Wednesday, August 2, 2023
Virtual Event

2023 NETL Multiphase Flow Science Workshop

ENABLING PREDICTIVE SIMULATIONS OF REACTING MULTIPHASE FLOWS VIA DATA-DRIVEN EMULATION

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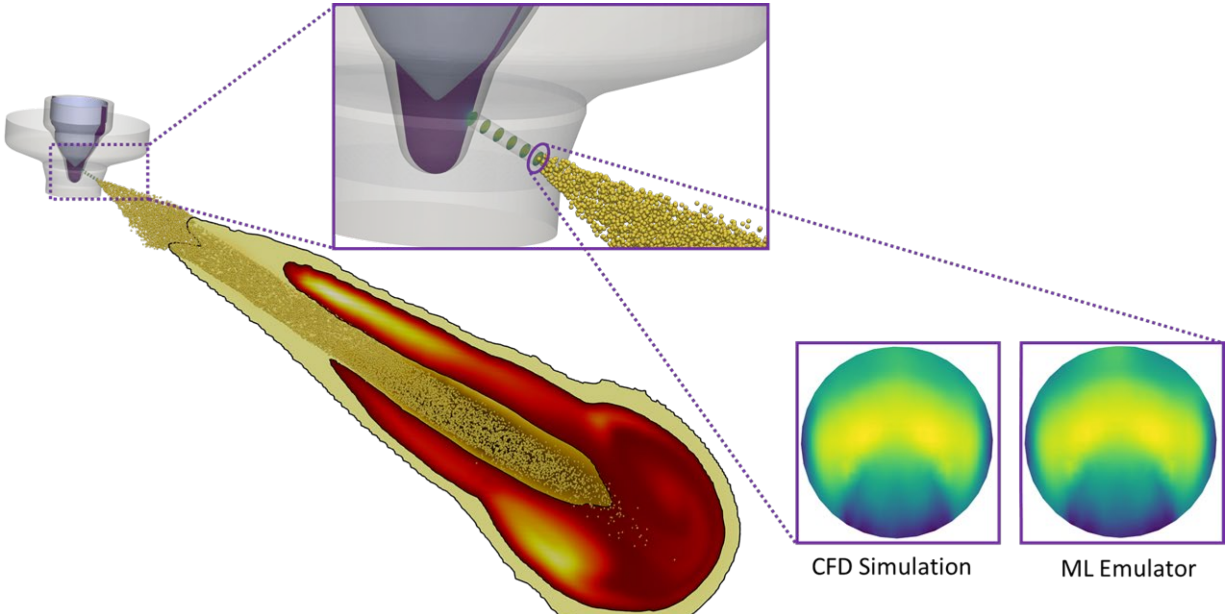


ACKNOWLEDGEMENTS

Sponsors

- Argonne's Laboratory Directed Research and Development (LDRD) program

Team members

- Roberto Torelli – Lead PI, Senior Research Scientist, Argonne National Laboratory
- Bethany Lusch – Co-PI, Computer Scientist, Argonne National Laboratory
- Gina M. Magnotti – Co-PI, Senior Research Scientist (*formerly at Argonne*)
- Sudeepta Mondal – Main Contributor, Postdoctoral Researcher (*formerly at Argonne*)

Computing resources

- Laboratory Computing Resource Center: Bebop HPC Cluster
- Argonne Leadership Computing Facility: Theta Supercomputer

Industry partners

- Convergent Science Inc. for licensing support

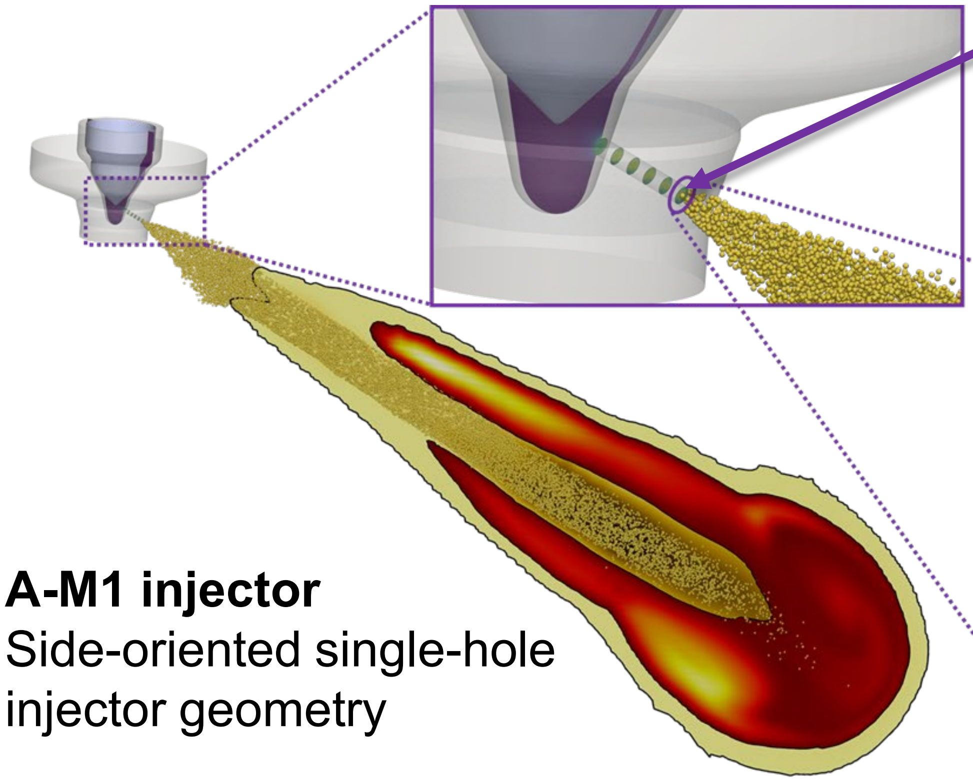
INJECTION INFLUENCES ENGINE PERFORMANCE[1]

Detailed injection simulations are too expensive at the industry level

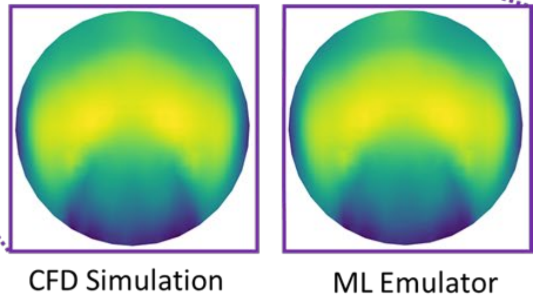
Emulated flowfields at orifice exit **for static-needle-lift Large Eddy Simulations at steady state[2]**:

- Gaseous volume fraction (α)
- Velocity components (u, v, w)
- Liquid mass (m_l)

