

A Comprehensive Machine Learning Framework for Benchmarking Complex Multiphase Flows

Harish Ramachandran - Björn Kimpel
Thomas Paula - Josef Winter - Steffen Schmidt - Nikolaus Adams

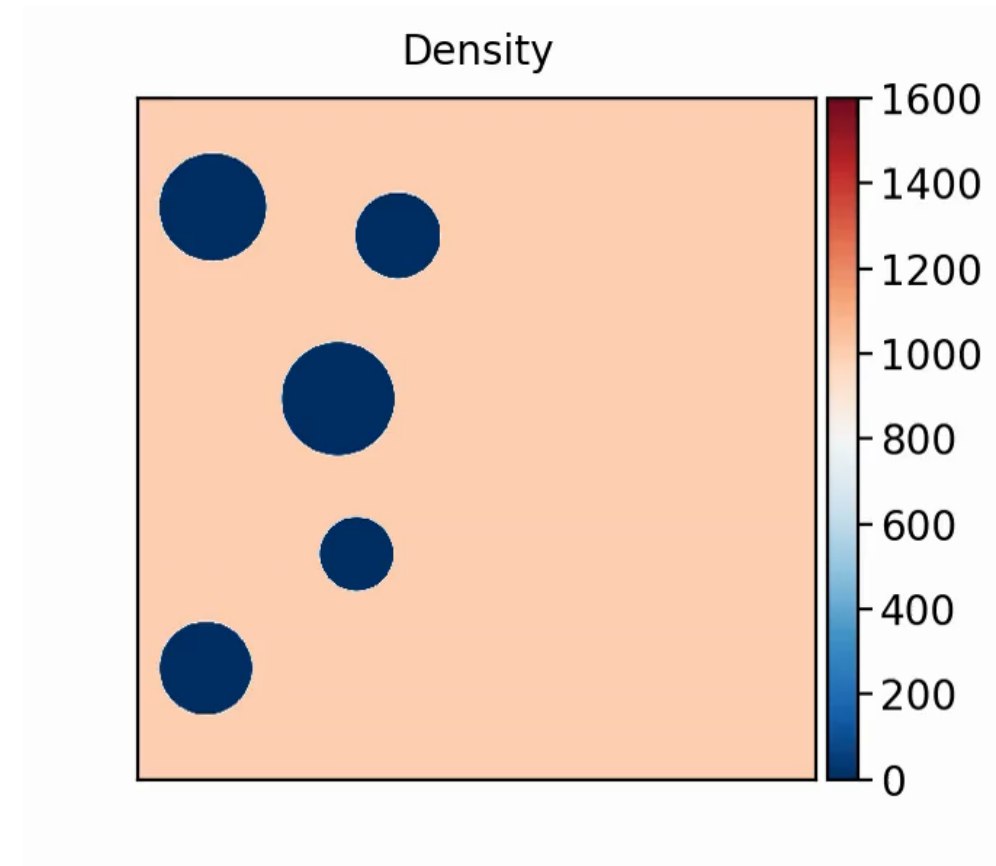
Technical University of Munich

NeurIPS 2026 - Evaluations & Datasets Track



Challenges for ML Surrogates

- Shock waves $\rightarrow$ sharp discontinuities
- Material interfaces $\rightarrow$ strong density jumps
- Interface deformation and breakup





