CCSI²
Carbon Capture Simulation for Industry Impact

ML Based CFD Model Reduction for Rapid Computational Screening

Phan Nguyen & Brian Bartoldson
Lawrence Livermore National Laboratory

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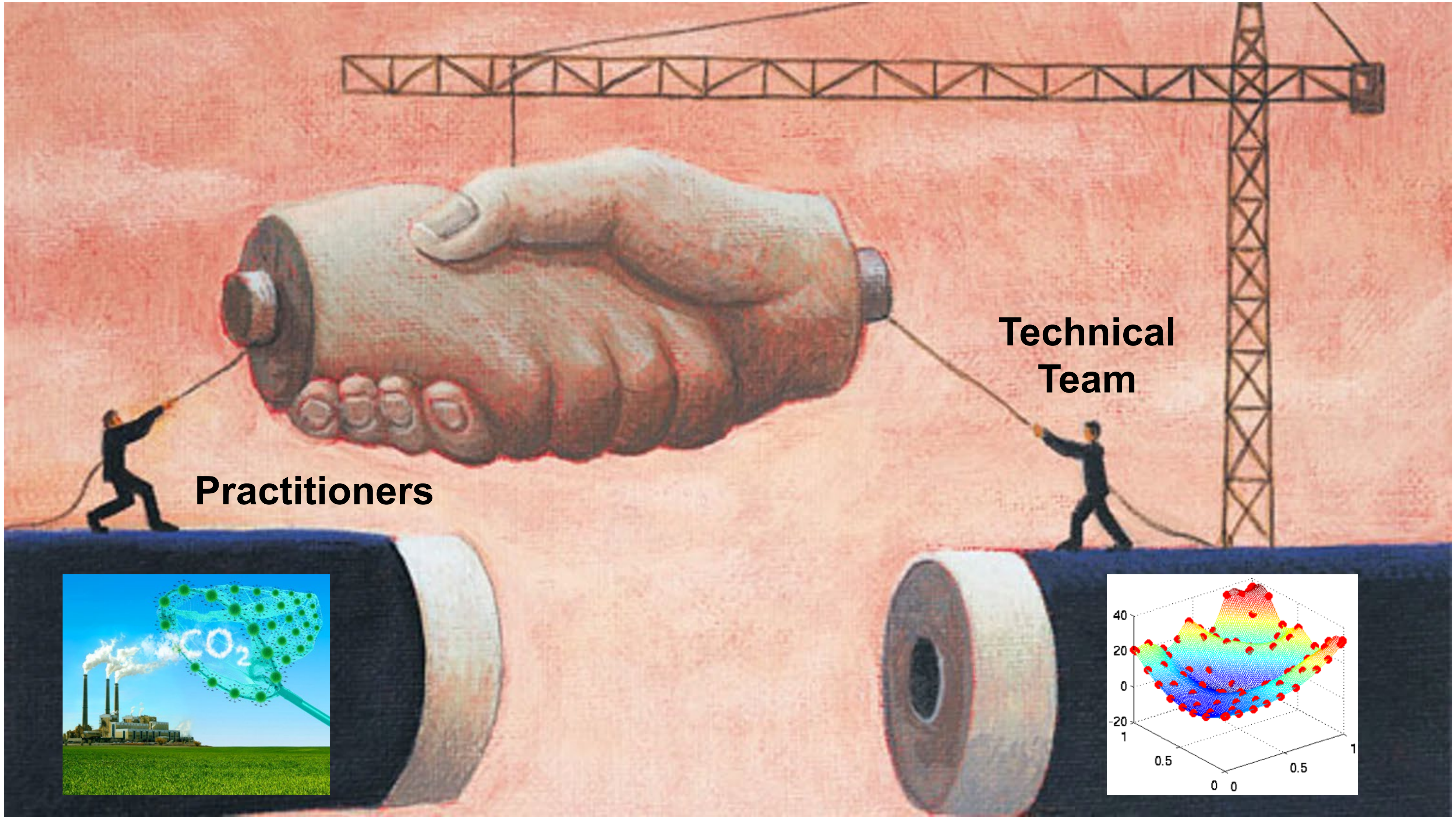
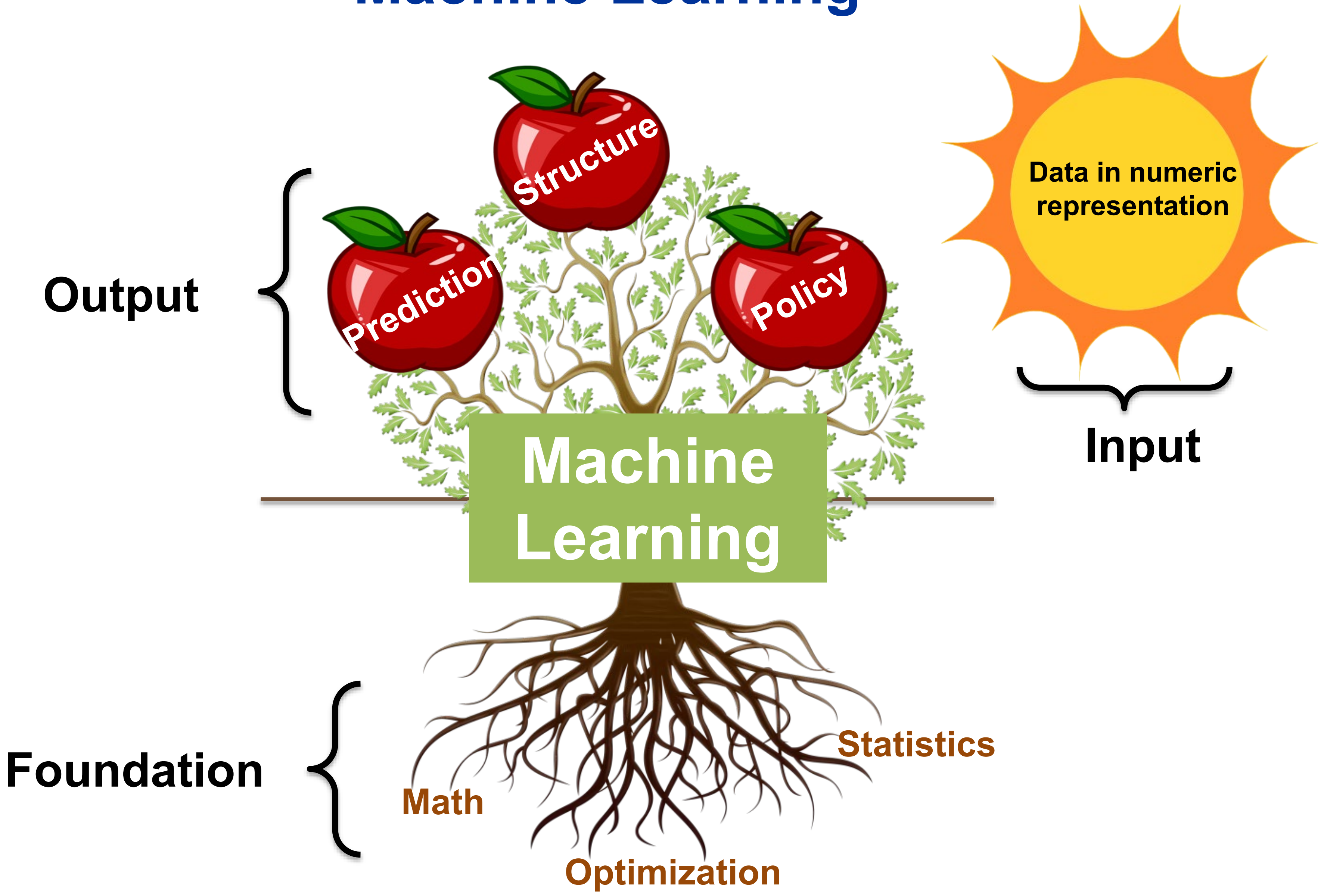
Machine Learning Team:
Jose Cadena (LLNL)
Amar Saini (LLNL)
Yeping Hu (LLNL)

LLNL-PRES-838660

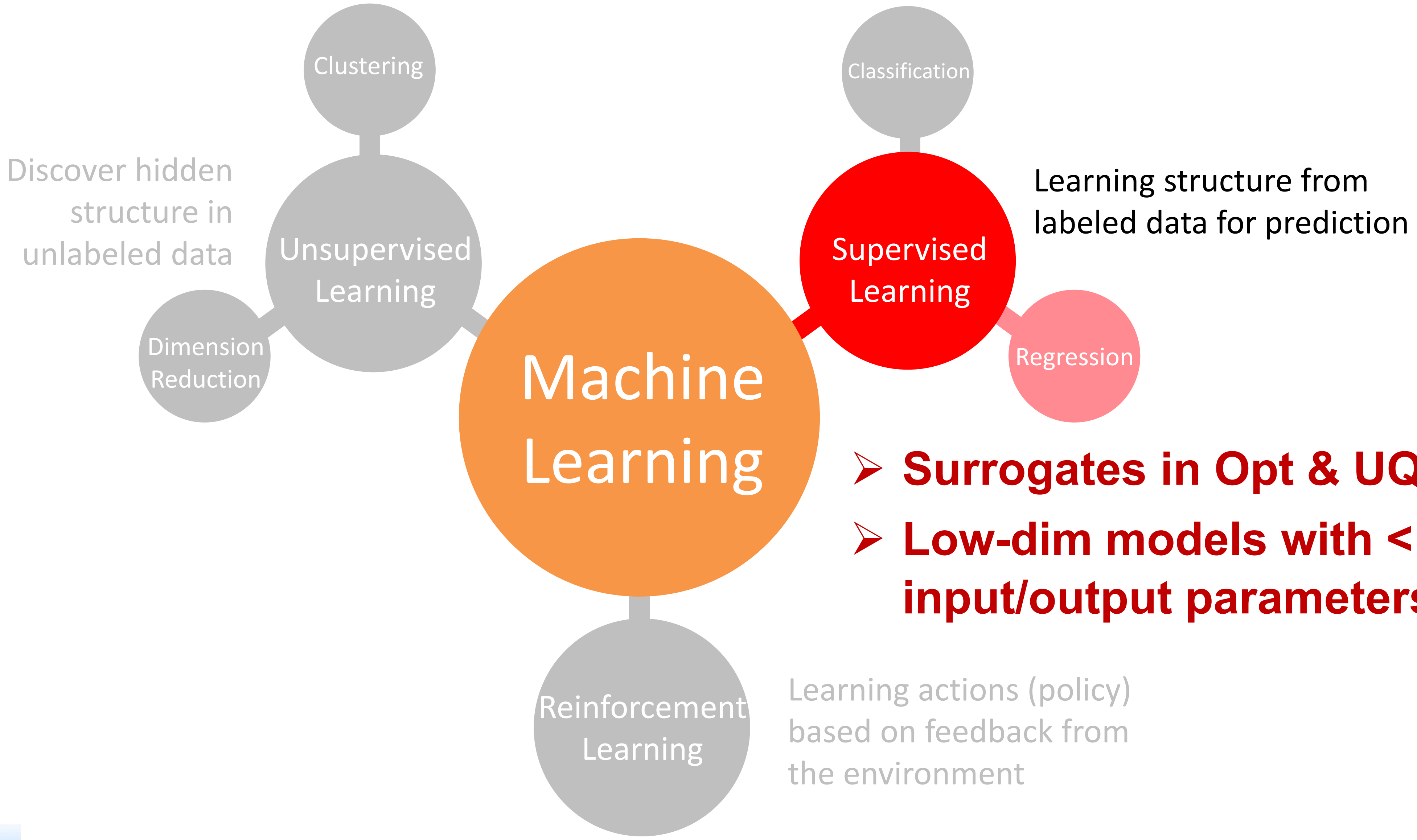
CCSI²: Carbon Capture Simulation for Industry Impact



Machine Learning



History of ML in CCSI



- **Surrogates in Opt & UQ**
- **Low-dim models with <100 input/output parameters**

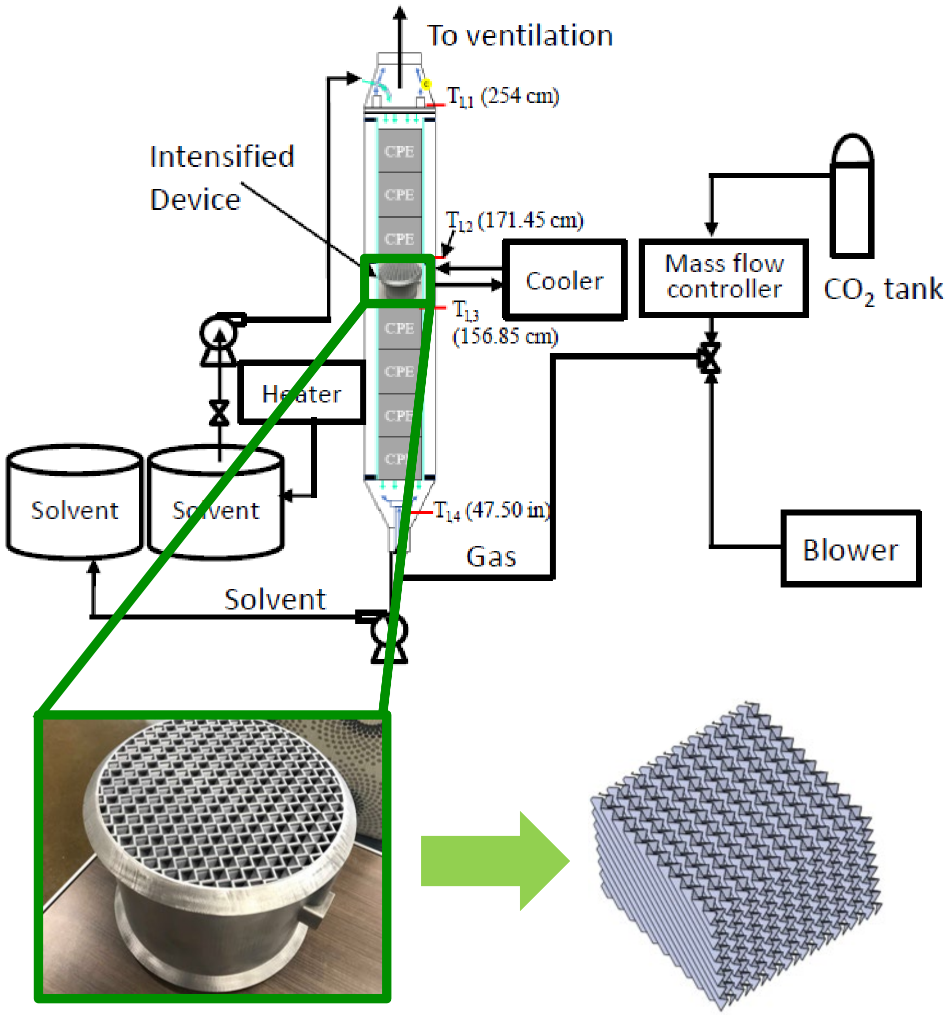
How do we use ML for $CCSI^2$?

CFD is critical for the fundamental understanding, to inform process and system level modeling.

- **Need local information on transport phenomena** to understand driving forces
- **Can be incorporated into design optimization** to optimize the device

Simulation time is a bottleneck that impedes high-level modeling.

Machine learning surrogates, such as Deep Fluids (DF) and MeshGraphNets (MGN), can reduce the computational burden of time-consuming simulations.



