

Accelerating Barracuda Virtual Reactor Workflow with AI-Powered ROMs

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CPFD Software

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What CPFD Is Building: ML-ROM Capability Layers

1

Eulerian Field ROM

Fast prediction of fixed-mesh fields such as particle volume fraction and gas species.

2

Lagrangian Field ROM

Particle/parcels-aware ROM for transient solids motion, bed evolution, and regime behavior.

3

Parameter-Conditioned ROM

Interpolation across operating conditions such as velocity, air flow, injection rate, and material settings.

4

Interactive Engineering Layer

Snapshot queries, what-if studies, design exploration, calibration, and digital twin support.

MAIN TAKEAWAY

CPFD is not replacing Barracuda. CPFD is building acceleration layers around Barracuda-generated physics.

Why Acceleration Matters in Industrial Multiphase CFD

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Acceleration Drivers



Design Space Exploration

Evaluate more geometries, operating conditions, and physics models



Optimization & Calibration

Systematic parameter tuning across high-dimensional spaces



Digital Twins

Real-time virtual replicas requiring continuous simulation updates



Turnaround Time

Compress weeks of analysis into hours for faster decision-making

AI is Shifting Toward



Transient Trajectory Learning

Capturing time-dependent behaviors across simulation runs



Parameter + Time Conditioning

Models that generalize across operating conditions and timesteps



Industrial-Scale Focus

Moving beyond academic benchmarks to real-world complexity



AI as Augmentation

Enhancing — not replacing — physics-based simulation tools

Why ML for CFD is Hard to Trust — and What it Must Satisfy

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Sources of Skepticism



Conservation + Stability Risk

Small errors can blow up over long transients or stiff regimes



Out-of-Distribution Behavior

Models interpolate well but extrapolate poorly without clear warning



Validation Burden

Trust requires reproducibility across operating envelopes, not single-case agreement



Deployment Constraints

Industrial workflows demand large-mesh compatibility, solver integration, and traceability

Engineering Requirements

Solver-Consistent Target

Learn the behavior of validated CFD — not replace governing equations

Predictable Failure Modes

Known envelopes and guardrails for safe deployment boundaries

Clear Validation Pathway

Metrics tied to decision variables (e.g., lift, pressure drop, etc.)

Non-Intrusive Integration

Drop-in inference on existing meshes and fields, preserving solver workflows

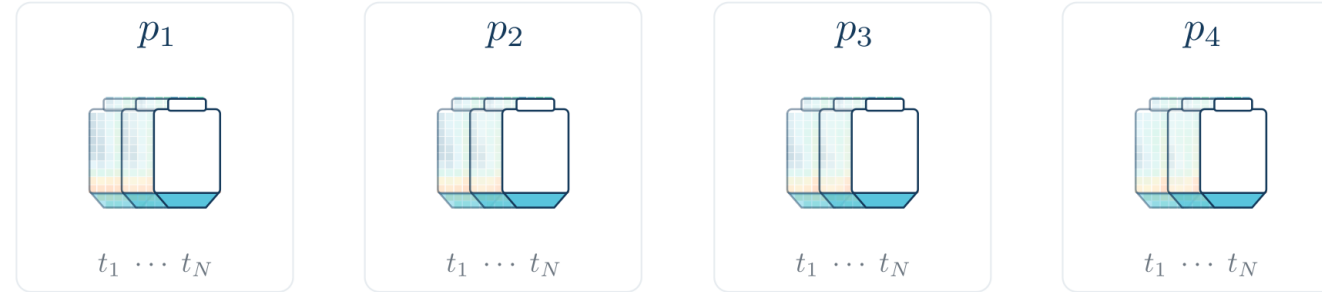
The objective is not solver replacement — it is accelerating validated CFD with controlled, deployable surrogates.

Method Tradeoffs Under Industrial-Scale Constraints

	Main Strength	Industrial Limitation	Why CPFD chose Graph-ROM
 POD	Fast	Limited generalization	Useful baseline
 PINNs	Physics residuals	Expensive at large mesh scale	Not deployment-ready yet
 Neural Operators	Promising	Active research for complex industrial geometry	Future direction
 Graph-ROM	Mesh-aware and scalable	Needs high-quality training data	Current practical path