The Datasets

6

Datasets

2D & 3D

Dimensions

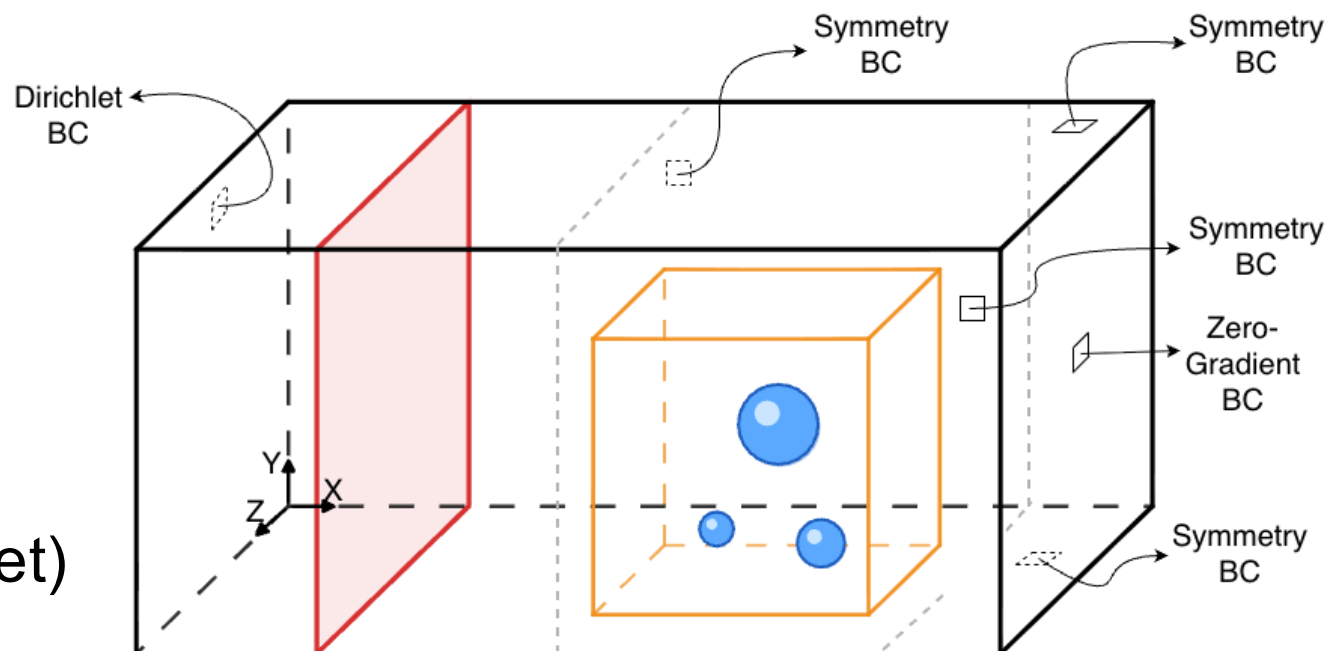
OOD & ID

Test splits

~ 3 TB

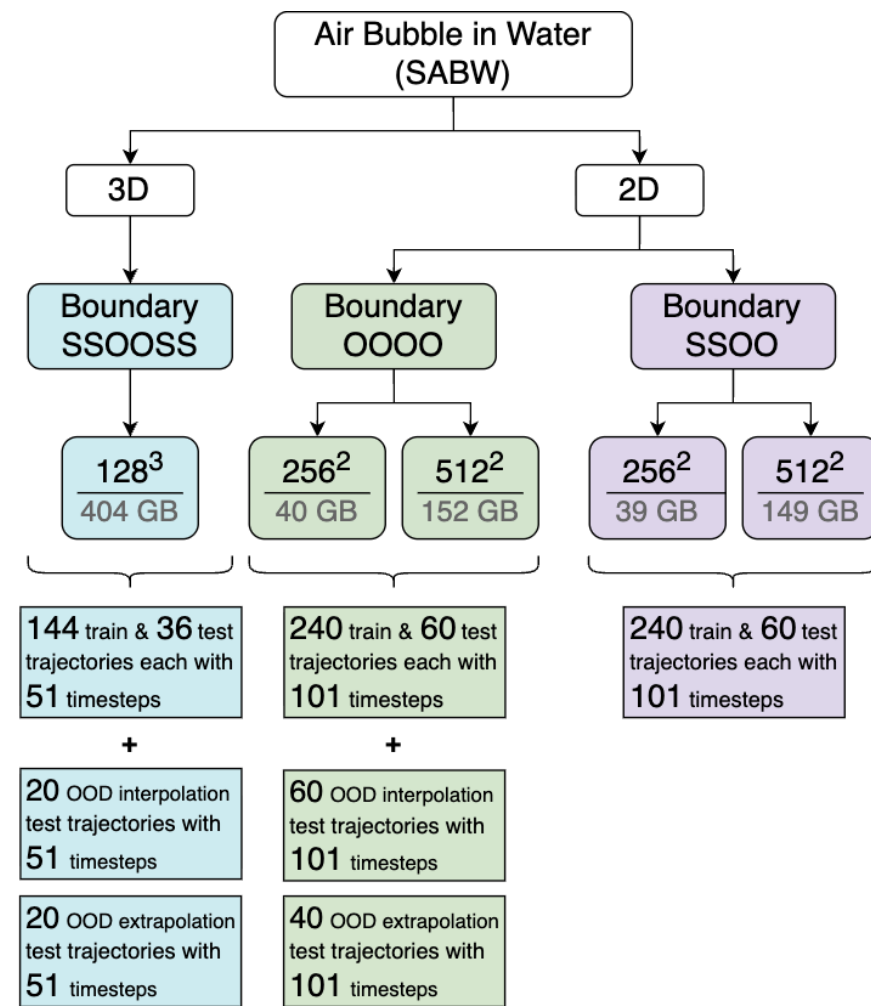
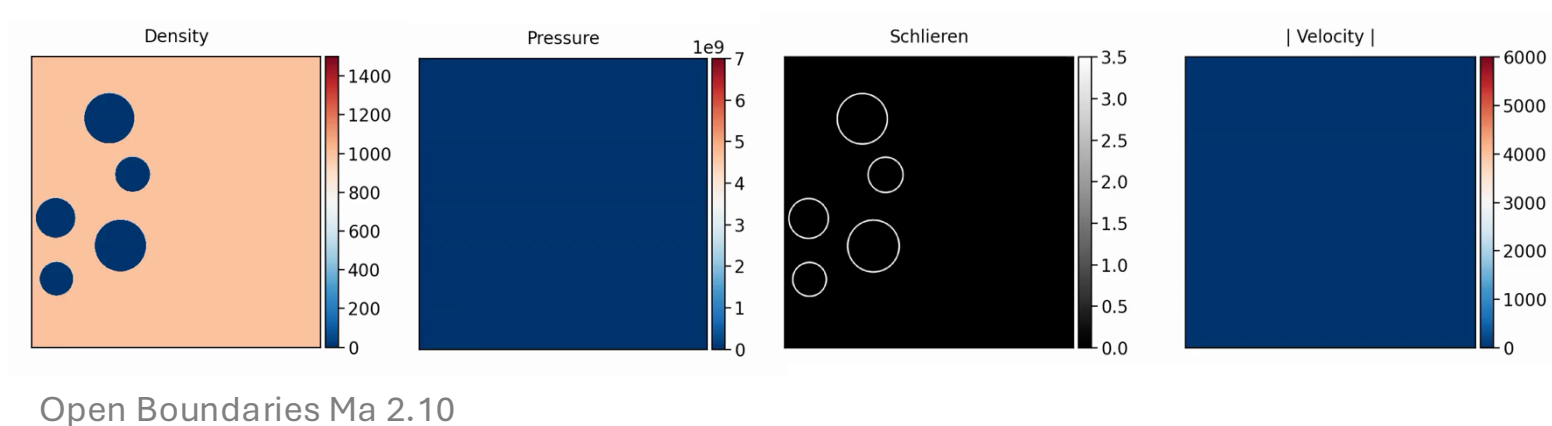
Size

- Varying Parameters
 - Shock Mach number
 - Bubble / Droplet Count
 - Bubble / Droplet Radius
 - Bubble / Droplet Position
 - Weber number (only for droplet)