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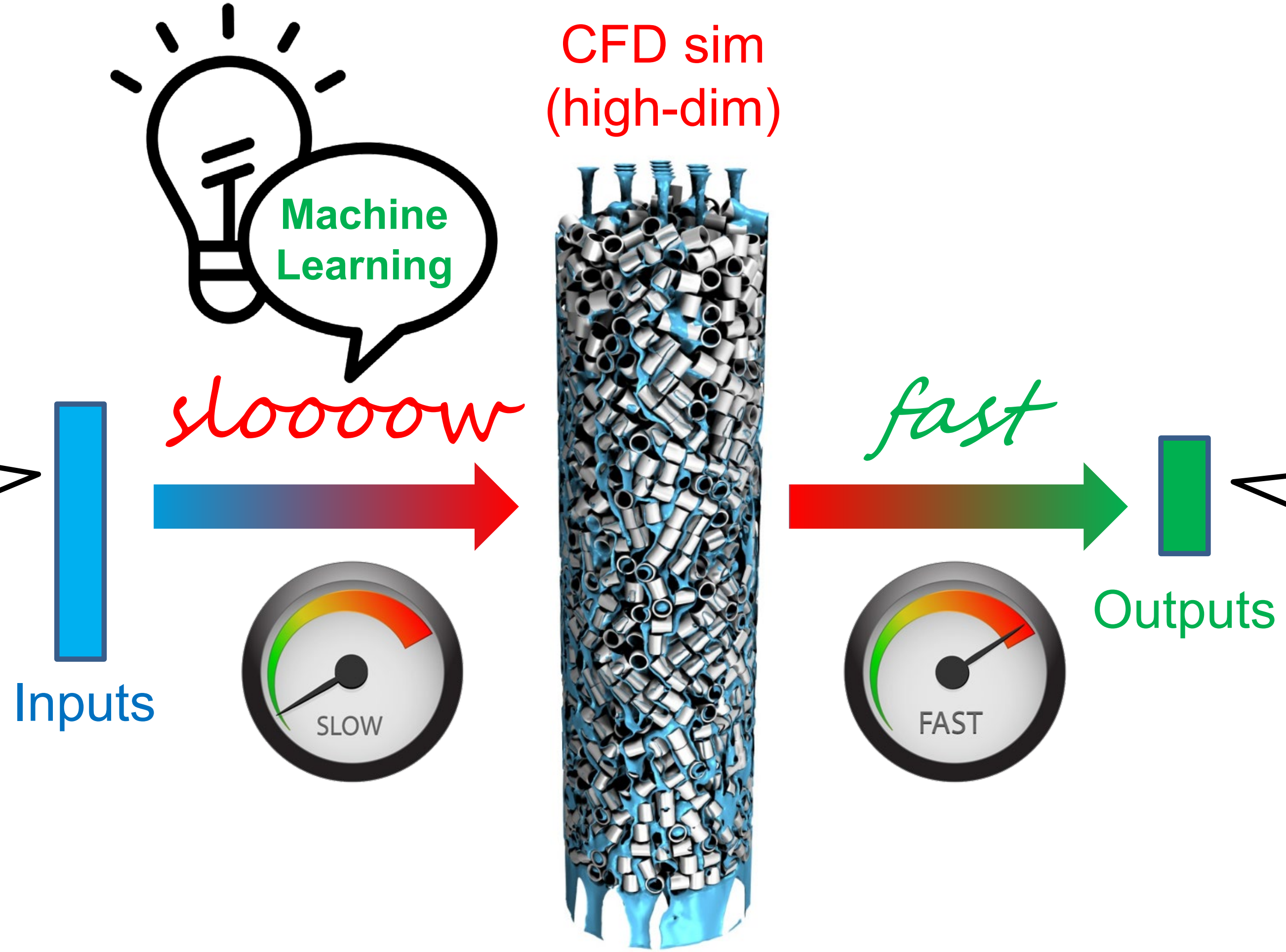
Fast Surrogates for CFD Simulation Model

Raschring random packing config
Raschring element properties
Liquid flow rate
Gas flow rate
Liquid viscosity
Liquid density
Surface tension
Contact angle
Packed ring surface to volume ratio



Interfacial area
Liquid holdup
Pressure drop
Effective mass transfer

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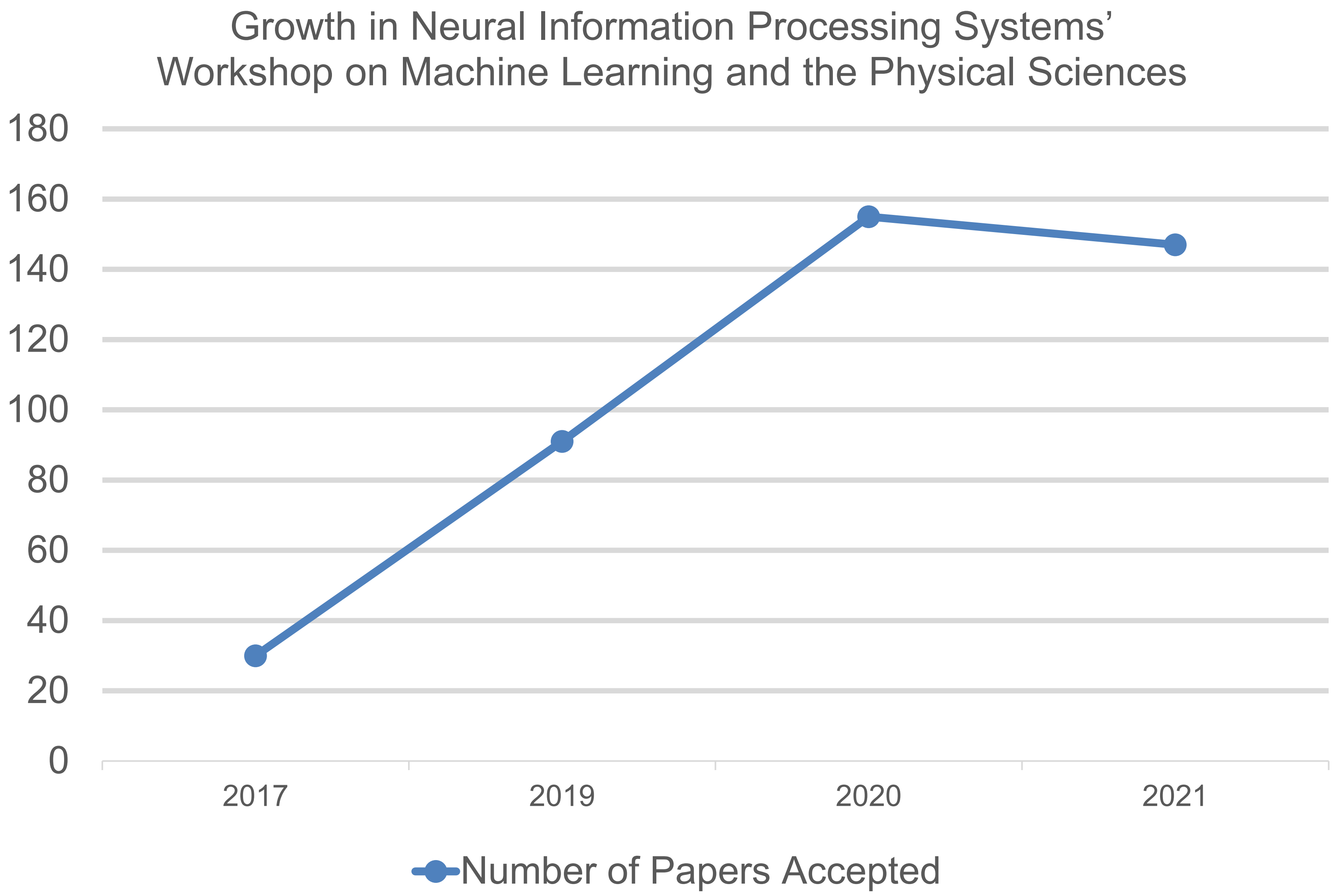
Computational approaches to screening parameters

Metric	Computational Fluid Dynamics (CFD)	Machine Learning (ML) Surrogates
Speed	*Slow*: 2D model **takes 1 hour** to simulate	*Fast*: 2D model **takes 1 second** to simulate
Effort to construct	*High*: Equations, assumptions, numerical methods, software packages, …	*Low*: Common architectures across problems reduce effort required for a ‘good’ model
Accuracy	*Variable:* Depends on the model/effort	*Variable:* Depends on accurate CFD training data and surrogate’s ability to bridge from ”toy” problems in literature to our large-scale data
Downstream modeling/problems	*Ill-suited:* Generally, **too slow to scale** to large, 3D simulations	*Well-suited:* **Scaling made feasible** by speed of reduced models

Growth in Machine Learning and the Physical Sciences



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We explore a range of ML surrogates

DeeperFluids

- Builds on Kim et al., 2019
- Interpolates CFD mesh onto regular grid
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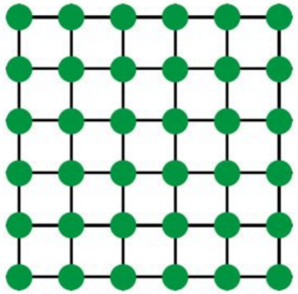

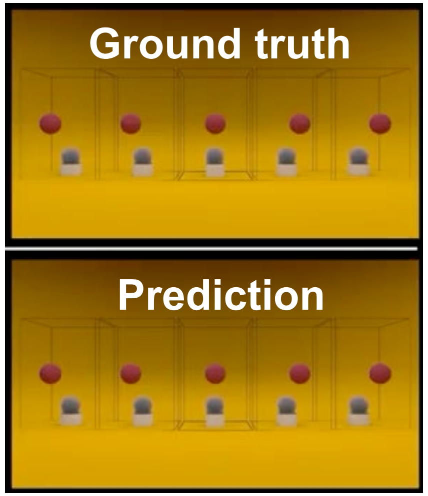

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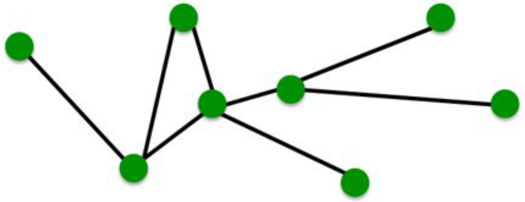

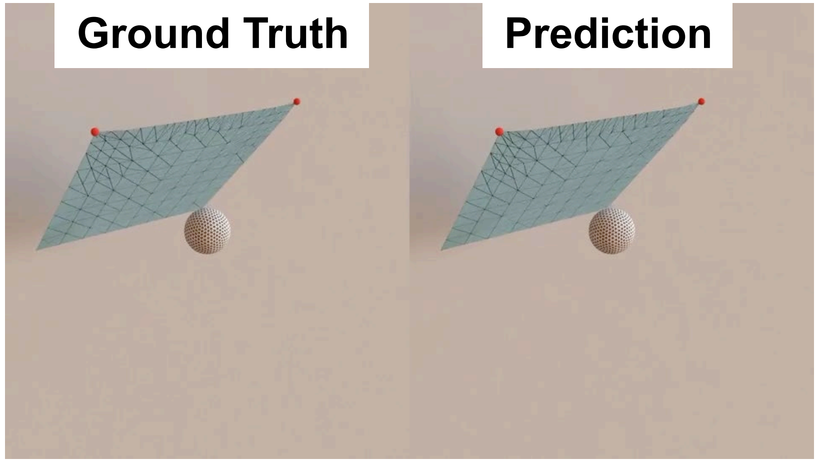

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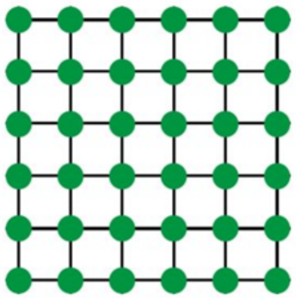

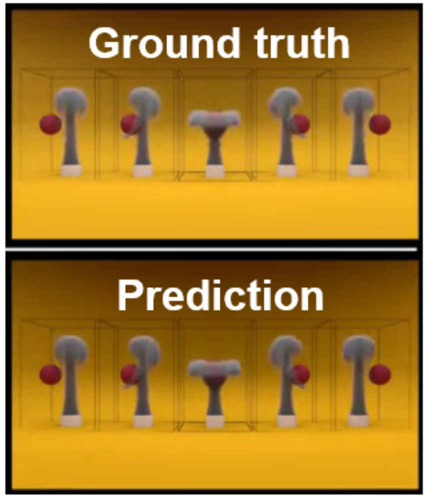

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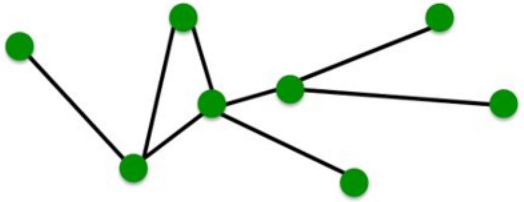

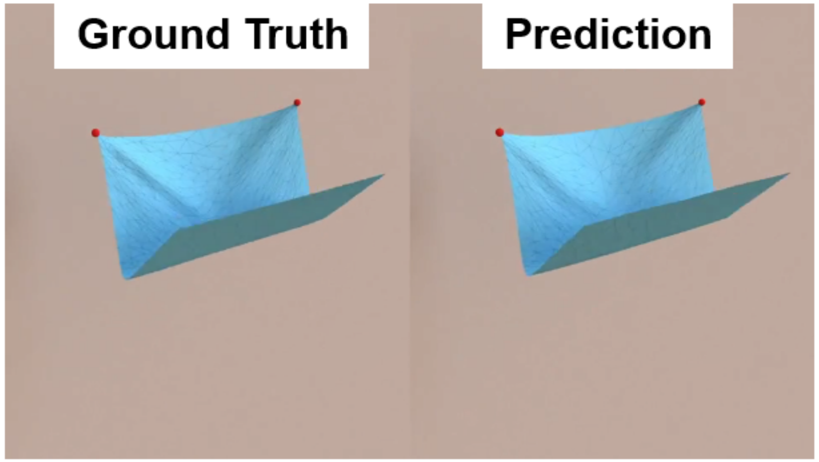

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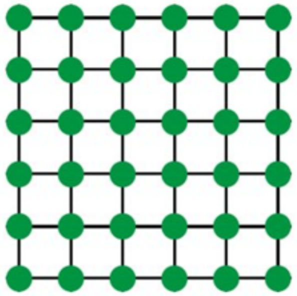

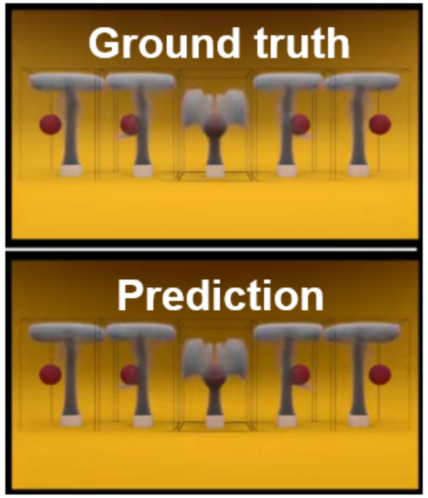

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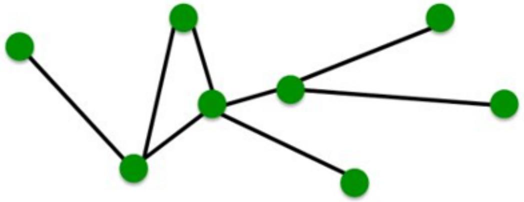

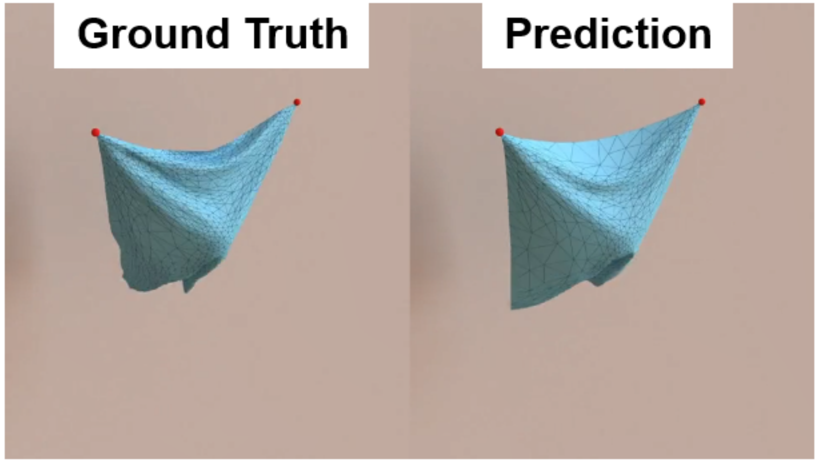

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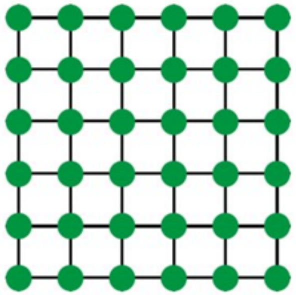

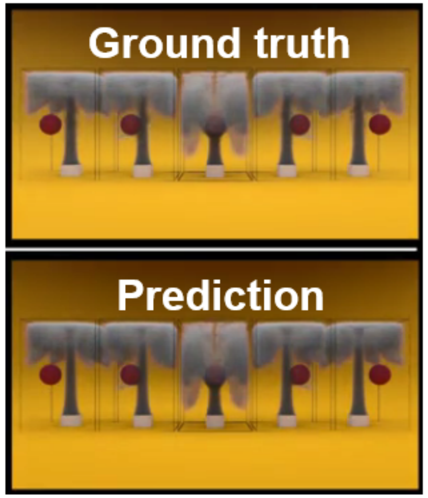

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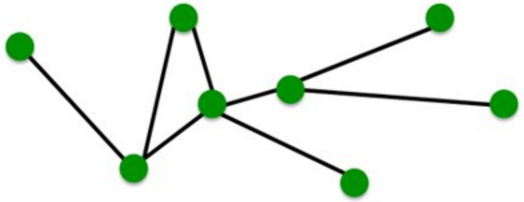

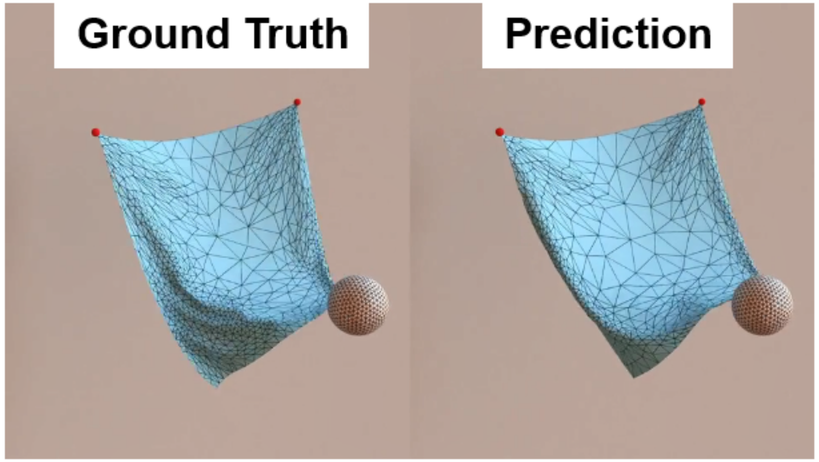

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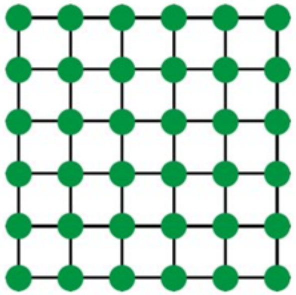