GNN-ROM: Continuous-Time Graph Operator

TRANSIENT TRAINING DATA



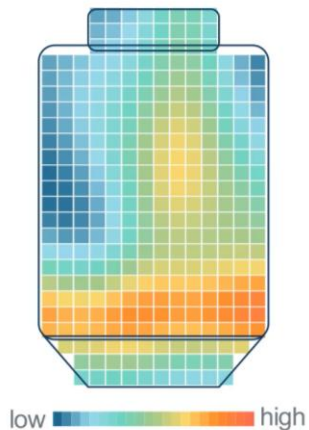
Offline Training

$$\{G(p_i, t_k)\} \rightarrow \theta$$

Unseen query: p^*, t^*

Eulerian Snapshot

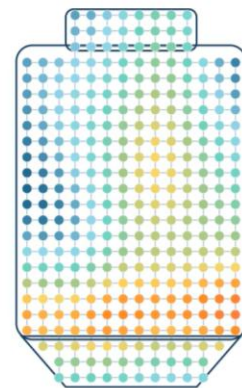
$$S(p_i, t_k)$$



same mesh connectivity

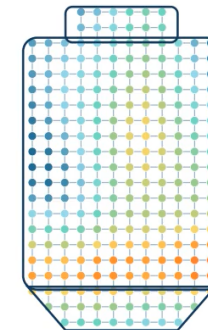
Graph Sample

$$G(p_i, t_k)$$



Inference Graph

$$G^*$$



Trained GNN-ROM θ

GAT Layer 1

GAT Layer 2

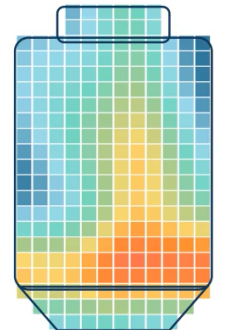
GAT Layer 3

GAT Layer 4

128 hidden features / layer

Predicted Field

$$\hat{Y}(p^*, t^*)$$



Nodes, Edges fixed
topology reused

Features vary
field, p_i, t_k

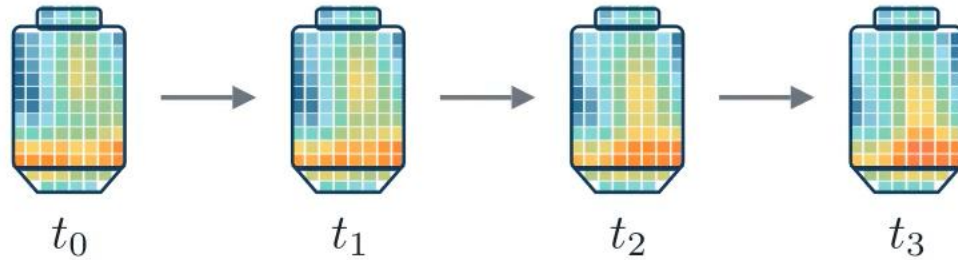
Graph sample
used in training

Single-shot prediction at unseen parameter

GNN-ROM: Fourier conditioned time

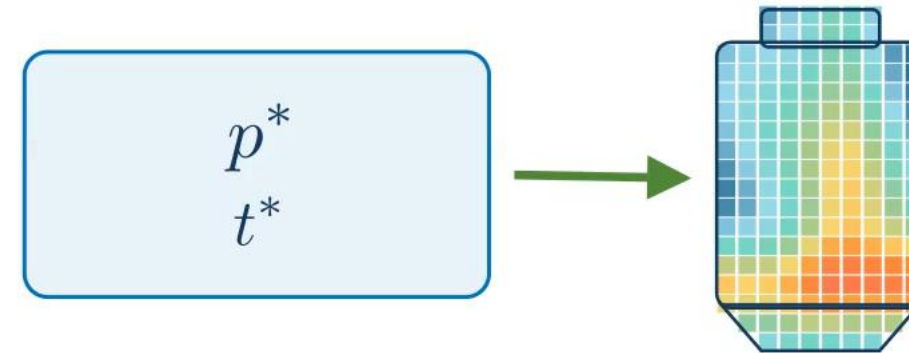


Sequential



Error accumulates

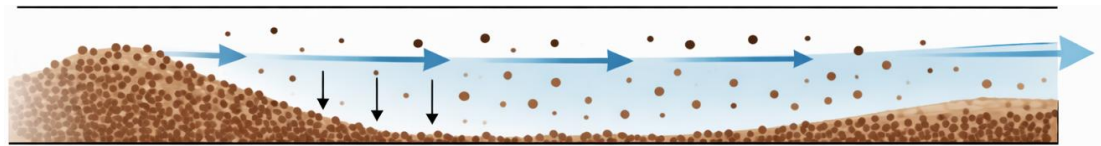
Trained GNN-ROM



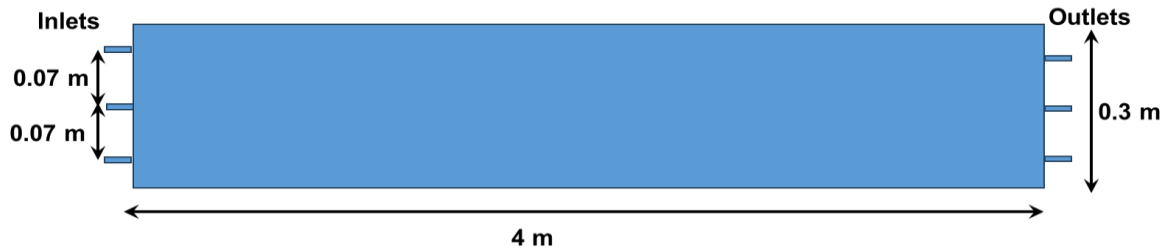
Single forward pass

No autoregressive error accumulation

Application 1: Hydraulic Fracture (Validation)



Gravity-driven settling + advection in a single fracture



Laboratory Scale Experiment (Zhou et al., 2025)

Physical Configuration

Geometry

- 4.0 m x 0.3 m x 0.01 m
- Rectangular slot fracture

Fluid

- Slick water (~ 2.5 mPa-s)
- Shear-thinning behavior

Proppant

- 40/70 mesh ceramsite
- Initial particle vol frac = 6%
- Gaussian size distribution

Barracuda Virtual Reactor (CFD Model)

- $\sim 170,000$ Eulerian cells ($470 \times 36 \times 10$)
- 9 million Lagrangian parcels
- MP-PIC formulation
- Modified Beetstra drag (Chhabra adaptation)

ROM Scope

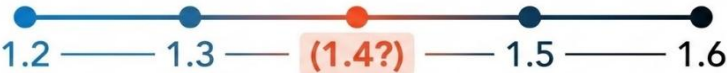
- Non-intrusive Eulerian ROM
- Input/Output: Particle volume fraction | Fixed mesh connectivity

Training Envelope

1.2 | 1.3 | 1.5 | 1.6
Inlet velocities (m/s)

Unseen Test Condition

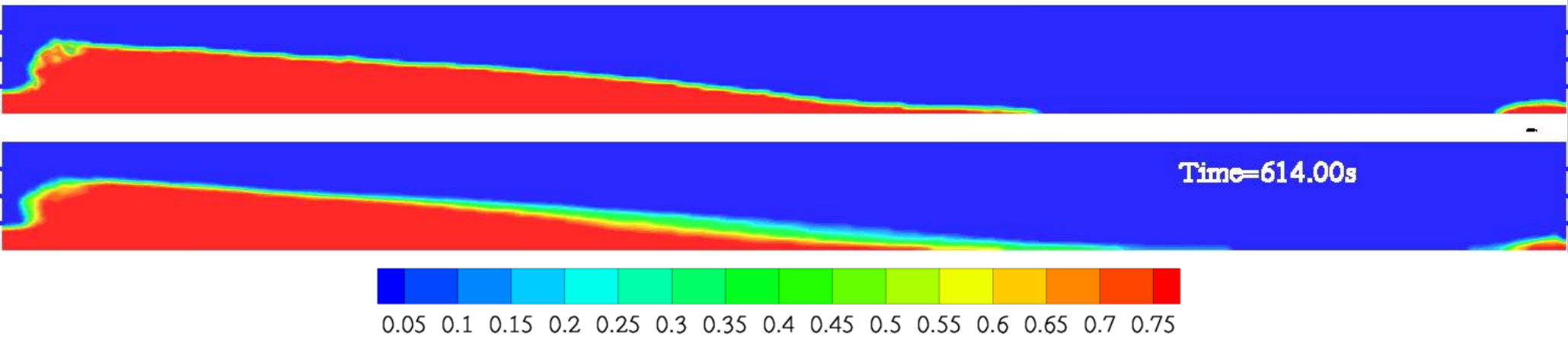
1.4 m/s
Not used in training



Application 1: Hydraulic Fracture (Validation)