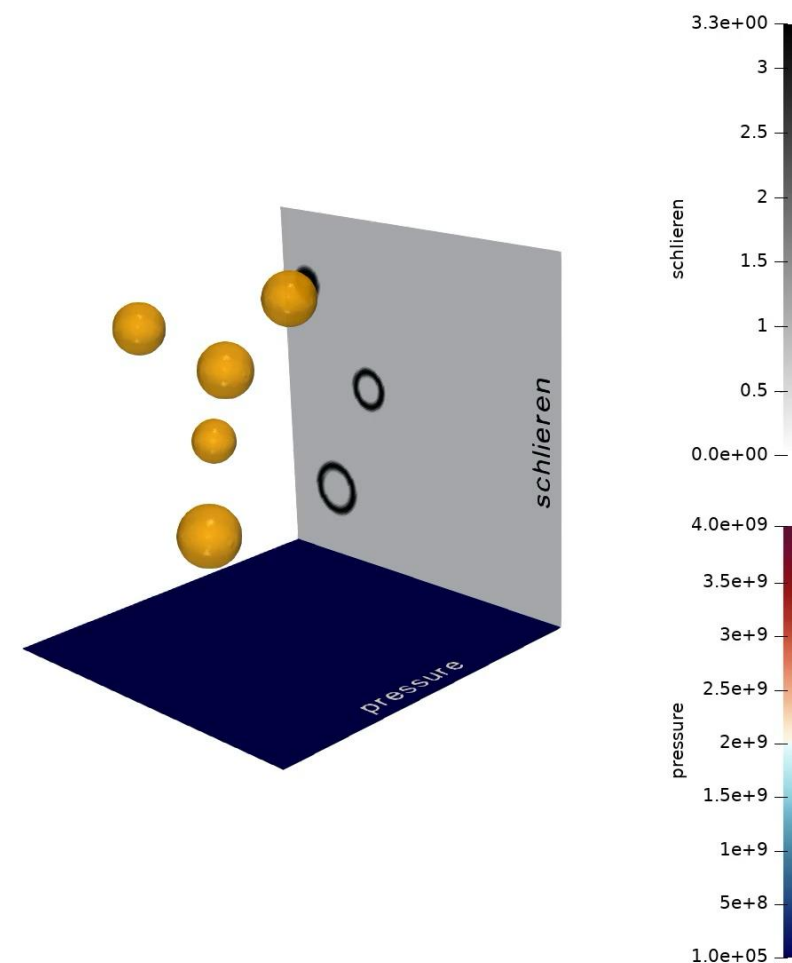
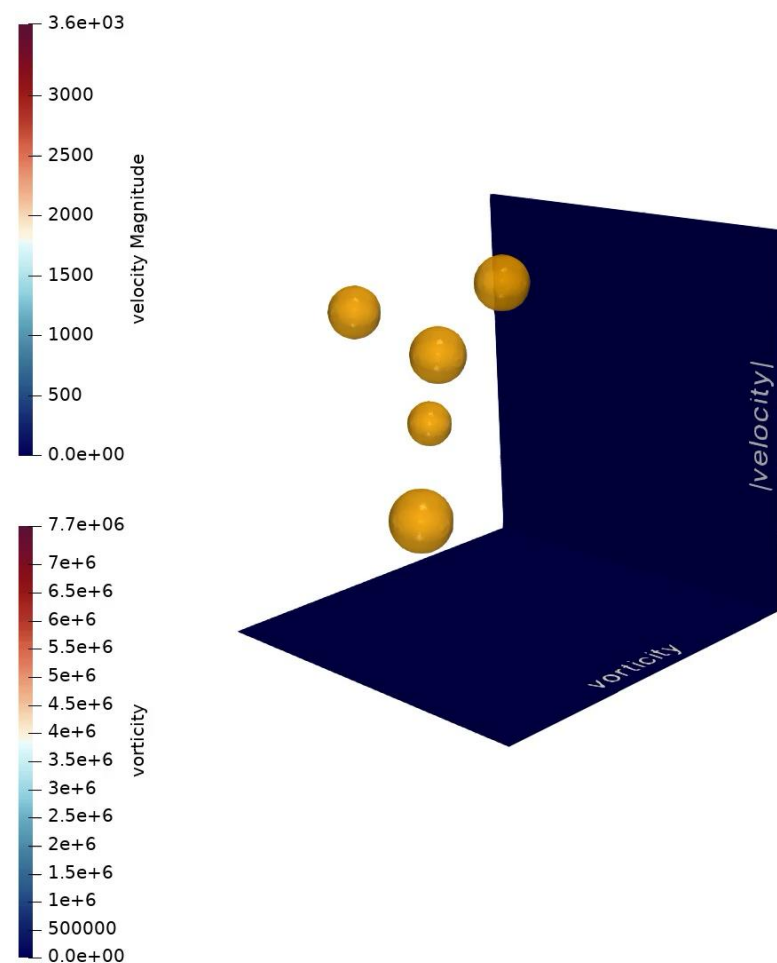
Air Bubble Collapse in Water

- Strong compression and energy focusing
- Jet formation and violent collapse
- Interacting shockwaves
- Reflecting and open boundaries





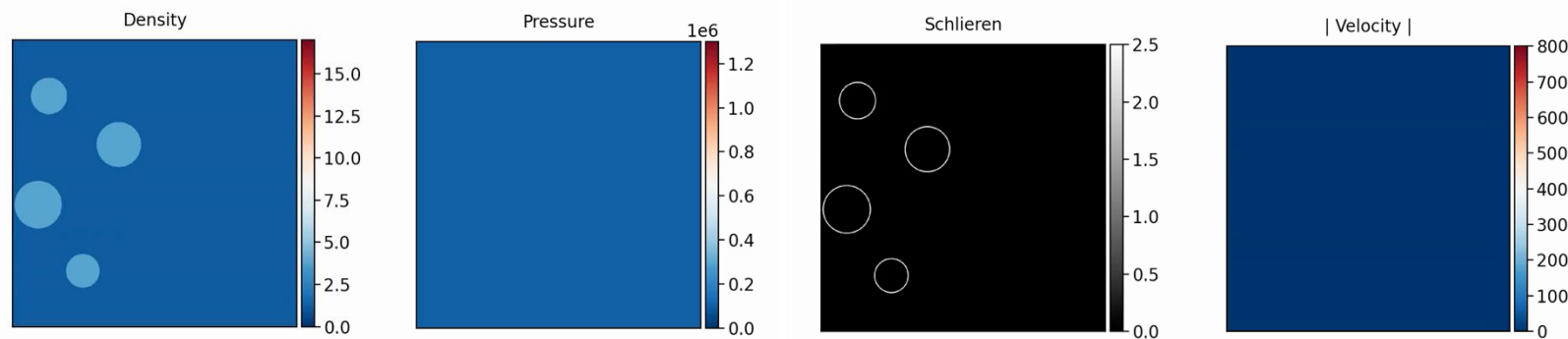
Air Bubble Collapse in Water



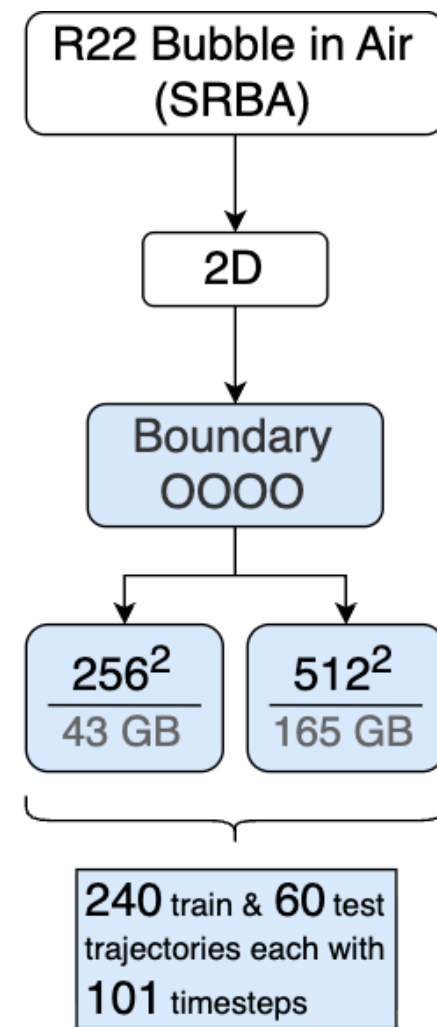
Reflecting Boundaries Ma 1.70

R22 Bubble Collapse in Air

- Gas-gas interaction
- No liquid surface tension
- Mushroom shaped deformation
- Open boundaries

