Machine Learning Approaches to Accelerate CFD Analyses

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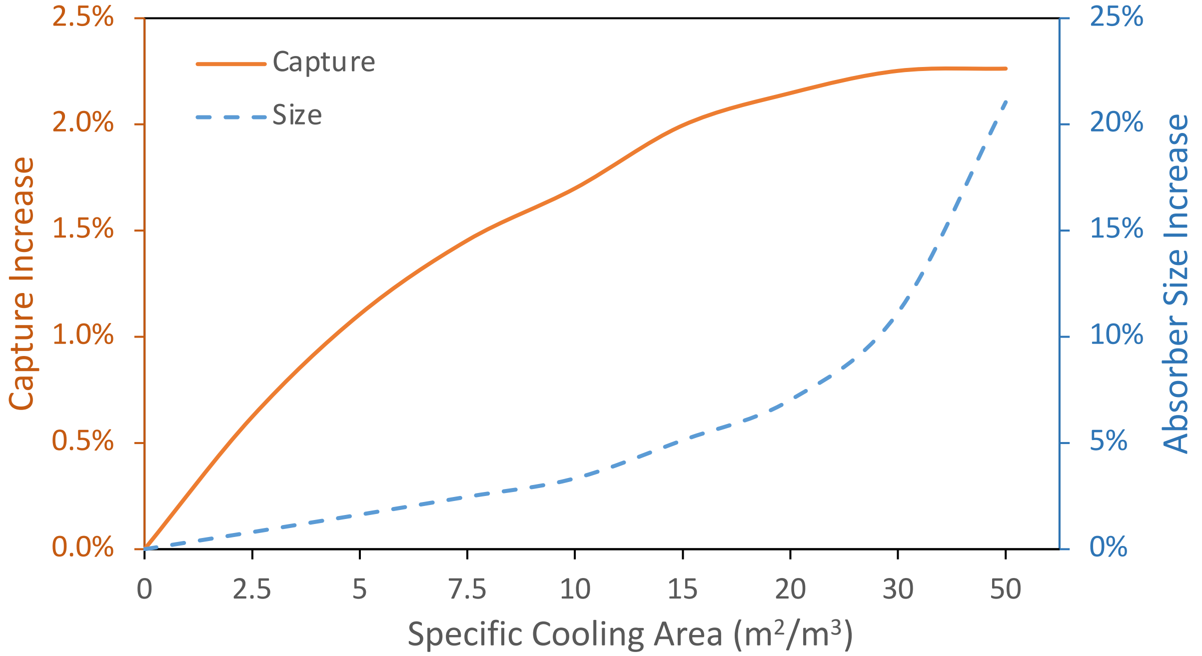
Vision

CCSI^2 has a vision to leverage Machine Learning methods on high-dimensional data from CFD models to:

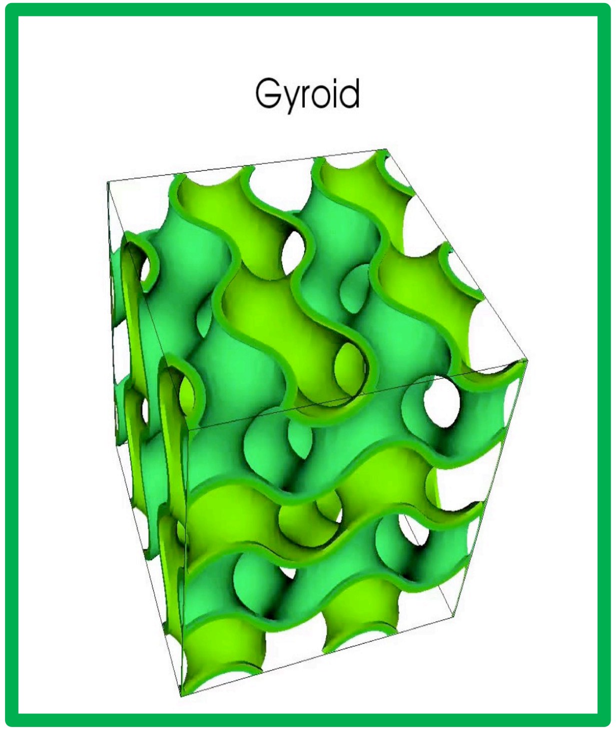
1. **Reduce computational burden** of expensive CFD models
2. **Inform process models** with knowledge derived from CFD results
3. **Establish control methodologies** of the Absorption/Desorption processes

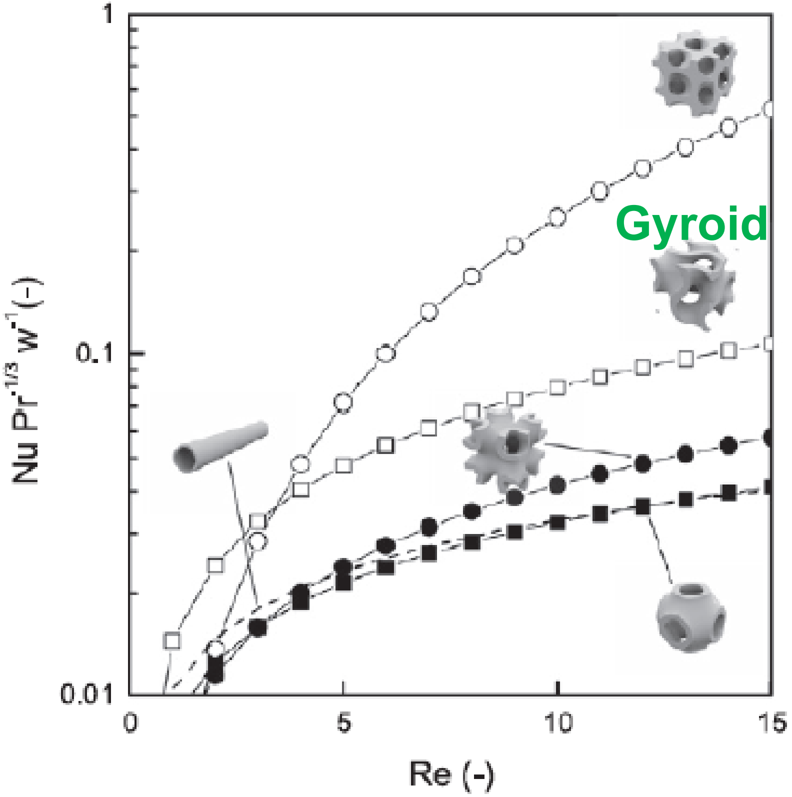
How to improve carbon capture rate while reducing absorber size?



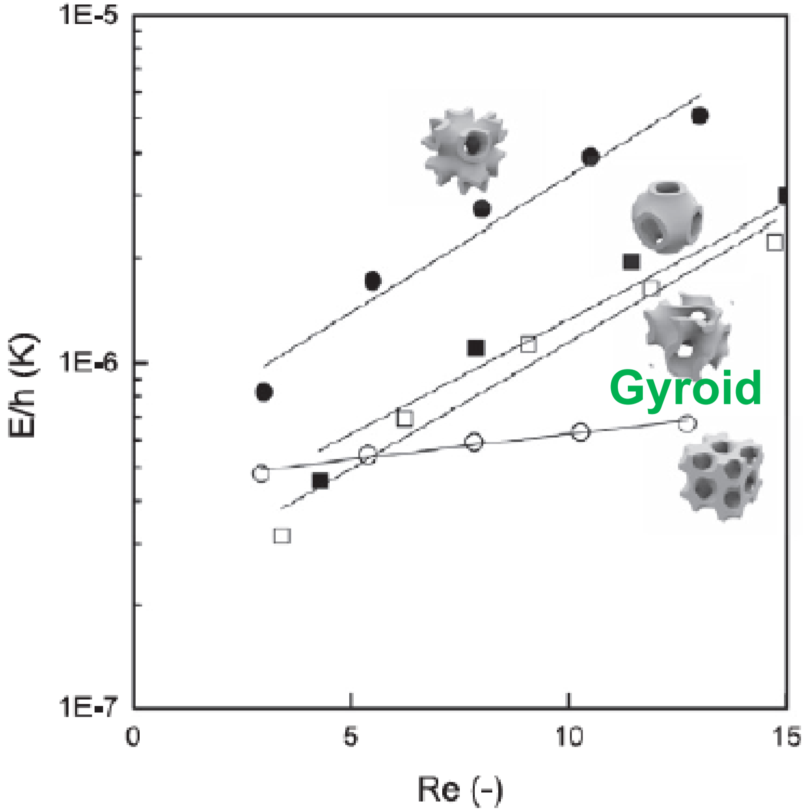
- Investigate the trade-off between increase in absorption performance and the increase in equipment size
- ***Geometry*** of shell and tube type heat exchanger

Why does geometry matter?





Heat transfer per unit surface area

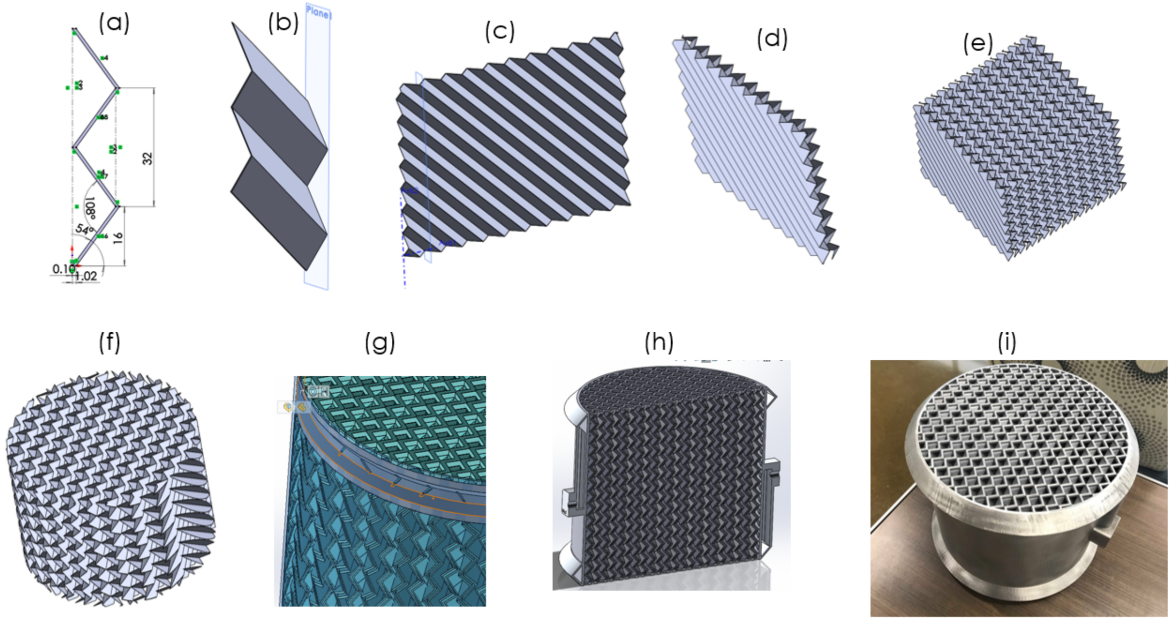


Friction loss per unit heat transferred at $\Delta T = 1 \circ C$

T. Femmer et al. *Chemical Engineering Journal* 273 (2015).

Why do we need CFD?