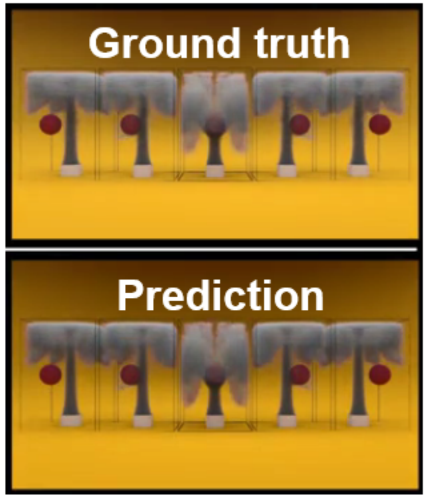

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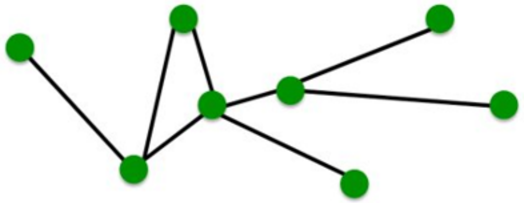

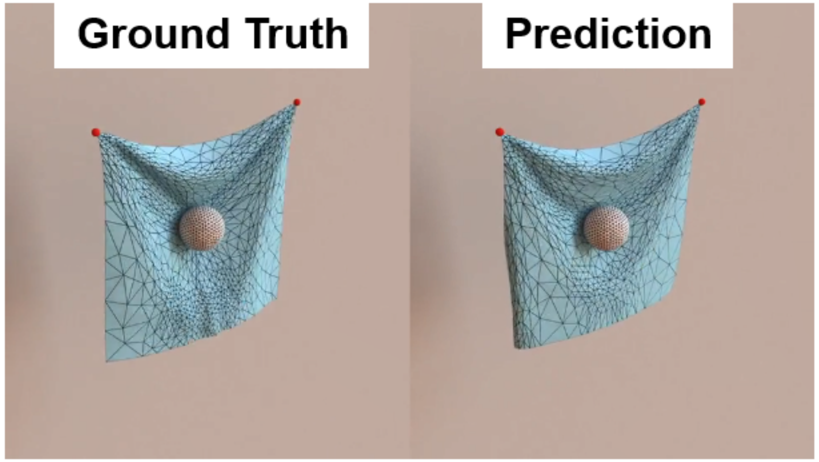

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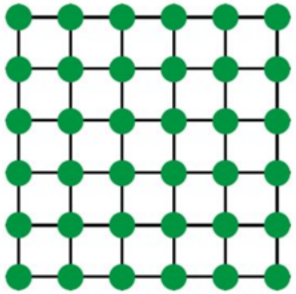

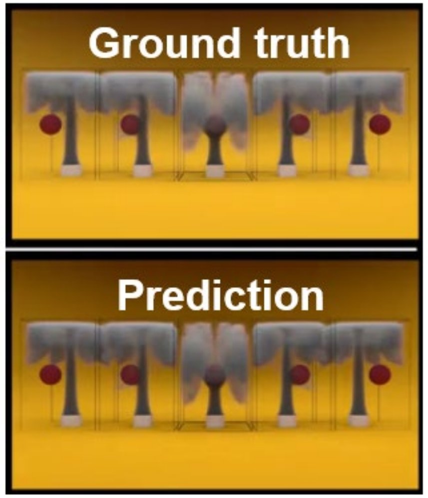

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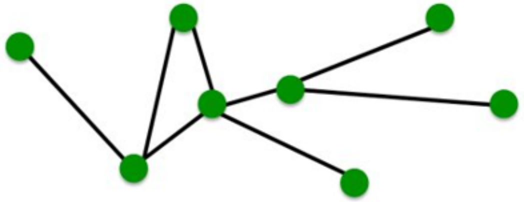

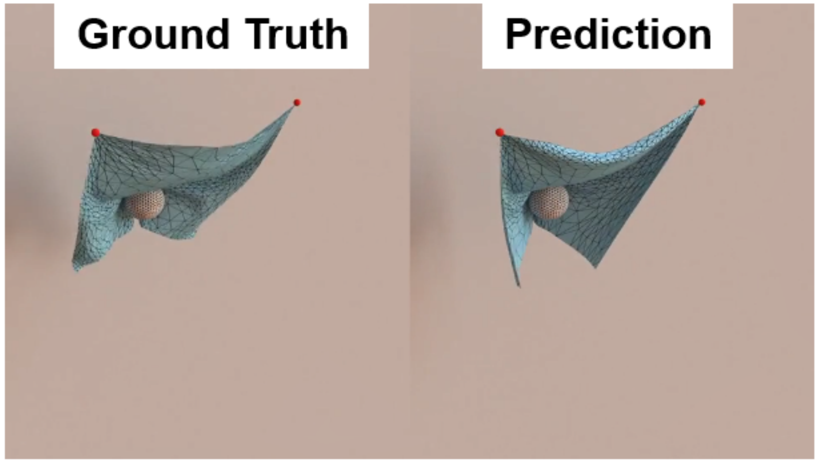

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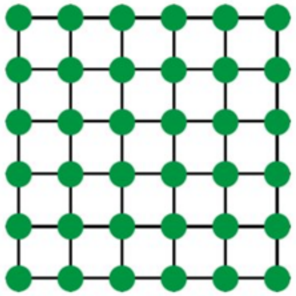

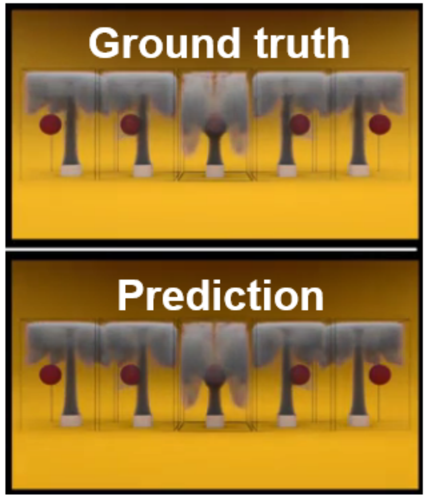

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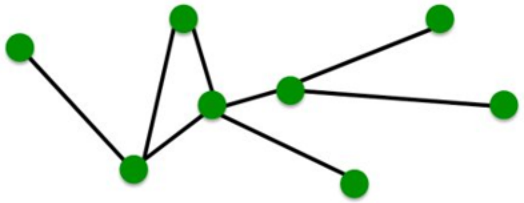

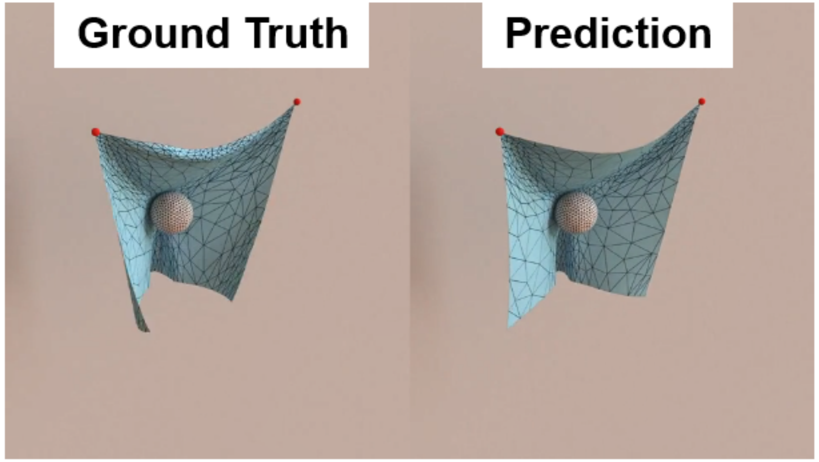

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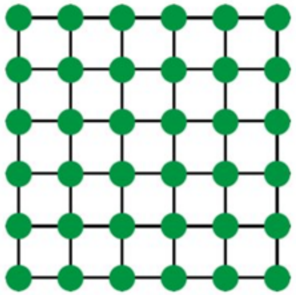

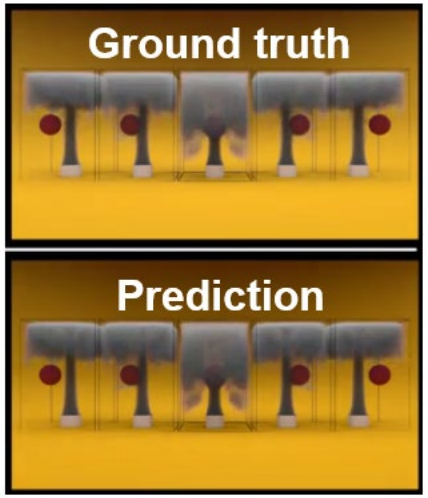

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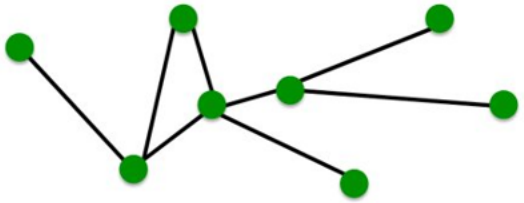

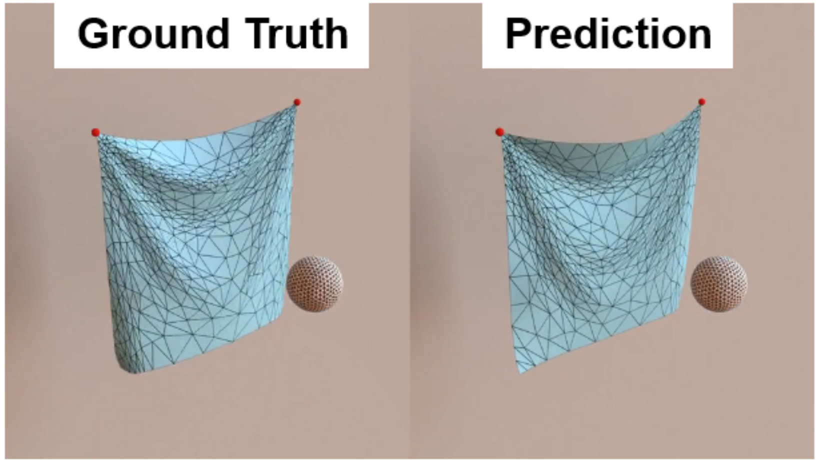

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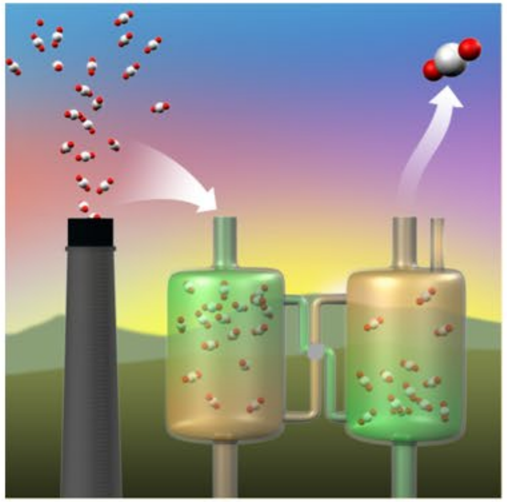
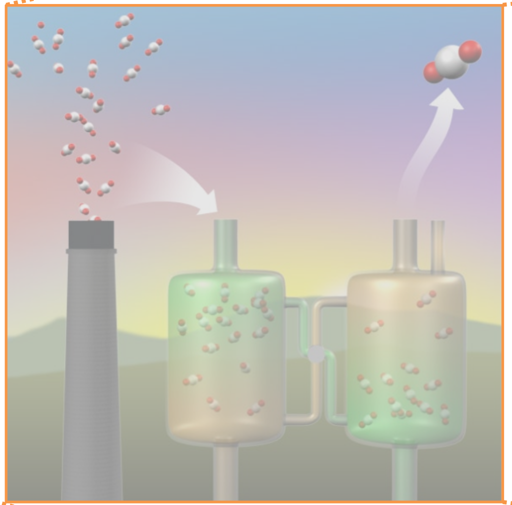
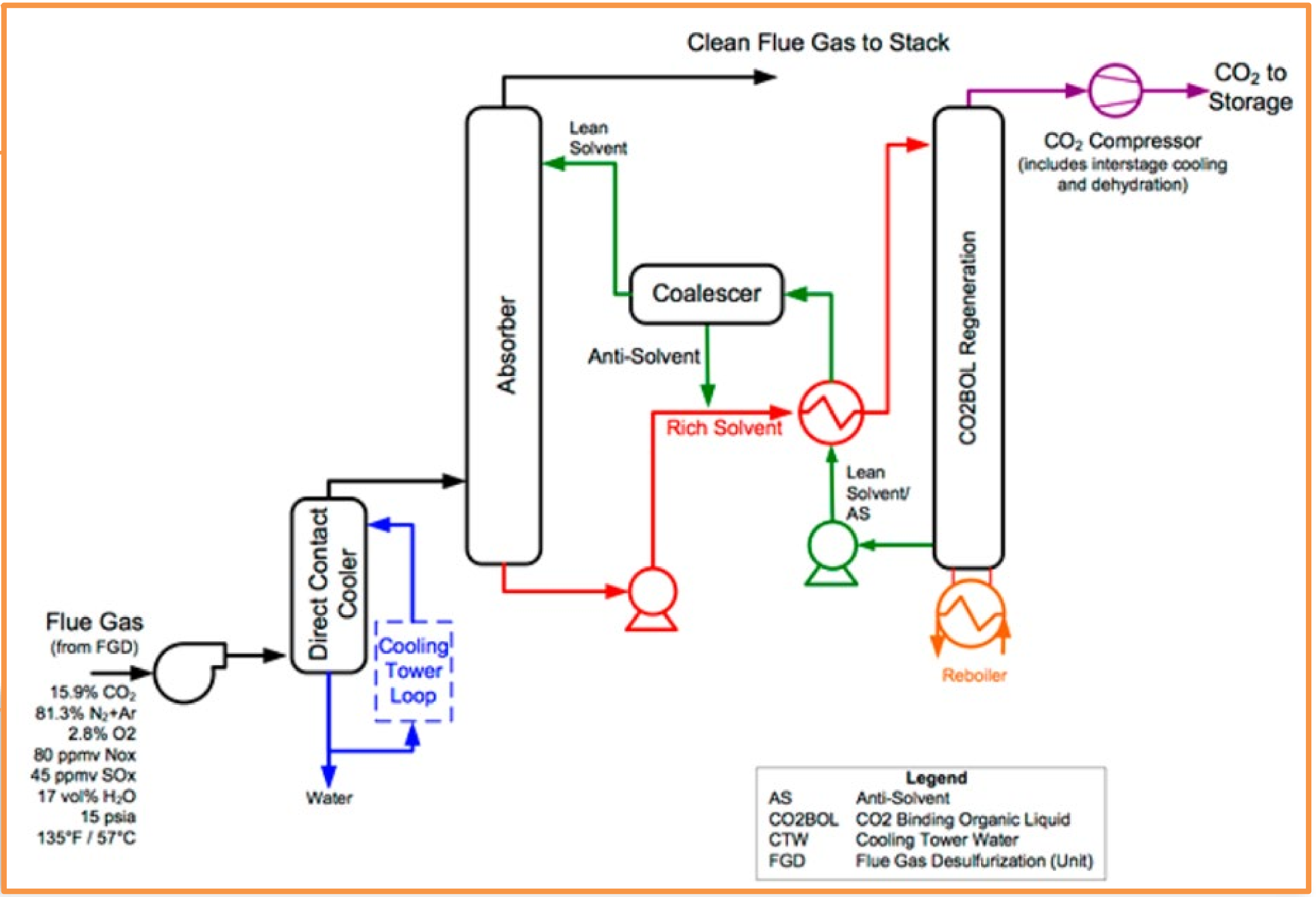