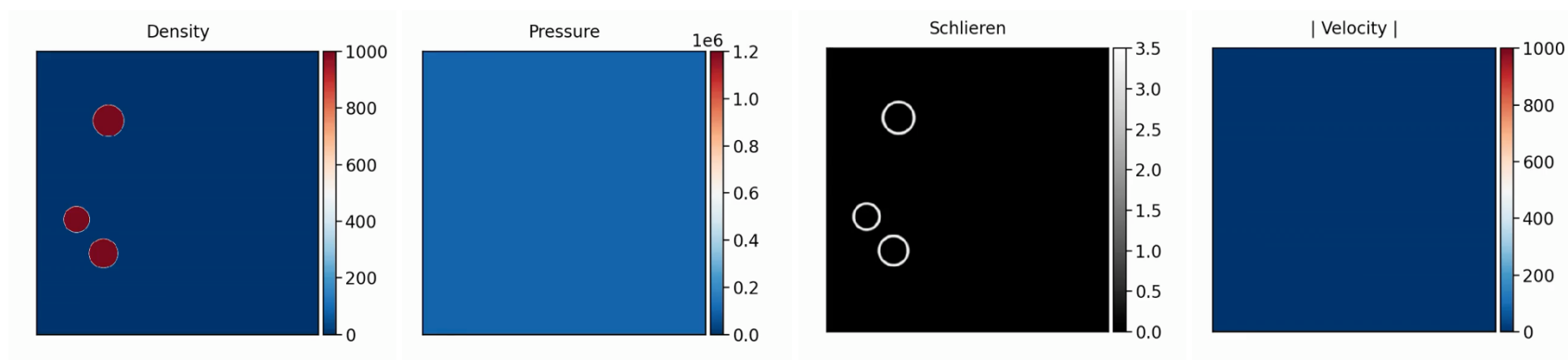


Open Boundaries Ma 2.10

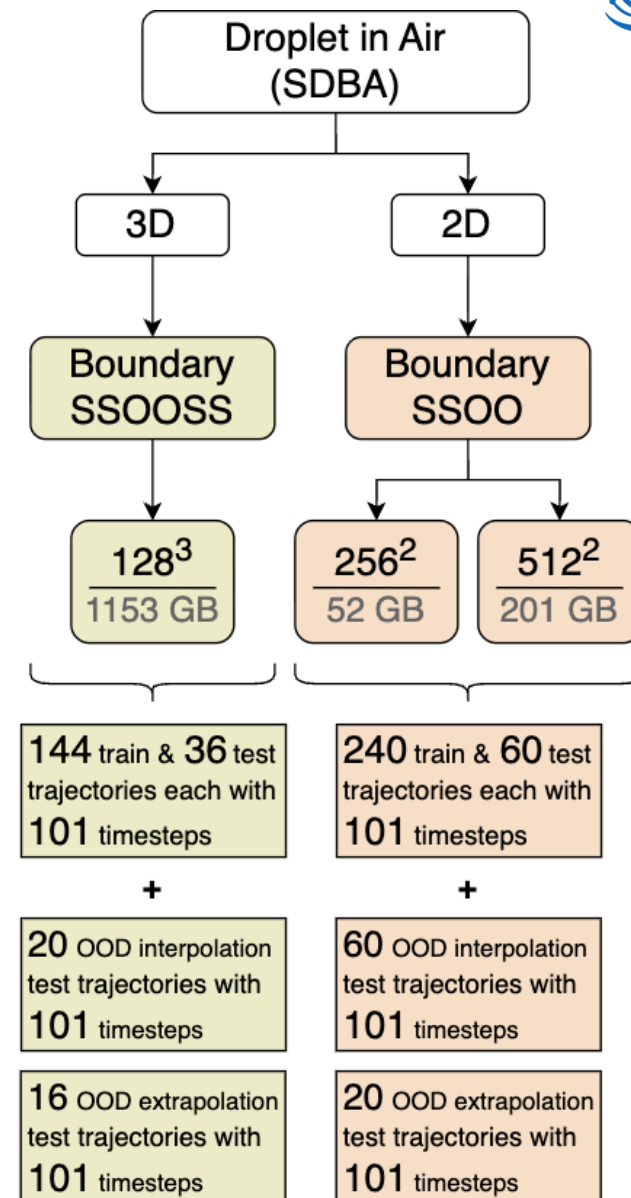


Shock Droplet Fragmentation in Air

- Two breakup regimes
 - Shear-Induced Entrainment (SIE)
 - Rayleigh-Taylor Piercing (RTP)
- Weber Number determines the breakup mode
- Reflecting Boundaries