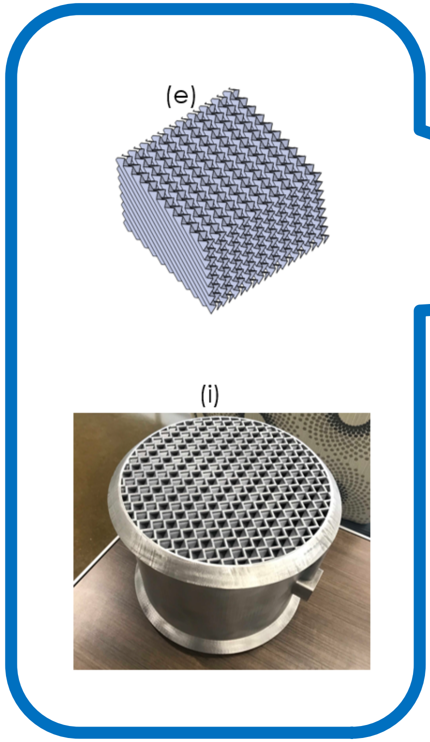
- **CFD captures the effects of changing the geometry**
- **Need local information on transport phenomena** to understand driving forces

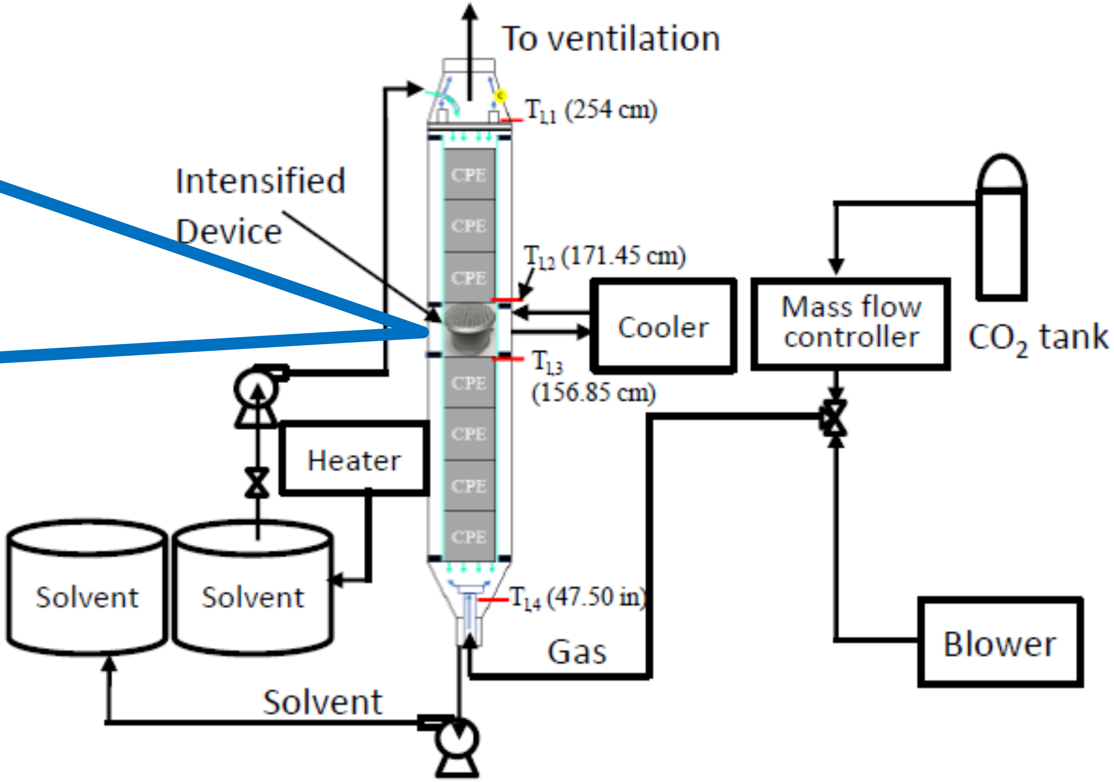


Why do we need CFD in $CCSI^2$?

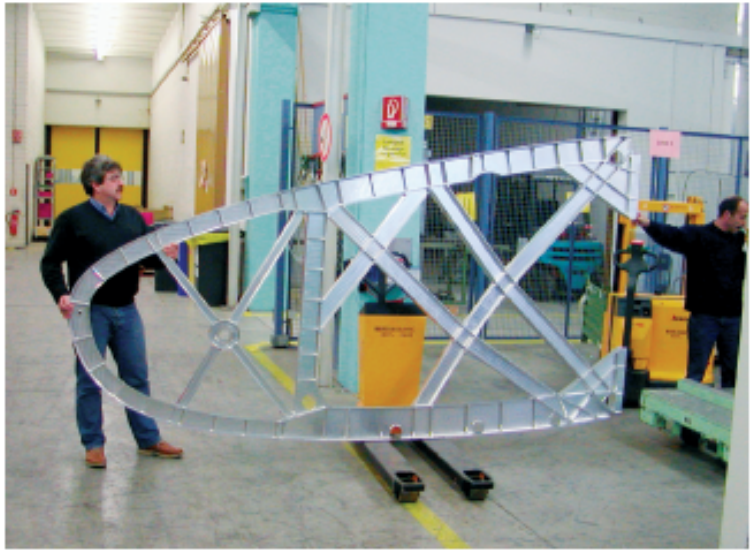
- **CFD captures the effects of changing the geometry**
- **Need local information on transport phenomena** to understand driving forces
- **Can be incorporated into design optimization** to optimize the device

CFD is critical for the fundamental understanding that will inform process and system level modeling





Topology Optimization in Aircraft Design



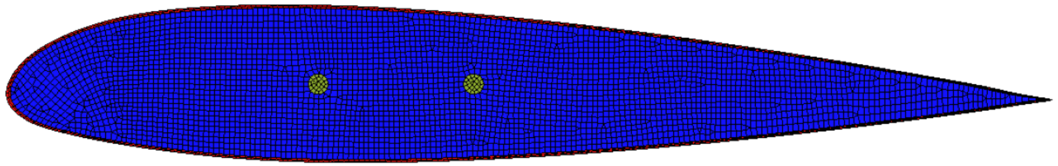


Figure 5.a. Topology optimization design space for 2D airfoil test case.

Figure 5.b Topology optimization results for simple 2D airfoil test case.

“Airbus researches use of topology optimization on aircraft wing ribs. It is stated that usage of topology optimization results in around 1000 kg of weight savings per aircraft…”

https://topologyoptimization.wordpress.com/2011/03/11/airbus/

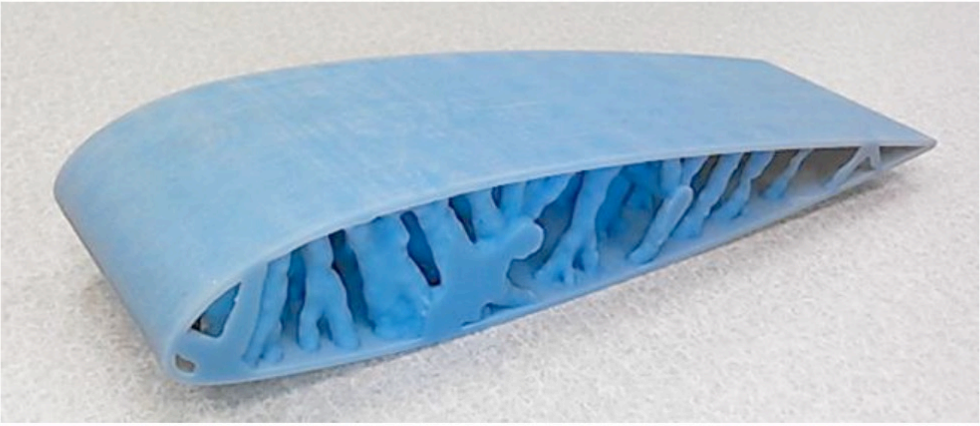
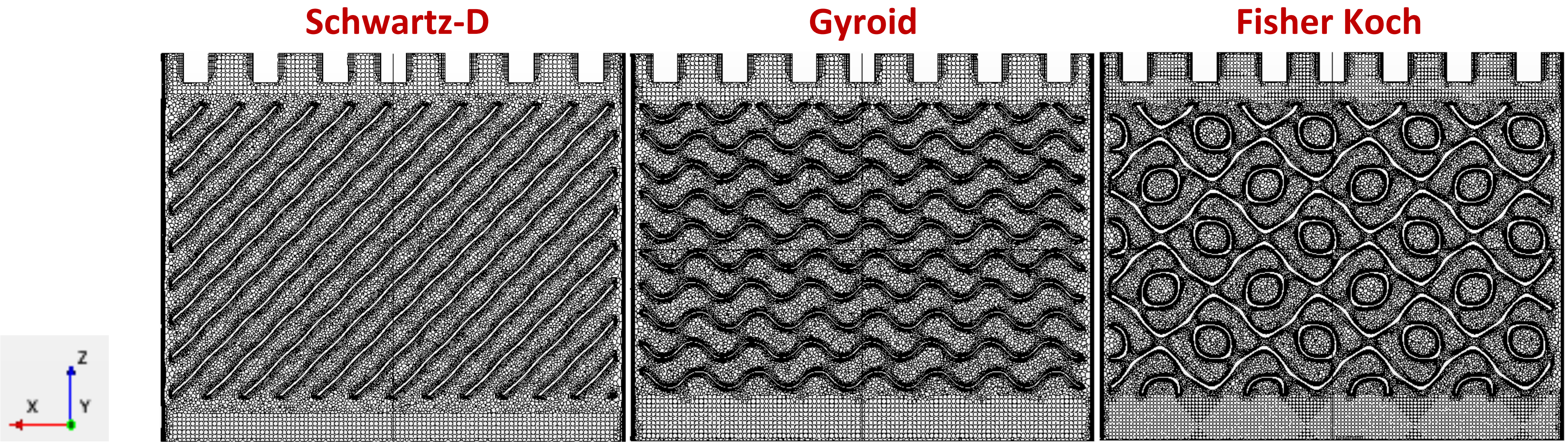


Figure 7. 3D printed wing section for a NACA 23015 airfoil.