Image source: Heldebrant et al., 2019

Carbon capture systems have many parameters to tune





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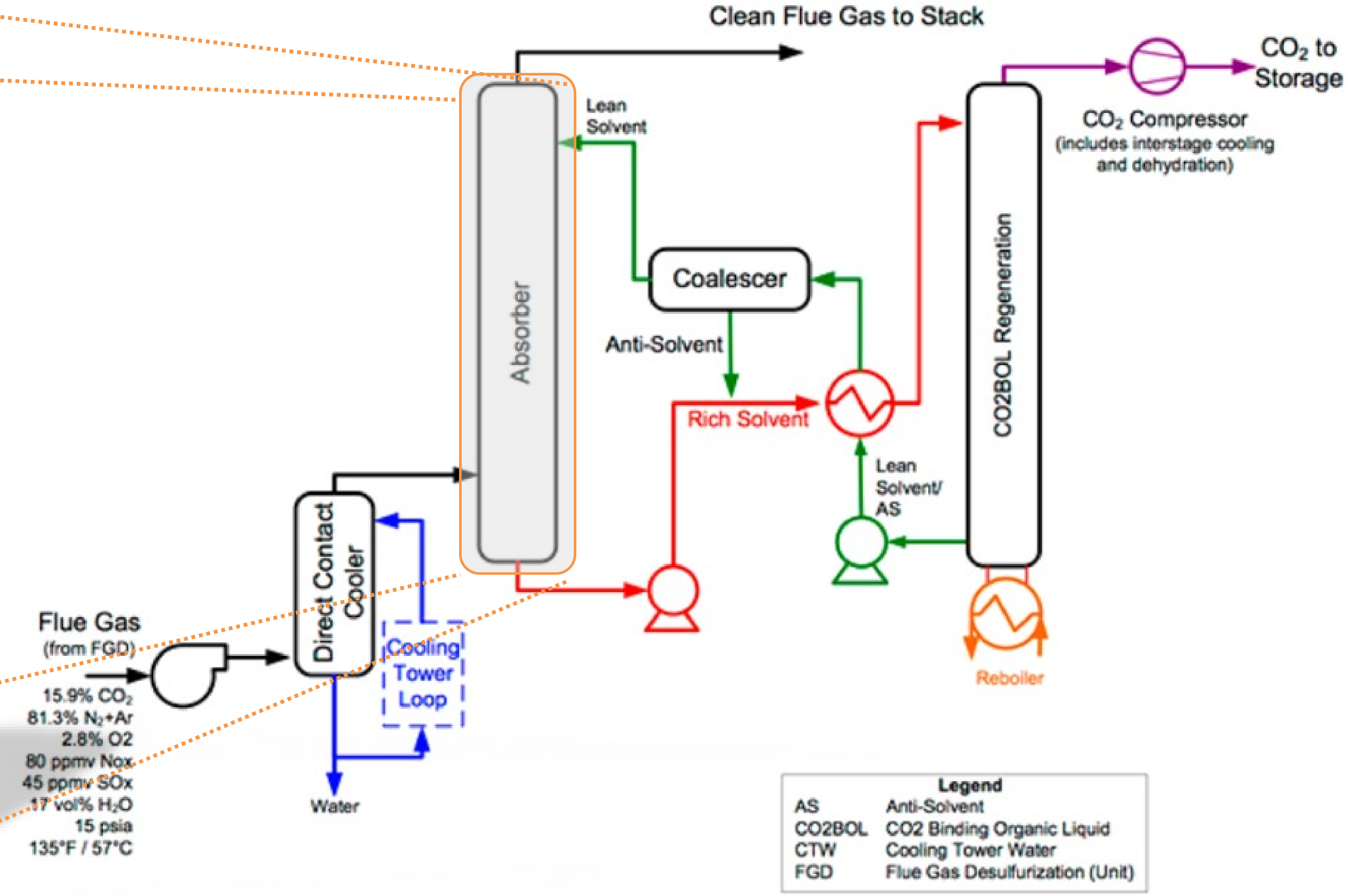
Potential approach: Run a CFD simulation to understand effect of each parameter…



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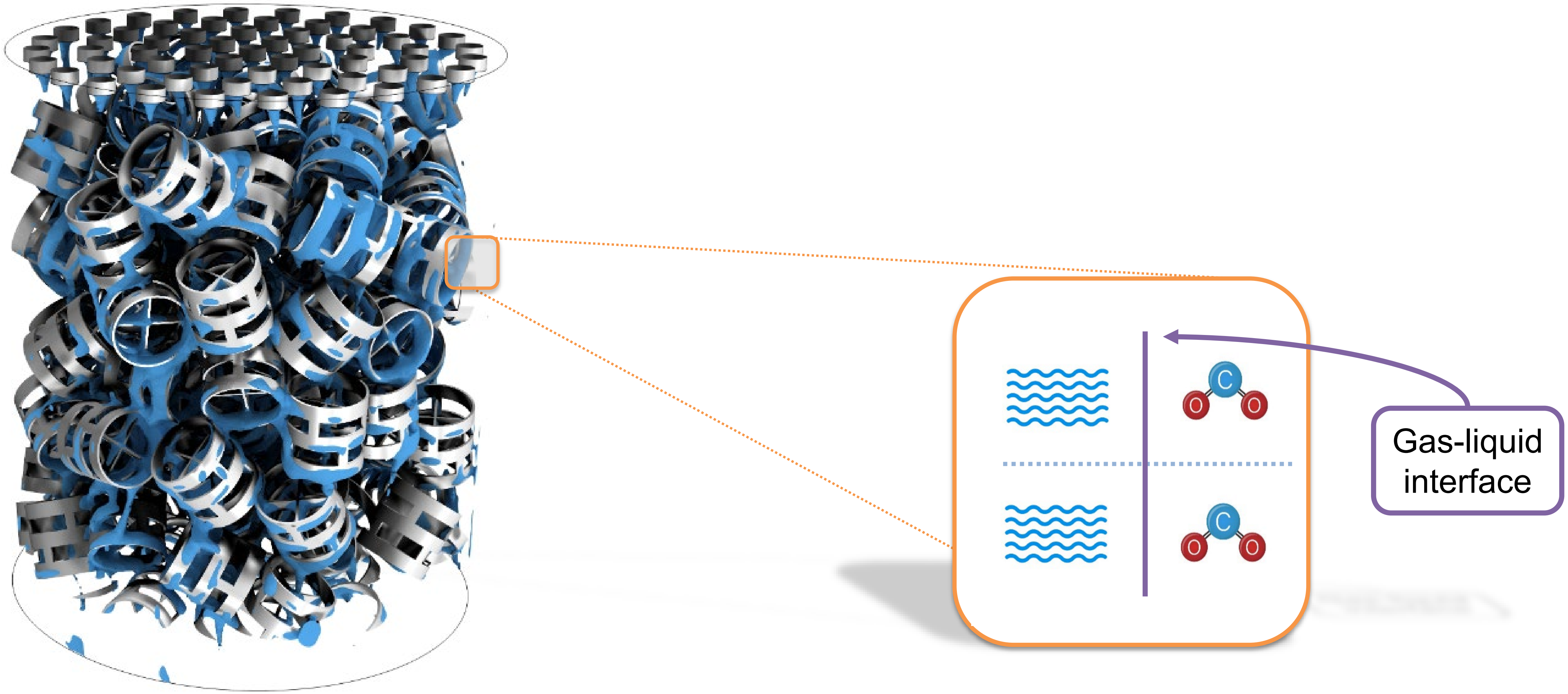
Screen parameter settings to optimize efficiency---interfacial area (IA), liquid holdup, pressure drop, etc.



Problem: CFD is too slow to fully explore parameter space

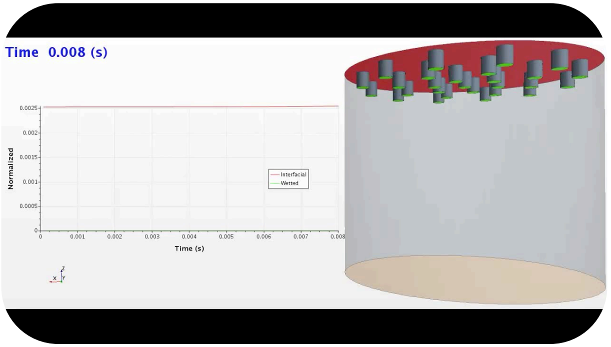
Computational fluid dynamics (CFD) modeling

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{F}_\sigma$$

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot (\mathbf{u}\alpha) = 0$$

Numerical methods/software for CFD



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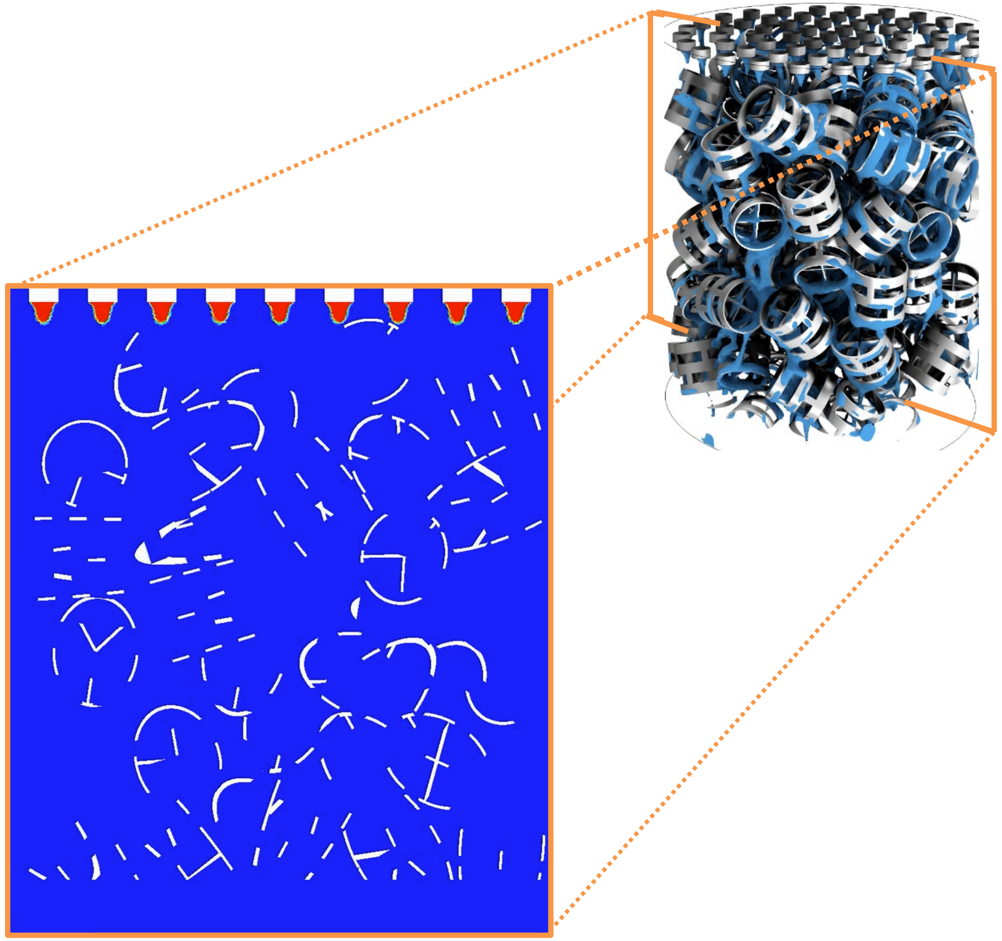

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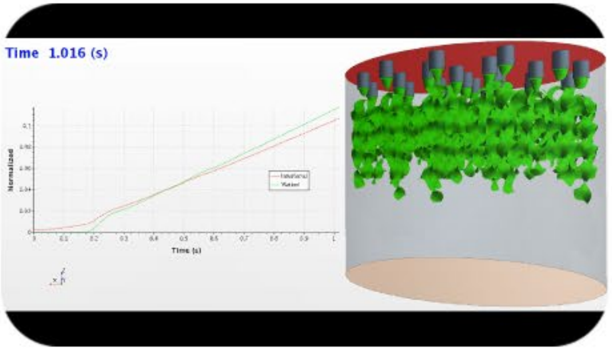

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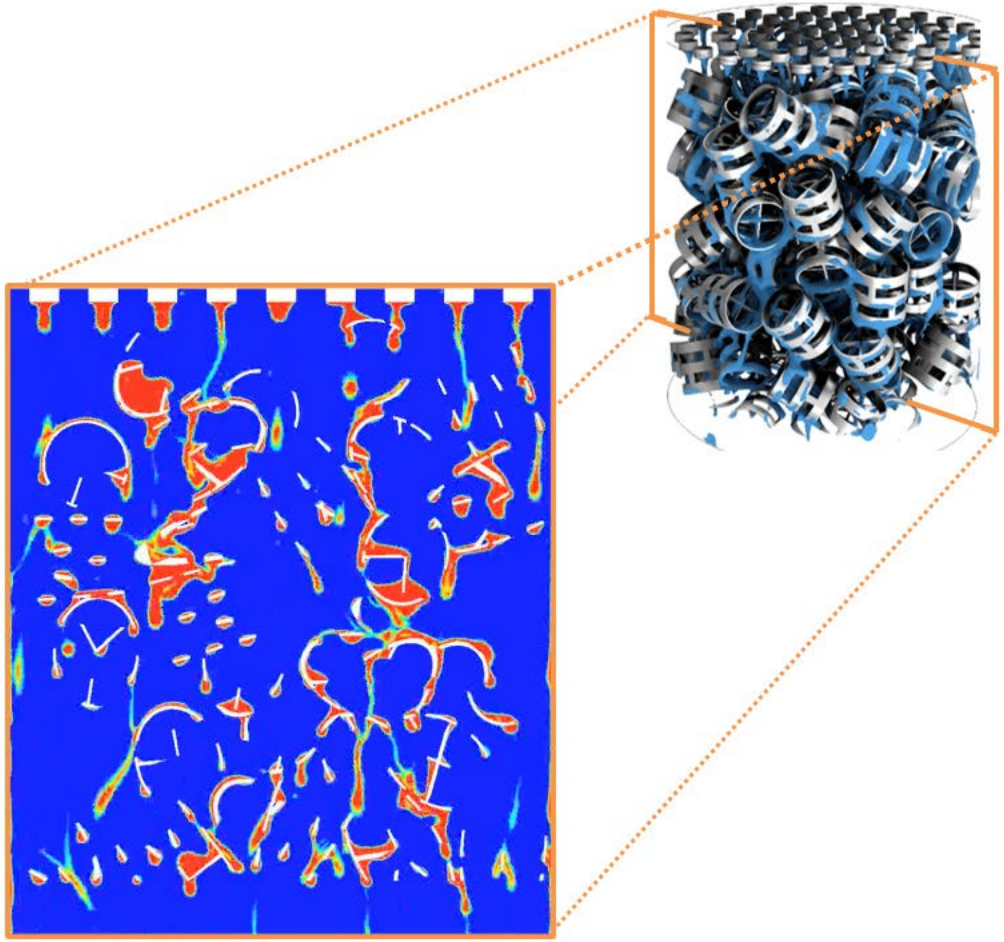

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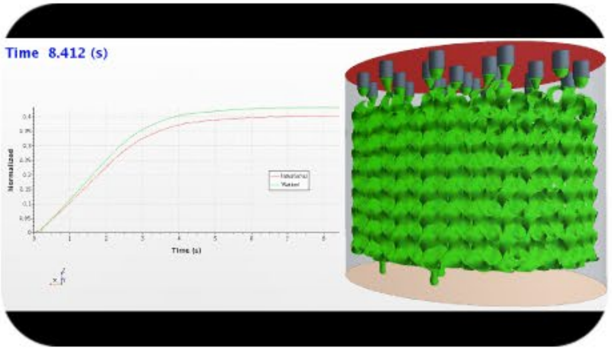