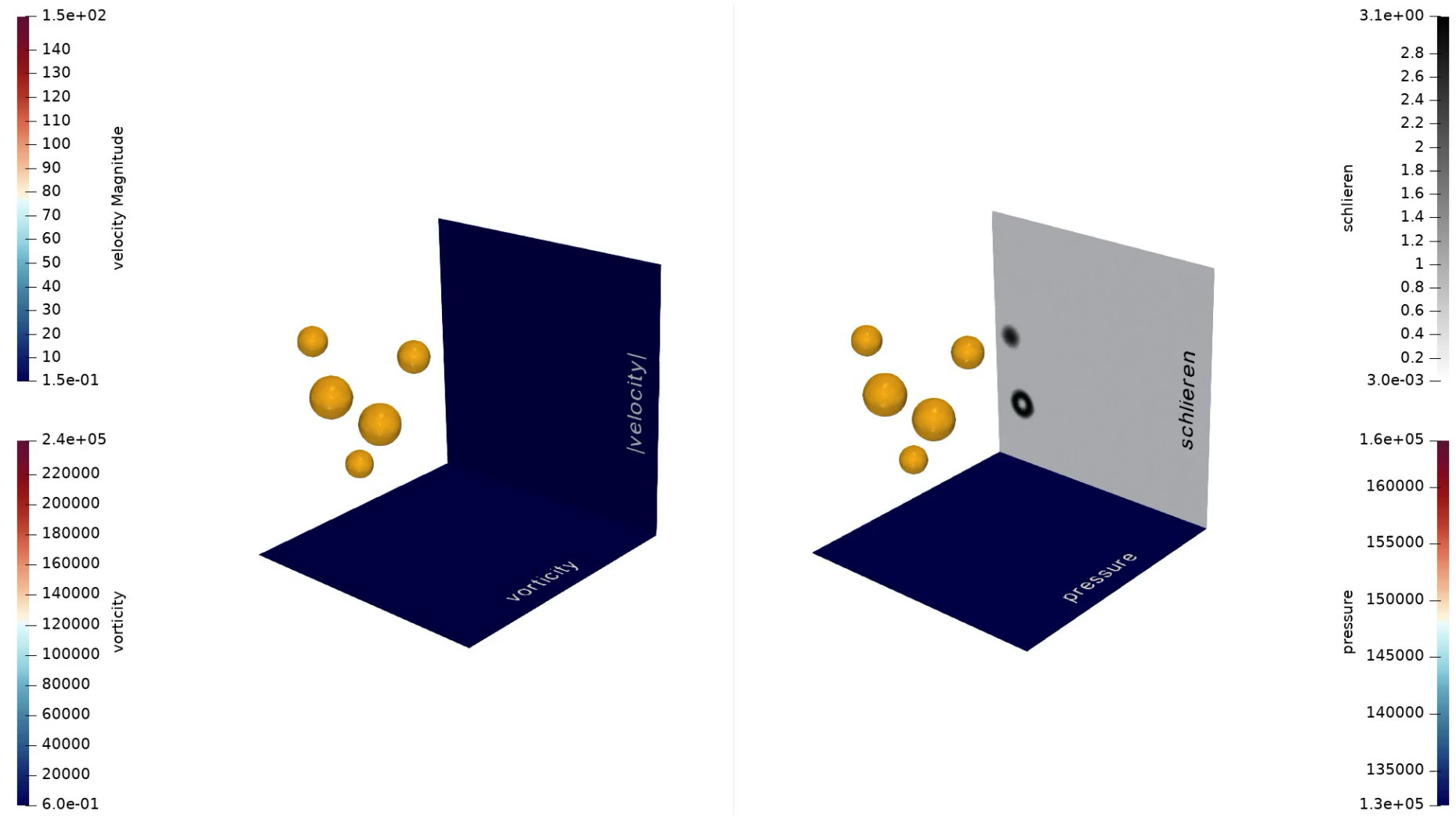


Reflecting boundaries RTP breakup Ma 2.00





Shock Droplet Fragmentation in Air



Reflecting boundaries SIE breakup Ma 1.20



Models and Training

Baselines

Randomly Initialized

- ConvNeXt
- CNO
- FFNO
- ScOT

Pre-trained

- Poseidon-B
- DPOT-M



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Standard

- MSE

Composite Loss

- MSE
- IRMSE
- H1
- SSIM

+

SA

GN



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Composite Loss

- MSE
- IRMSE
- H1
- SSIM

+

SA

GN

Evaluation

Pointwise

MSE

VRMSE

MAE

H1 / H2

Structure-aware

PCC

SSIM

Spectral

wfRMSE

MLW

Physics-informed

iqRMSE-mass

iqRMSE-momentum

iqRMSE-entrophy

iqRMSE-KE

iqRMSE-COM

Feature-focused

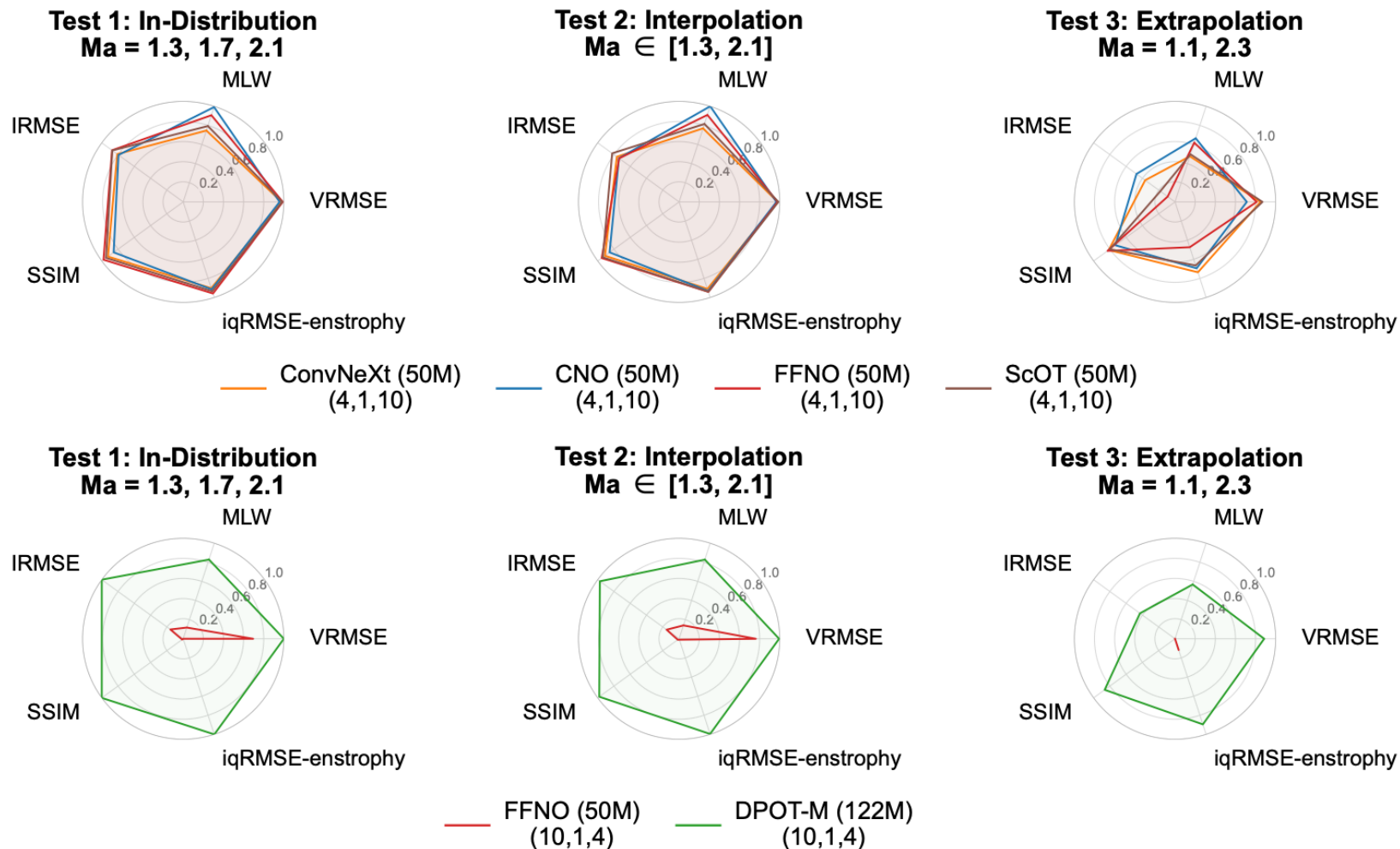
IRMSE

SRMSE



Results

2D-SABW (0000) Evaluation — MSE Training Loss

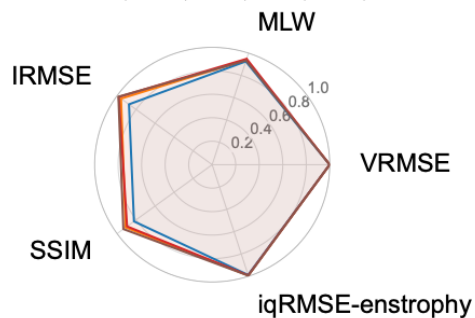




Results

2D-SDBA (SSOO) Evaluation — MSE Training Loss

Test 1: In-Distribution
Ma = 1.2, 1.6, 2.0, 2.4, 2.8, 3.2



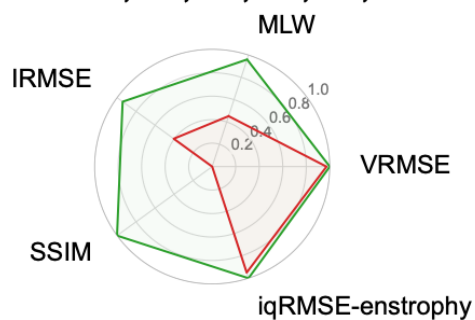
— ConvNeXt (50M)
(4,1,10)