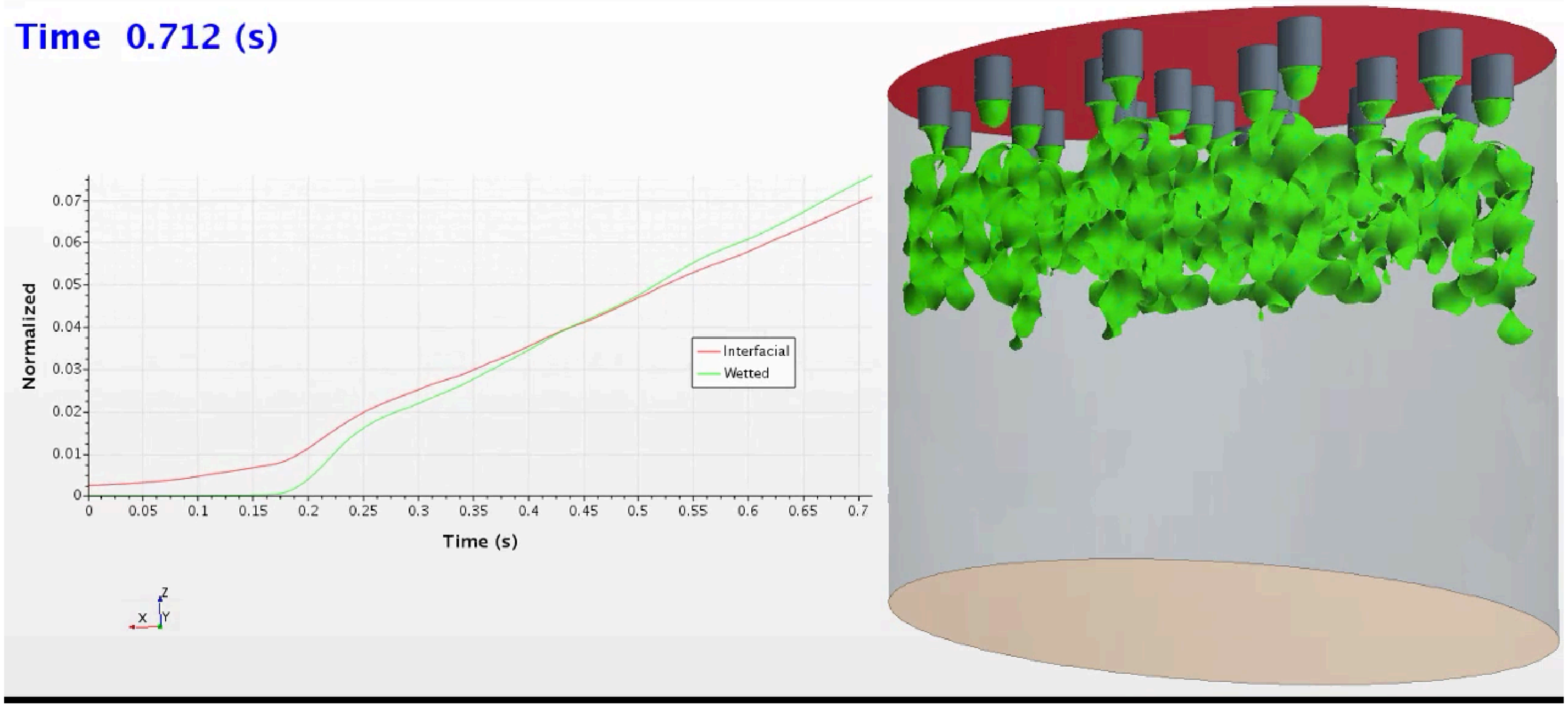
D. Walker et al. *Topology Optimization of an Aircraft Wing, 56th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*

Meshing, Timestep and Simulation Time

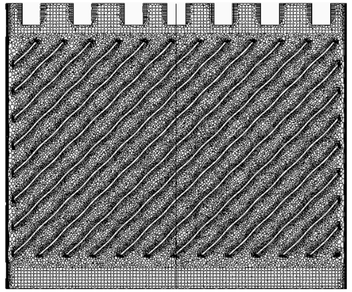
- Range of number of cells: 6 – 9 M
- $\Delta t = 10^{-5} - 10^{-04}\ sec$
- 3 - 6 days with 360 cores for 5-20 seconds simulation time

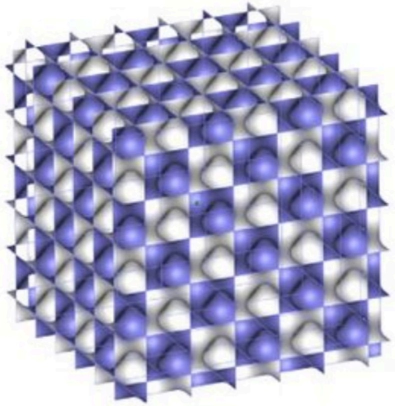


Flow Development for Schwarz-D with CO_2BOL Solvent



Schwartz-D





Simulation times is a bottleneck that impedes higher-level modeling

Deep Learning for Fluid Flow Prediction in the Cloud

Random Shape Generator	OpenFOAM simulations	Post-processing	Neural Network
Random shapes are generated for a diverse simulation data set	CFD simulations are executed. We use the OpenFOAM steady-state solver **SimpleFOAM**	Extract relevant data from the simulations	Neural Network implementation in TensorFlow (GPU)

Glue-code implemented using CAEML (a CAE Python Library developed by Renumics)

Figure 1: Deep Learning workflow.

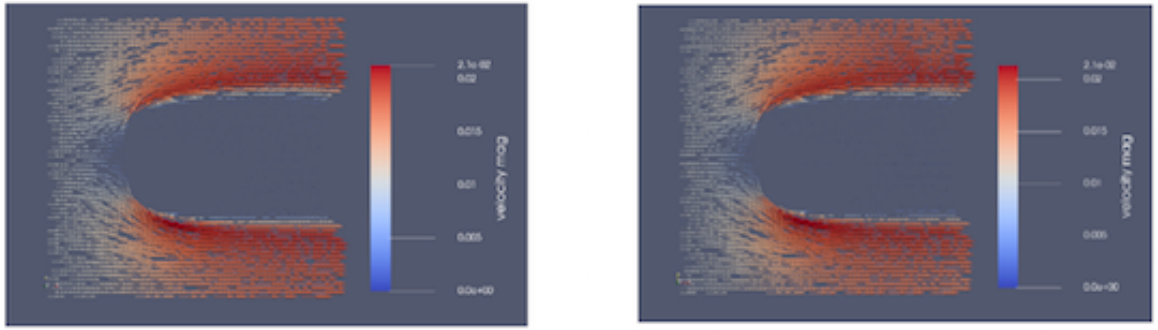


Figure 3: Simulated flow field (left image) and predicted flow field (right image).

- Performance for generating the flow field data set and Tensorflow training

Setup	2-D external flow	3-D internal flow
Time for 10.000 simulations	13.2 h	152.5 h
Time for training	23.7 h	48.5 h

- Neural network prediction of flow field

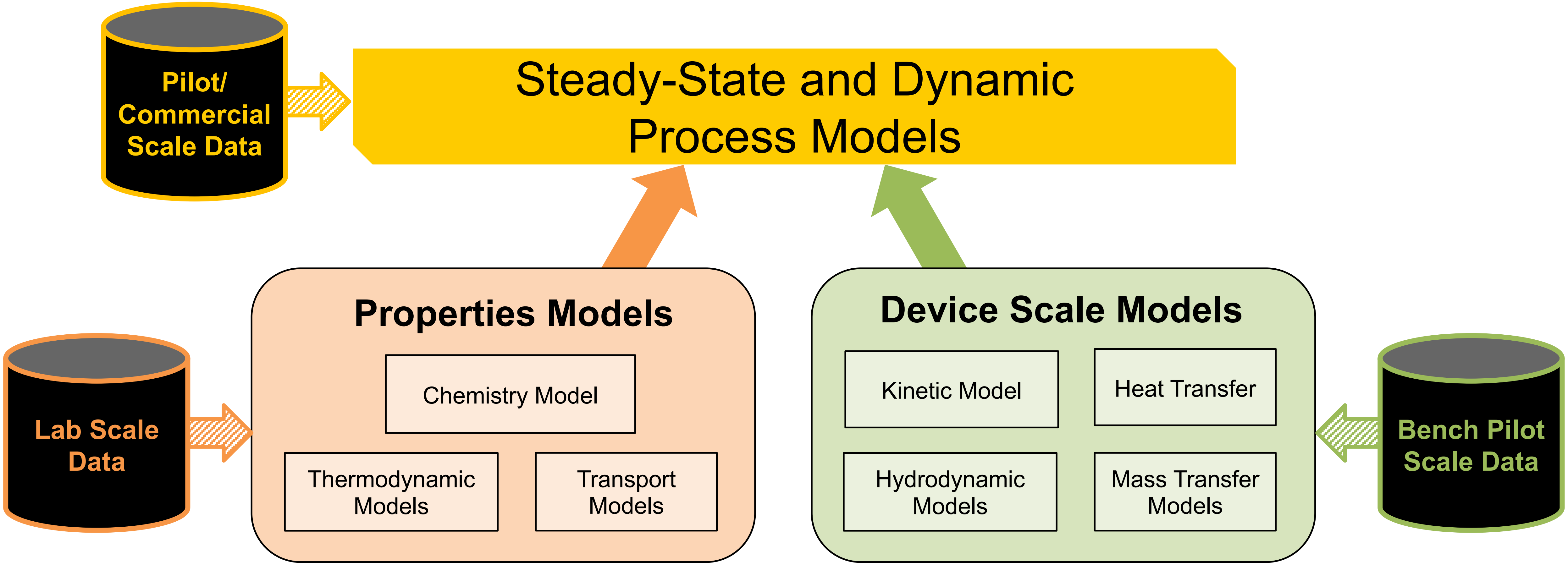
Setup	2-D external flow	3-D internal flow
Time for CFD solver	4.7 s	55.0 s
Time of neural network prediction	3 ms	120 ms
Speedup factor w/ deep learning	**1566**	**458**