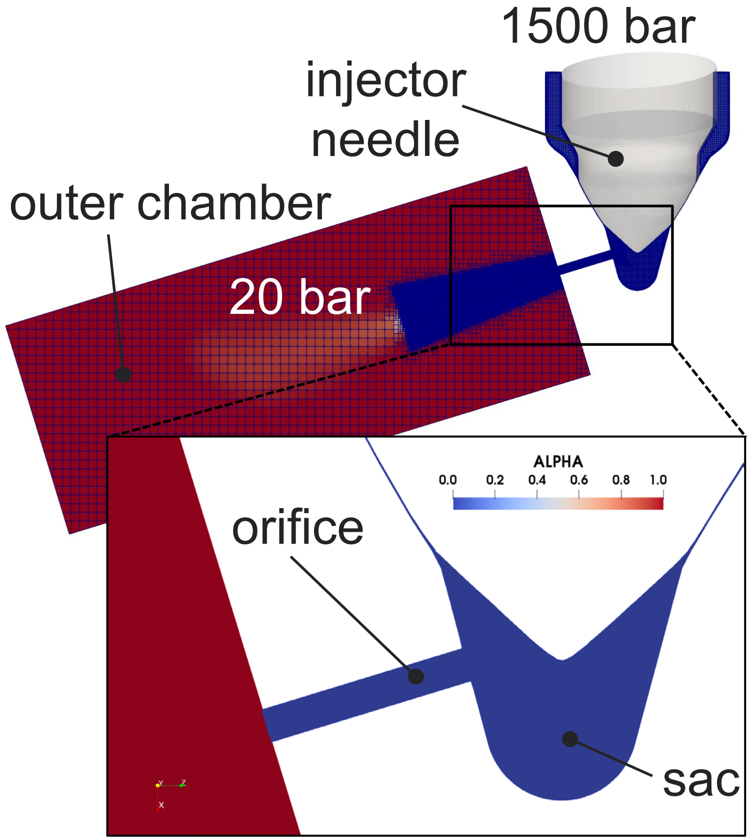
- Machine Learning models emulate internal flow fields at orifice exit
- Emulated flowfields coupled with Lagrangian spray simulations using static one-way coupling



A-M1 injector
Side-oriented single-hole injector geometry



Fuel: n-Dodecane - $P_{sat} = 0.0013$ bar

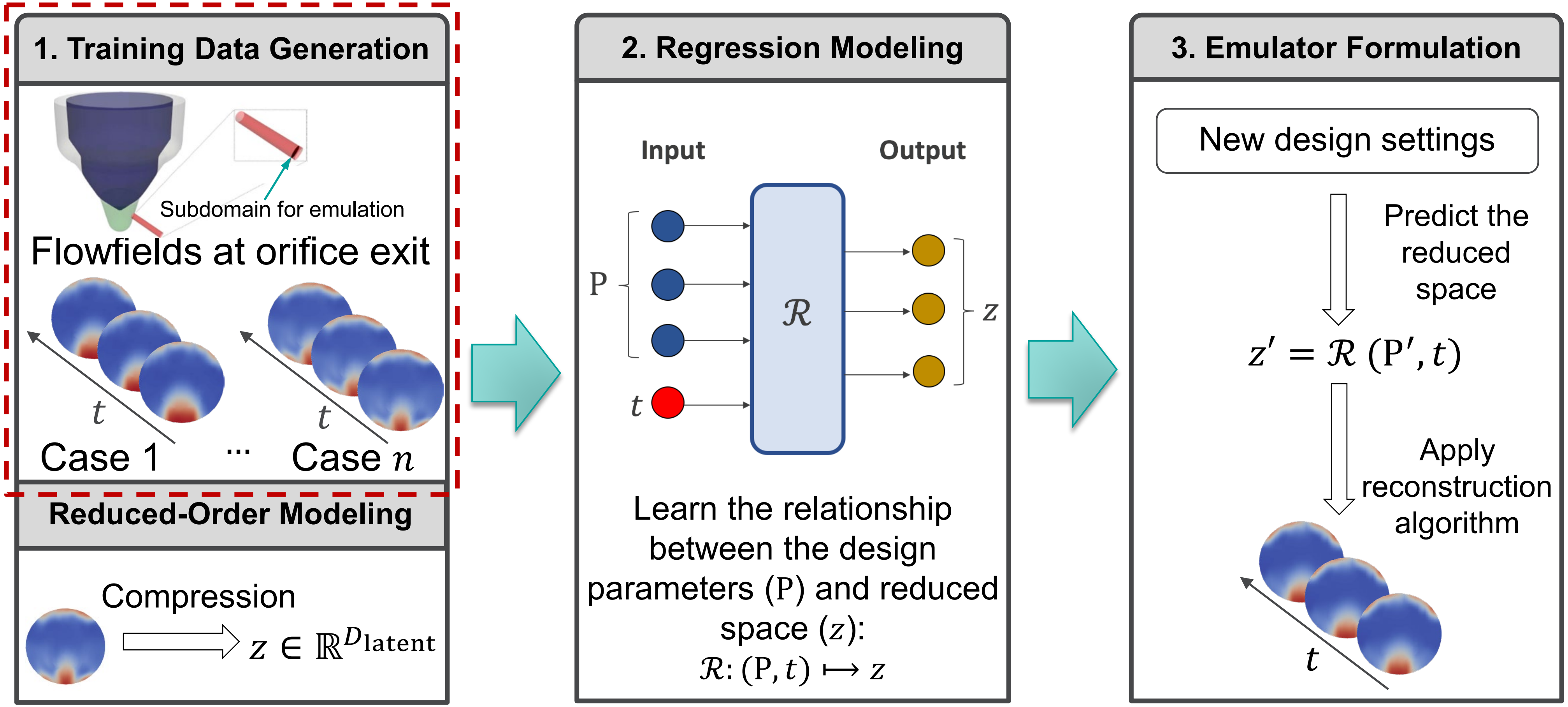


1400 – 2000 CPU-hours per 10 μs of simulated time[3]

[1] Torelli, Pei, Zhang, Som, *Communications Engineering*, 2022
[2] Mondal, Torelli, Lusch, Milan, Magnotti, SAE Technical Paper 2021-01-0550, 2021
[3] Milan, Torelli, Lusch, Magnotti, *Atomization and Sprays* 30(6), 2020

EMULATOR FRAMEWORK

Three phases to deconstruct the emulator formulation



81 snapshots per CFD case extracted at the **orifice exit** between $t = 20\text{-}40\ \mu s$, for steady-state flow conditions with static needle lift. Each snapshot contains 4,214 grid points

[1] Milan, Torelli, Lusch, Magnotti, *Atomization and Sprays* 30(6), 2020

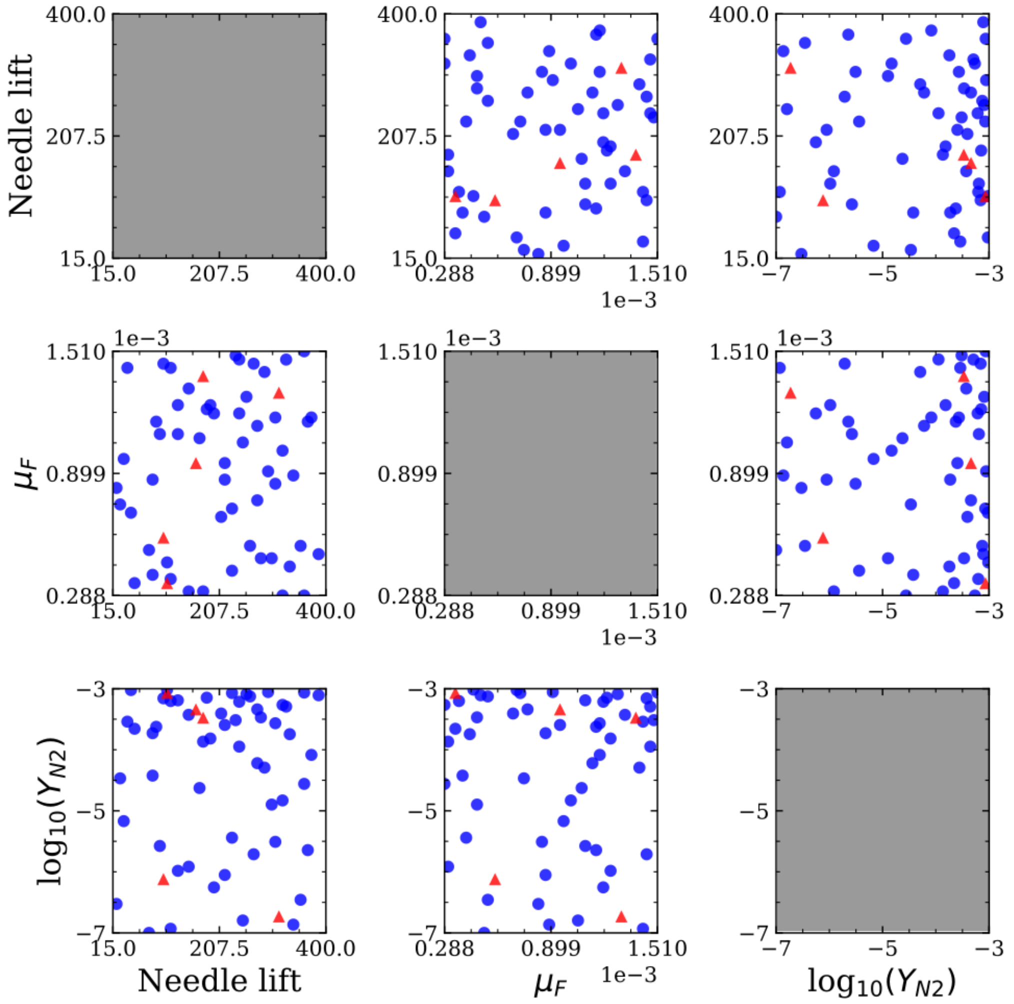
DESIGN OF EXPERIMENTS (DOE)