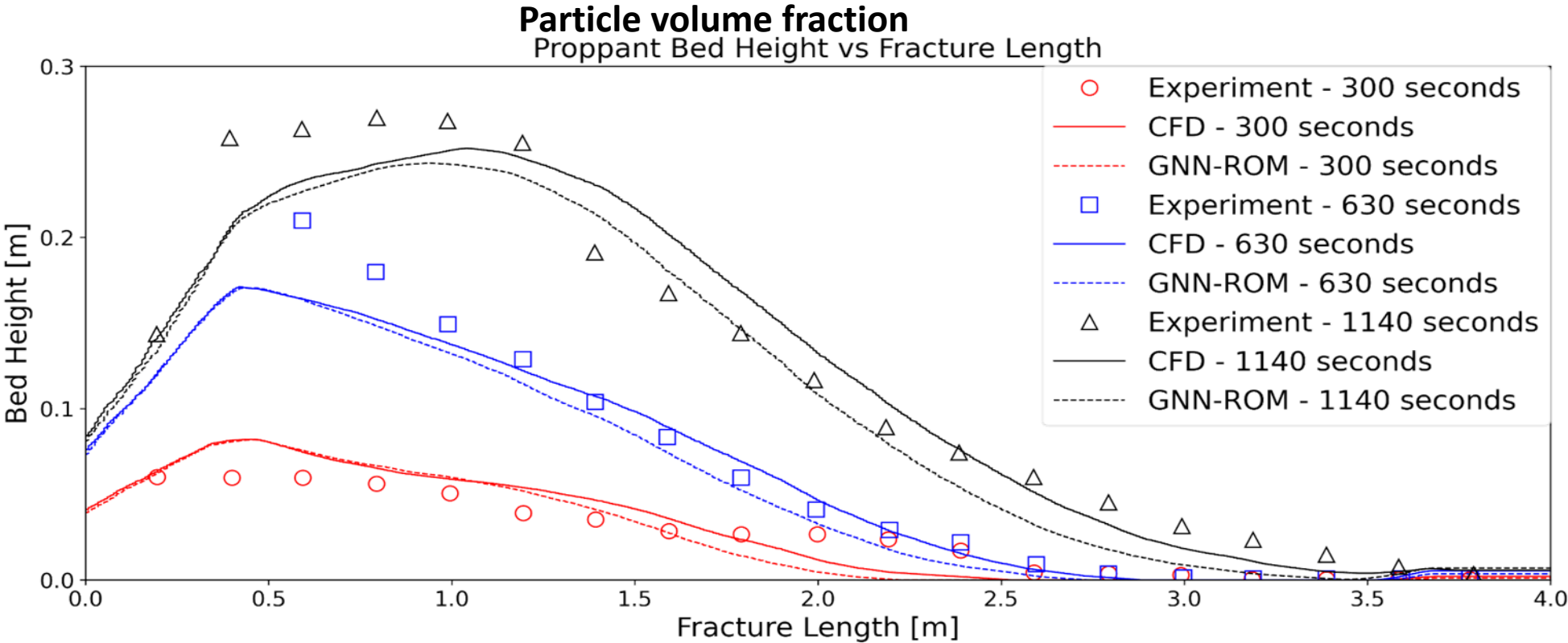
CFD – Reference

GNN-ROM – Prediction



$MAE_{bed_height} < 0.02\text{ m}$

ROM tracks spatial deposition profile



Geometry-Aware ROM: Multiple-Fracture Proppant Transport

Built on the PhysicsNeMo framework — joint research between CPFD and NVIDIA

ROM Capability Demonstrated

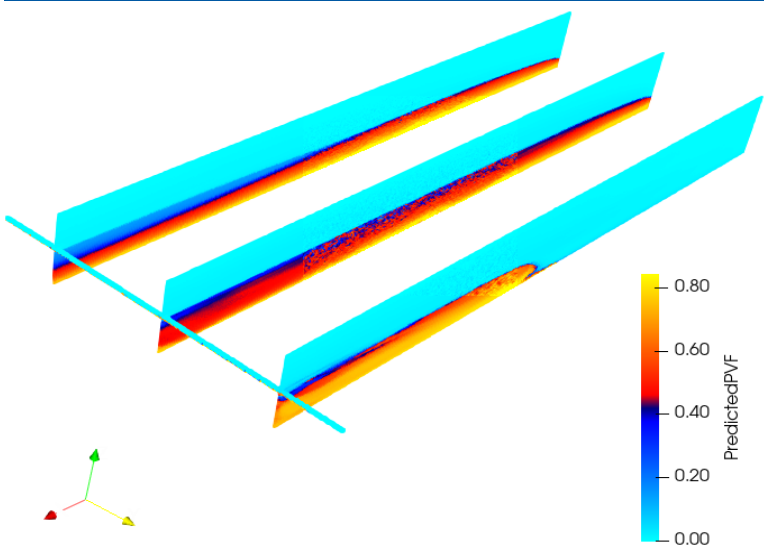
- ✓ Geometry-aware ROM prediction for multi-fracture proppant transport
- ✓ Trained across multiple fracture spacings: **3–30 m**
- ✓ Generalization across fracture spacing: **10 m and 18 m**
- ✓ CFD-like particle volume fraction fields
- ✓ Inference time: **< 1 second per query**
- ✓ Supports fast screening of alternative geometry layouts and flow conditions

Collaboration with NVIDIA

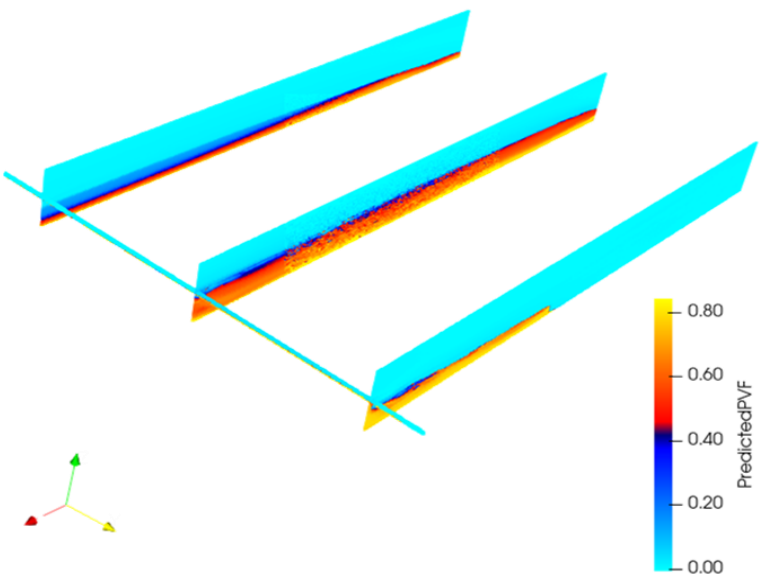
PhysicsNeMo is NVIDIA's open-source physics-ML framework



PhysicsNeMo (ROM)