— CNO (50M)
(4,1,10)

— FFNO (50M)
(4,1,10)

— ScOT (50M)
(4,1,10)

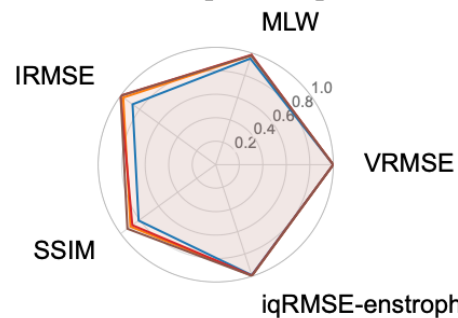
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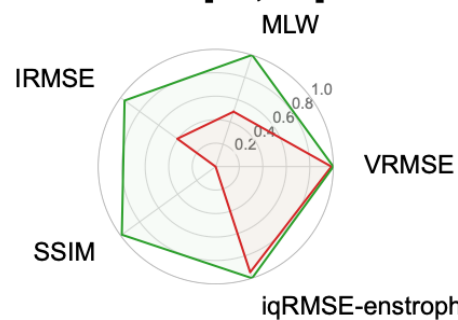
— FFNO (50M)
(10,1,4)

— DPOT-M (122M)
(10,1,4)

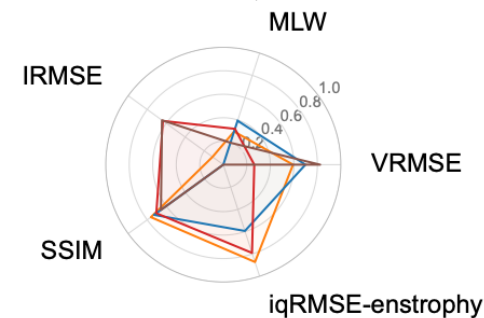
Test 2: Interpolation
Ma ∈ [1.2, 3.2]



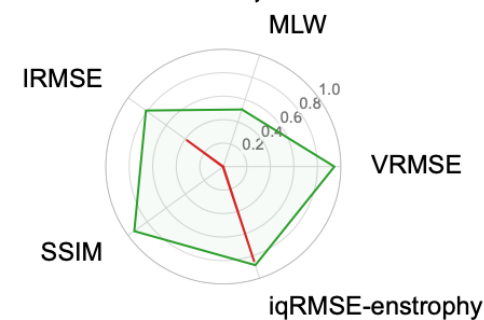
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Test 3: Extrapolation
Ma = 1.05, 3.35

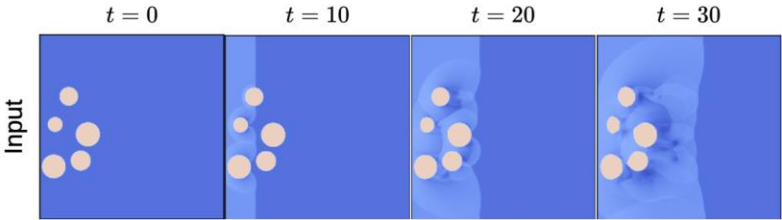


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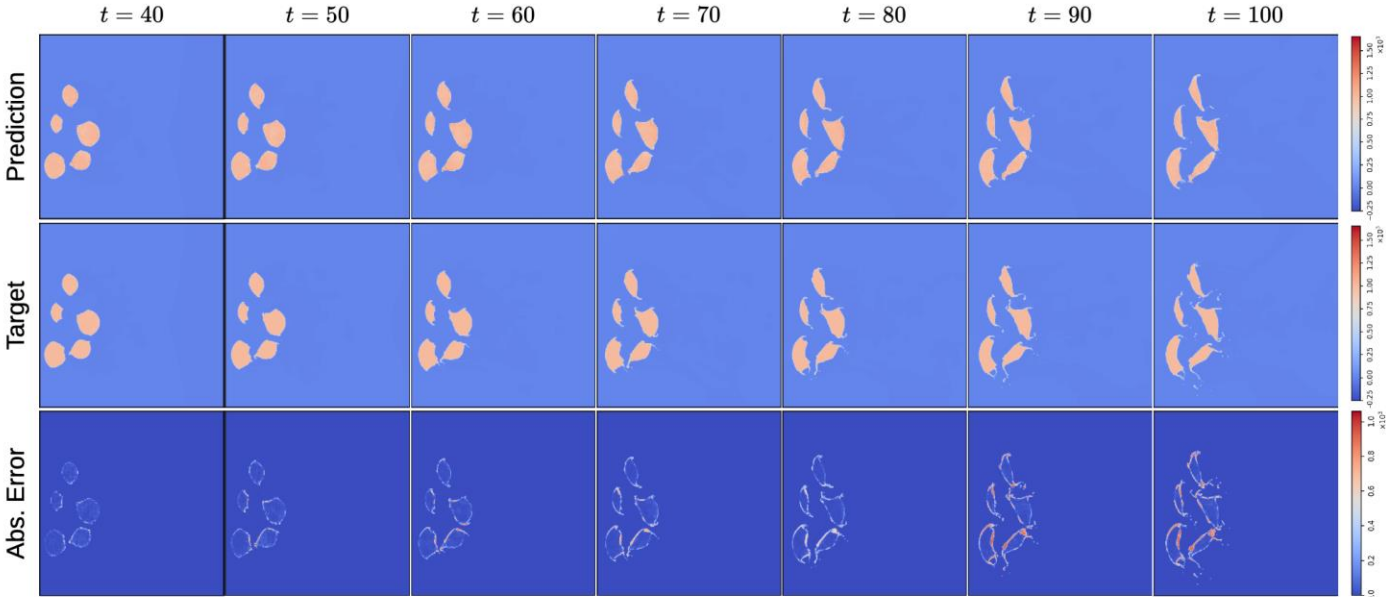