Input space of parameters that affect cavitation is efficiently explored

Design Parameters	Range		
Needle lift, δ [μm]	15	400	[1]
Fuel viscosity, μ_F [(N s) /m^2]	2.88×10^{-4}	1.51×10^{-3}	[2]
Level of dissolved gas Y_{N_2} [-]	1.0×10^{-7}	1.0×10^{-3}	[3]

- Design of Experiments (DoE)
  - ❑ Variant of Latin Hypercube Sampling
  - ❑ **60 samples in total in 3-D design parameter space**
- The blue dots (55) represent operating conditions seen during training, and the red dots (5) correspond to new operating conditions (test cases)

The test cases are chosen to encompass the different flow structures of the gas phase in the design space through input sensitivity analysis



[1] Guo, Torelli et al., *SAE Int. J. Advances & Curr. Prac. in Mobility*, 2020
[2] Magnotti and Som, ASME ICEF2019-7269, 2019
[3] Battistoni et al., *Atomization and Sprays* 25(6), 2015

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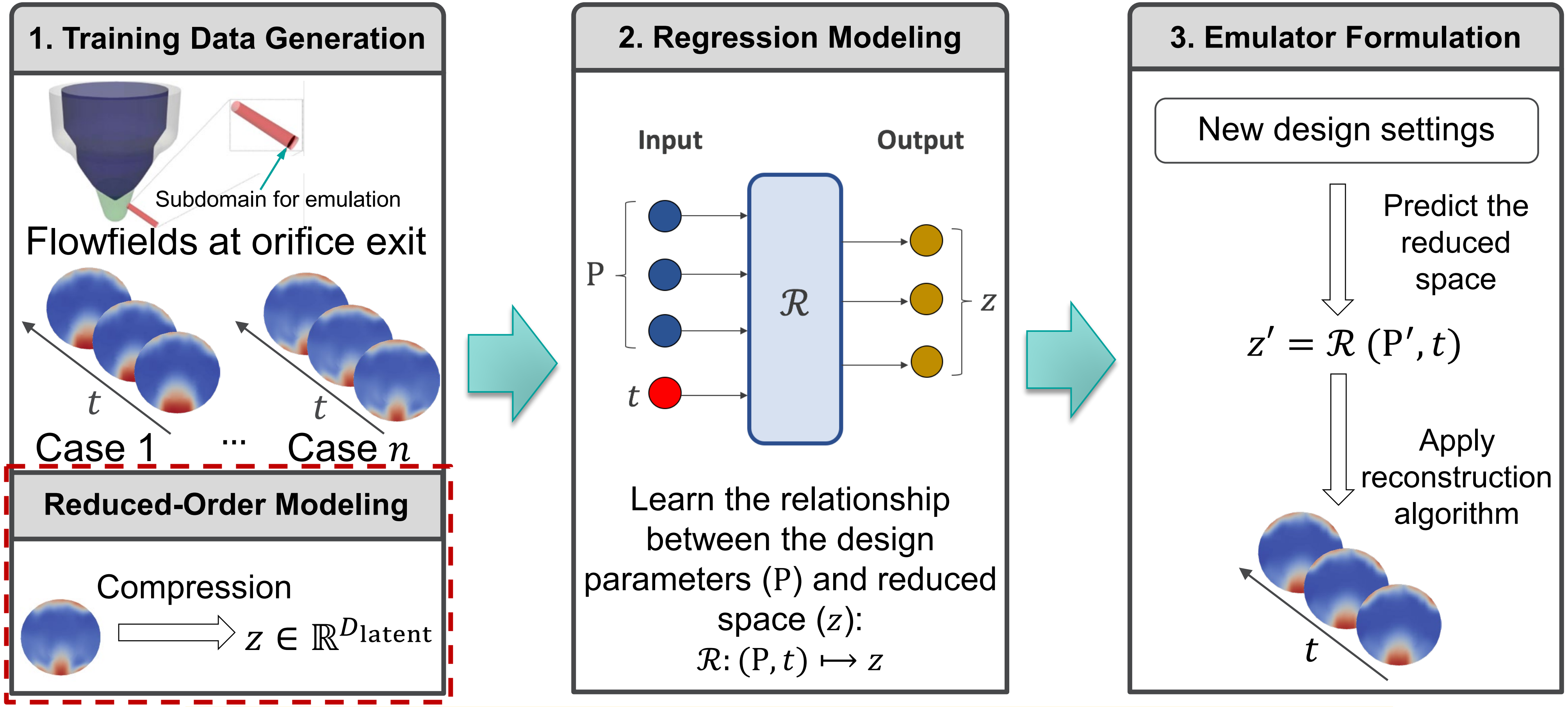
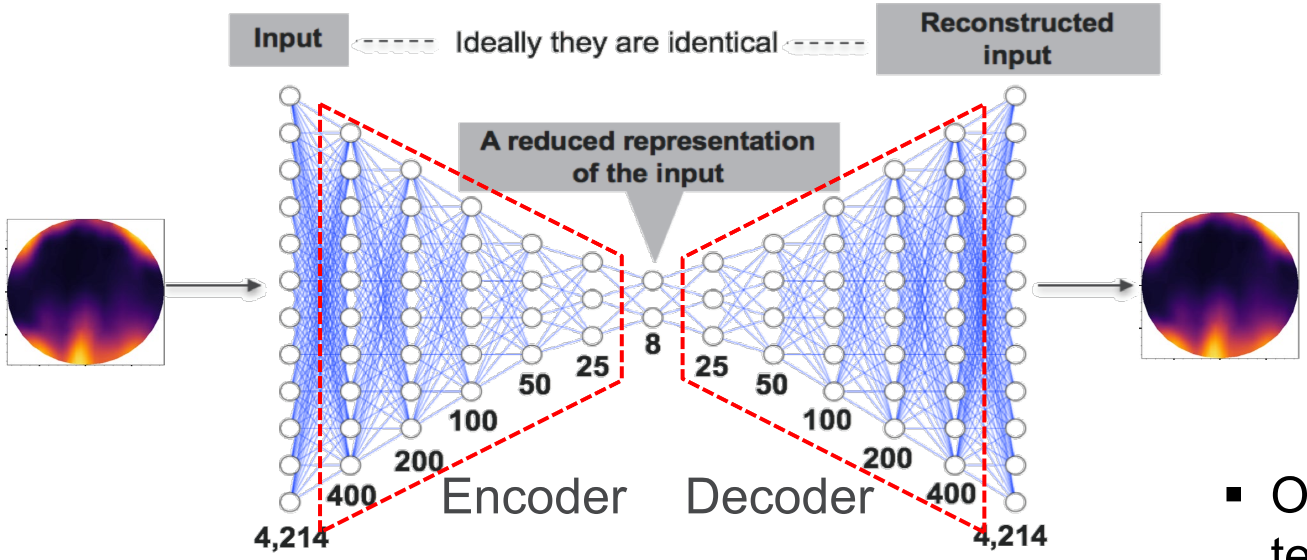


