{L}(\mathcal{C}(\mathcal{P}_S(\mathcal{T}\mathbf{r}_t)), \mathcal{T}\mathbf{r}_{t+1}) < \mathcal{L}(\mathcal{P}_S(\mathcal{T}\mathbf{r}_t), \mathcal{T}\mathbf{r}_{t+1})$
- Deep neural network model: $\mathcal{C}(\mathbf{s}|\theta)$
- Recursive application of solver
 - $\mathbf{s}_{t+n} = \mathcal{P}_S(\mathcal{P}_S(\cdots \mathcal{P}_S(\mathcal{T}\mathbf{r}_t) \cdots)) = \mathcal{P}_S^n(\mathcal{T}\mathbf{r}_t)$
 - $\tilde{\mathbf{s}}_{t+n} = \mathcal{C}(\mathcal{P}_S(\mathcal{C}(\mathcal{P}_S(\cdots \mathcal{C}(\mathcal{P}_S(\mathcal{T}\mathbf{r}_t)) \cdots)))) = \mathcal{P}_S \mathcal{C}^n(\mathcal{T}\mathbf{r}_t)$



Related work

- Negiar et al., *Learning differentiable solvers for systems with hard constraints*, ICLR 2023
- Kochkov et al., *Machine learning-accelerated computational fluid dynamics*, PNAS 2021
- Holl et al., *Learning to control PDEs with differentiable physics*, ICLR 2020
- Bar-Sinai et al., *Learning data-driven discretizations for partial differential equations*, PNAS 2019
- Raissi and Karniadakis, *Hidden physics models: Machine learning of nonlinear partial differential equations*, JCP 2018
- Chen et al., *Neural ordinary differential equations*, NeurIPS 2018
- Long et al., *PDE-Net: Learning PDEs from data*, ICML 2018
- ...

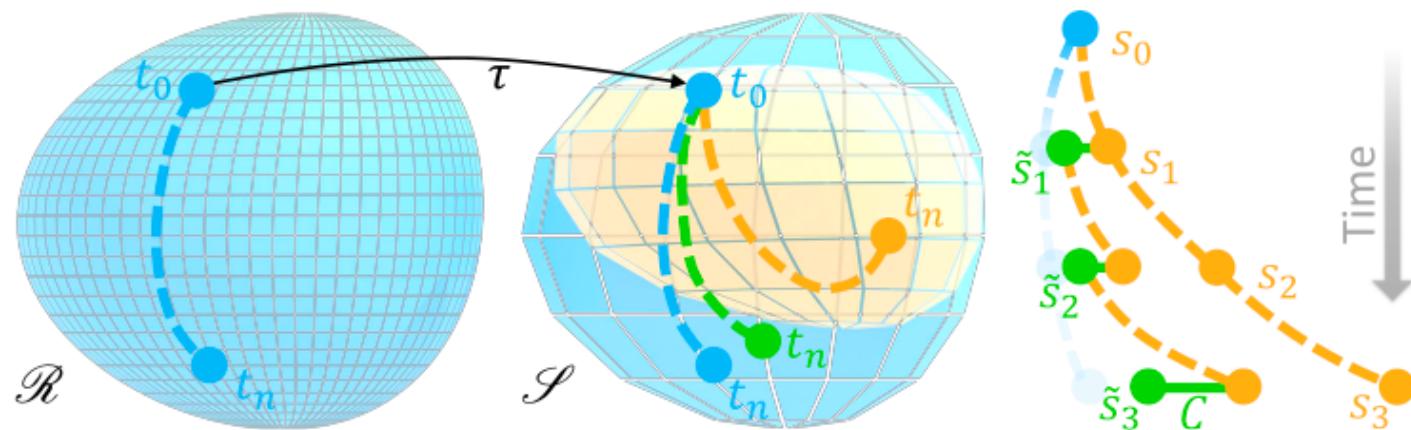
Highlight

- Efficiency & accuracy
 - Use low-resolution setups, i.e., less amount of resources
 - Generate solutions as accurate as possible