Figure 2: Performance and speedup with neural network prediction.

1 week → 6 to 20 min

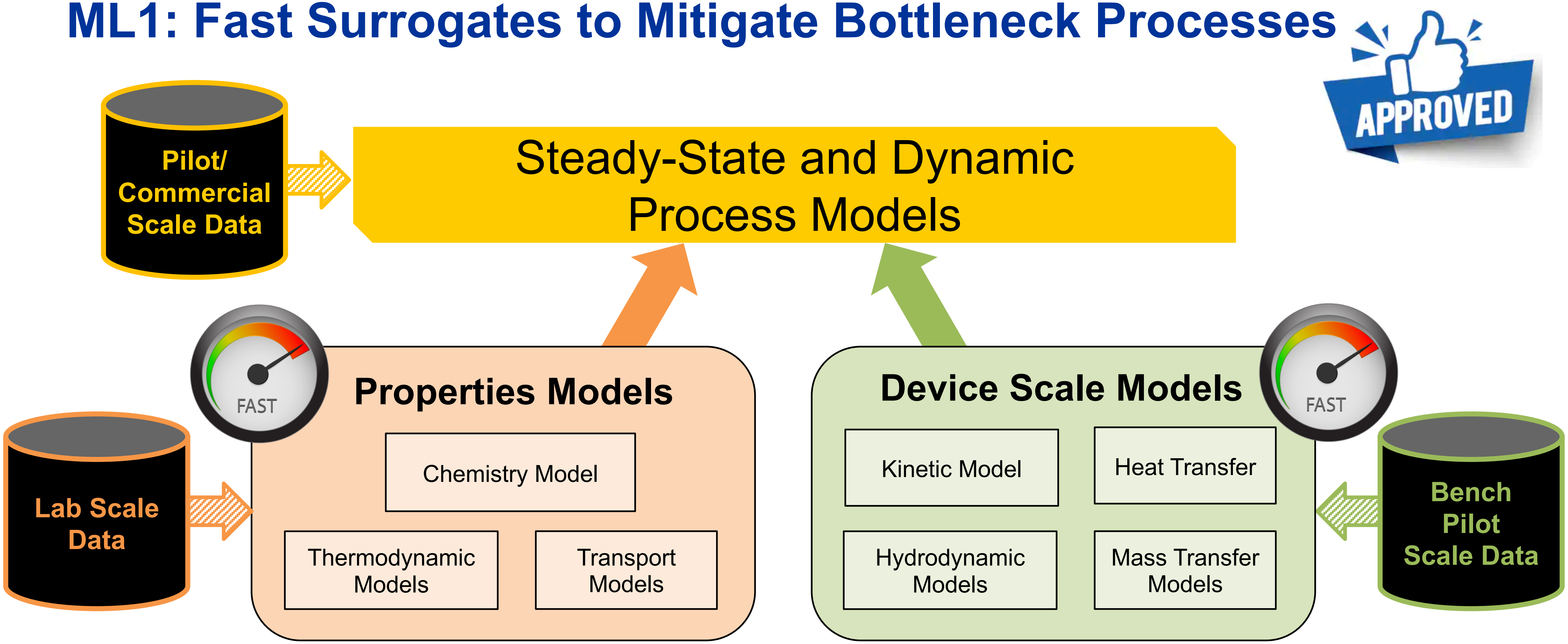
https://insidehpc.com/2019/01/case-study-deep-learning-for-fluid-flow-prediction-in-the-cloud/

Machine Learning Roadmap



CCSI² has a vision to leverage Machine Learning methods to accelerate high-dimensional CFD models.

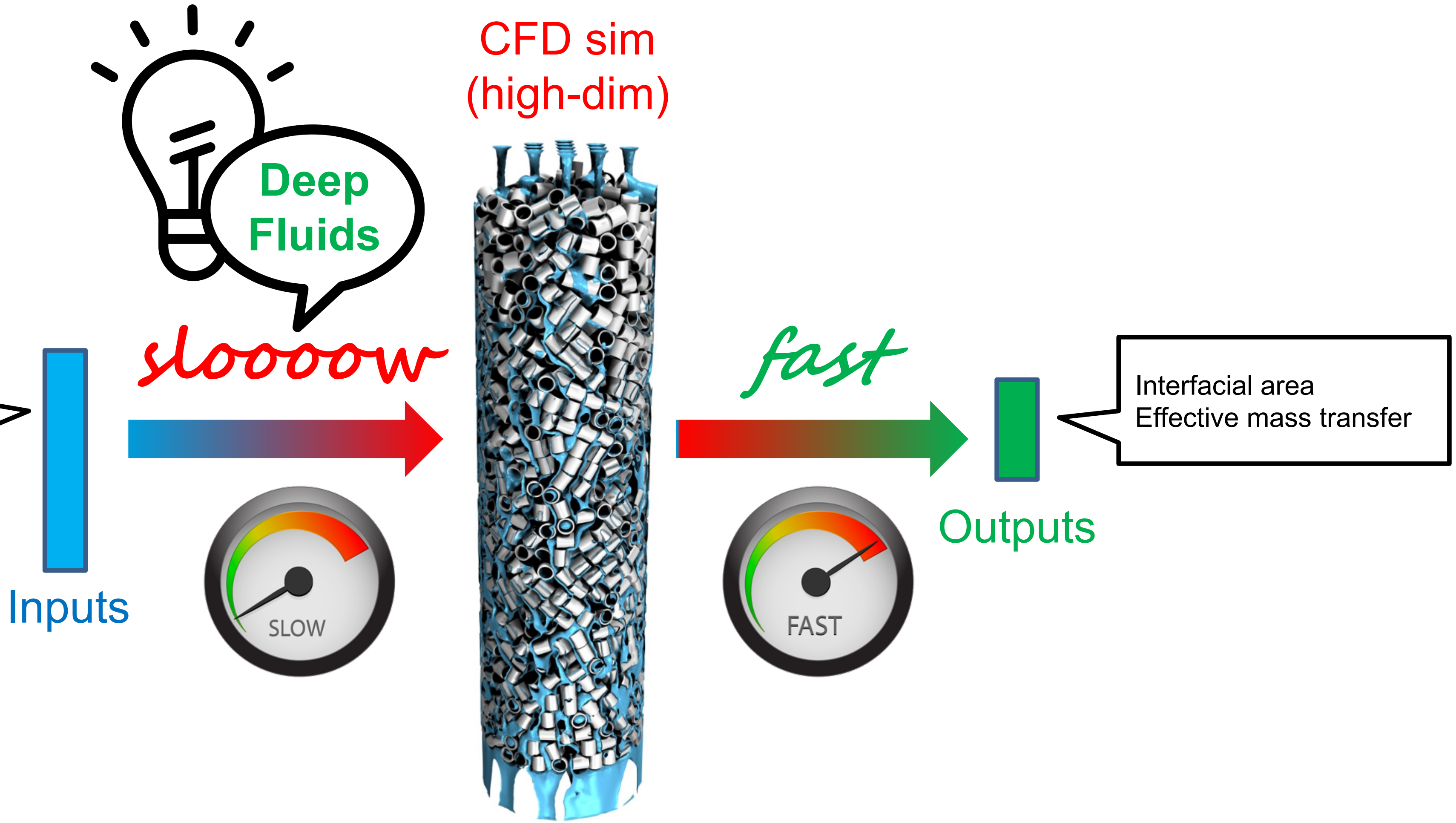
ML1: Fast Surrogates to Mitigate Bottleneck Processes