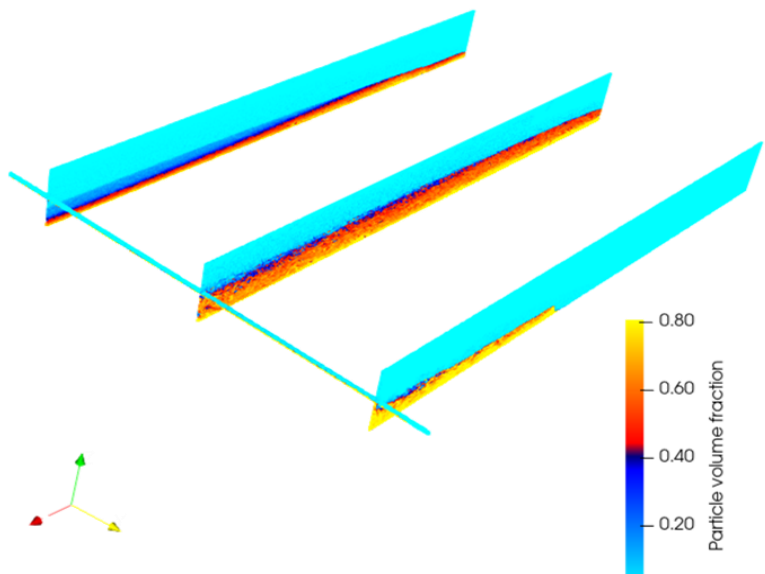
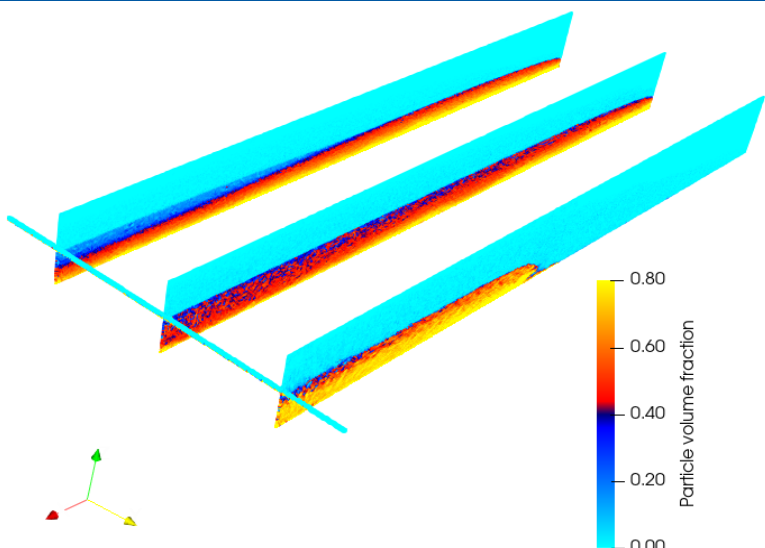


10 m

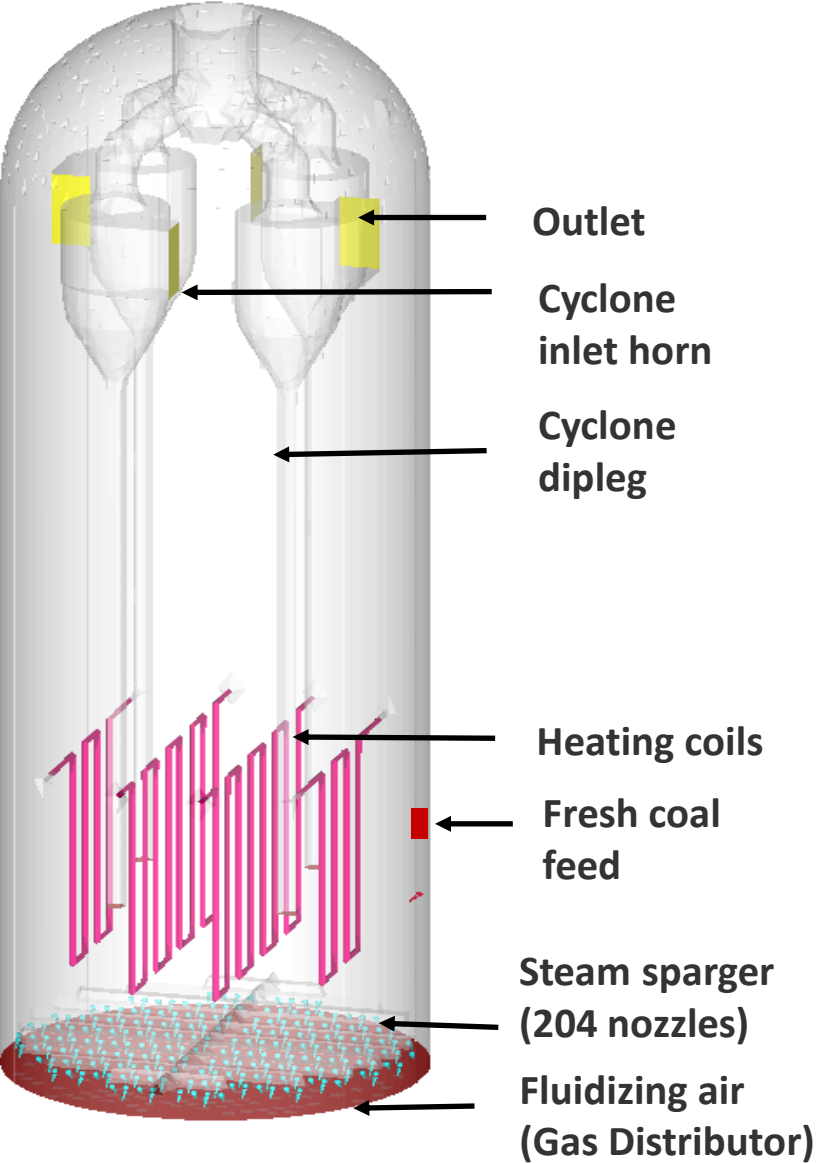


18 m

Barracuda CFD (Reference)



Application 2: Fluidized-Bed Gasifier (Generalization)

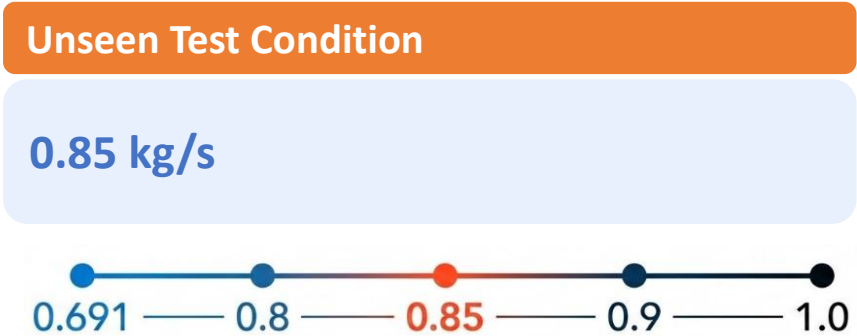


Baseline Operating Conditions	
Fluidizing Air Flow	0.691 kg/s
Air Temperature	700 K
Air Composition	77% N ₂ / 23% O ₂
Steam Flow	0.296 kg/s
Steam Temperature	900 K
Steam Injection	204 nozzles
Wall Temperature	~1300 K
Outlet Pressure	200 kPa