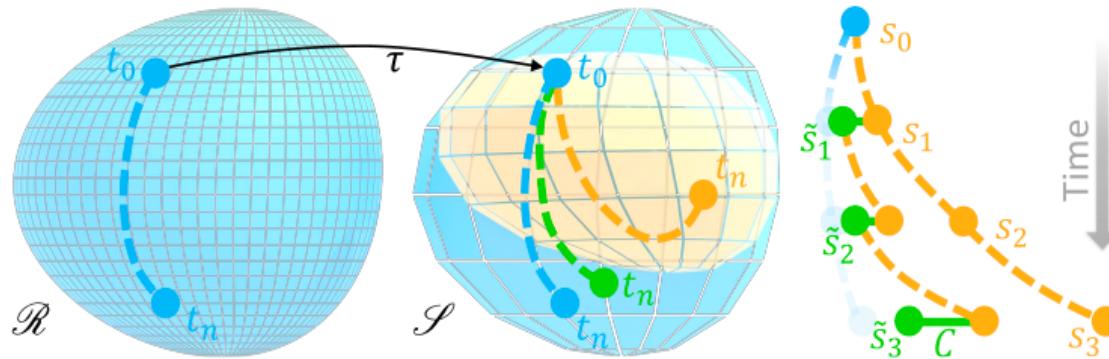
Models

- Non-interacting model, **NON**
- Pre-computed interaction model, **PRE**
- Solver-in-the-loop model, **SOL**



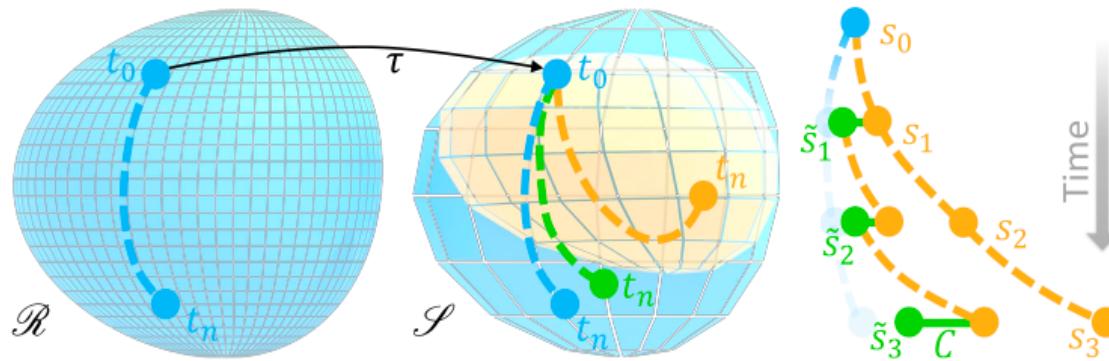
Non-interacting (NON)

- Learn from the unaltered PDE trajectories
 - $\mathbf{s}_{t+k} = \mathcal{P}_S^k(\mathcal{T}\mathbf{r}_t)$
- Model will not see any states deviated from the original solutions.
 - Learn *difference between orange and blue trajectories*
- $\arg \min_{\theta} \sum_{i=0}^n \|\mathbf{s}_{t+i} + \mathcal{C}(\mathbf{s}_{t+i} | \theta) - \mathcal{T}\mathbf{r}_{t+i}\|^2$



Pre-computed interaction (PRE)

- Learn from the pre-computed correction function, \mathcal{C}_{pre}
 - $\tilde{\mathbf{s}}_{t+k} = (\mathcal{P}_S \mathcal{C}_{\text{pre}})^k(\mathcal{T} \mathbf{r}_t)$
 - *How to pre-compute? ... coming soon*
- Model will see the corrected states, which are not influenced by the learning process.
- $\arg \min_{\theta} \sum_{i=0}^n \|\mathbf{c}_{t+i} - \mathcal{C}(\tilde{\mathbf{s}}_{t+i} | \theta)\|^2$



Training data for PRE model

- Assume the *perfect* correction \mathbf{c}_R
- Given a high-res. correction \mathbf{c}_R , solve for \mathbf{c}_S (on low-res.):

$$\underset{\mathbf{c}_S}{\operatorname{argmin}} \|\mathbf{W}\mathbf{c}_S - \mathbf{c}_R\|^2 \quad \text{subject to} \quad \mathbf{M}\mathbf{c}_S = 0$$