81 snapshots per CFD case extracted at the **orifice exit**.
Each snapshot contains 4,214 grid points

[1] Milan, Torelli, Lusch, Magnotti, *Atomization and Sprays* 30(6), 2020

AUTOENCODER FRAMEWORK

Using deep learning to reduce the dimensionality of flowfields



Autoencoders:
Reduce the dimension of the flowfields

Make the problem of predicting flowfields for unknown operating conditions tractable

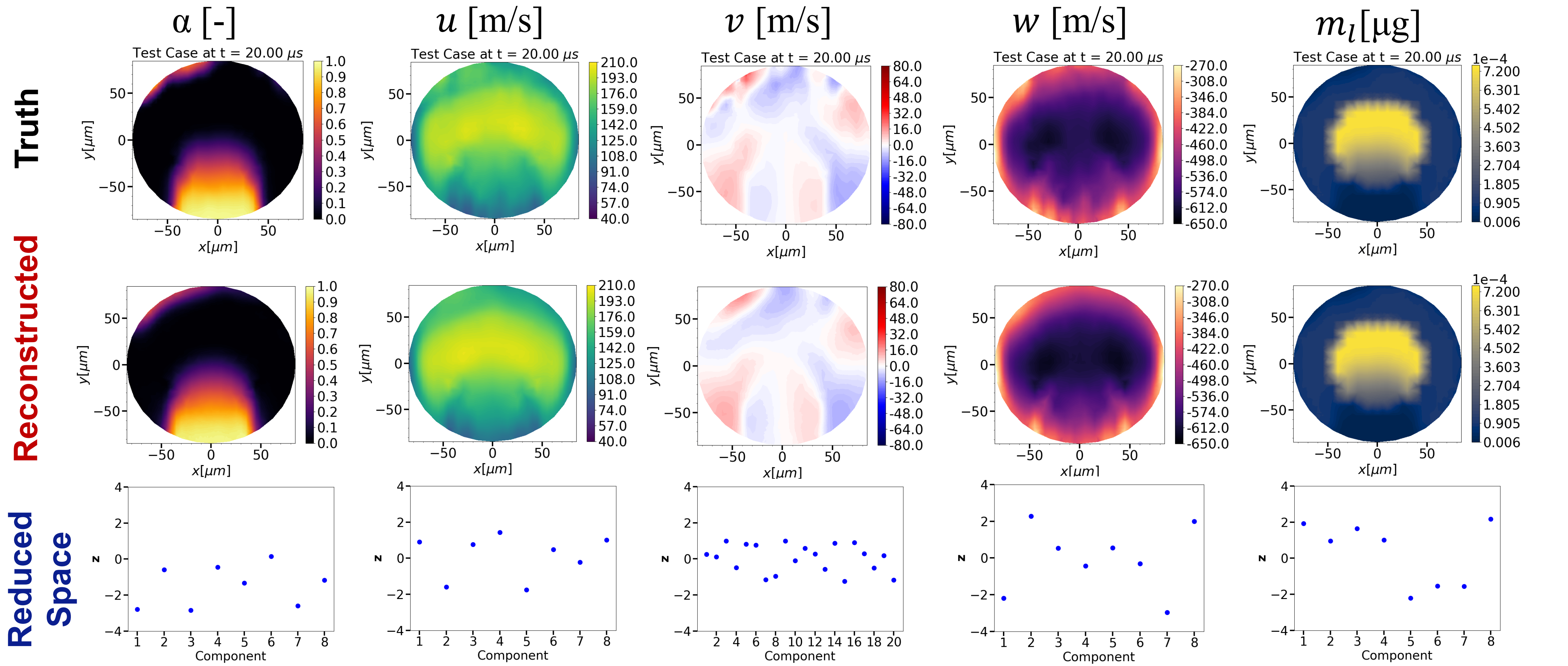
- Other dimensionality reduction techniques like Proper Orthogonal Decomposition (POD) were also explored [1]
- Deep autoencoders are chosen as the preferred dimensionality reduction tool because the complex non-linear transformations allow high representation power with low latent space dimensions

Hyperparameters (grid-search-based)

Hyperparameter	Value
Number of hidden layers	10 (5 each for $\mathcal{T}_{enc}$ and $\mathcal{T}_{dec}$)
$\mathcal{T}_{enc}$	[400, 200, 100, 50, 25]
$\mathcal{T}_{dec}$	[25, 50, 100, 200, 400]
D_{code}	8 (for α, u, w, m_l), 20 (for v)
Optimizer algorithm	Adam
Learning rate of optimizer	2×10^{-5}
Number of epochs	1000
Batch size	25
L_2 Regularization parameter	5×10^{-5}

[1] Milan, Torelli, Lusch, Magnotti, *Atomization and Sprays* 30(6), 2020
[2] Mondal et al., SAE Technical Paper 2021-01-0550, 2020.
[3] Milan et al., AIAA SciTech Paper 2021-1016, 2021.