Barracuda Virtual Reactor	
80,010 Eulerian control volumes	
1.1 million Lagrangian parcels	
MP-PIC formulation	
Tang drag correlation	
Volume-averaged chemistry	
Chemistry: Devolatilization, Char oxidation, Steam gasification	

Strongly coupled hydrodynamics + reactions + transport

Training Envelope	
	0.691 kg/s
	0.8 kg/s
	0.9 kg/s
	1.0 kg/s



Fluidizing air mass flow rates

Application 2: Fluidized-Bed Gasifier (Time-Average Fields)

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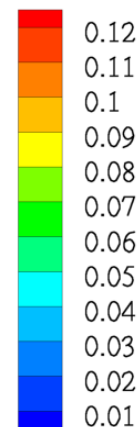
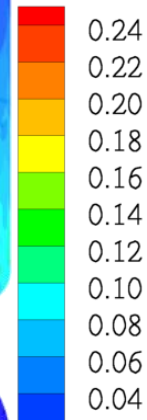
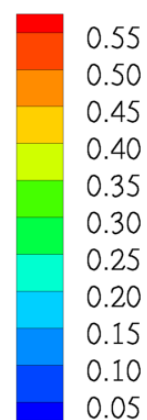


Particle Volume-fraction

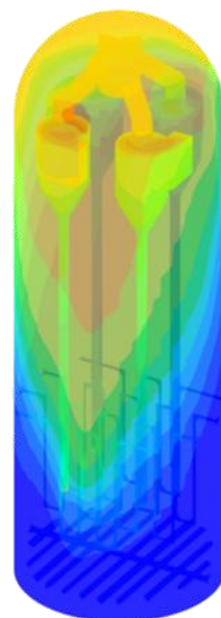
CH₄ (g)

CO₂ (g)

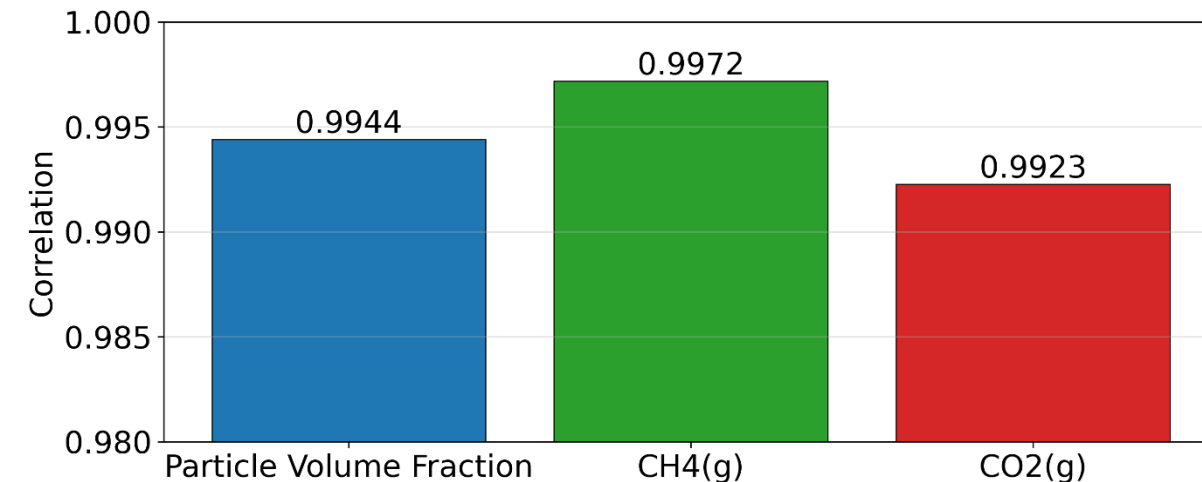
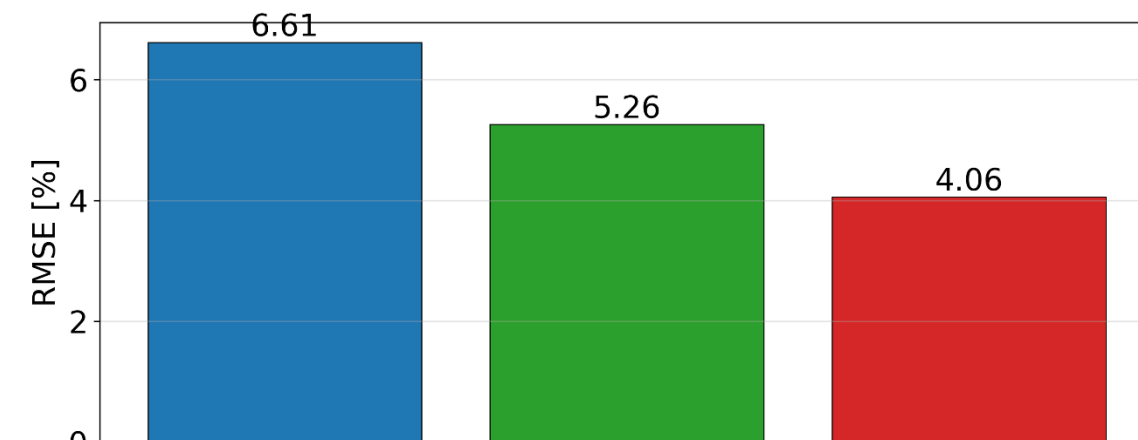
CFD – Reference



GNN-ROM – Prediction



Unseen Operating Condition: Air Flow = 0.85 kg/s (Not Used in Training)



Generalizes to unseen operating condition with <7% RMSE and >0.99 spatial correlation

Application 2: Fluidized-Bed Gasifier (Transients)

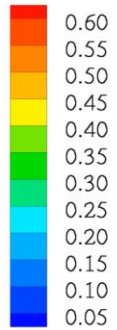
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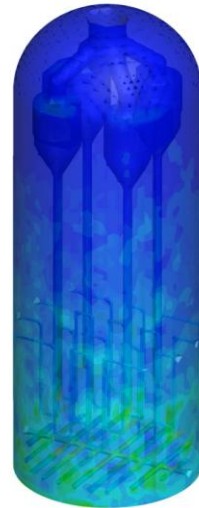
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Time=48.80 s

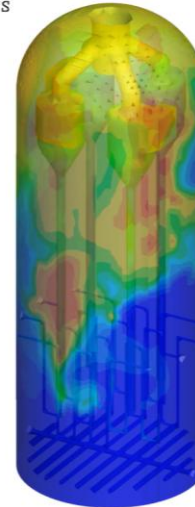
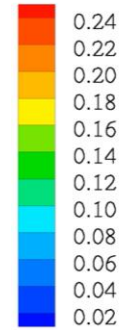