- \mathbf{W} : transform \mathcal{S} to \mathcal{R} , e.g., *interpolation*
- \mathbf{M} : constraints, e.g., *divergence* $\nabla \cdot$ for the Navier-Stokes scenario
- Linear system with Lagrange multiplier: λ

$$\begin{bmatrix} \mathbf{W}^\top \mathbf{W} & -\mathbf{M} \\ -\mathbf{M}^\top & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c}_S \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{W}^\top \mathbf{c}_R \\ 0 \end{bmatrix}$$

- Simplify with the Schur complement

$$\begin{aligned} \mathbf{M}^\top (\mathbf{W}^\top \mathbf{W})^{-1} \mathbf{M} \lambda &= \mathbf{M}^\top (\mathbf{W}^\top \mathbf{W})^{-1} \mathbf{W}^\top \mathbf{c}_R \\ \mathbf{c}_S &= (\mathbf{W}^\top \mathbf{W})^{-1} (\mathbf{W}^\top \mathbf{c}_R - \mathbf{M} \lambda) \end{aligned}$$

- In our example, $\mathbf{c}_t = (\mathbf{W}^\top \mathbf{W})^{-1} (\mathbf{W}^\top (\mathbf{r}_t - \mathbf{W}\mathbf{s}_t) - \mathbf{M} \lambda)$

Temporal regularization

- Very chaotic corrections despite smoothly changing inputs
 - Need to make the corrections smooth as well
 - *Why?* ... hoping the model can learn better
- Updated objective function:

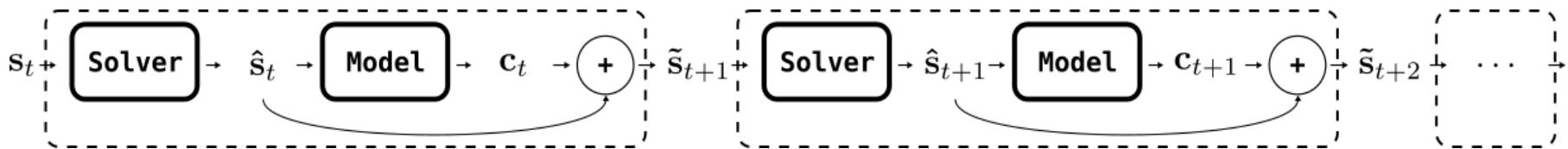
$$\operatorname{argmin}_{\mathbf{c}_S} \left(\|\mathbf{W}\mathbf{c}_S - \mathbf{c}_R\|^2 + \beta \left\| \frac{d\mathbf{c}_S}{dt} \right\|^2 \right) \text{ subject to } \mathbf{M}\mathbf{c}_S = 0$$

- Linear system with the regularization

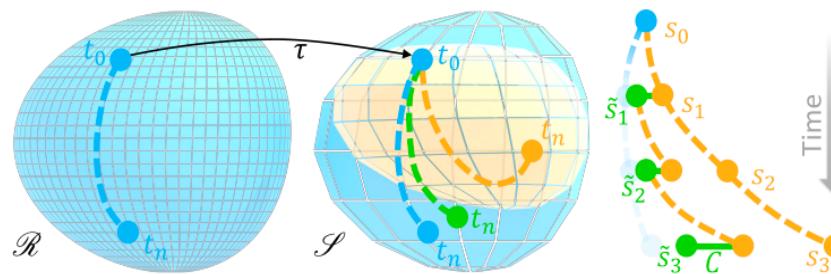
$$\begin{bmatrix} \mathbf{W}^\top \mathbf{W} + \beta \frac{2}{\Delta t} \mathbf{I} & -\mathbf{M} \\ -\mathbf{M}^\top & 0 \end{bmatrix} \begin{bmatrix} \mathbf{c}_S \\ \lambda \end{bmatrix} = \begin{bmatrix} \mathbf{W}^\top \mathbf{c}_R + \beta \frac{2}{\Delta t} \mathbf{c}_S^{t-1} \\ 0 \end{bmatrix}$$

Solver-in-the-loop (SOL)

- The learning process interacts with the correction function, \mathcal{C} .
 - $\tilde{\mathbf{s}}_{t+k} = (\mathcal{P}_S \mathcal{C})^k(\mathcal{T} \mathbf{r}_t)$
 - Similar to PRE, but what differences?
 - ... \mathcal{C} interacts with the physical system.
 - Need a *differentiable physics solver!*