REDUCED SPACE CAPTURES FLOW COMPLEXITIES



Reconstruction error of time-averaged flowfields

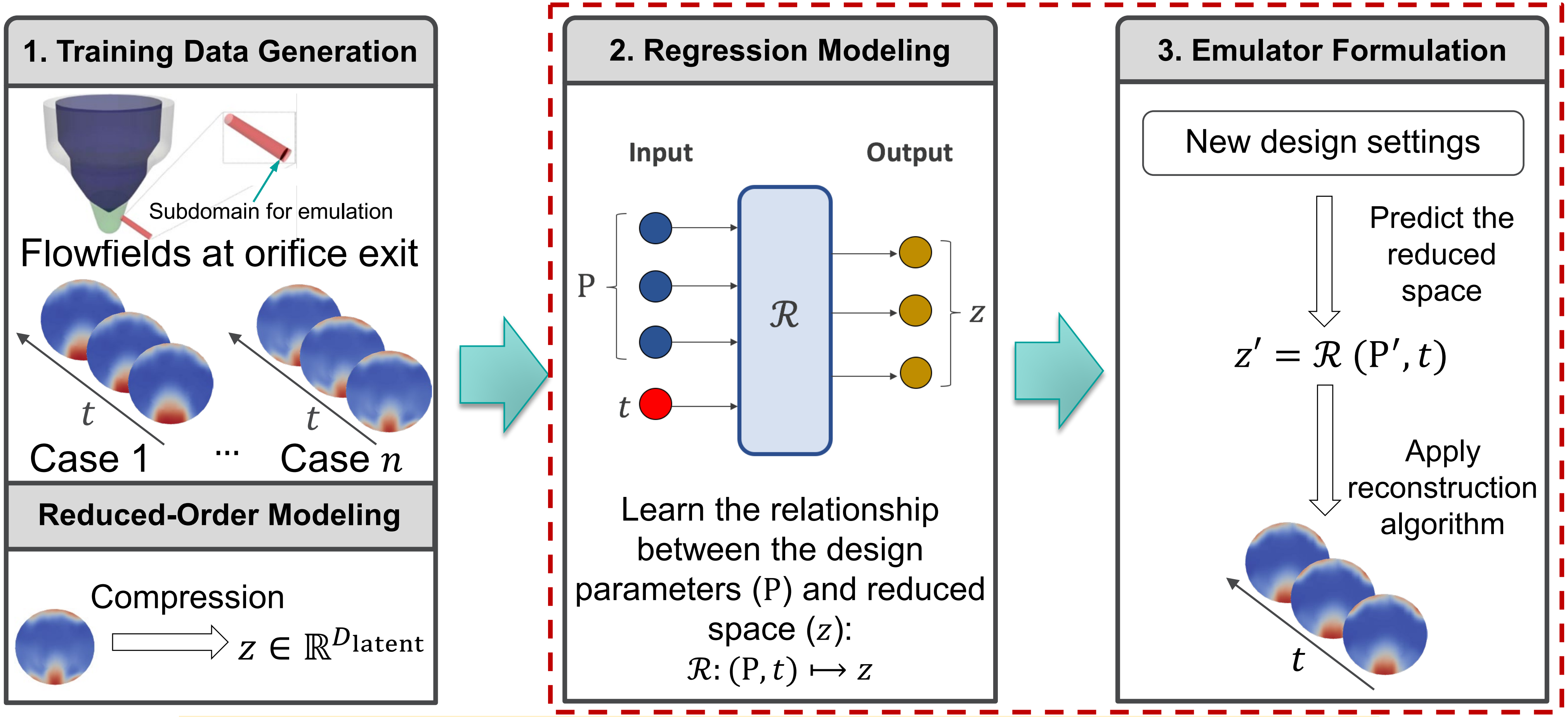
Flowfield	α	u	v	w	m_l
Error	2%	1%	8%	1%	1%

Errors averaged over 5 test cases

Demonstrations shown for Case 51

EMULATOR FRAMEWORK

Three phases to deconstruct the emulator formulation



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Each snapshot contains 4,214 grid points

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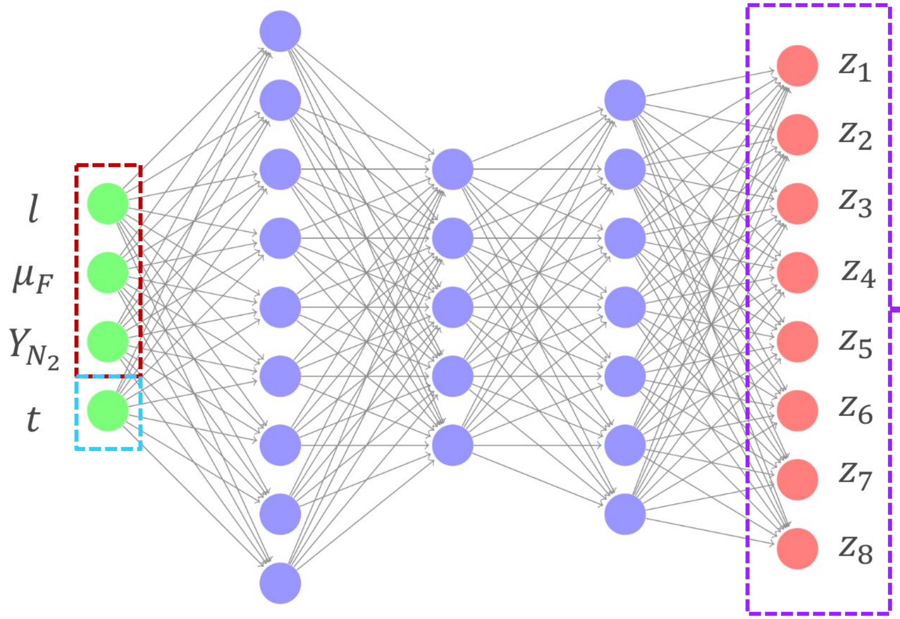
REGRESSION AND EMULATION PERFORMANCE

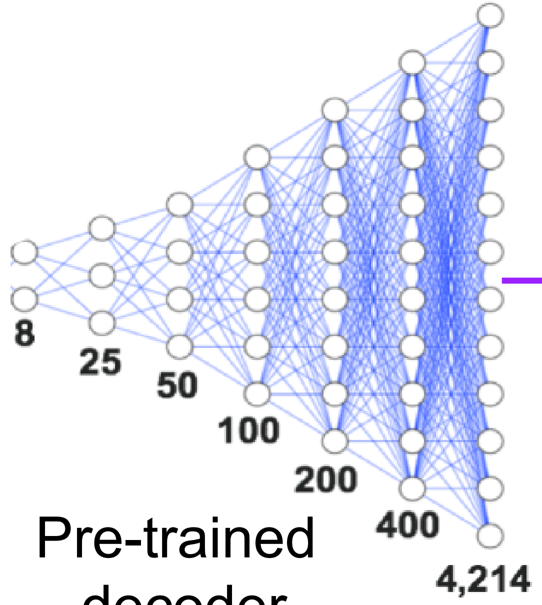
Deep Learning to relate design parameters to reduced space



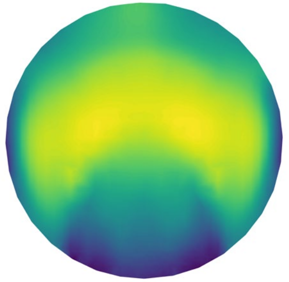
The regression model is another deep neural network that maps the design variables and time to the reduced dimensional latent space

Hyperparameters

Hyperparameter	Value
Number of hidden layers	4
$\mathcal{J}_{enc}$	[8, 16, 32, 32]
Optimizer algorithm	Adam
Learning rate of optimizer	1×10^{-4}
Number of epochs	500
Batch size	25
L_2 Regularization parameter	2×10^{-3}