Approach: Leverage neural networks to learn fast surrogates for CFD models

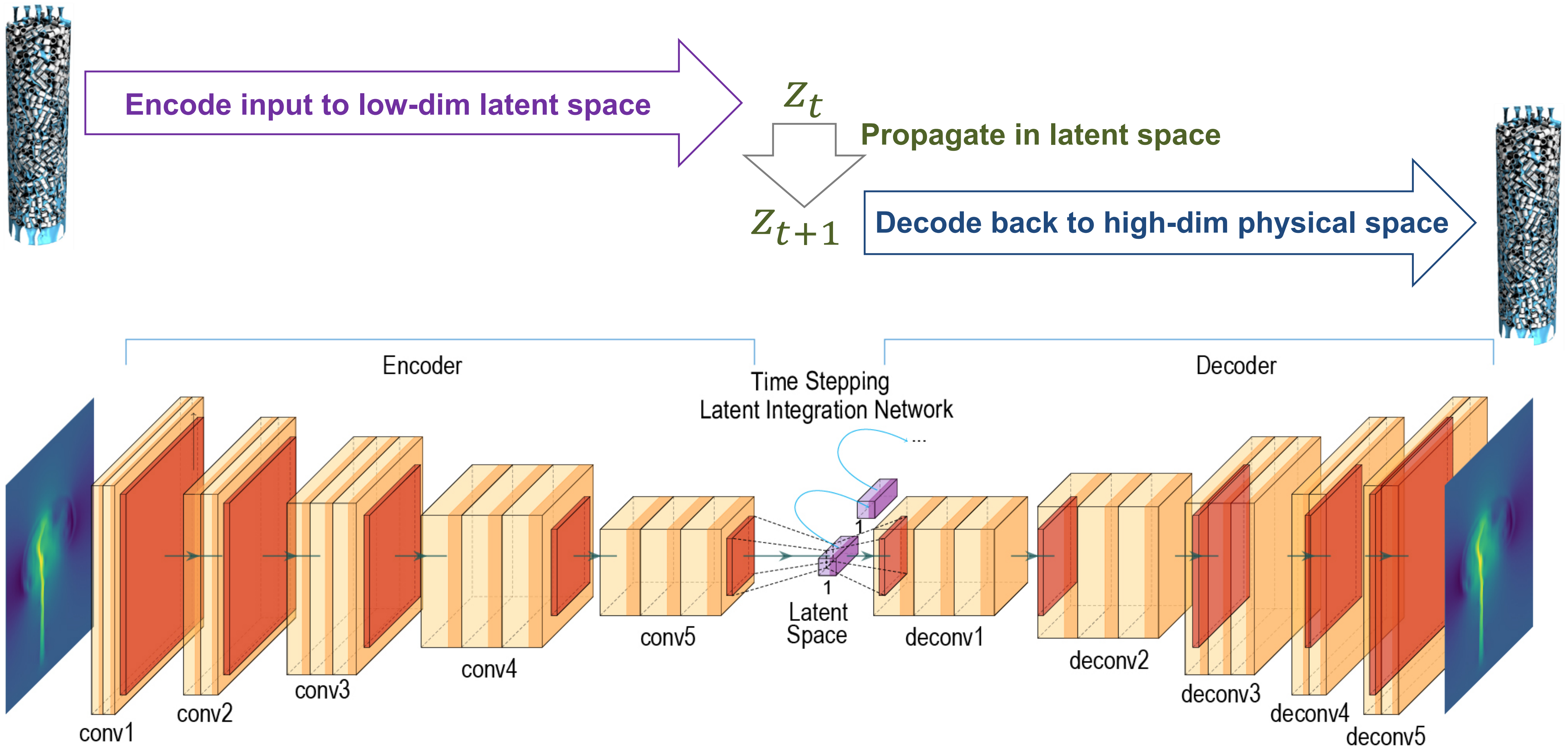
ML1 Progress: Fast Surrogate for CFD Simulation Model

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

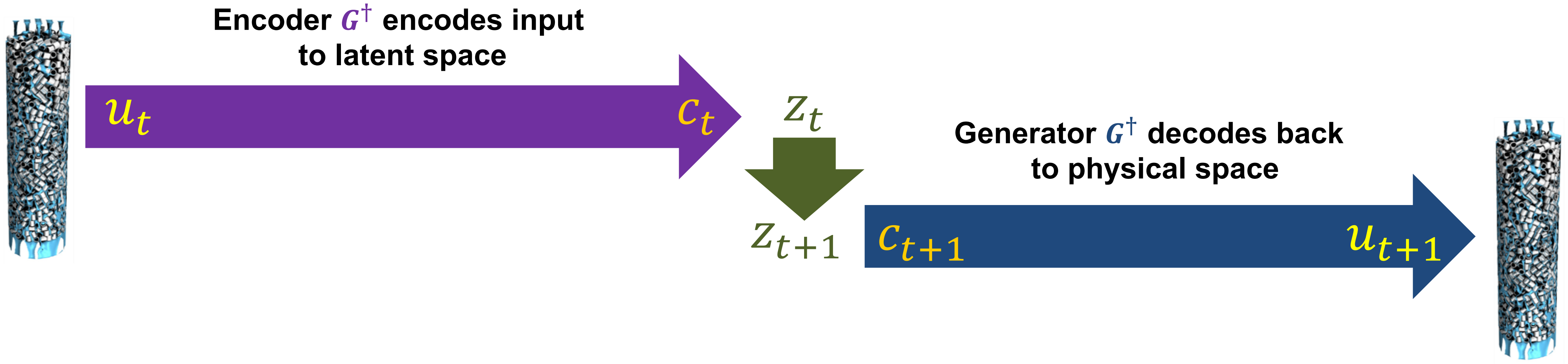


*Kim et al. (2019), "**Deep Fluids: A Generative Network for Parametrized Fluid Simulations**"*

ML1 Approach: DeepFluids



ML1 Approach: DeepFluids



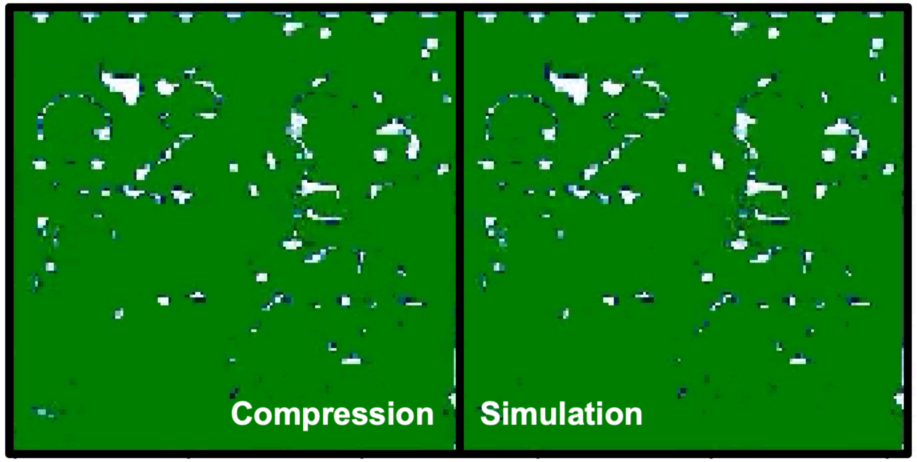
Algorithm 1 Simulation with the Latent Space Integration Network

$\mathbf{c}_0 \leftarrow G^{\dagger}(\mathbf{u}_0)$
while simulating from t to $t+1$ **do**
  $\mathbf{x}_t \leftarrow [\mathbf{c}_t; \Delta\mathbf{p}_t]$ // $\mathbf{c}_t$ from previous step, $\mathbf{p}$ is given
  $\mathbf{z}_{t+1} \leftarrow \mathbf{z}_t + T(\mathbf{x}_t)$ // latent code inference
  $\mathbf{c}_{t+1} \leftarrow [\mathbf{z}_{t+1}; \mathbf{p}_{t+1}]$
  $\mathbf{u}_{t+1} \leftarrow G(\mathbf{c}_{t+1})$ // velocity field reconstruction
end while

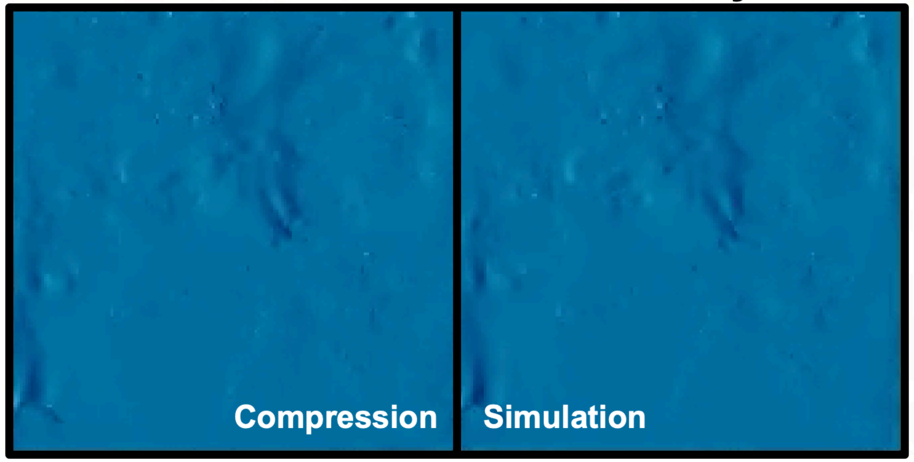
Scene	Grid Resolution	# Frames	Simulation Time (s)	**Speed Up** ($\times$)
Smoke Plume	96×128	21,000	0.033	635
Smoke Obstacle	$64 \times 96 \times 64$	6,600	0.491	513
Smoke Inflow	$112 \times 64 \times 32$	3,750	0.128	128
Liquid Drops	$96 \times 48 \times 96$	7,500	0.172	125
Viscous Dam	$96 \times 72 \times 48$	600	0.984	**716**
Rotating Smoke	$48 \times 72 \times 48$	500	0.08	308
Moving Smoke	$48 \times 72 \times 48$	80,000	0.08	308