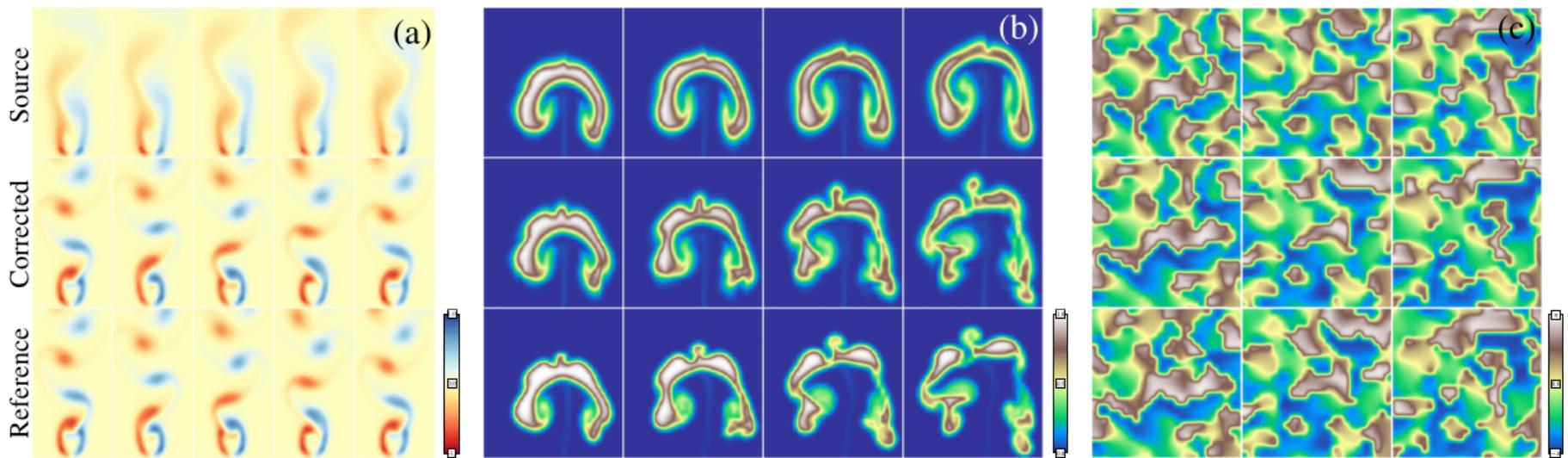


- Model will see the corrected states and influence the evolution of trajectories.
- $\arg \min_{\theta} \sum_{i=0}^{n-1} \|\mathcal{P}_S(\tilde{\mathbf{s}}_{t+i}) + \mathcal{C}(\mathcal{P}_S(\tilde{\mathbf{s}}_{t+i})|\theta) - \mathcal{T} \mathbf{r}_{t+i+1}\|^2$



Experiments

- 5 complex examples
 - Unsteady wake flow^(a)
 - Buoyancy-driven flow^(b)
 - Forced advection-diffusion^(c)
 - Conjugate gradient solver
 - Three-dimensional fluid flow