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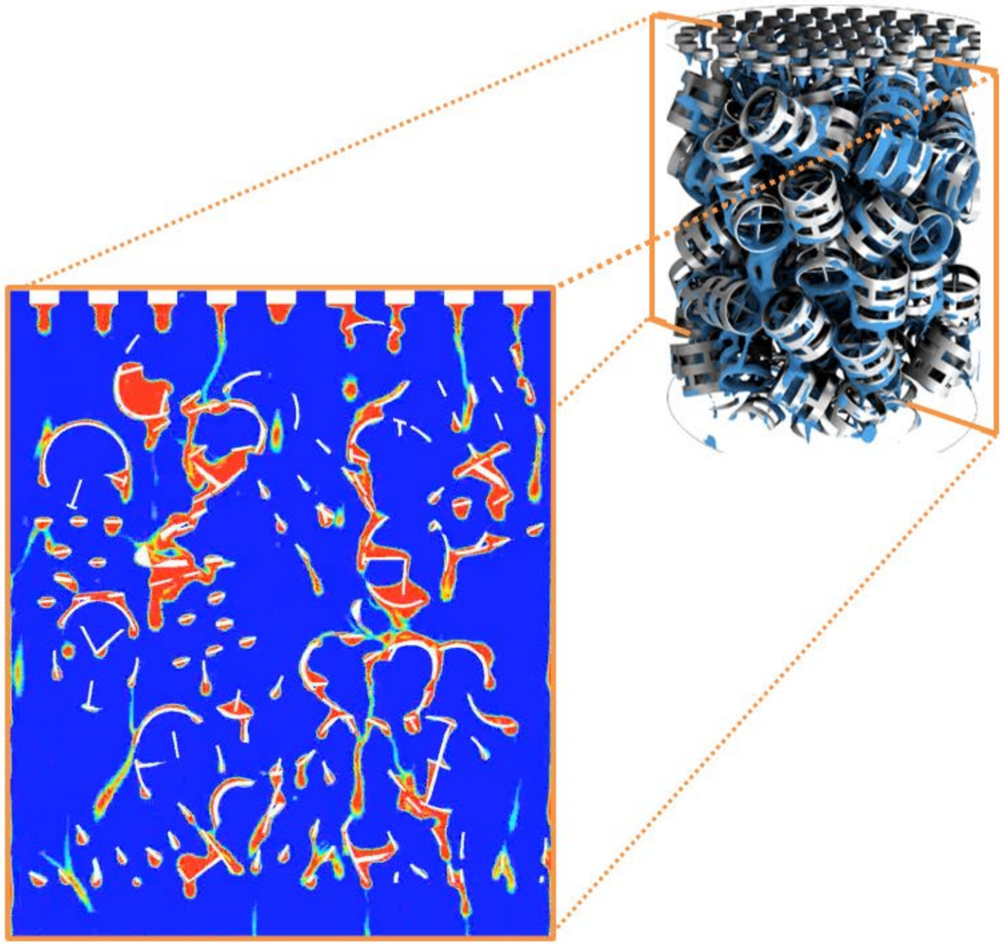
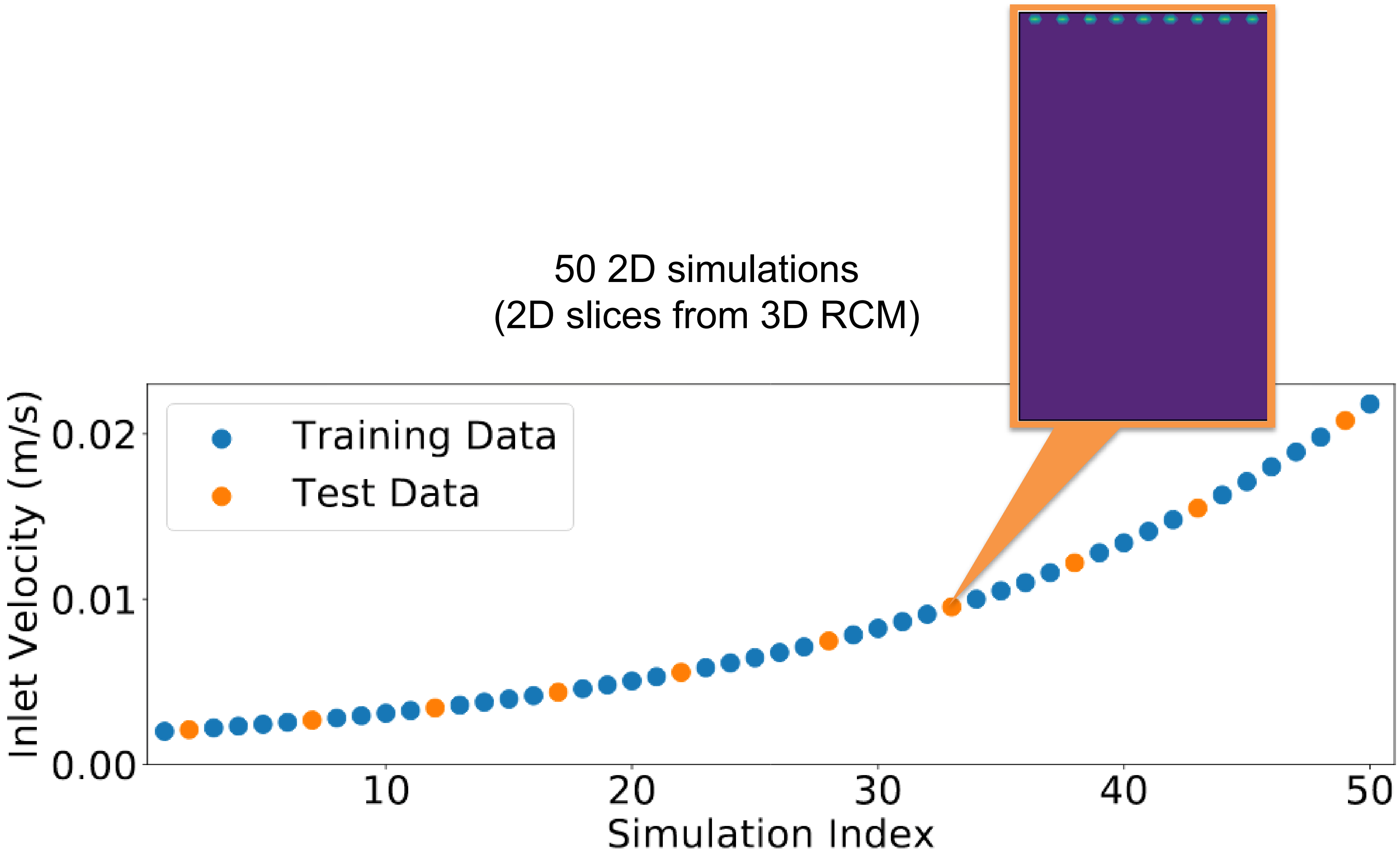


Surrogates learn from CFD data, are tested against CFD data

50 2D simulations
(2D slices from 3D RCM)



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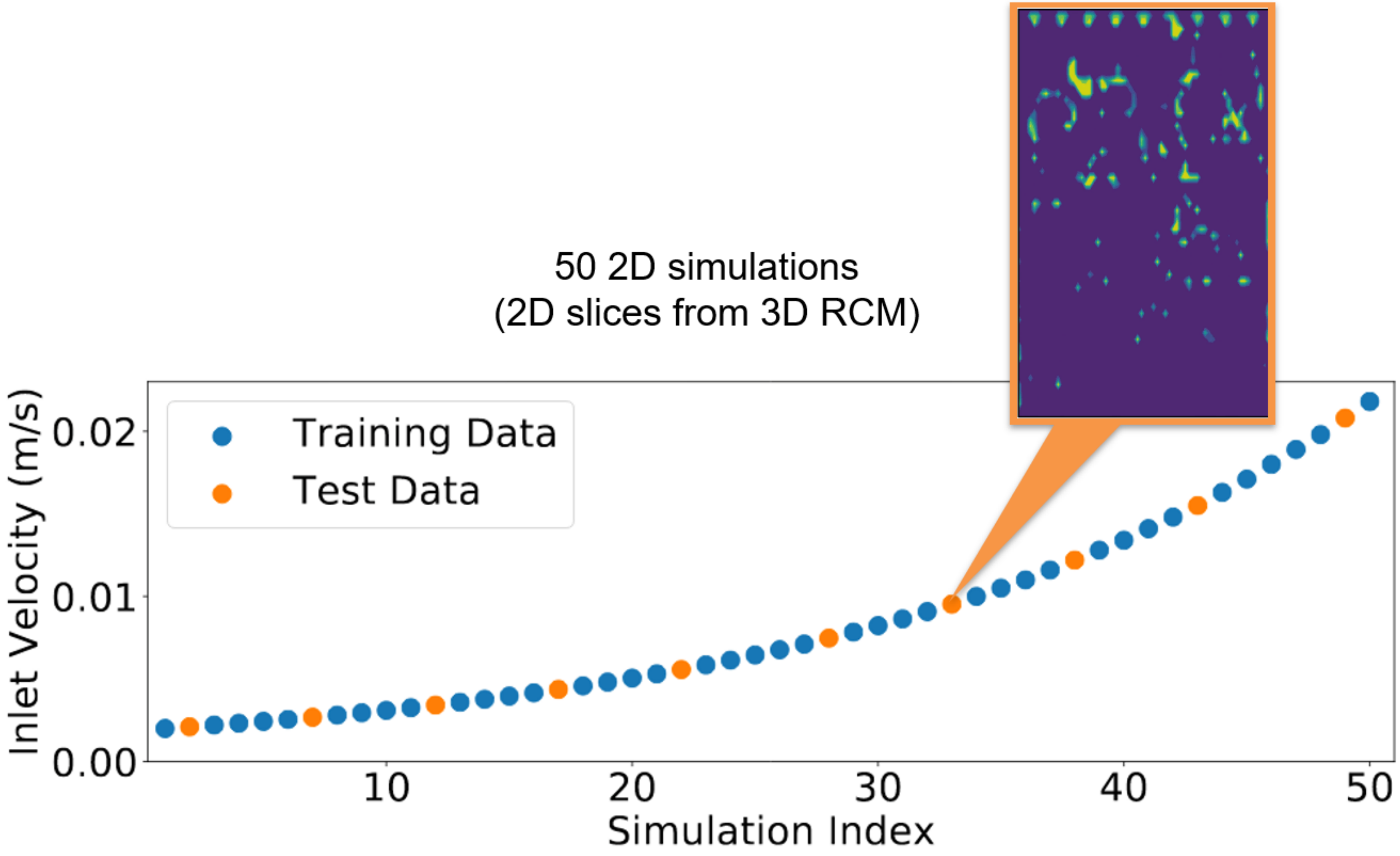

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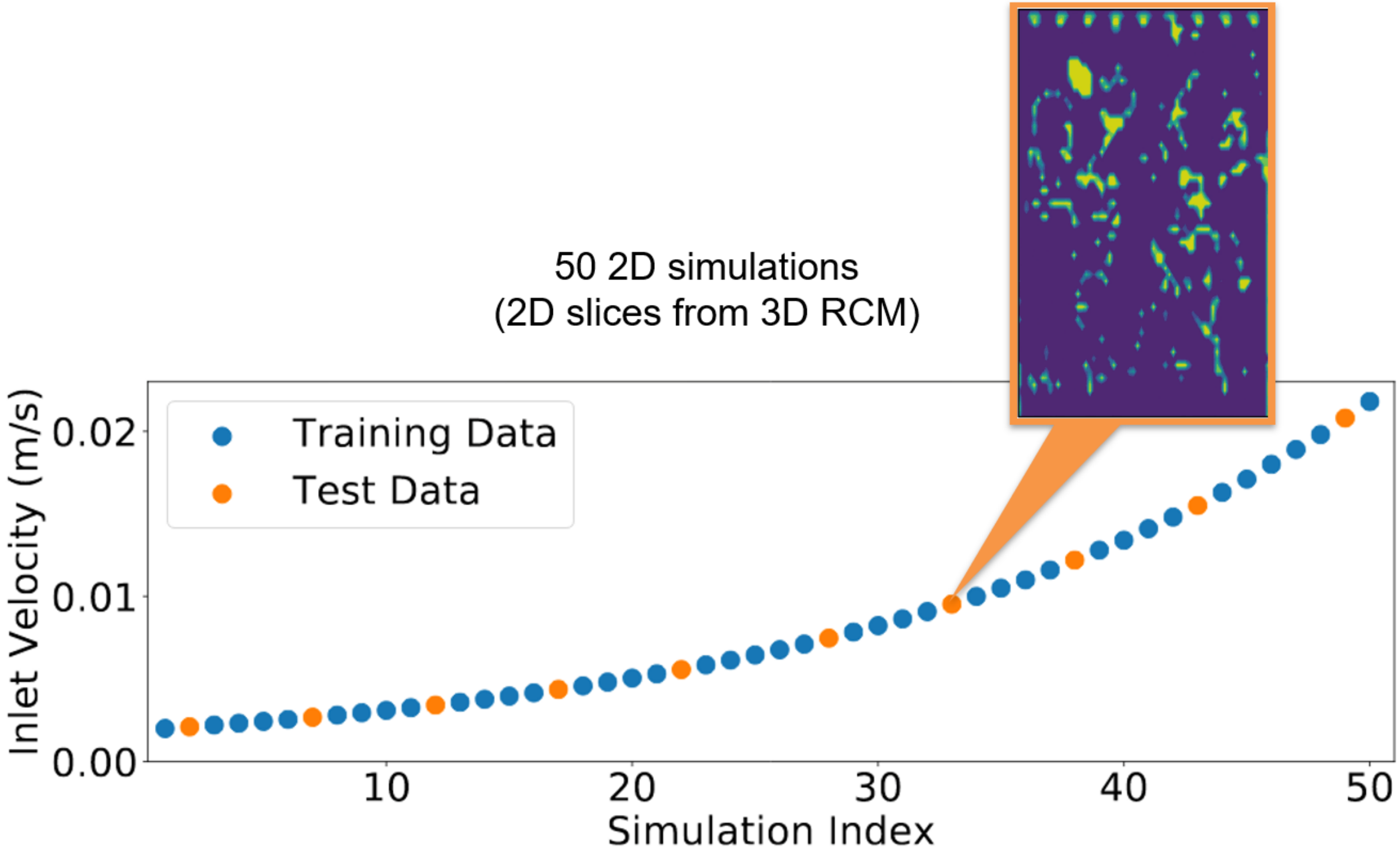

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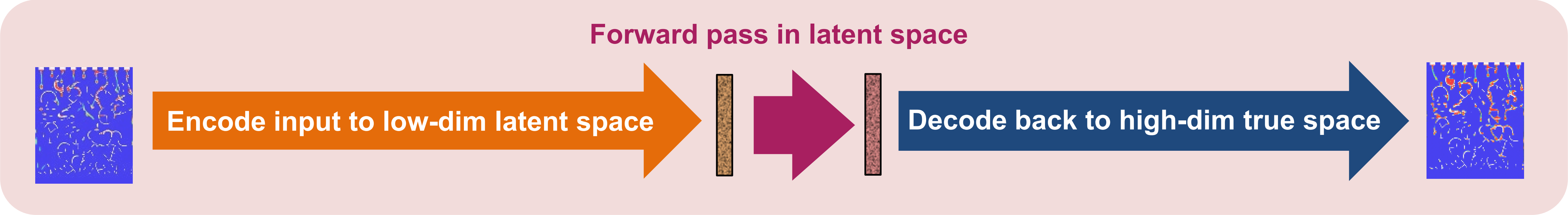
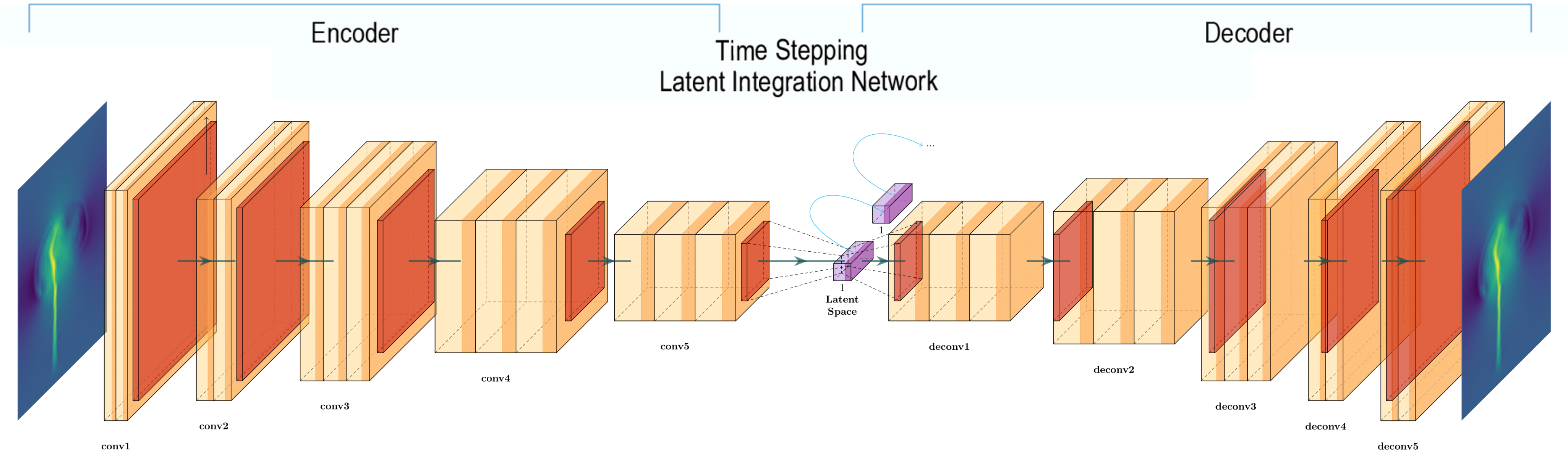
Deep Fluids (DF)





CCSI2
Carbon Capture Simulation for Industry Impact

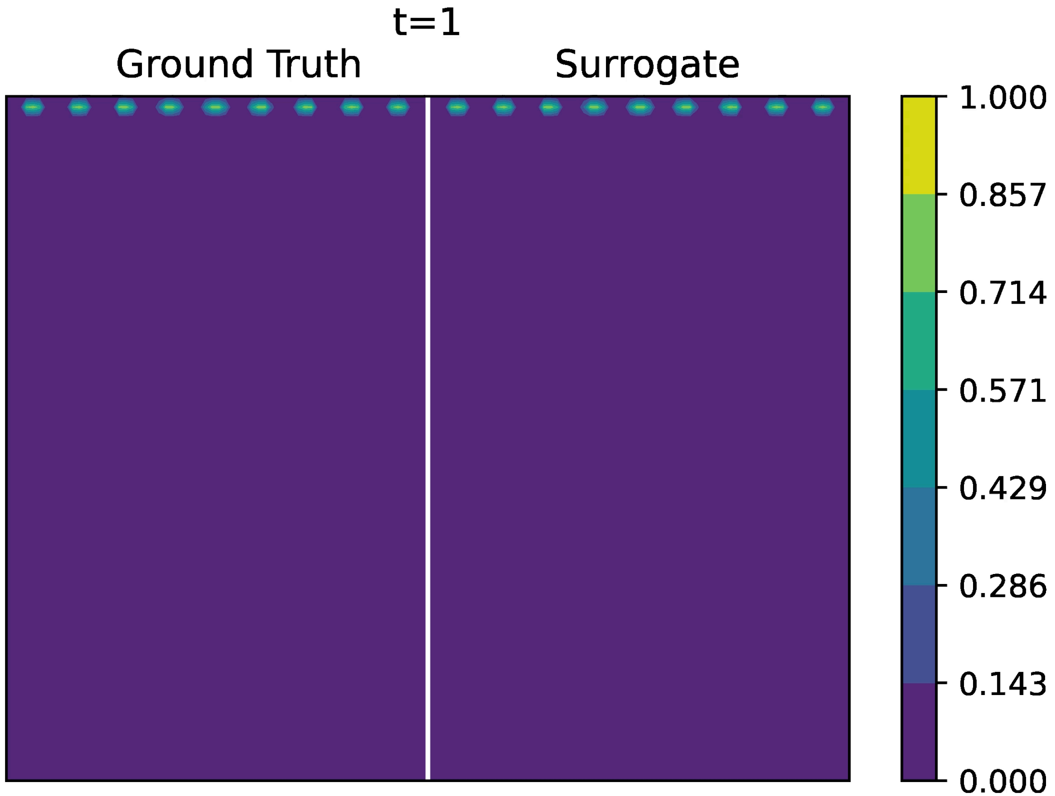
LLNL's Deeper Fluids Surrogates

Building on the original surrogates…

H	$Error_{IA}$ w=20	50	150	200	300	499
1024, 512	0.33 (0.14)	0.08 (0.00)	0.09 (0.00)	0.10 (0.00)	0.11 (0.00)	2.53 (0.26)
128, 128, 128	0.64 (0.11)	0.08 (0.01)	0.08 (0.00)	0.07 (0.00)	**0.06** (0.00)	2.25 (0.18)

We find better performance!