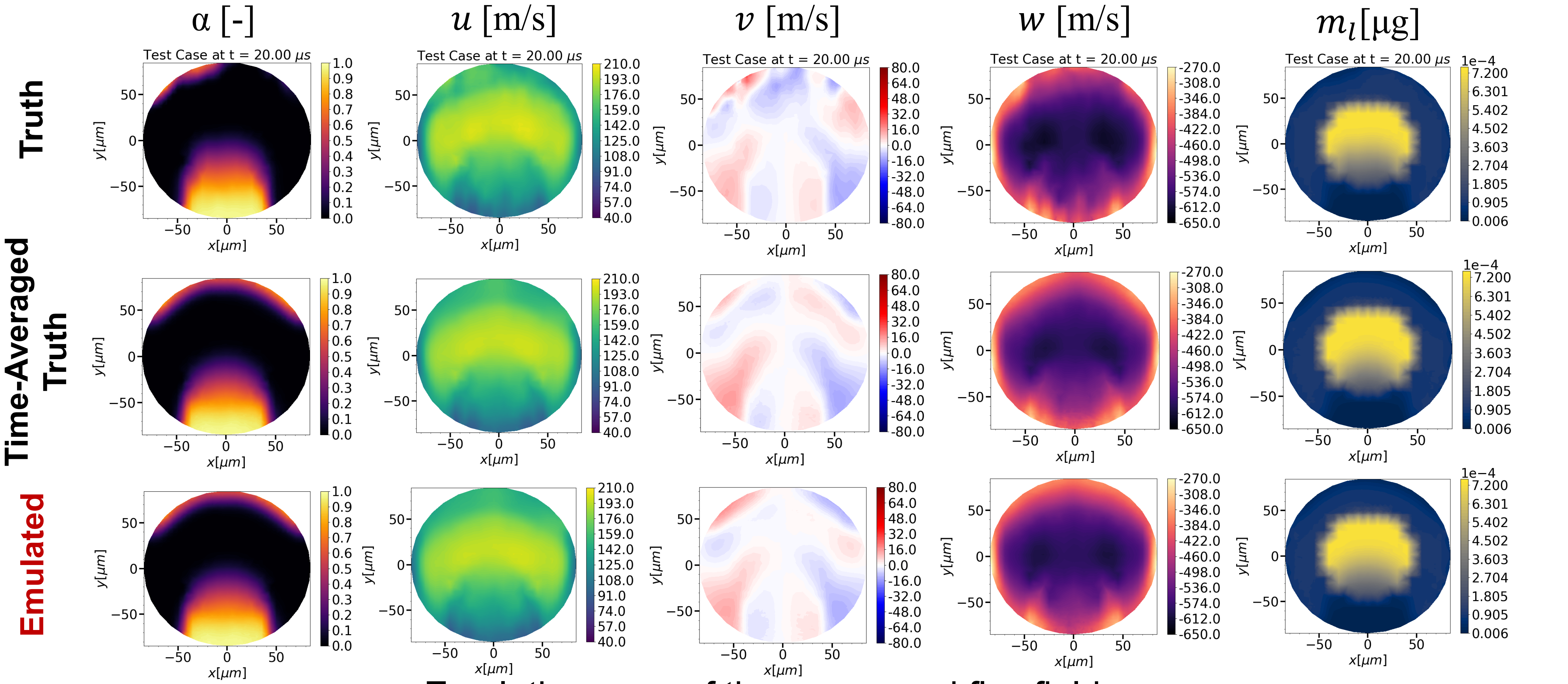


Pre-trained decoder



Emulated flowfield of Interest

PREDICTIONS OF TIME-AVERAGED FLOWFIELDS



Errors averaged over 5 test cases

Emulation error of time-averaged flowfields

Flowfield	α	u	v	w	m_l
Error	8%	2%	22%	2%	2%

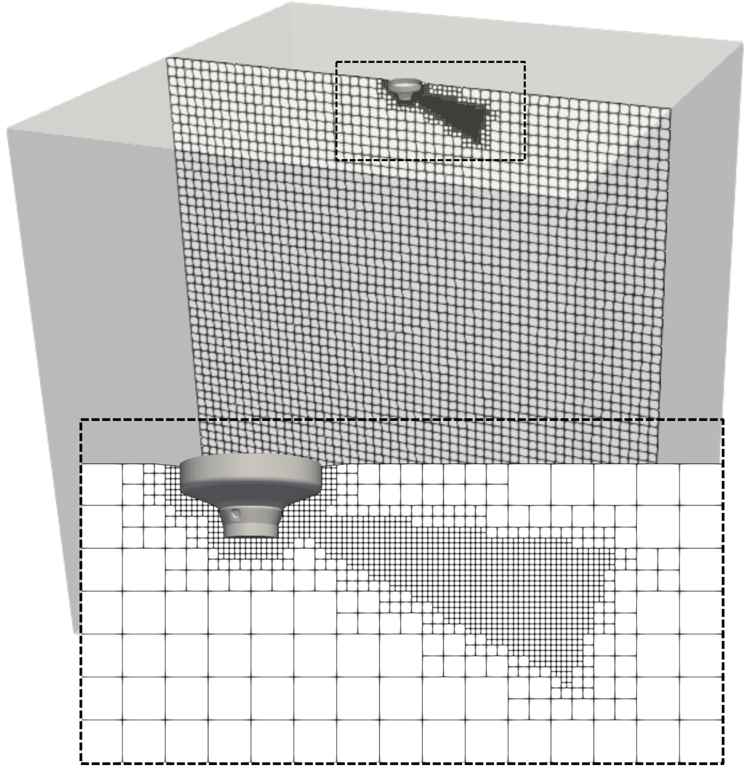
Demonstrations shown for Case 51

APPLICATION OF EMULATED FLOWFIELDS

Injector-exit predictions to study the spray and combustion behavior

Fuel	Fuel Temperature [K]	Fuel Pressure [bar]	Chamber Temperature [K]	Chamber Density [kg/m^3]
n-dodecane	323	1500	900	22.8

Model Set-up	
Software	CONVERGE
Parcel Initialization	Static coupling, LVF threshold = 0.1,TKE = 3000 m^2/s^2 [1]
Spray breakup	KH-RT, No collisions
Turbulence	RANS, RNG κ-ε
Combustion	UFPV – 4D tabulation (χ, c, $\widetilde{Z''^2}$, $\tilde{Z}$) [2] LLNL mechanism (2,755 species + 11,173 reactions)
Mesh spacing	2 mm base grid size 250 μm min grid size (AMR + Embedding) Peak cell count: 940,000 cells
Run time	~20 core-hours per 10 μs of simulated time Max convective-based CFL = 1.0, dt ~ 1e-07 s