CFD - Reference

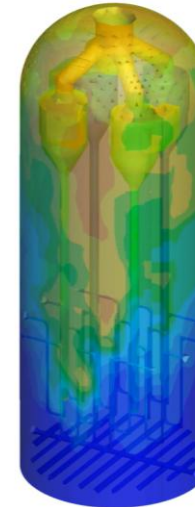


GNN-ROM - Prediction

Time=49.40 s

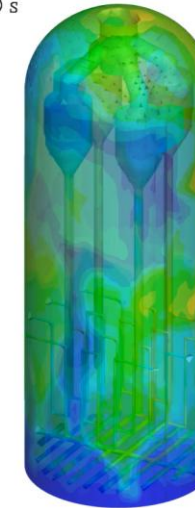
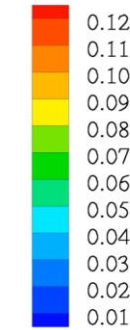


CFD - Reference



GNN-ROM - Prediction

Time=48.80 s



CFD - Reference



GNN-ROM - Prediction

Particle Volume-fraction

CH4 (g)

CO2 (g)

Unseen Operating Condition: Air Flow = 0.85 kg/s (Not Used in Training)

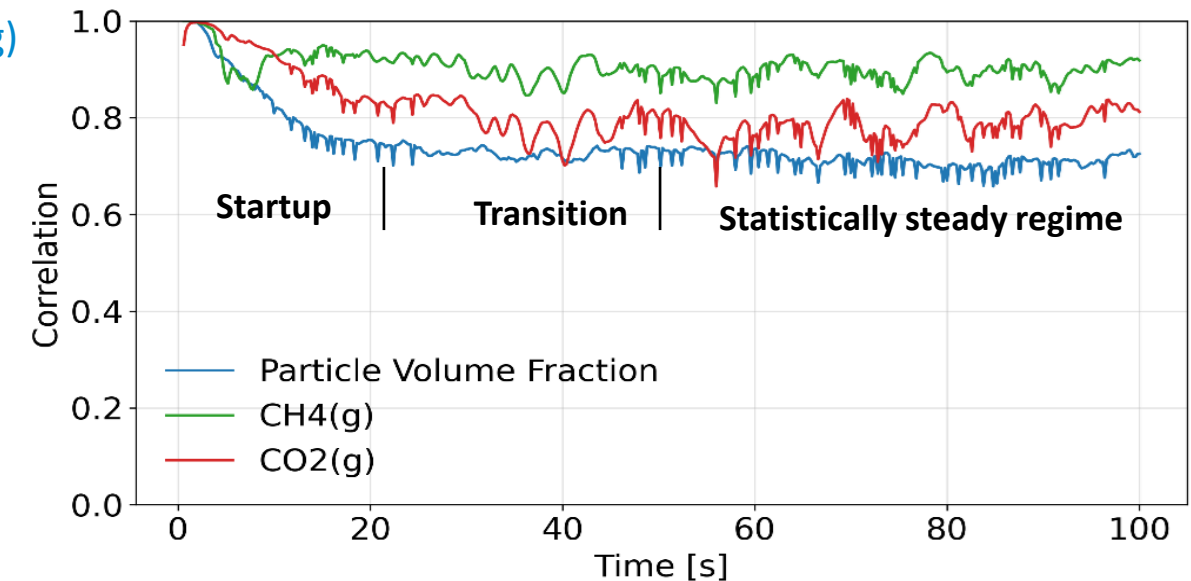


Key Observations:

Startup reorganization captured

Large-scale circulation preserved

Evolution of reaction fronts captured



Why Lagrangian ROM Matters

Foundation: Barracuda already maps particles onto Eulerian cells → particle volume fraction & solids motion as field data

Eulerian GNN-ROM

Accelerates field prediction

- ✓ Speeds up Barracuda's **fixed-mesh field** predictions
- ✓ Returns **volume-fraction & velocity fields** on the Eulerian grid
- ✓ Familiar **mesh-aware** output format for CFD users

Lagrangian PointNet-GNN-ROM

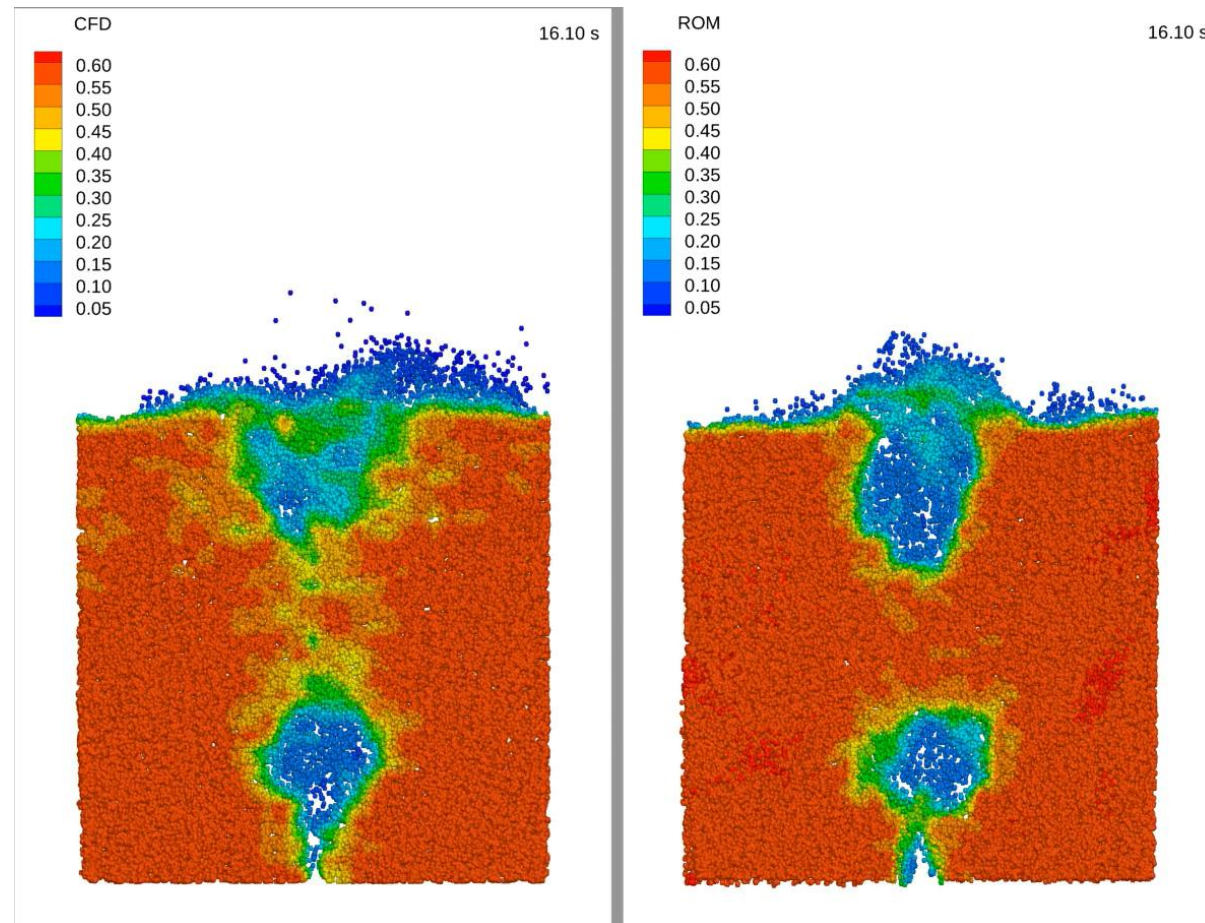
Adds particle-cloud awareness — native to MP-PIC