		$Error_{IA}$		$Error_{VF}$	
LIN	s	L_{RE}	RMSE	L_{RE}	RMSE
ARC	1	0.12	0.09	0.53	0.55
	6	0.15	0.14	0.51	0.53
LSTM	1	0.12	0.06	0.56	0.54
	6	0.09	0.09	0.52	0.54
MLP	1	0.07	0.07	0.53	0.55
	6	0.08	0.12	**0.49**	0.52
Transformer	1	0.08	**0.04**	0.53	0.55
	6	0.06	0.22	0.53	0.80



And big speedups!

LIN	$Error_{IA}$	$Error_{VF}$	S_W
ARC	0.07 (0.00)	0.49 (0.00)	4800
LSTM	0.08 (0.01)	0.49 (0.01)	2700
MLP	**0.06** (0.00)	**0.47** (0.00)	5400
Transformer	0.08 (0.04)	0.51 (0.00)	4300

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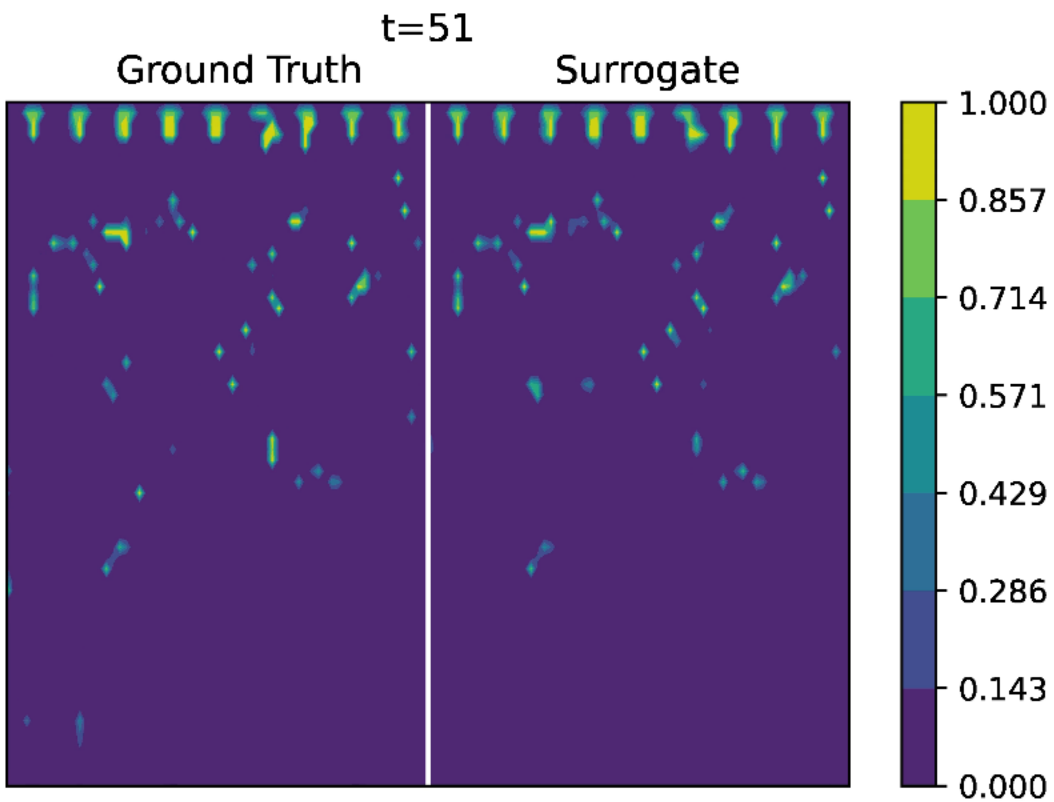

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CCSI^2 Carbon Capture Simulation for Industry Impact

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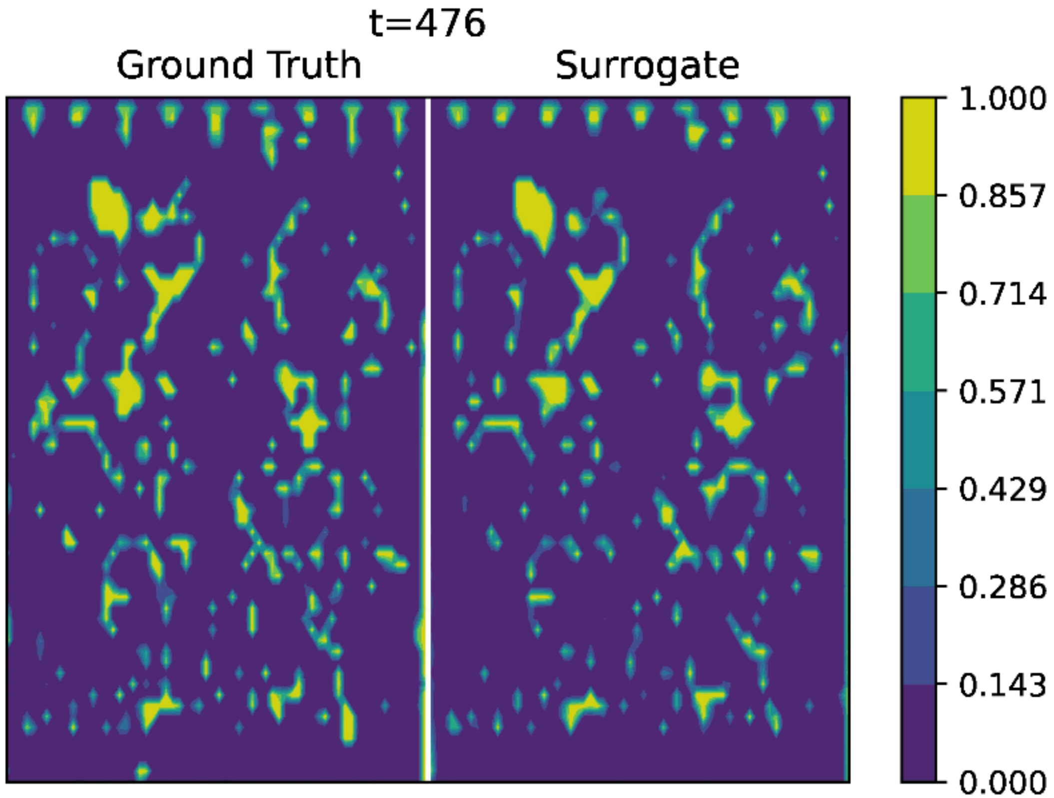

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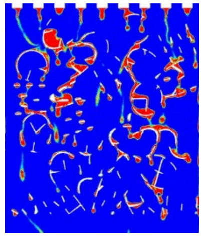
CCSI²
Carbon Capture Simulation for Industry Impact

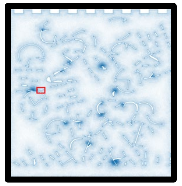
MeshGraphNets (MGN)

t = 0



MeshGraphNets (MGN)

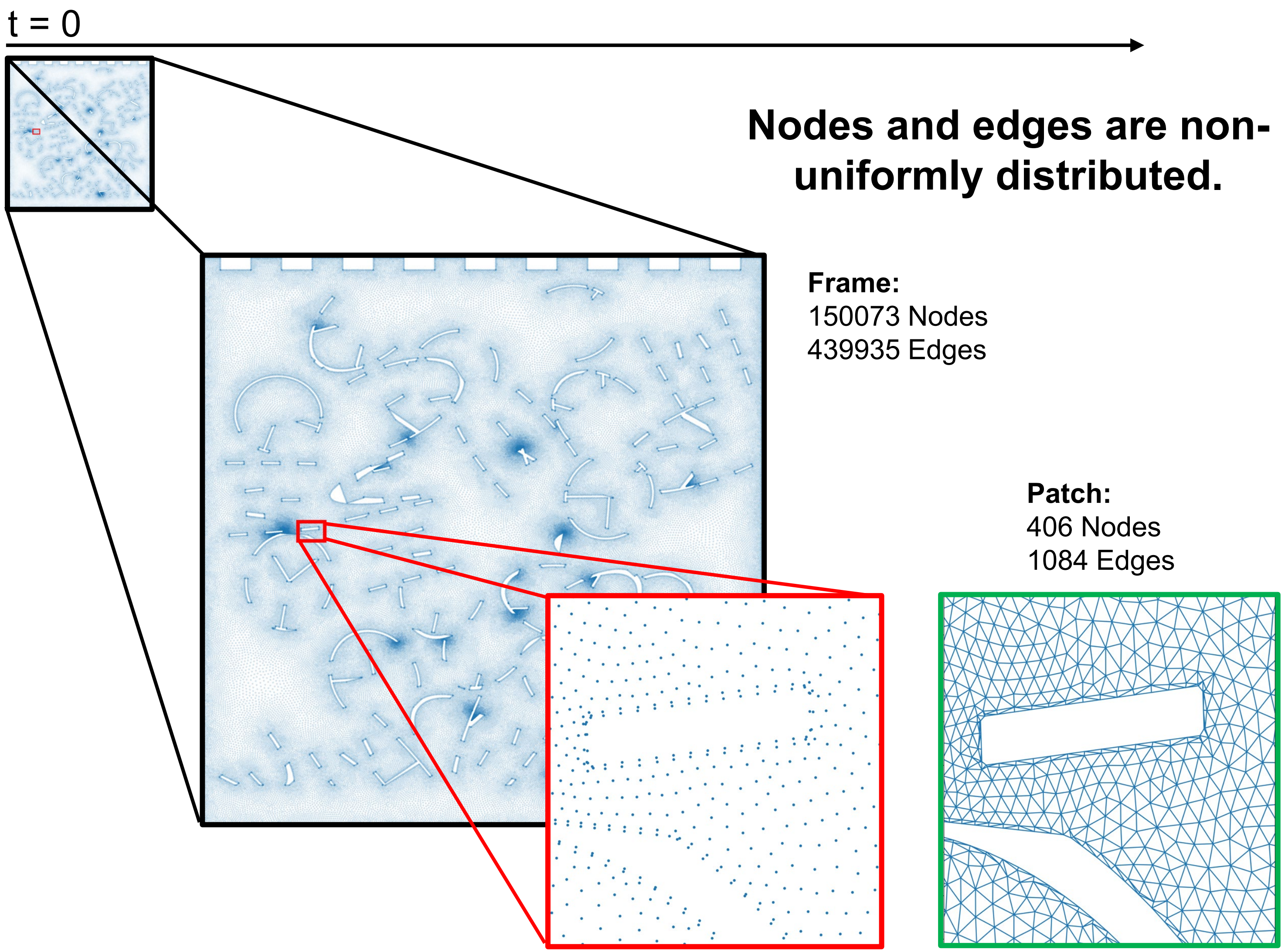
t = 0



MeshGraphNets (MGN)

Input

A patch within the original frame



MeshGraphNets (MGN)

Input
A ***mesh*** within the original frame

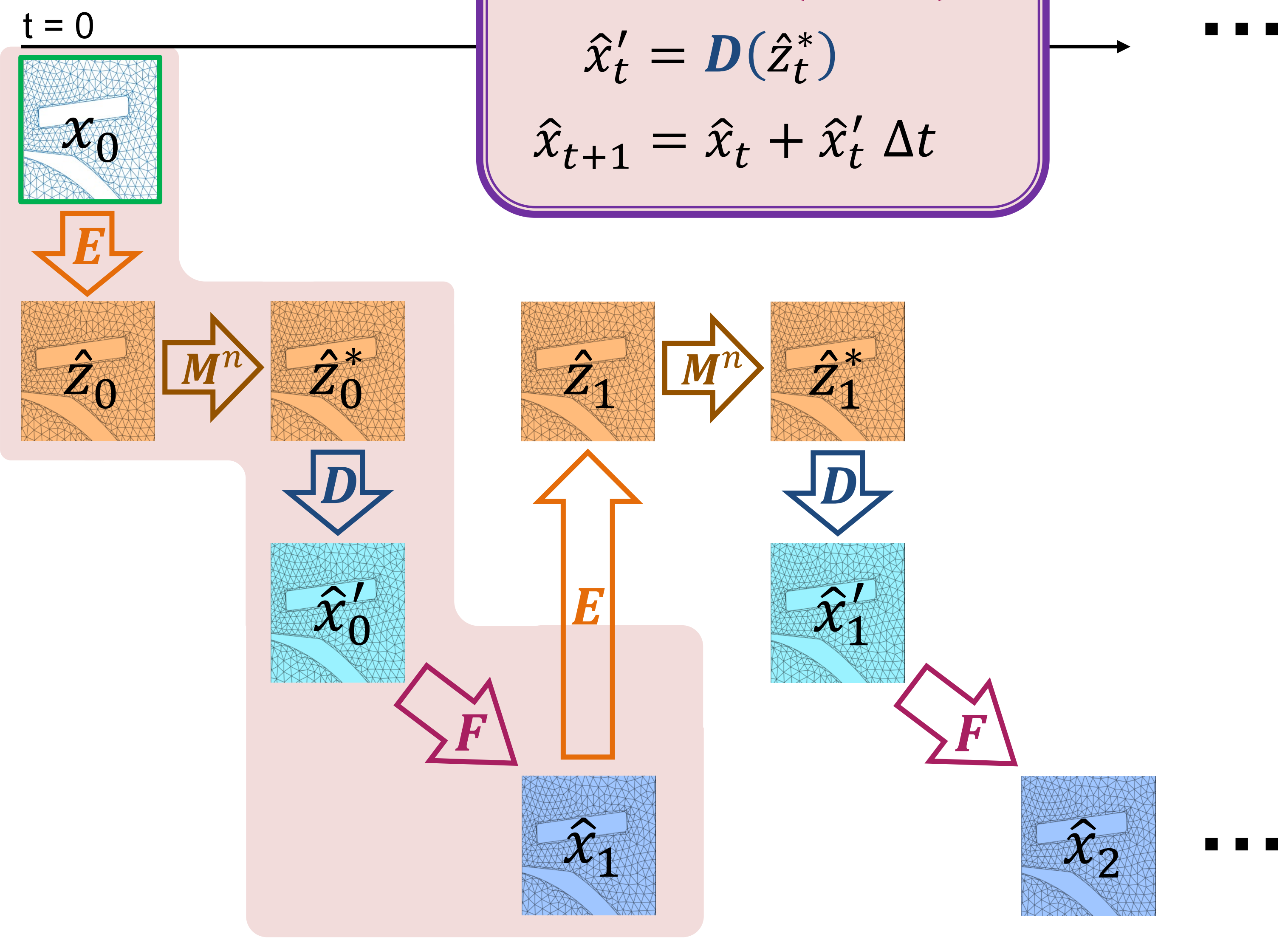
Encoding *E*
Each node and edge has its own embedding.

Message Passing *M*
Neighboring edges and nodes exchange info to update embeddings.

Decoding *D*
Updated embeddings are decoded, which represent the gradient in physical space.