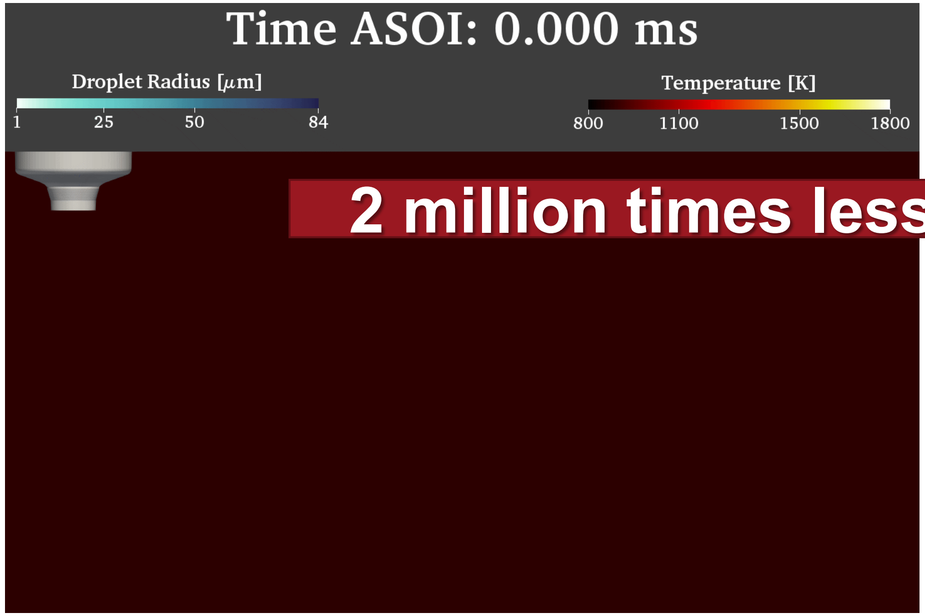


[1] Nocivelli et al., ASME ICEF2019-7258, 2019
[2] Nunno et al. AEC, 2020

APPLICATION OF EMULATED FLOWFIELDS

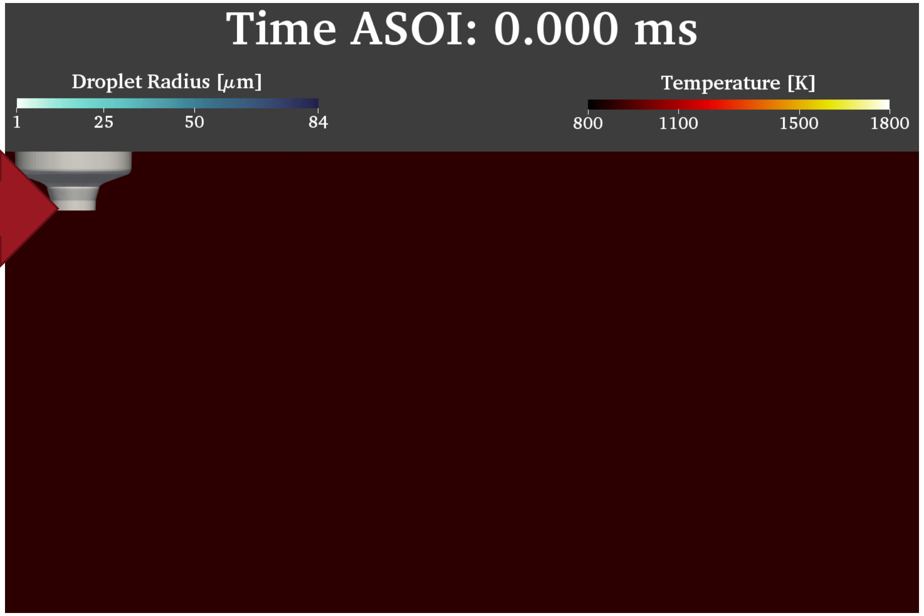
Accurate spray combustion predictions at a fraction of the cost

Injection Map from CFD ("Truth")



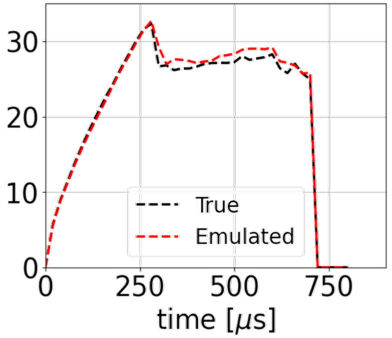
2 million times less expensive

Injection Map from Emulator



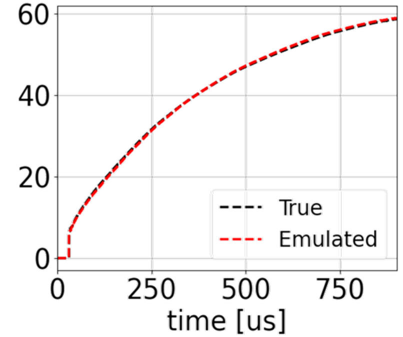
Liquid Penetration [mm]

Error < 4%



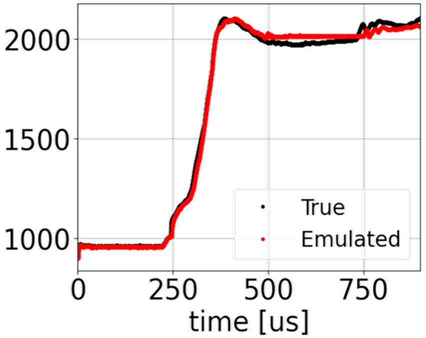
Vapor Penetration [mm]

Error < 1%



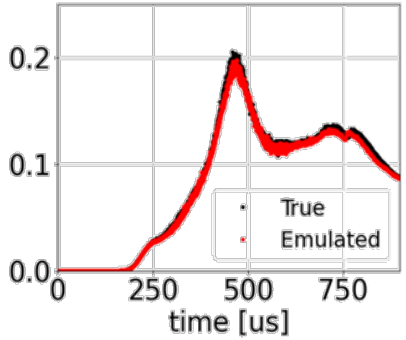
Max Temperature [K]

Error < 2%



Heat Release Rate [MJ/s]

Error < 2%



[1] Mondal, Torelli, Lusch, Milan, Magnotti, SAE World Congress, 2021

NEED FOR TRANSFER LEARNING[1]

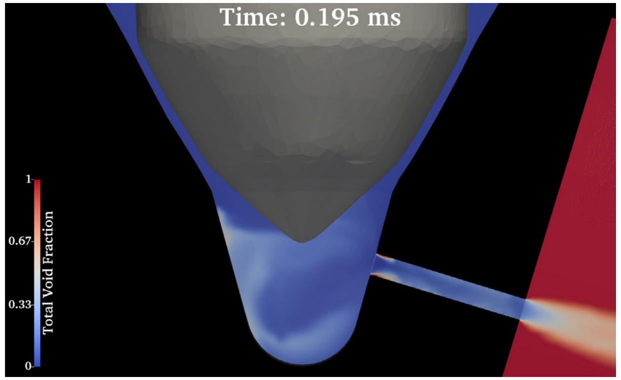
Addressing data scarcity in transient injection simulations

Typical turn-around time	
Internal flow simulations	Engine simulations
~ weeks	**~ days**

Need to accelerate internal flow simulations to have comparable turn around time with engine simulations

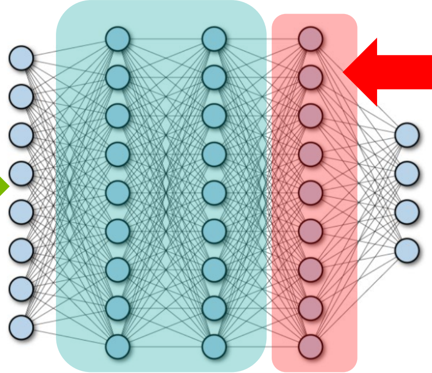
Transient injection simulations are expensive ⇒ Scarcity of data for training machine learning models

Expedite training for transient injector simulations using transfer learning



Static-Needle simulations **(Source domain)**

Freeze



Retrain

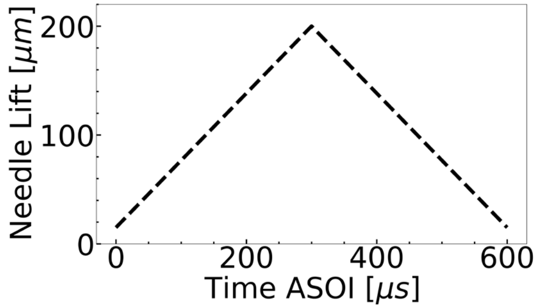
Moving-needle simulations **(Target domain)**