ML1 Results: Latent Representation Learning

PNNL Data: Volume Fraction

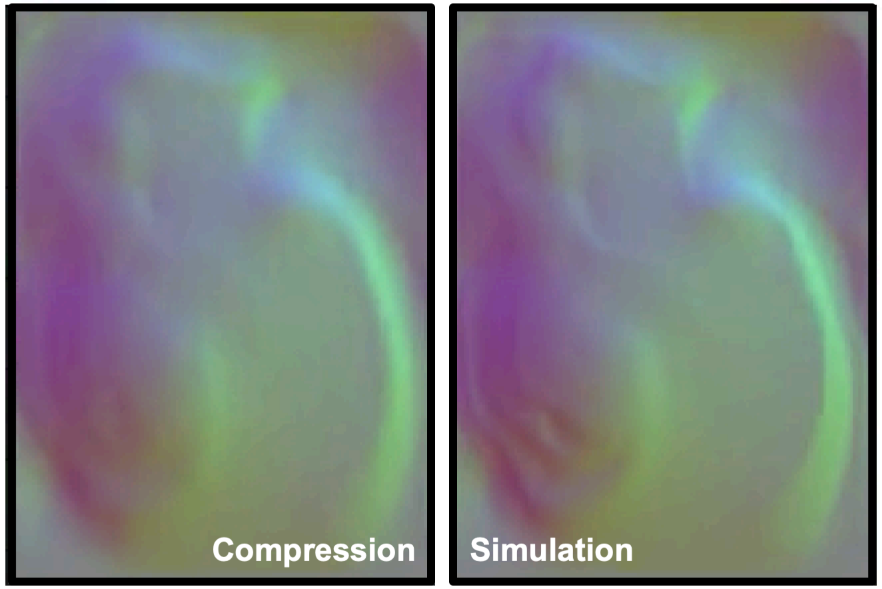


PNNL Data: Vertical Velocity



- **[TOP]** Trained on StarCCM simulations
  - 4 output channels: volume fraction, pressure, flow x- and y-velocities
  - Initial velocity at top boundary layer set to 6.45e-3 m/s
- **[RIGHT]** Trained on MantaFlow Smoke Source simulations

MantaFlow Smoke Source



CCSI2 Carbon Capture Simulation for Industry Impact
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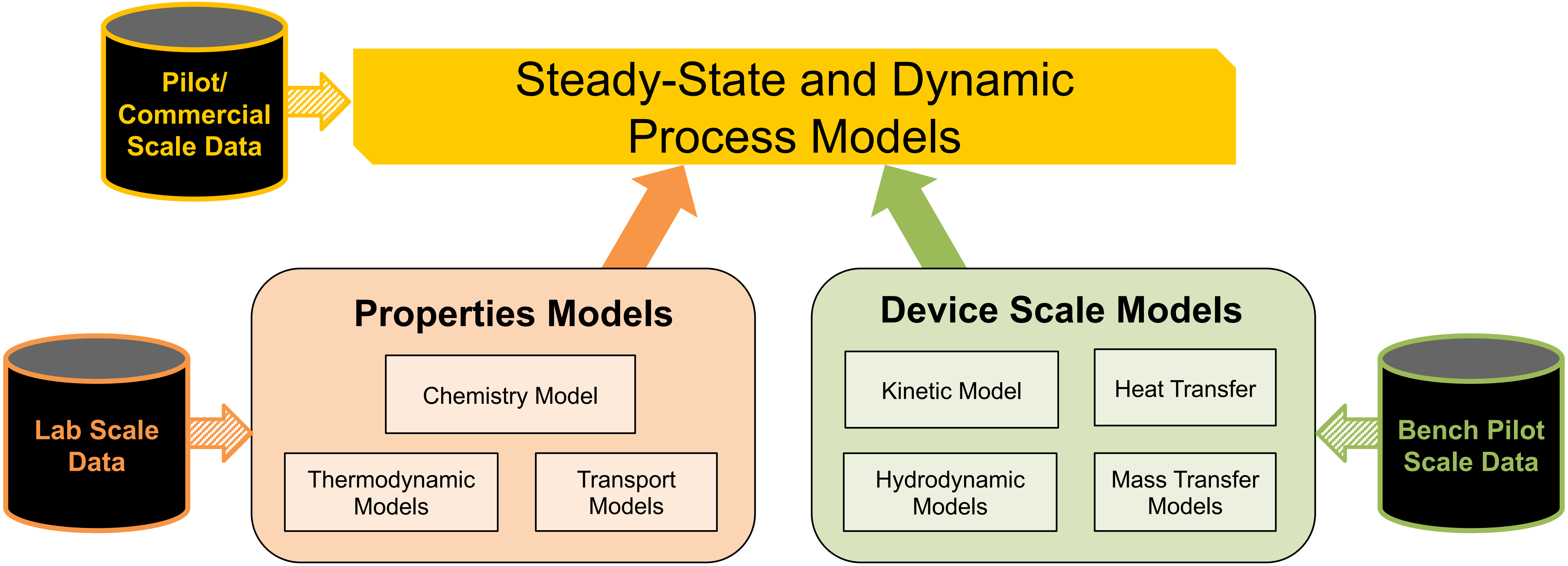
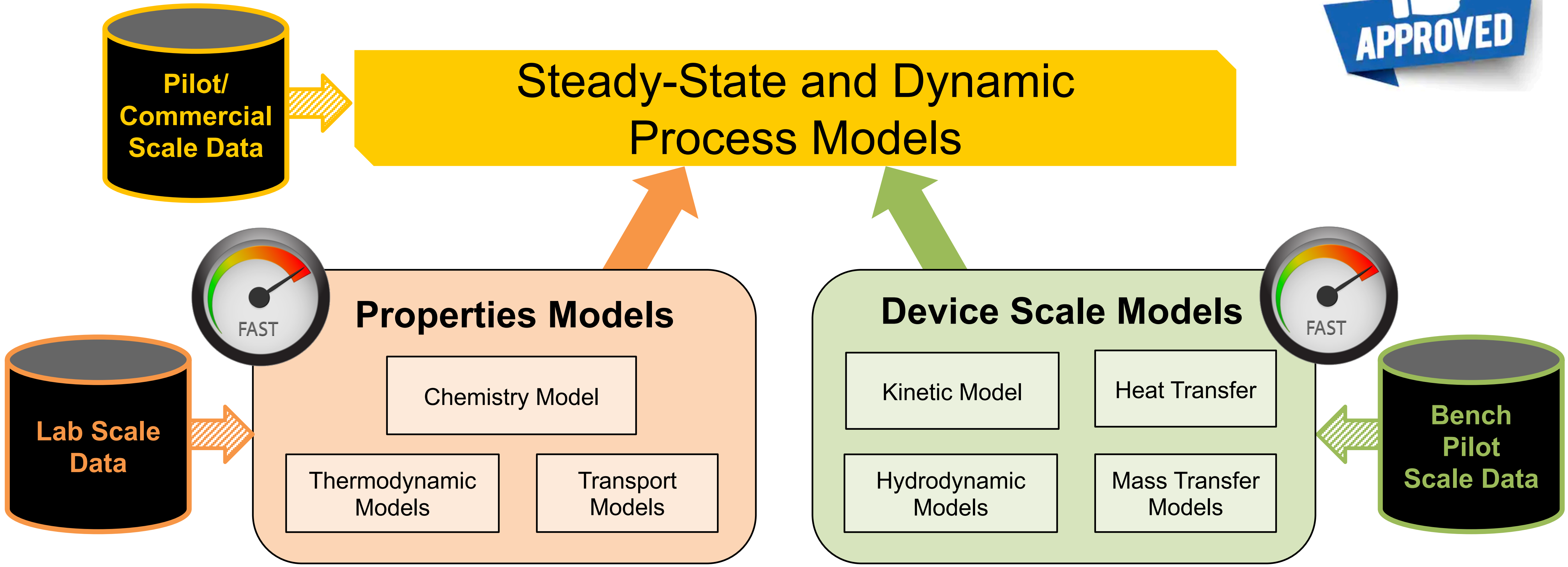
Returning back to the Machine Learning Roadmap…

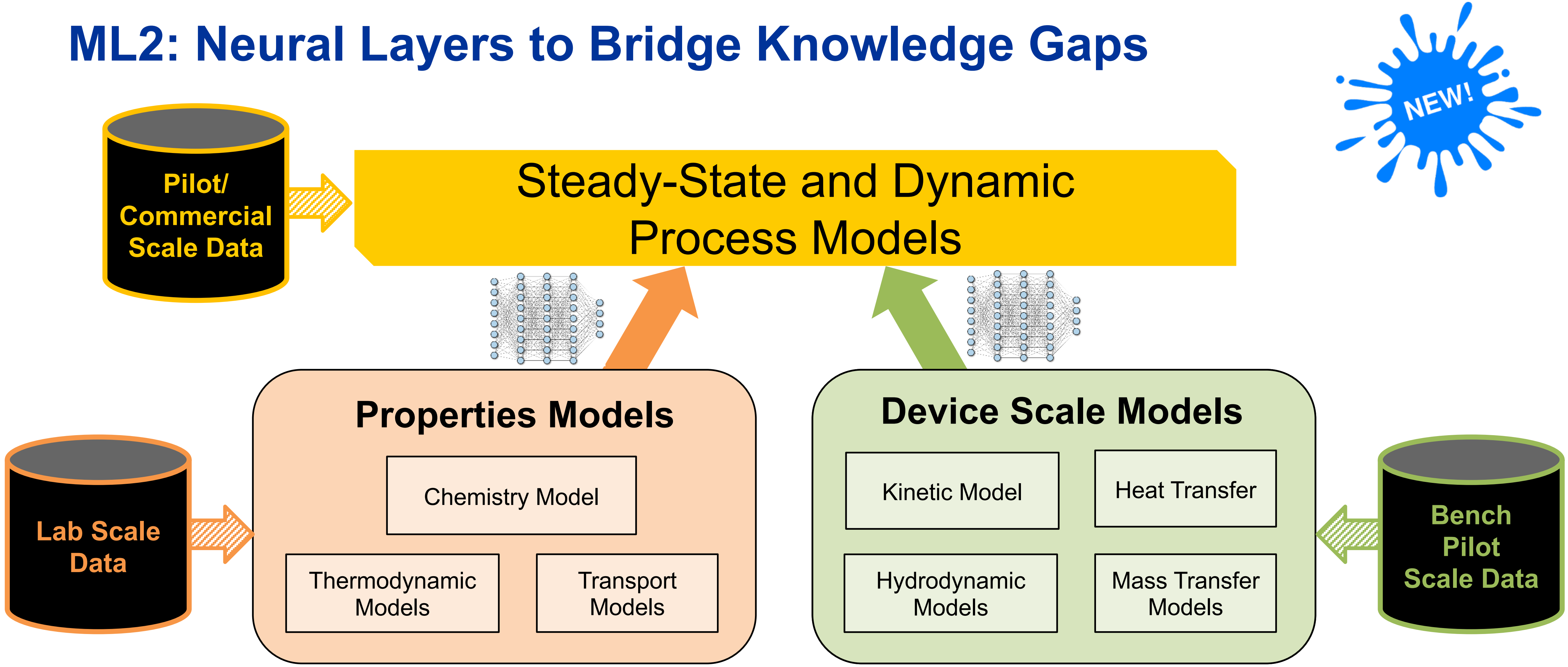


ML1: Fast Surrogates to Mitigate Bottleneck Processes



Approach: Leverage neural networks to learn fast surrogates for CFD models

ML2: Neural Layers to Bridge Knowledge Gaps



Approach: Mix and match (traditional) neural network layers with PDEs

ML2: Neural Layers to Bridge Knowledge Gaps

NEW!