- ◆ **Architecture:** PointNet captures global cloud state; GNN message passing captures local interactions
- ◆ **Unlocks engineering descriptors:** bed height & expansion, center of mass, solids spread, spout structure, segregation, regime-change indicators
- ◆ **Parameter-conditioned:** predicts cloud descriptors at unseen operating conditions

TAKEAWAY

Eulerian ROM accelerates field prediction. **Lagrangian ROM** turns particle-cloud evolution into fast engineering descriptors for fluidization, spouting & solids transport.

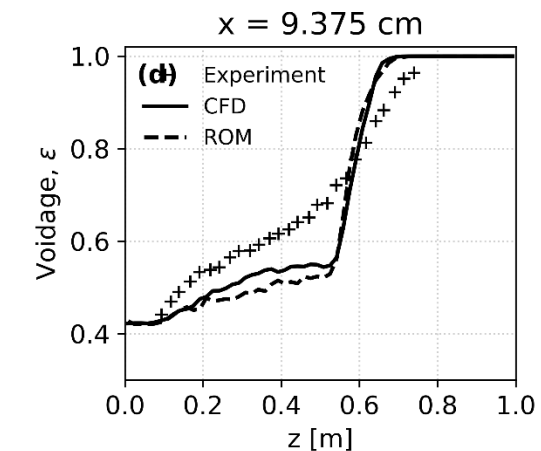
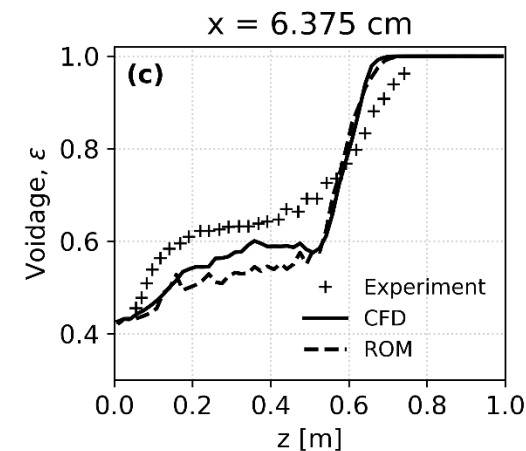
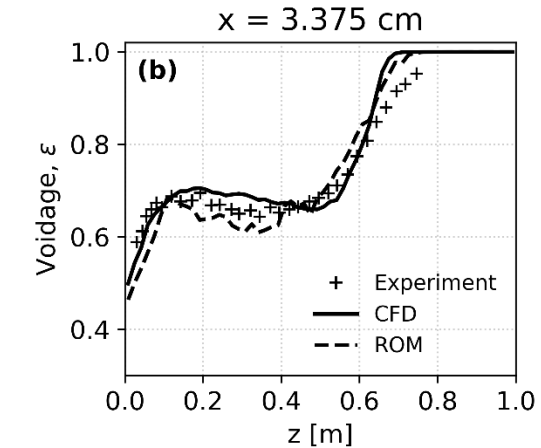
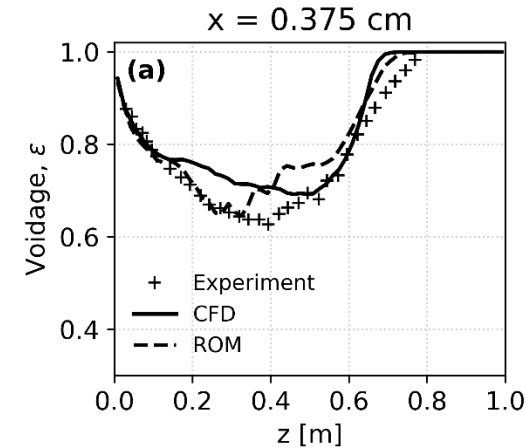
Application 3: Kuiper's Bed (Validation)