Forward pass *F*
Via forward Euler

$$\hat{z}_t^* = M^n\left(E(\hat{x}_t)\right)$$
$$\hat{x}_t' = D(\hat{z}_t^*)$$
$$\hat{x}_{t+1} = \hat{x}_t + \hat{x}_t' \,\Delta t$$

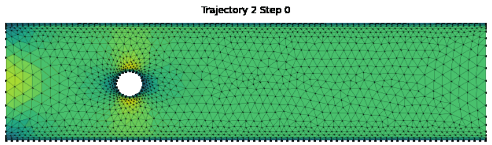


CCSI² Carbon Capture Simulation for Industry Impact

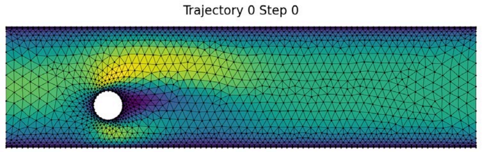
LLNL’s MGN Surrogates

Implemented the first public version of MGN in PyTorch

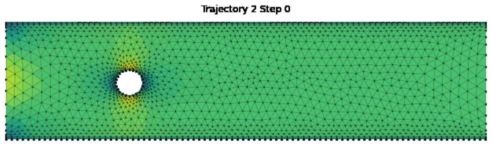
MGN:



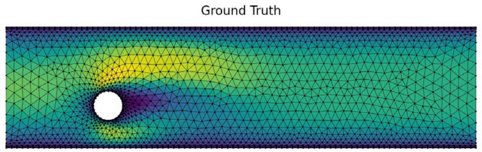
MGN:



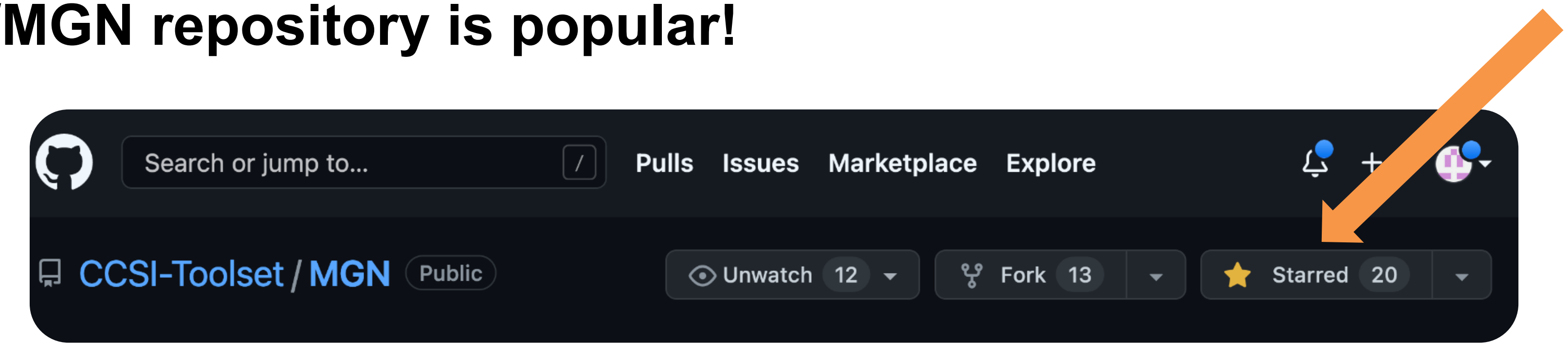
CFD:



CFD:



CCSI-Toolset/MGN repository is popular!



CCSI²
Carbon Capture Simulation for Industry Impact

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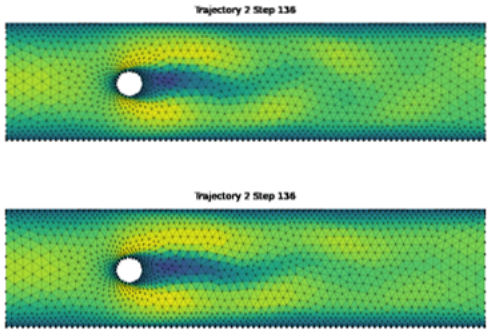

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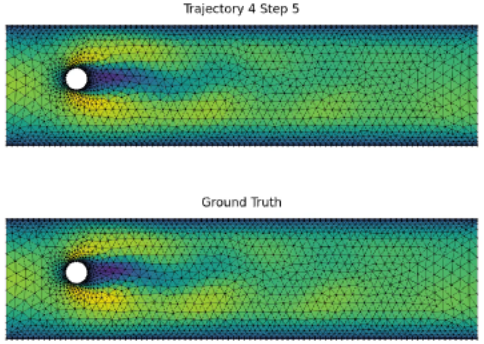

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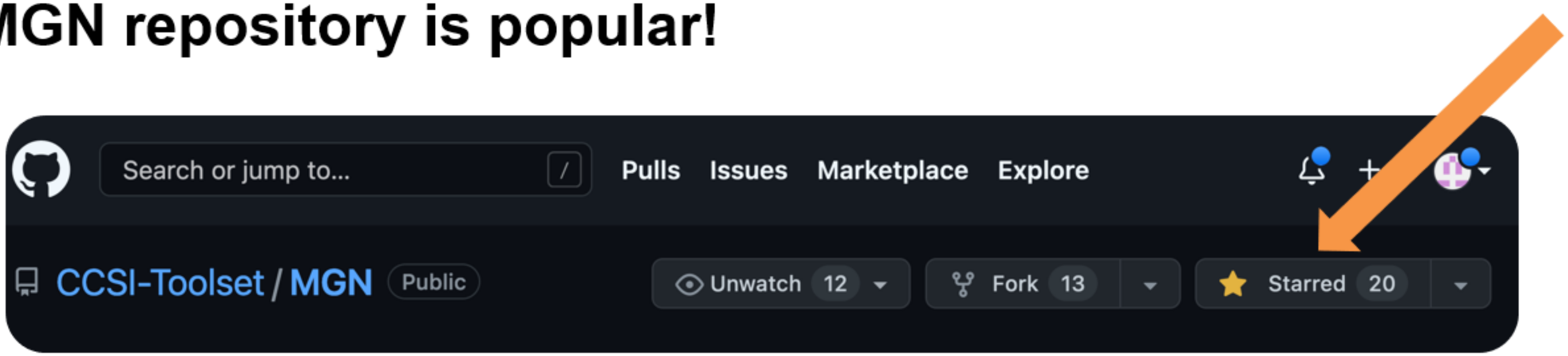

CCSI2
Carbon Capture Simulation for Industry Impact

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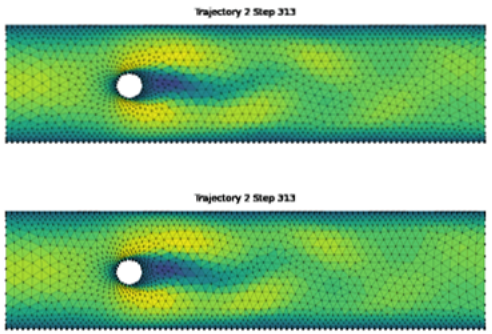

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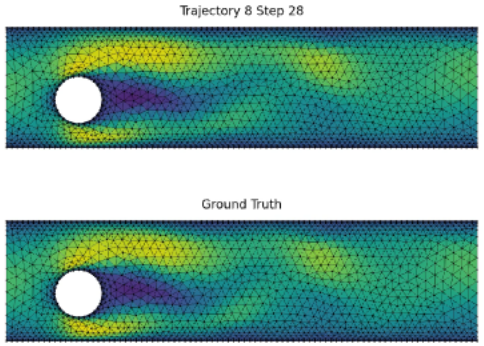

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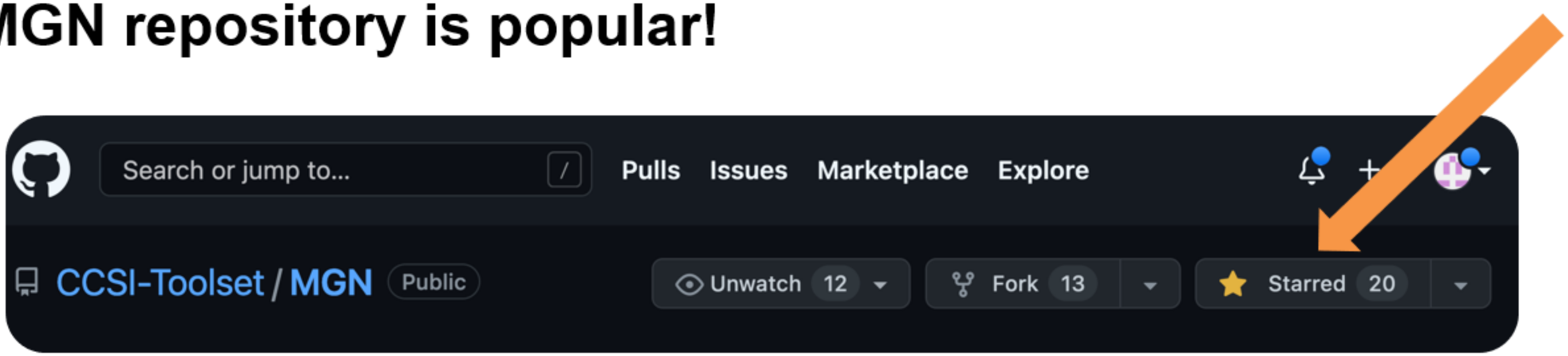

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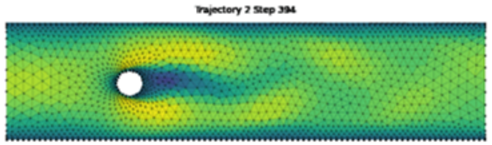

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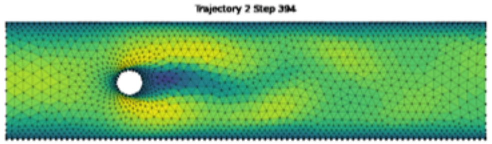

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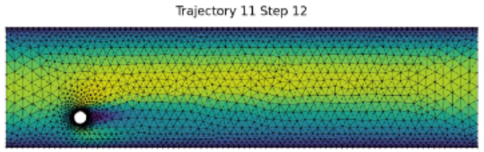

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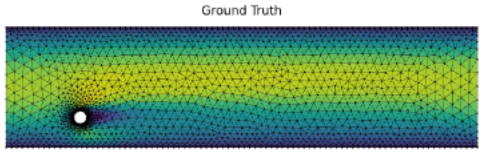

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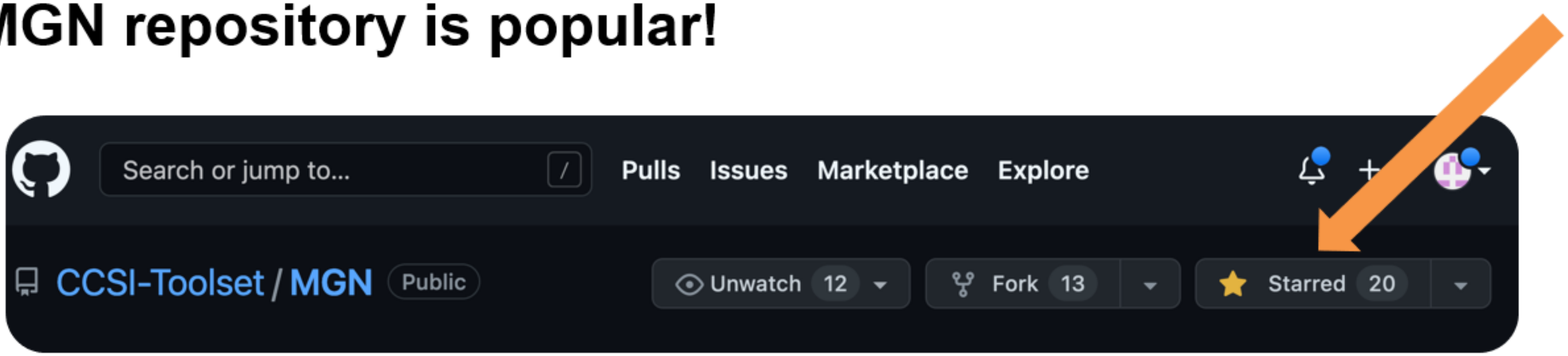

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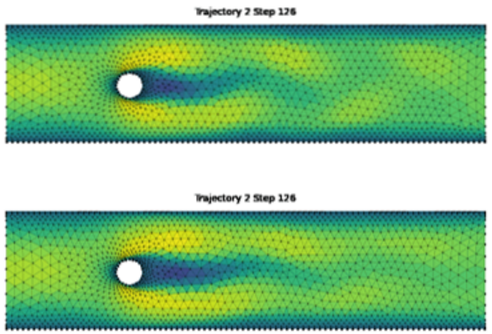

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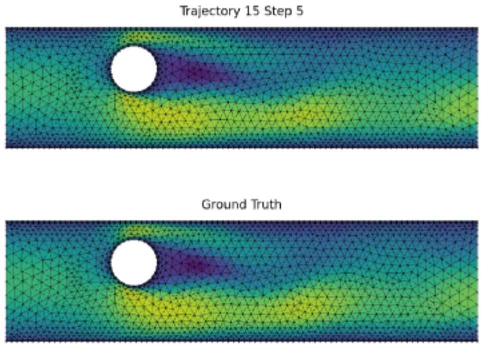

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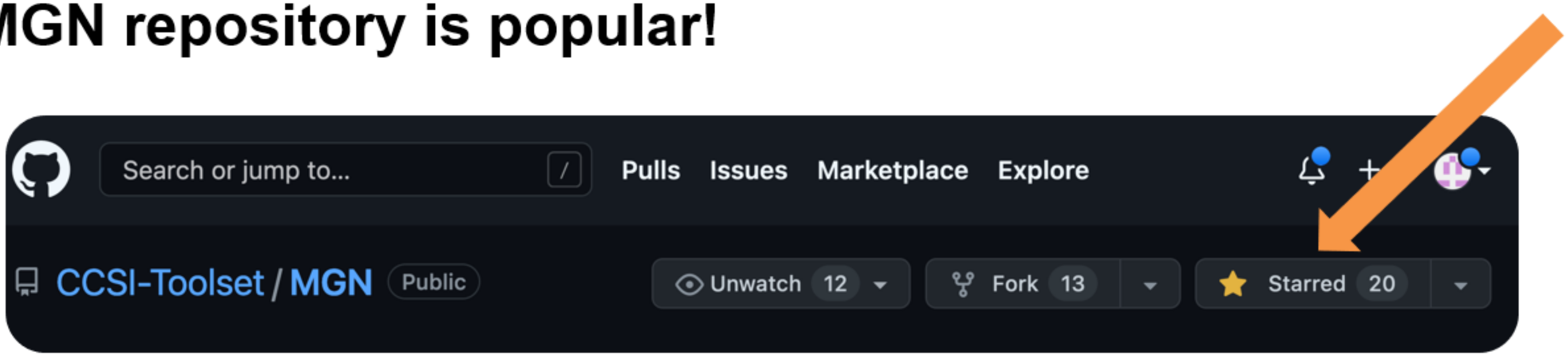
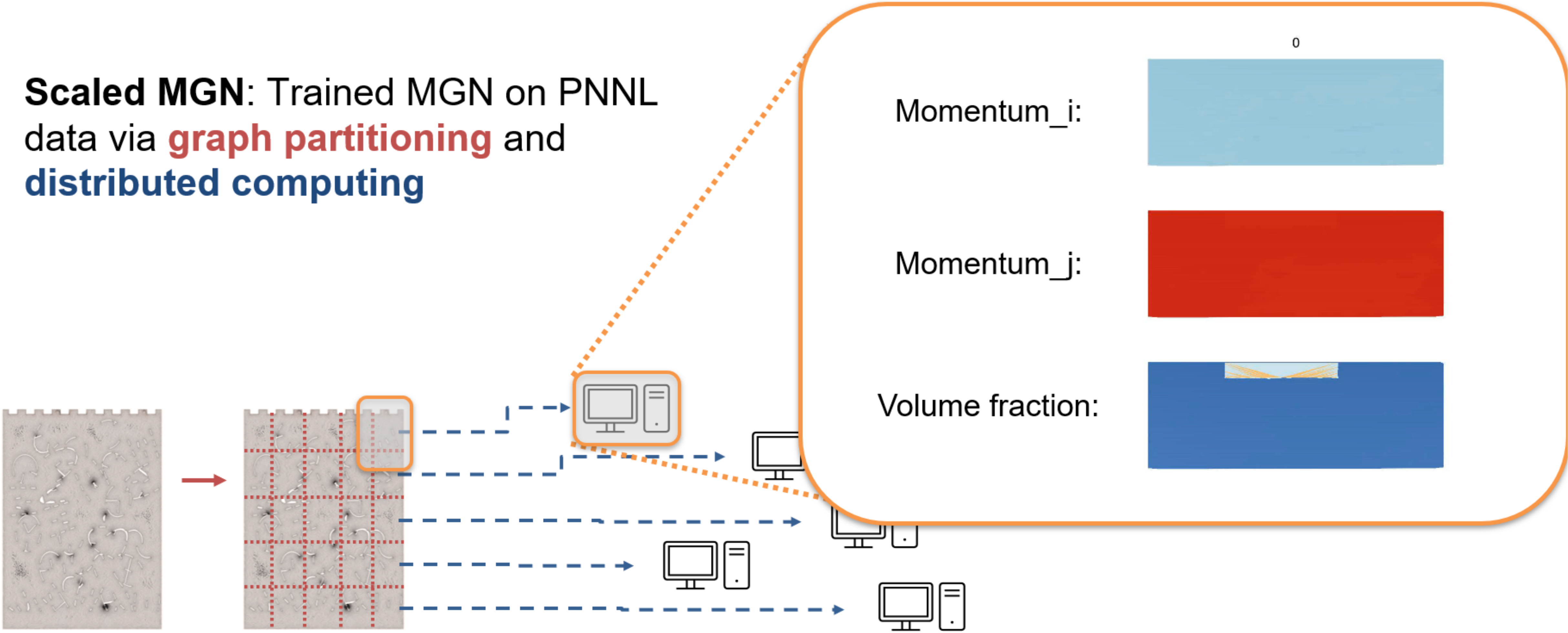