Dandekar & Barbastathis (2020), "Quantifying the Effect of Quarantine Control in COVID-19 Infectious Spread Using Machine Learning", medRxiv 2020.04.03.20052084

Quarantine population $T(t)$

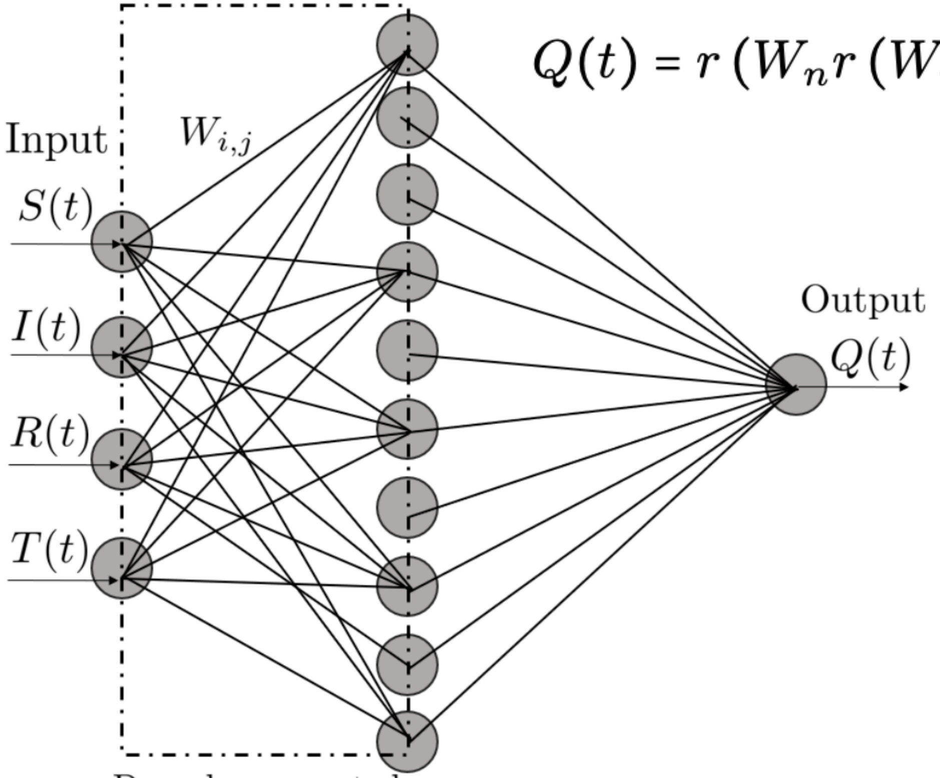
$$U = (S(t), I(t), R(t), T(t))$$

$$\frac{\mathrm{d}S(t)}{\mathrm{d}t} = -\frac{\beta\, S(t)\, I(t)}{N}$$

$$\frac{\mathrm{d}I(t)}{\mathrm{d}t} = \frac{\beta\, S(t)\, I(t)}{N} - \left(\gamma + Q(t)\right) I(t) = \frac{\beta\, S(t)\, I(t)}{N} - \left(\gamma + \mathrm{NN}(W,U)\right) I(t)$$

$$\frac{\mathrm{d}R(t)}{\mathrm{d}t} = \gamma I(t)$$

$$\frac{\mathrm{d}T(t)}{\mathrm{d}t} = Q(t)\, I(t) = \mathrm{NN}(W,U)\, I(t).$$



Quarantine strength $Q(t)$

$$Q(t) = r\left(W_n r\left(W_{n-1} \ldots r\left(W_1 U\right)\right)\right) \equiv \mathrm{NN}(W,U)$$

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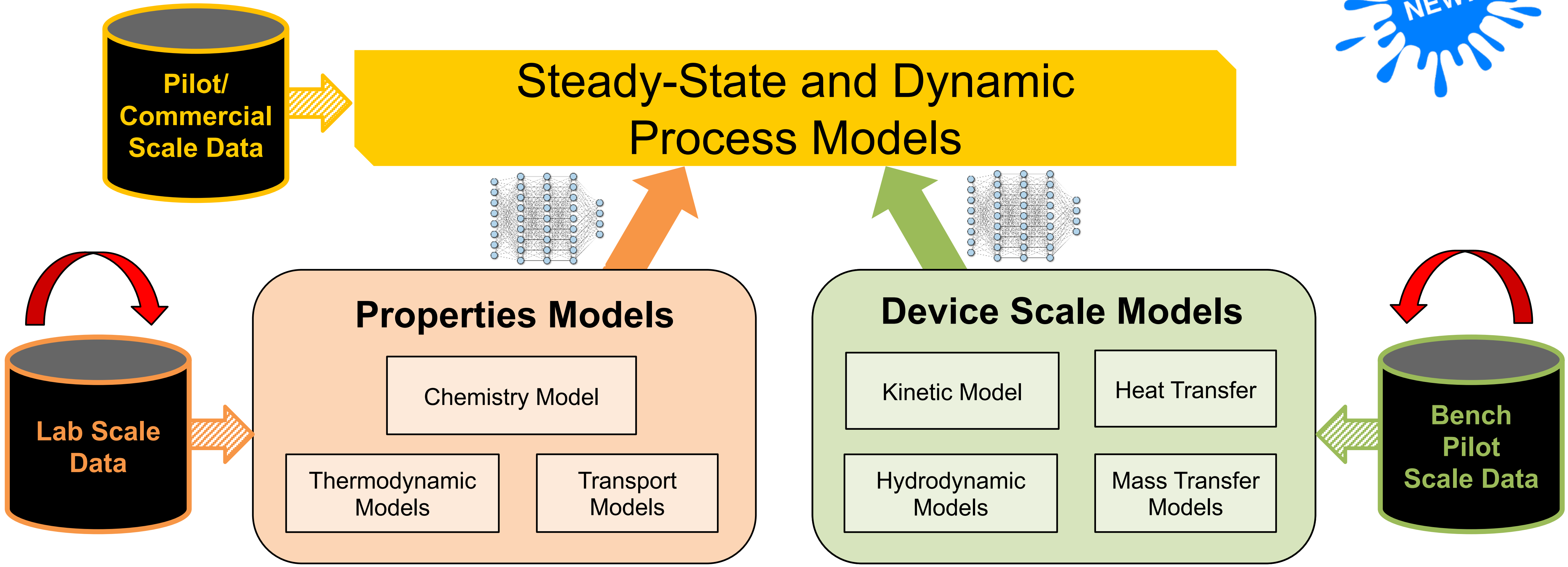
ML3: Reinforcement Learning for Optimal Control

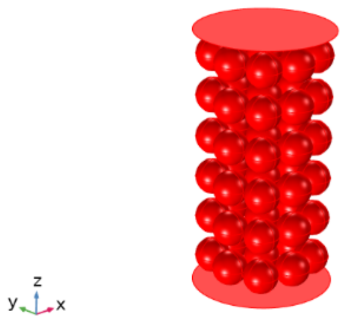
NEW!

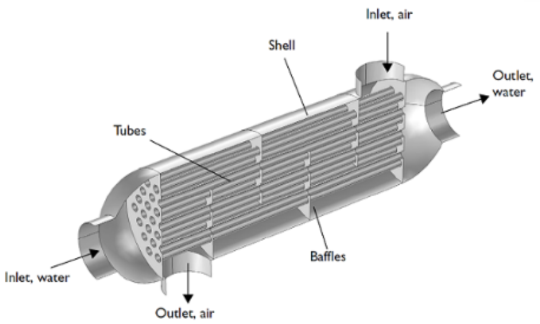


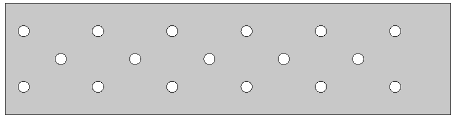
Approach: Apply reinforcement learning to optimize device configuration to drive performance

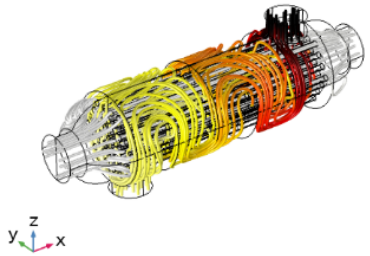
ML3: Control Problems for Absorption/Desorption Processes

- Changes in flue gas flow rate
- Changes in flue gas inlet CO_2 concentration
- Changes in the inlet flue gas temperature