CFD – Reference

PointNet-GNN-ROM – Prediction

Particle Volume-fraction



Training Envelope

8 m/s

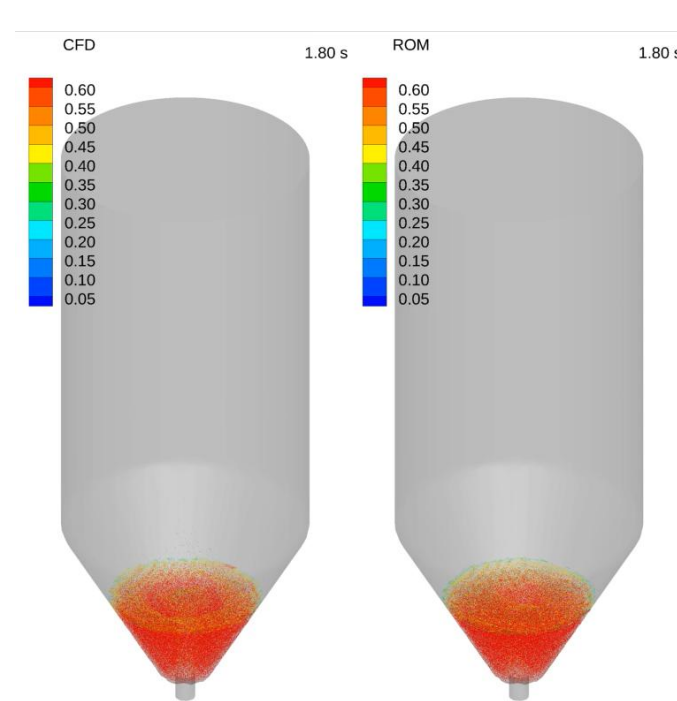
12 m/s

Unseen Test Condition

10 m/s

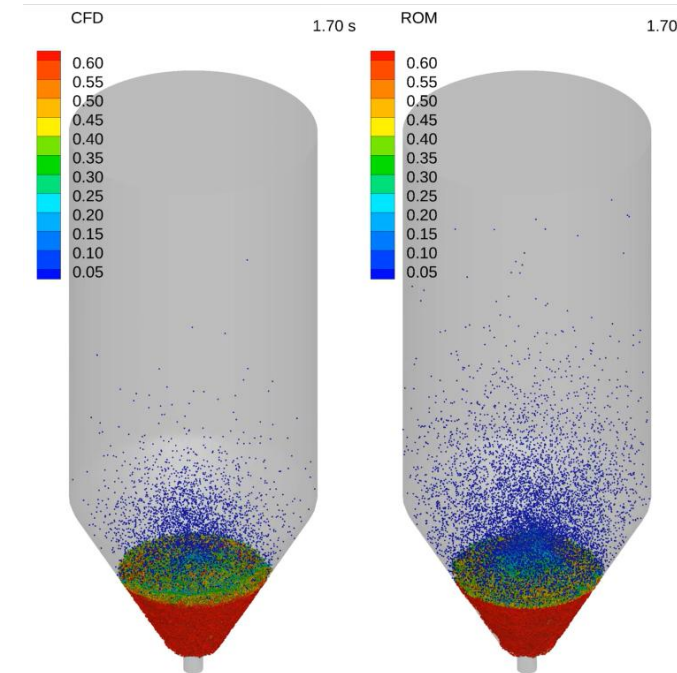
(Not used in training)

Application 4: Spouted Bed (Testing Regime Change)



CFD – Reference PointNet-GNN-ROM – Prediction

Regime 1 – Center-jet velocity = 40 m/s



CFD – Reference PointNet-GNN-ROM – Prediction

Regime 2 – Center-jet velocity = 52 m/s

Training Envelope

10 m/s

30 m/s

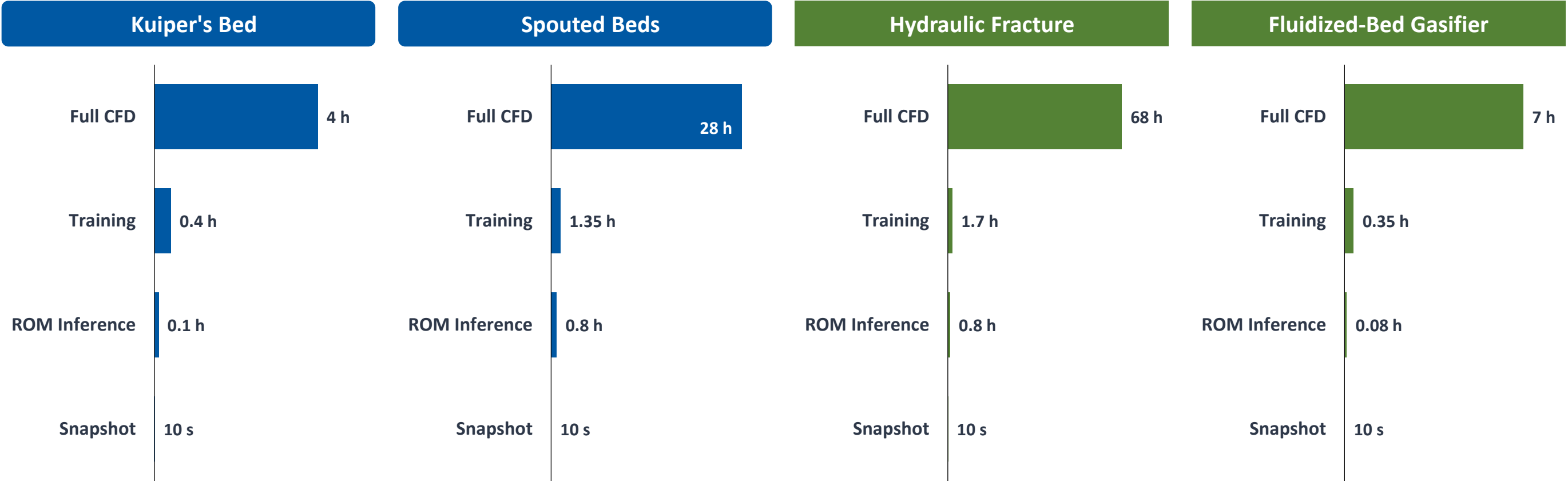
60 m/s

Unseen Test Condition

40 m/s (Not used in training)

52 m/s (Not used in training)

Reduced Order Models Boost Performance & Efficiency



Key Findings

- ✓ Eulerian ROM: 80–90x Faster than full CFD (Hydraulic Fracture, Fluidized-Bed Gasifier)
- ✓ Lagrangian ROM: 35–40x Faster than full CFD (Kuiper’s Bed, Spouted Beds)
- ✓ Real-time snapshot queries (<10 s) on all geometries

GNN-ROM preserves MP-PIC physics while enabling deployment-scale transient prediction across diverse geometries.

Where CPFD's ROM Direction Differs

CPFD's differentiator: transient + multiphase + complex geometry ROMs built around validated Barracuda physics

Common AI-CFD demos	CPFD ROM direction
Slow training-data generation	GPU-accelerated Barracuda data pipeline
Broad generic training datasets	Targeted ROMs with lower training-data burden
Steady or time-averaged	Transient evolution
Single-phase or weak coupling	Dense gas/liquid-solid multiphase
Simple benchmark geometry	Industrial reactor / fracture geometries

BOTTOM LINE

This is not generic surrogate modeling. This is **ROM development for dense industrial multiphase CFD.**

From Validation to Deployment: What This Enables

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Rapid Parametric Exploration

- Evaluate 10–100 operating points in hours, not weeks
- Interpolate across air flow / injection rates
- Identify optimal regimes



Model Calibration

- Match plant data via fast surrogate evaluation
- Tune drag, reaction, closure models
- Embed into solver workflows



Digital Twin Infrastructure

- Real-time field queries
- Snapshot <10 seconds
- 99% less energy per evaluation



Interactive Engineering

- What-if scenarios
- Startup transients
- Sensitivity studies

AI as acceleration layer — not solver replacement.



Release Timeline

Roadmap through Q4 2026

► Features

- Eulerian field prediction: PVF, gas species, reacting-flow fields
- Lagrangian solids descriptors: bed height, COM, solids spread, spout structure
- Parameter-conditioned inference across operating envelopes
- Continuous-time snapshot queries
- ROM vs CFD validation reports
- Engineering metrics tied to design decisions
- What-if studies across flow conditions and geometries
- GUI-based ROM inference and visualization



Advanced Models

Collaboration with nVidia

- Geometry generalization
- More models via PhysicsNeMo
 - Transformers
 - Neural Operators
 - MeshGraphNet



Get In Touch

Connect with our team

Saurav Mitra

CPFD Software

cpfd-software.com

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