MGN Surrogate Innovations for Scaling to PNNL Data

Scaled MGN: Trained MGN on PNNL data via **graph partitioning** and **distributed computing**



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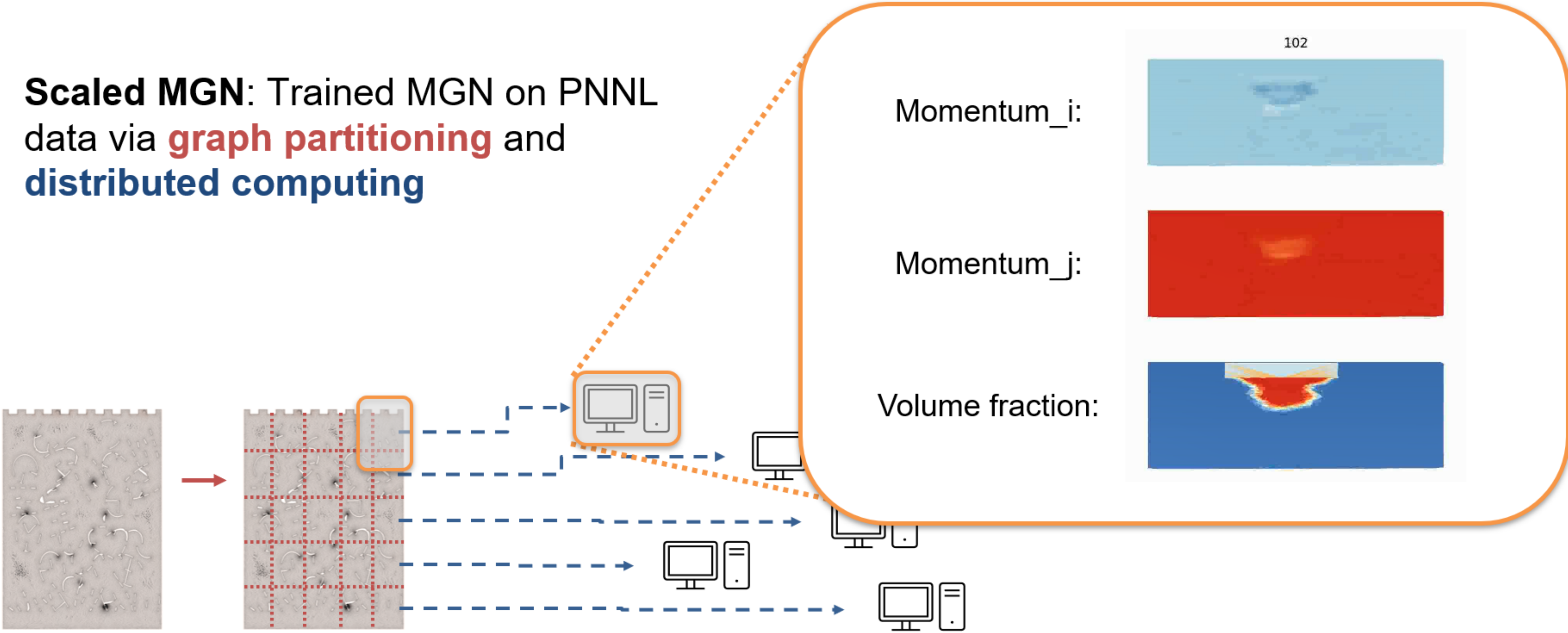

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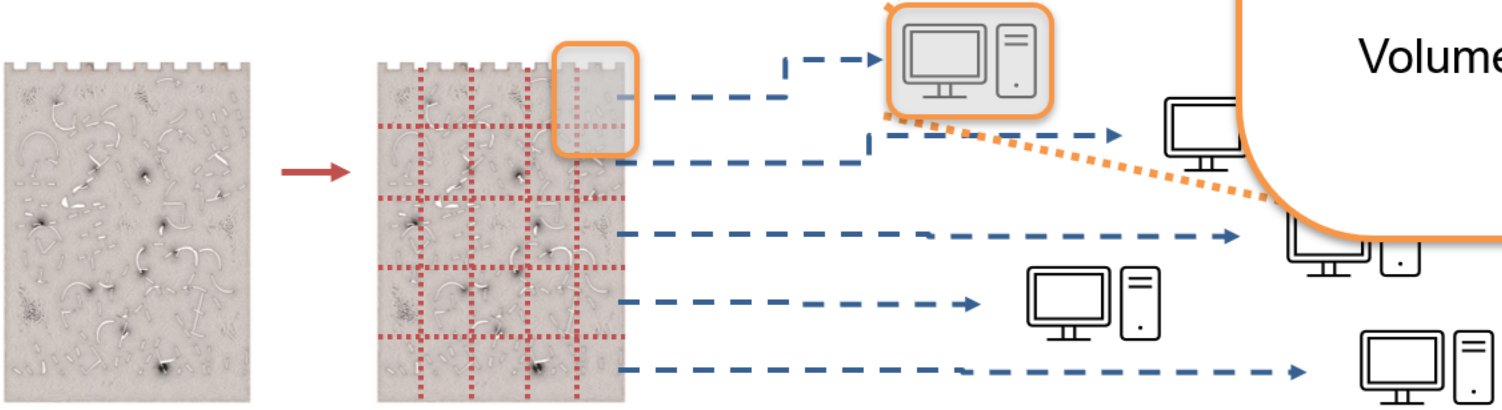
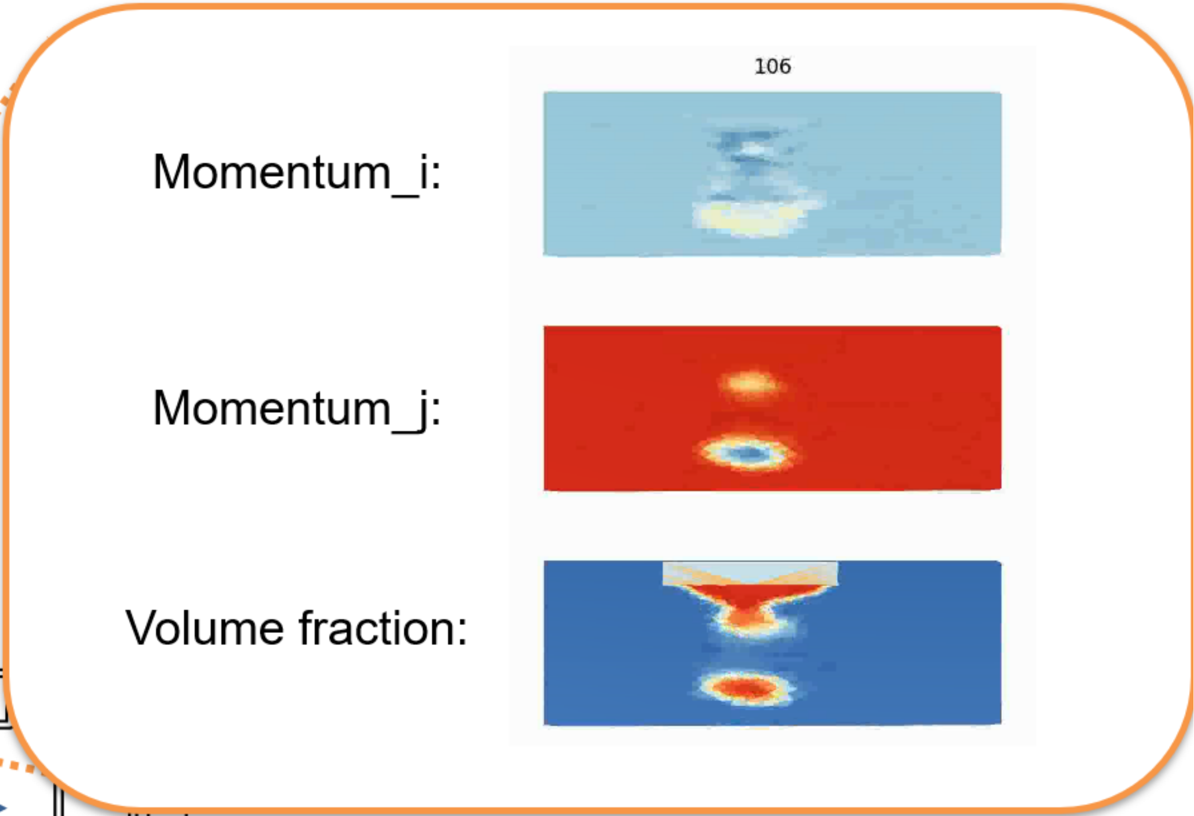
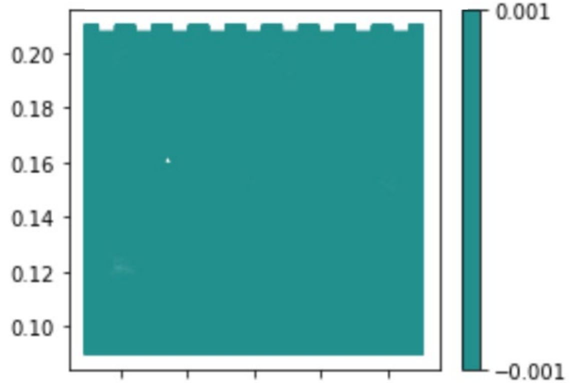




Physics-informed surrogates

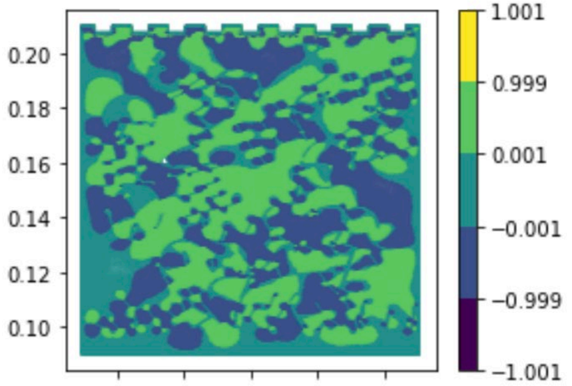
$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u}) = -\nabla p + \mu \nabla^2 \mathbf{u} + \rho \mathbf{g} + \mathbf{F}_\sigma$$

Velocity Model Input

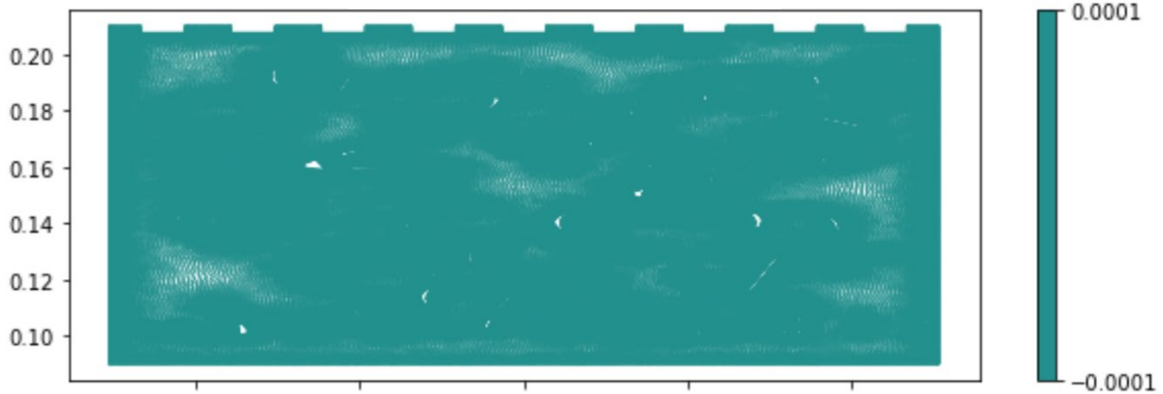


Difficult to predict next velocity state!

Desired Output

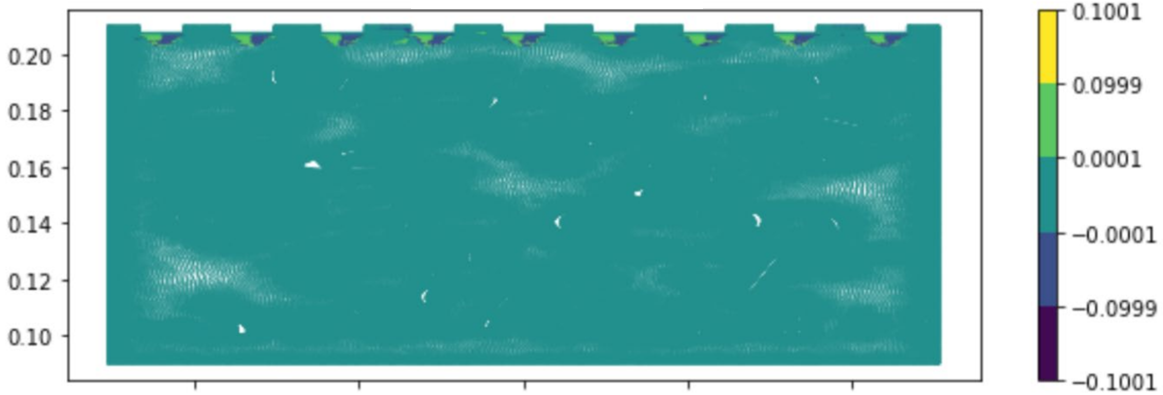


Momentum Model Input



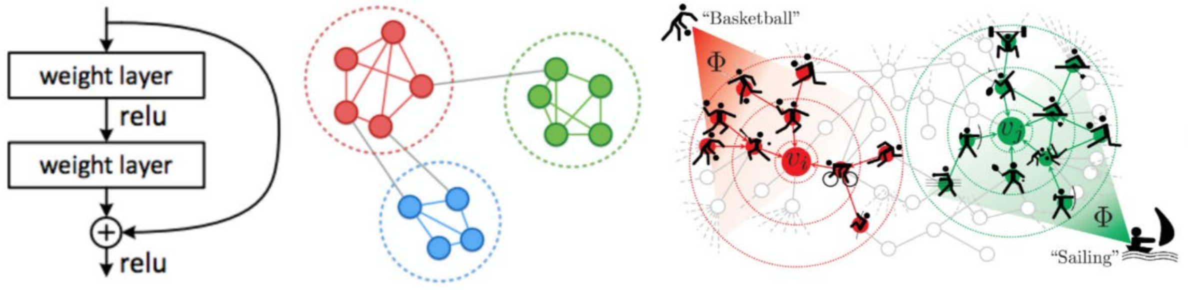
Easy to predict next momentum state!

Desired Output



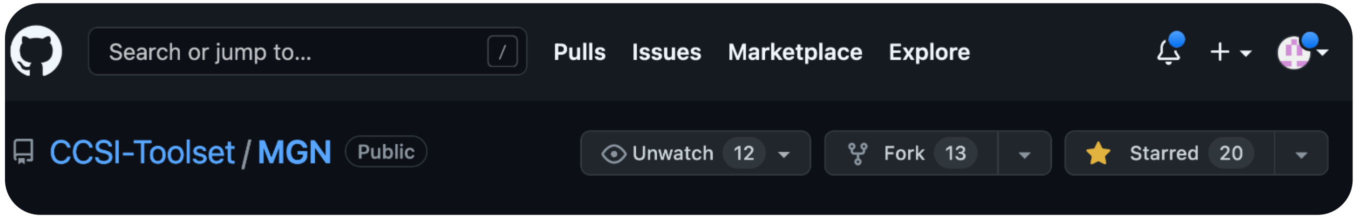
Work in progress

- MGN extensions/improvements
  - Improving scalability
  - Architectural improvements
  - Training/optimization improvements
    - Curriculum learning
    - Incorporating physics constraints/expert knowledge
  - Explainability methods
- Surrogate models with CMU/PNNL data
- Design optimization
  - Integrate MGN into FOQUS



(a) skip connection (b) clustering (c) explainability

https://github.com/CCSI-Toolset/MGN



CCSI^2 Carbon Capture Simulation for Industry Impact

Acknowledgements

CCSI^2 Machine Learning Team

Phan Nguyen
LLNL

Brian Bartoldson
LLNL

Jose Cadena
LLNL

Amar Saini
LLNL

Yeping Hu
LLNL

Subtask Collaborators

Jay Xu
PNNL

Jie Bao
PNNL

Yucheng Fu
PNNL

Grigorios Panagakos
CMU

Charles Finney
ORNL

CCSI^2 Carbon Capture Simulation for Industry Impact

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

Contact Info:

Phan Nguyen

nguyen97@llnl.gov

Questions