2D-SDBA-SSOO-SIE
ScOT-50M

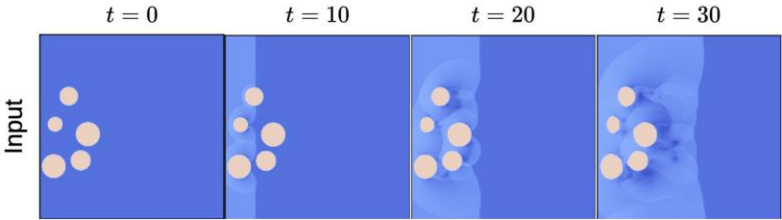


Density

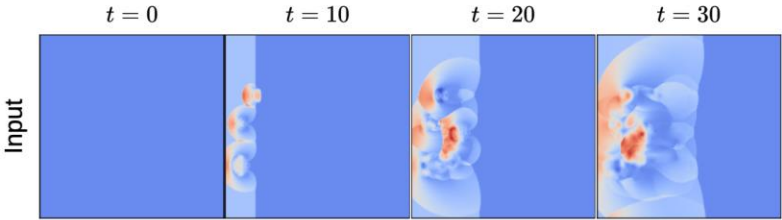




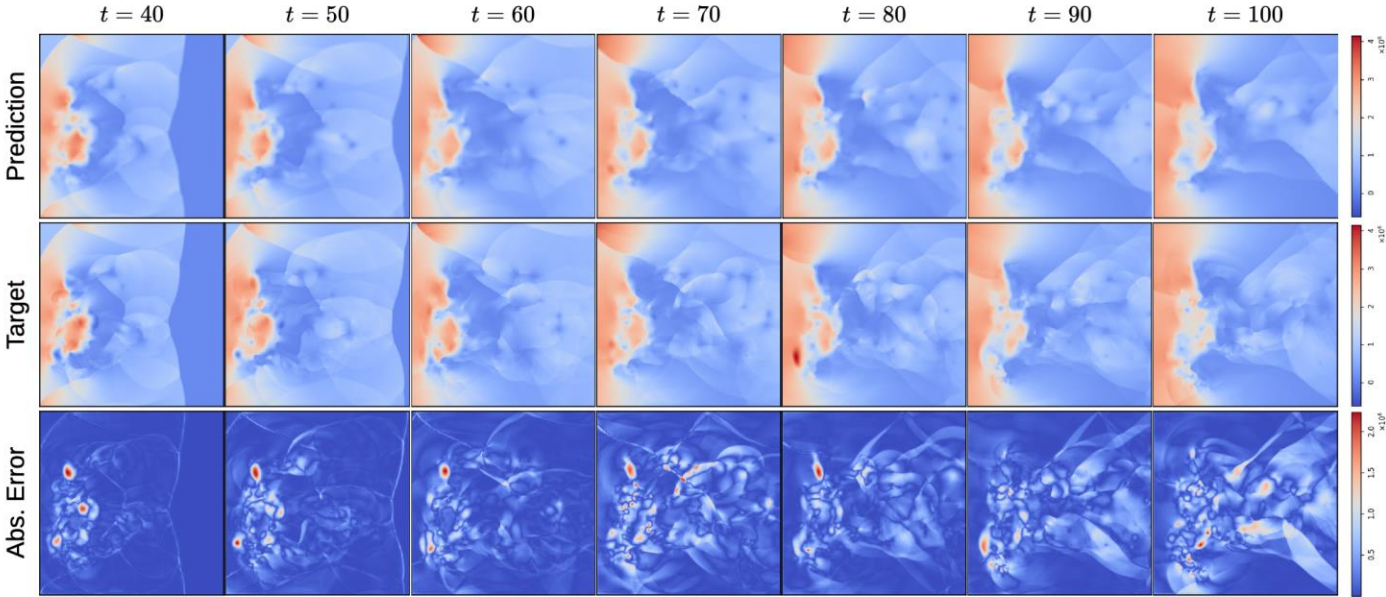
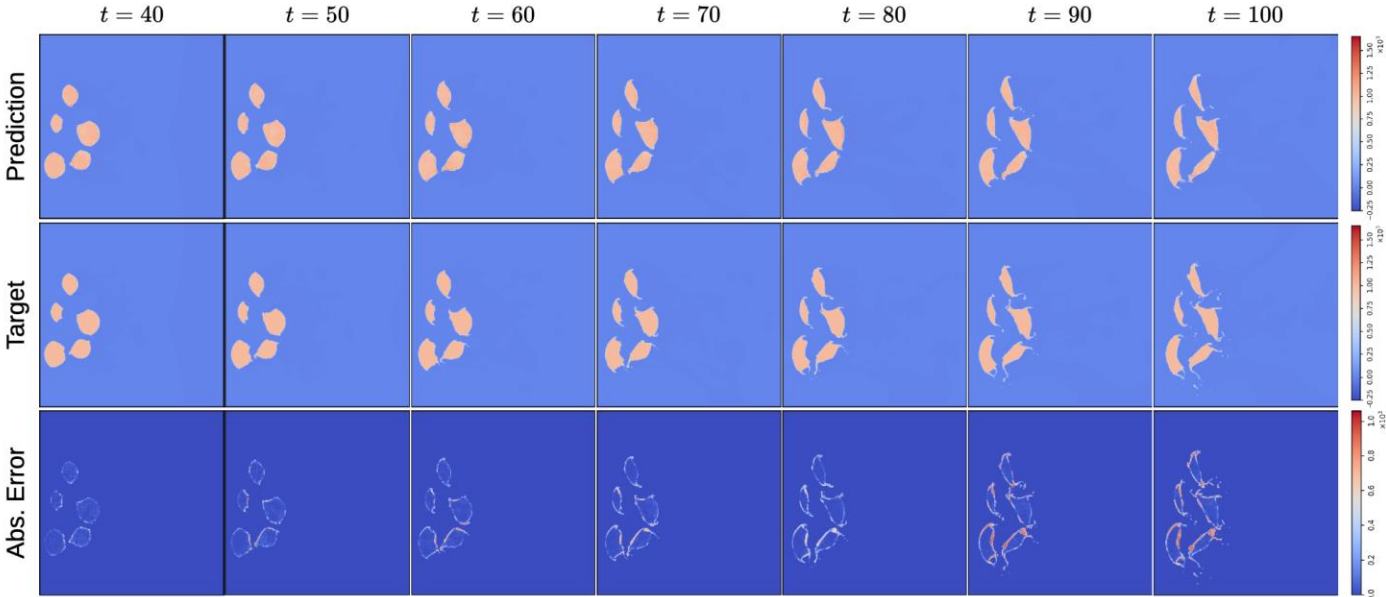
2D-SDBA-SSOO-SIE
ScOT-50M