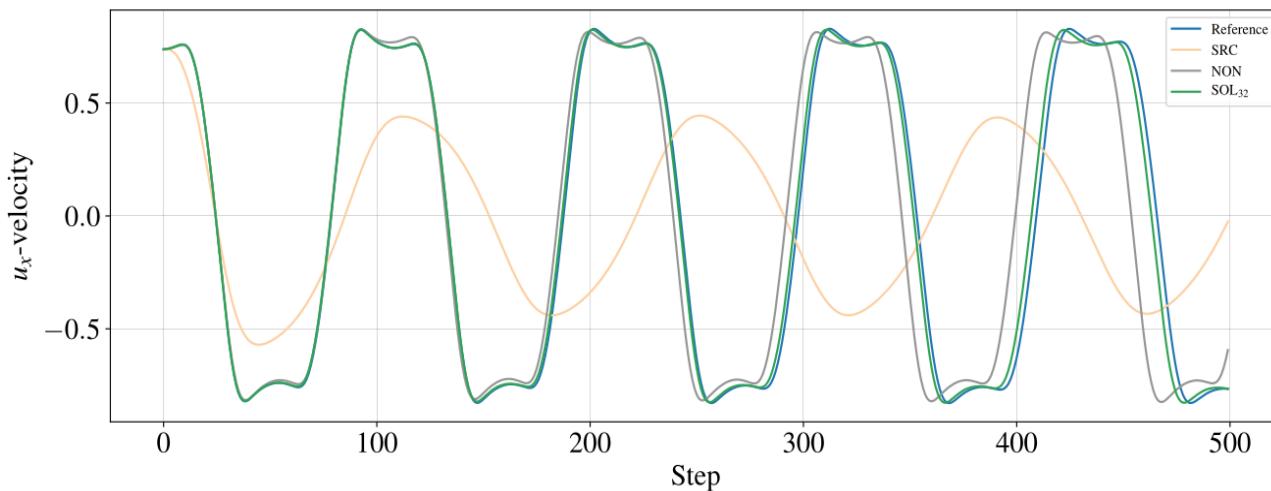
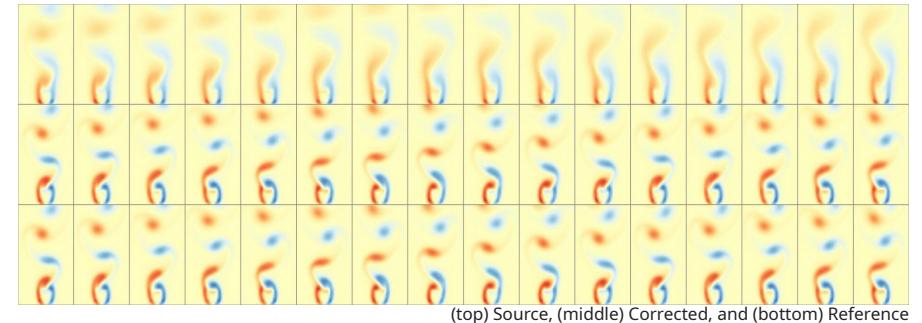
Unsteady wake flow

- Incompressible Navier-Stokes equations for Newtonian fluids:

$$\frac{\partial u_x}{\partial t} + \mathbf{u} \cdot \nabla u_x = -\frac{1}{\rho} \nabla p + \nu \nabla \cdot \nabla u_x$$

$$\frac{\partial u_y}{\partial t} + \mathbf{u} \cdot \nabla u_y = -\frac{1}{\rho} \nabla p + \nu \nabla \cdot \nabla u_y$$

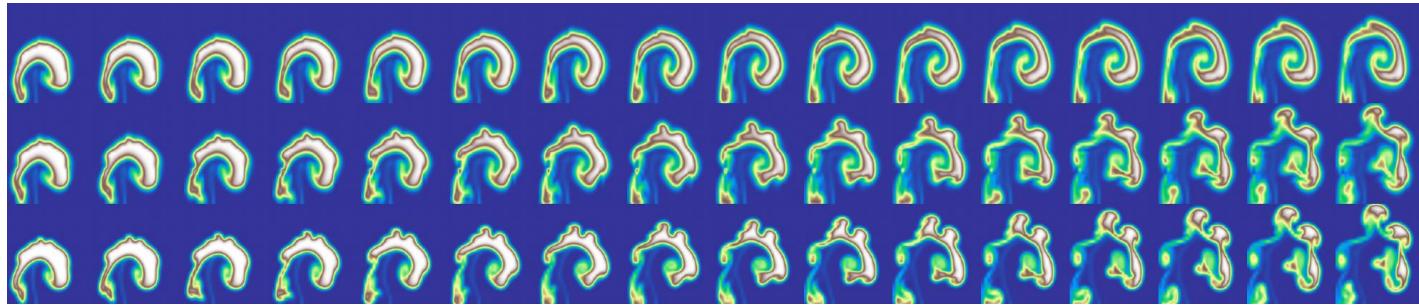
subject to $\nabla \cdot \mathbf{u} = 0$



Buoyancy-driven flow

- Incompressible N.-S. equations with a marker density field:

$$\frac{\partial u_x}{\partial t} + \mathbf{u} \cdot \nabla u_x = -\frac{1}{\rho} \nabla p, \quad \frac{\partial u_y}{\partial t} + \mathbf{u} \cdot \nabla u_y = -\frac{1}{\rho} \nabla p + \eta d \quad \text{subject to} \quad \nabla \cdot \mathbf{u} = 0$$
$$\frac{\partial d}{\partial t} + \mathbf{u} \cdot \nabla d = 0$$