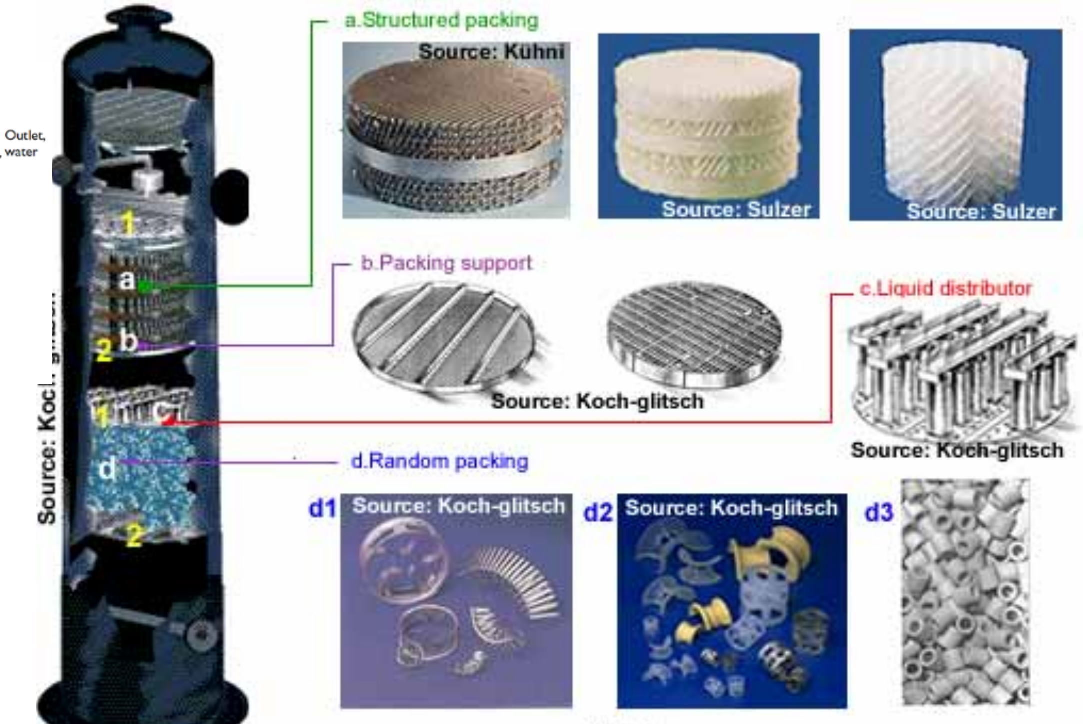
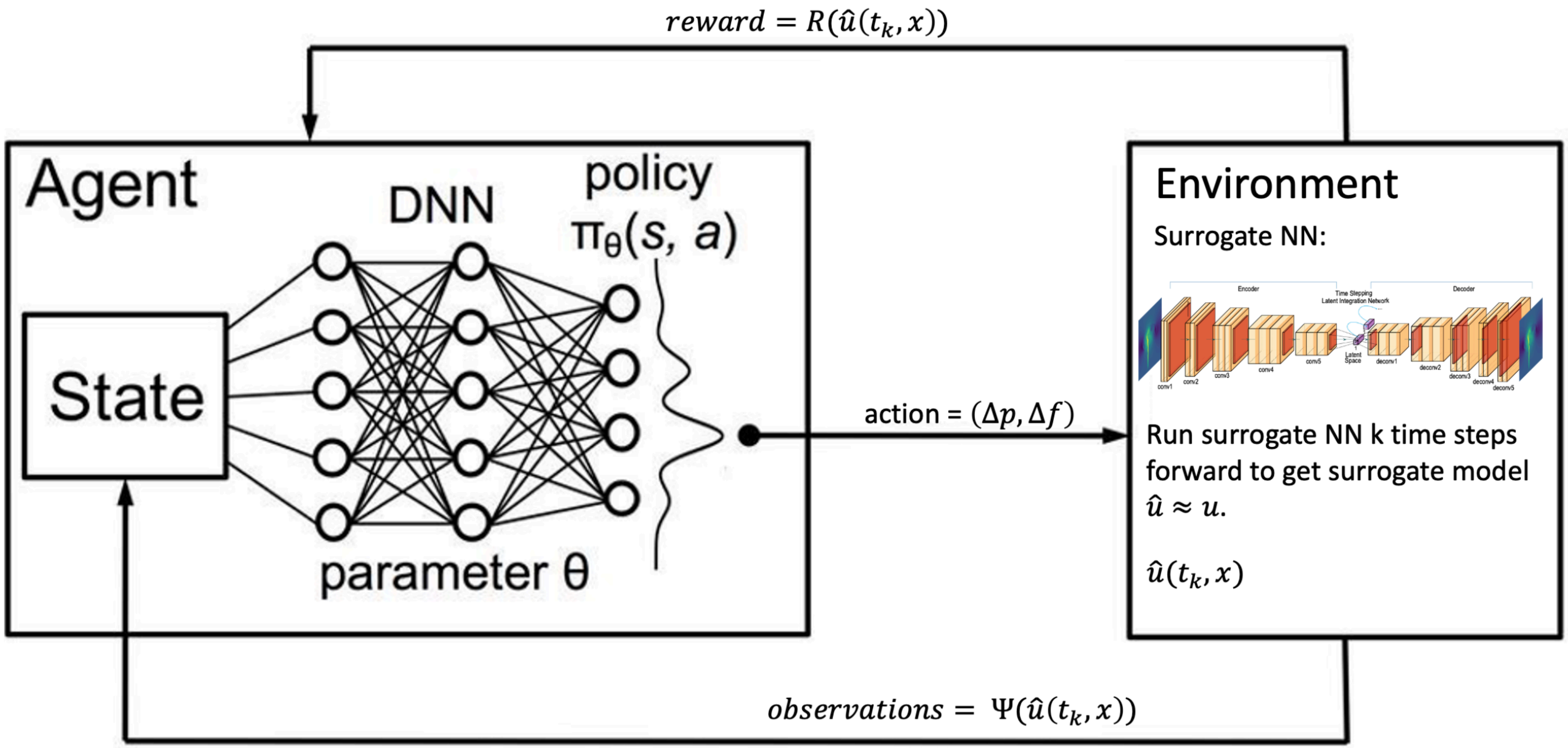


Fig.1

ML3: Reinforcement Learning for Optimal Control

- RL agent learns a policy to optimally explore CFD inputs



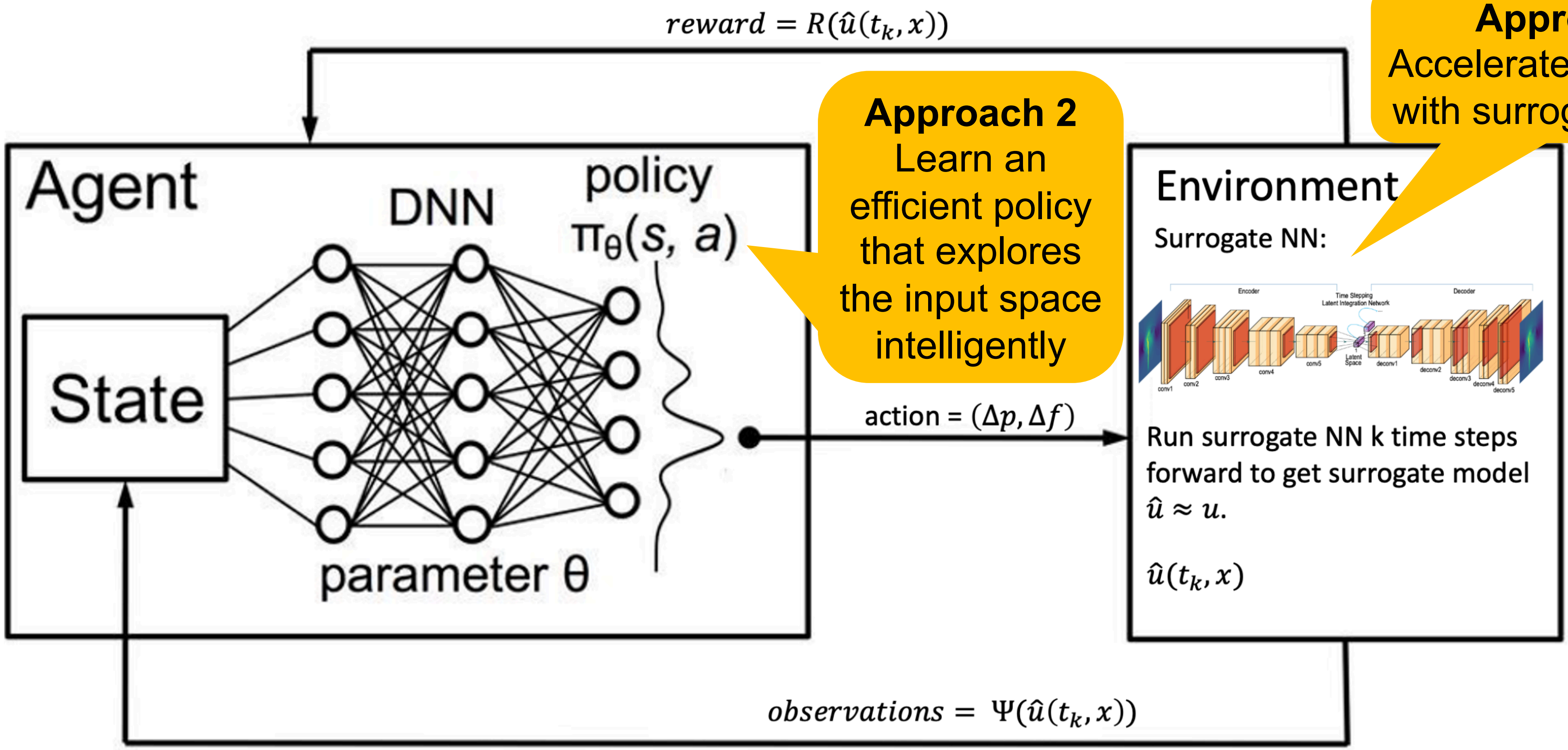
ML3: Reinforcement Learning for Optimal Control

- RL agent learns a policy to optimally explore CFD inputs

NEW!

Approach 1
Accelerate simulations with surrogate models

Approach 2
Learn an efficient policy that explores the input space intelligently



RL needs 1000s of simulations to train.

Use a surrogate to generate sim data.

Summary

CCSI² has a vision to leverage Machine Learning methods on high-dimensional data from CFD models to:

- **Reduce computational burden** of expensive CFD models
- **Inform process models** with knowledge derived from CFD results
- **Establish control methodologies** of the Absorption/Desorption processes

Our Machine Learning Roadmap will achieve these goals:

- ✓ Fast Surrogates to **Mitigate Bottleneck Processes**
- ✓ Neural Layers to **Bridge Knowledge Gaps**
- ✓ Reinforcement Learning for **Optimal Control**

CCSI²

Carbon Capture Simulation for Industry Impact

For more information

https://www.acceleratecarboncapture.org/

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