Density

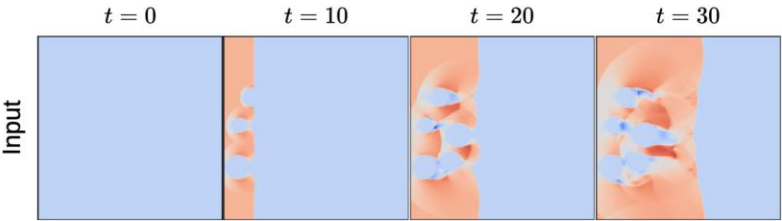


Pressure

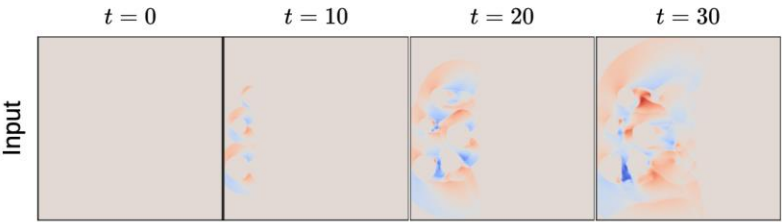




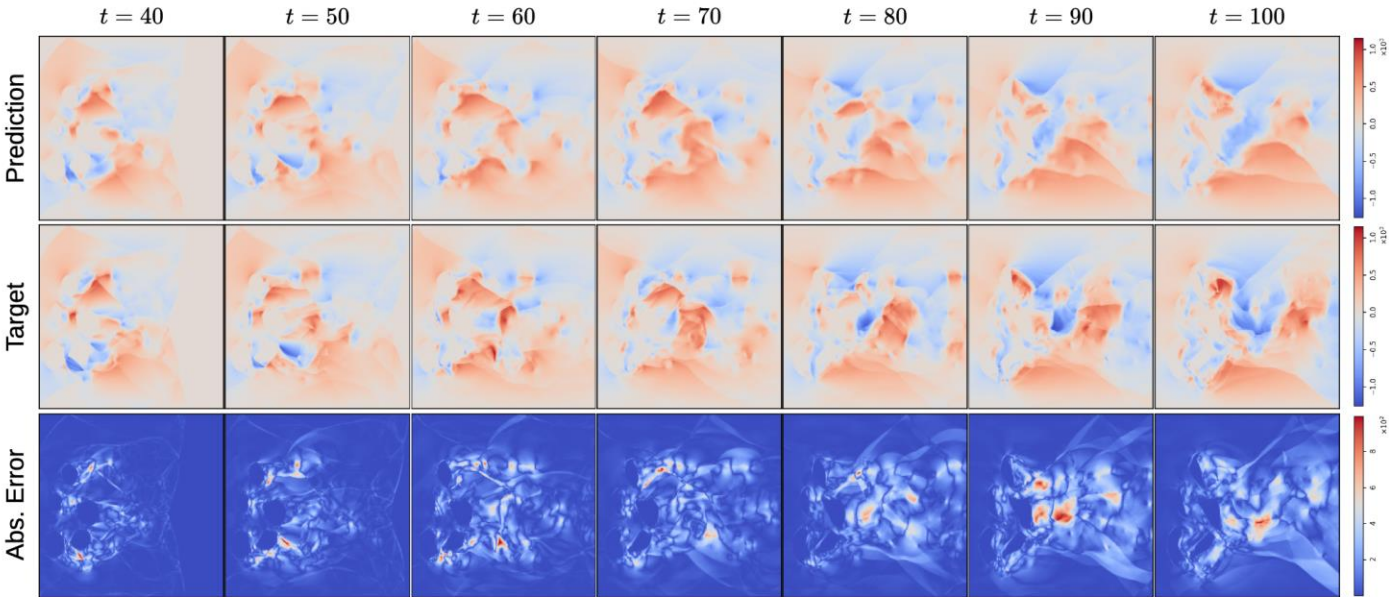
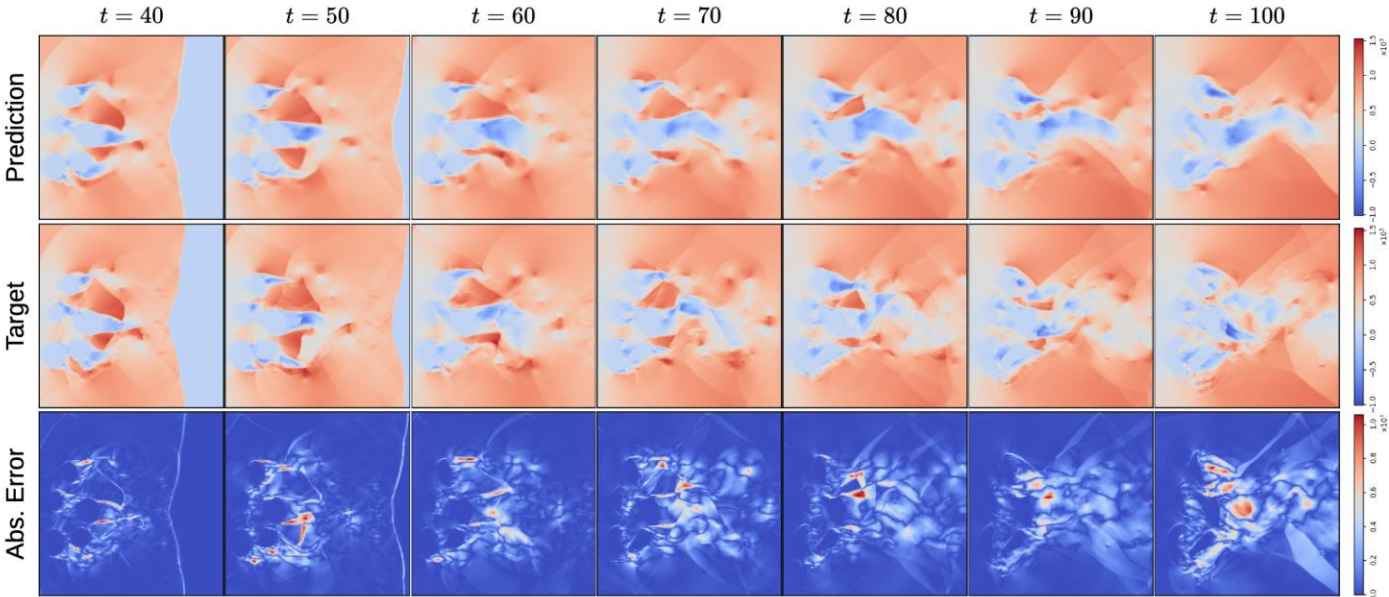
2D-SDBA-SSOO-SIE
ScOT-50M



VelocityX



VelocityY





Key Contributions

1. Neptuna extends SciML benchmarking to challenging 2D / 3D shock-driven compressible multiphase flows.



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2. No single baseline is universally best across datasets.
3. Training loss matters.
4. Reliability focused evaluation framework.



Thank you



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