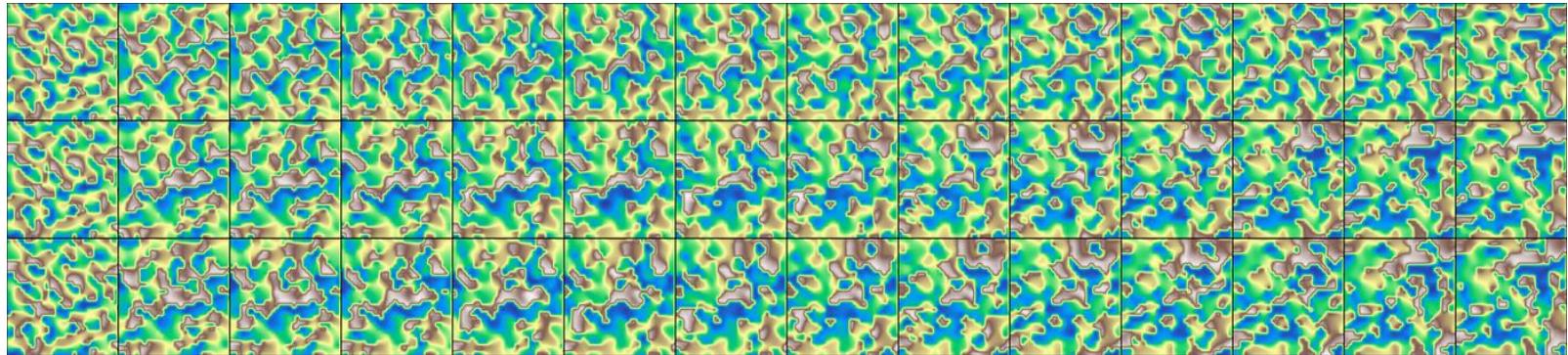


Quantity	MAE Velocity, Mean (std. dev.)							
	SRC	NON	PRE	SOL ₂	SOL ₁₆	SOL ₃₂	SOL ₆₄	SOL ₁₂₈
Velocity	1.590 (1.032)	1.079 (0.658)	1.373 (0.985)	1.027 (0.656)	0.859 (0.539)	0.775 (0.482)	0.695 (0.420)	0.620 (0.389)
Marker d	0.677 (0.473)	0.499 (0.336)	0.579 (0.409)	0.484 (0.325)	0.430 (0.281)	0.419 (0.277)	0.401 (0.262)	0.391 (0.253)

Forced advection-diffusion

- Burgers' equation

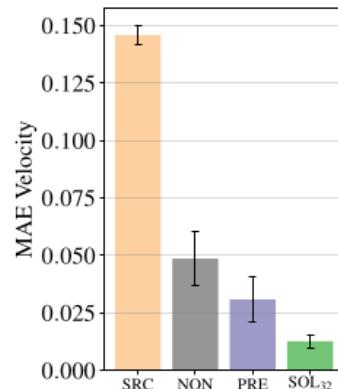
$$\frac{\partial u_x}{\partial t} + \mathbf{u} \cdot \nabla u_x = \nu \nabla \cdot \nabla u_x + g_x(t), \quad \frac{\partial u_y}{\partial t} + \mathbf{u} \cdot \nabla u_y = \nu \nabla \cdot \nabla u_y + g_y(t)$$



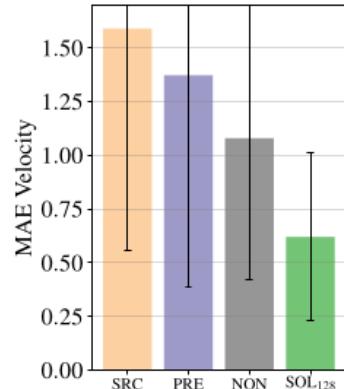
(top) Source, (middle) Corrected, and (bottom) Reference

MAE Velocity, Mean (std. dev.)						
With forcing	SRC	PRE	NON	SOL ₂	SOL ₄	SOL ₈
	0.248 (0.019)	0.218 (0.017)	0.159 (0.015)	0.148 (0.016)	0.152 (0.015)	0.158 (0.017)
Without forcing (×100)	SRC	NON	SOL ₄	SOL ₈	SOL ₁₆	SOL ₃₂
	0.306 (0.020)	0.272 (0.028)	0.276 (0.037)	0.277 (0.040)	0.268 (0.030)	0.253 (0.020)

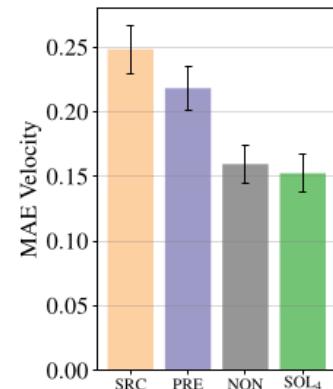
Errors and improvements



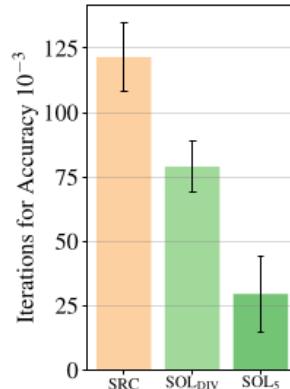
(a) Unsteady wake



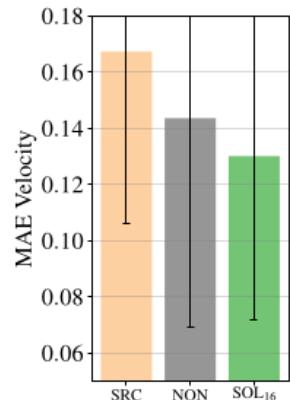
(b) Buoyancy-driven



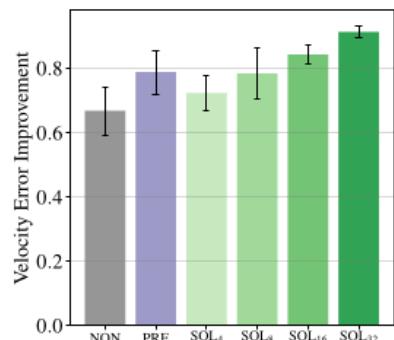
(c) Advection-diffusion



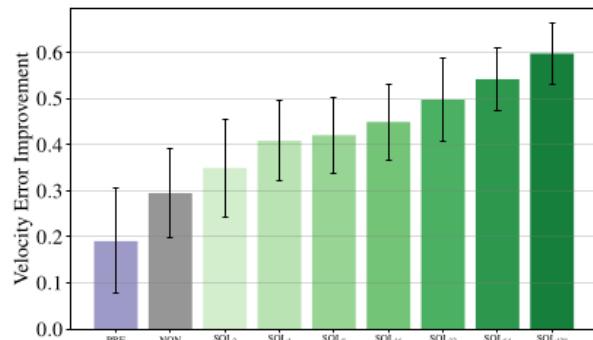
(d) CG solver



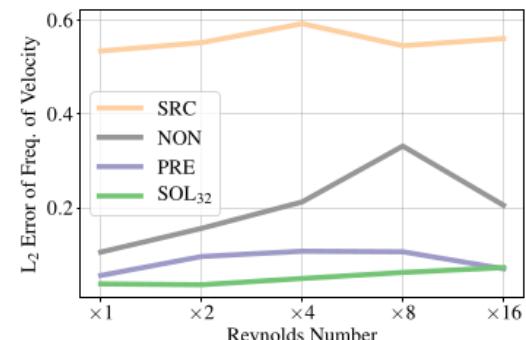
(e) 3D wake



(f) Unsteady wake, look-ahead



(g) Buoyancy-driven, look-ahead



(h) Unsteady wake, frequency error

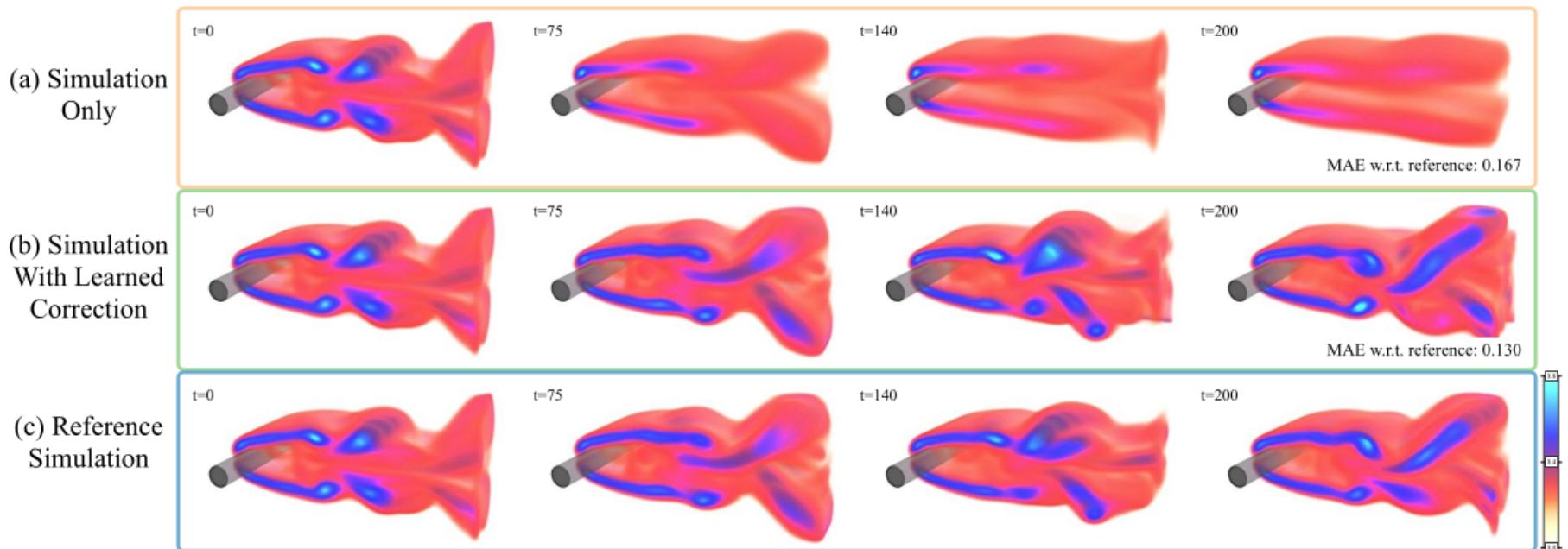
Quantitative summary

Exp.	Mean absolute error of velocity					Rel. improvement			
	SRC	PRE	NON	SOL _s	SOL	PRE	NON	SOL _s	SOL
Wake Flow	0.146±0.004	0.031±0.010	0.049±0.012	0.041±0.009	0.013±0.003	79%	67%	72%	91%
Buoyancy	1.590±1.033	1.373±0.985	1.080±0.658	0.944±0.614	0.620±0.390	19%	29%	41%	60%
Adv.-diff.	0.248±0.019	0.218±0.017	0.159±0.015	0.152±0.015	0.158±0.017	12%	36%	39%	36%
*CG Solver	121.6±13.44	-	-	79.03±10.02	29.59±14.83	-	-	35%	76%
3D Wake	0.167±0.061	-	0.144±0.074	-	0.130±0.058	-	14%	-	22%

- SOL_s: smaller model
- * Iterations to reach an accuracy of 0.001

Performance

- 3D Wake Flow: average cost for 100 time steps
- Reference simulation (CPU): 913.2 seconds
- Source simulation with the trained model: 13.3 seconds
- **Speed-up of ca. $68\times$**



Performance (cont'd)

Solver-in-the-Loop: Learning from Differentiable Physics to Interact with Iterative PDE-Solvers

NeurIPS 2020
Supplemental Video

Kiwon Um, Robert Brand, Yun Fei, Philipp Holl, Nils Thuerey



More details



Solver-in-the-Loop: Learning Physics to Interact with Iteration

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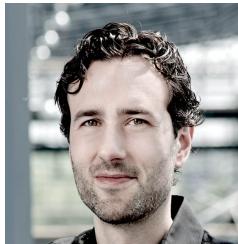
Thank you! Questions?

The online book, *Physics-based Deep Learning*,
and the codes are available!

<https://www.physicsbaseddeeplearning.org/>



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Philipp Holl