[1] Mondal, Magnotti, Lusch, Maulik, Torelli, *JEGTP* 145(4), 2022

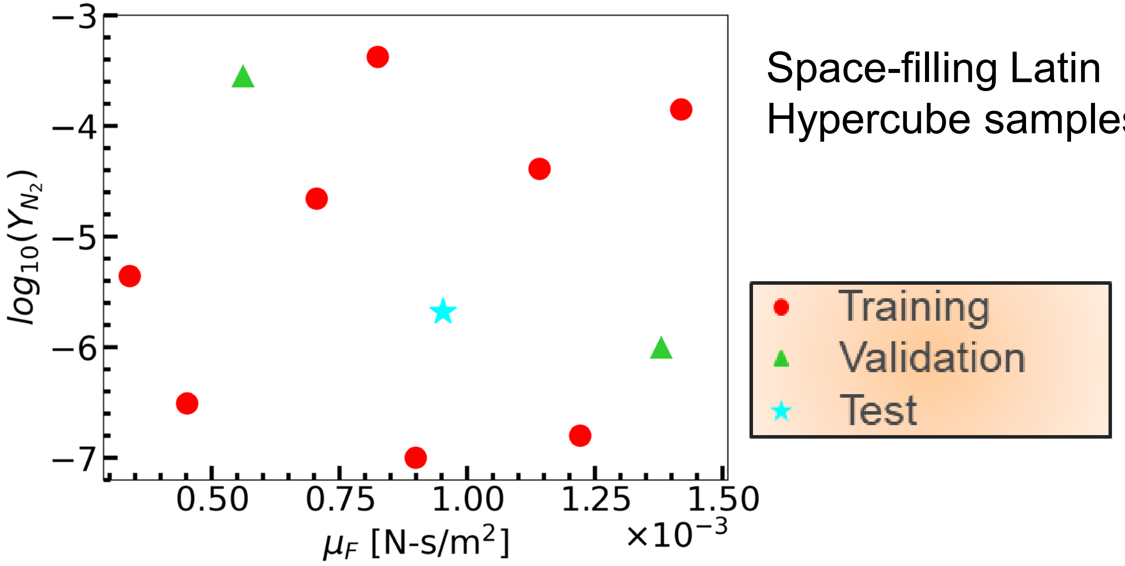
DESIGN OF EXPERIMENTS (DOE)

Input space of parameters that affect cavitation is efficiently explored

Design Parameters	Range		
Needle lift, δ [µm]	15	400	[1]
Fuel viscosity, μ_F [(N s) /m^2]	2.88×10^{-4}	1.51×10^{-3}	[2]
Level of dissolved gas Y_{N_2} [-]	1.0×10^{-7}	1.0×10^{-3}	[3]

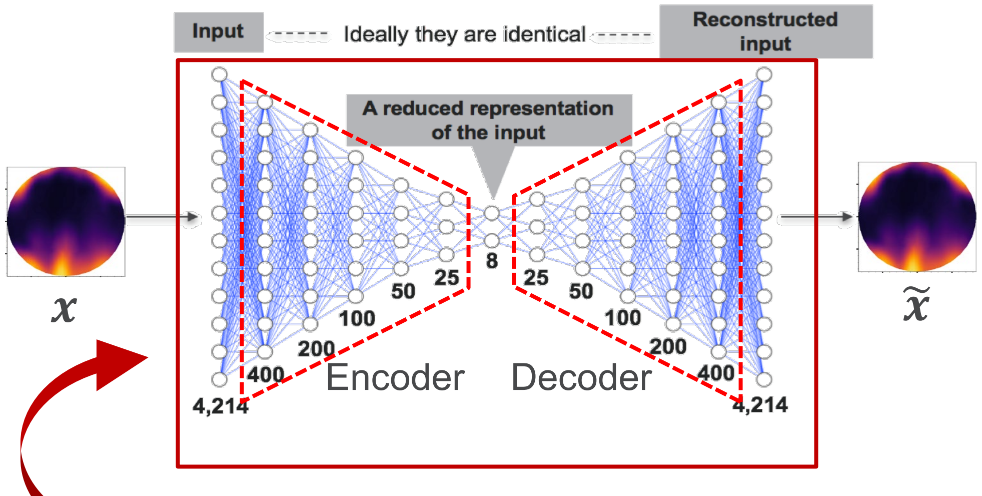


Needle lift profile[1]



Space-filling Latin Hypercube samples

11 samples in total in 2-D design parameter space



Weights and biases of the autoencoder framework initialized from the trained static needle autoencoder

[1] Guo, Torelli et al., *SAE Int. J. Advances & Curr. Prac. in Mobility*, 2020
[2] Magnotti and Som, ASME ICEF2019-7269, 2019
[3] Battistoni et al., *Atomization and Sprays* 25(6), 2015

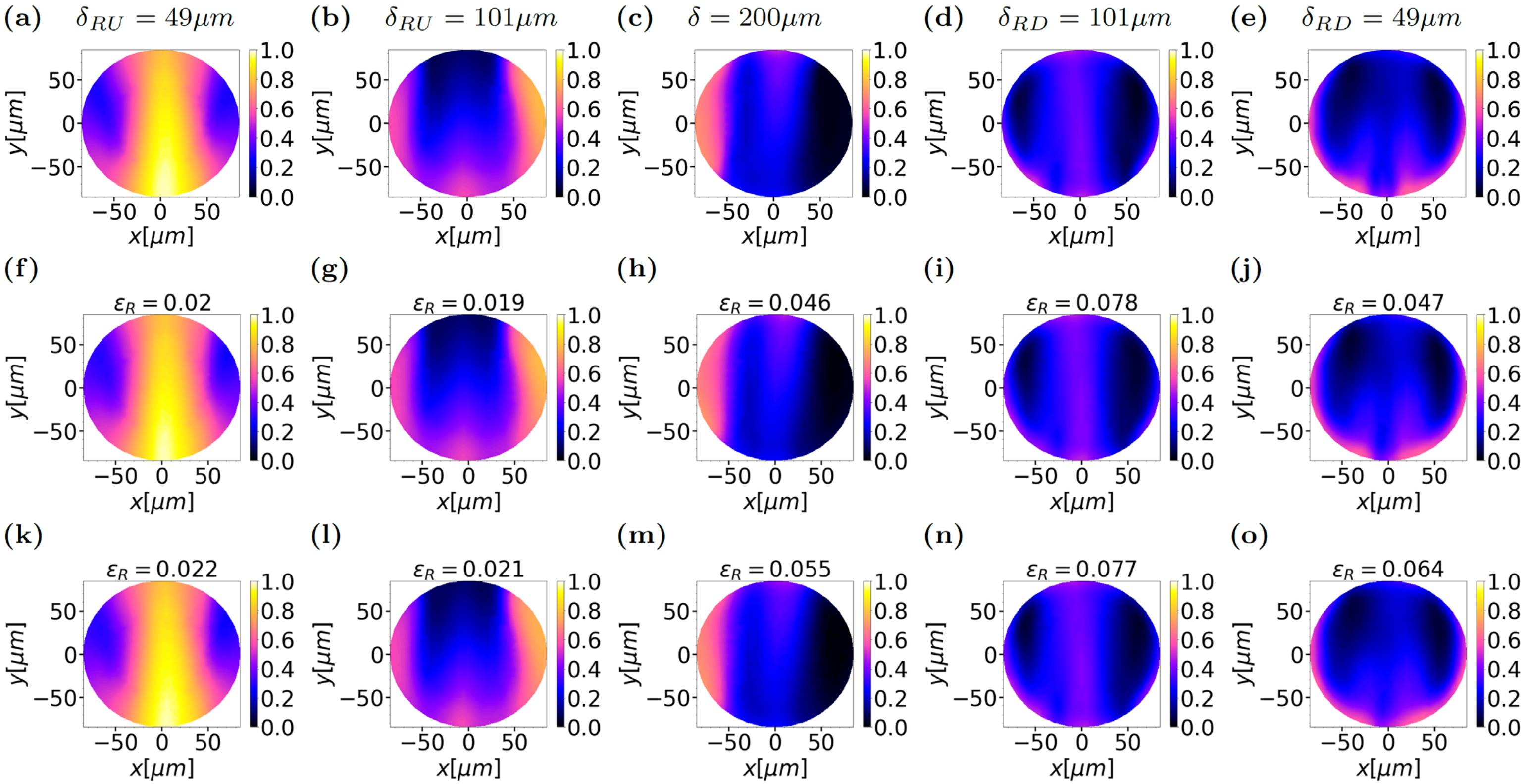
IMPACT OF TRANSFER LEARNING

Performance evaluated on reconstruction error for total void fraction

Truth (CFD)

Reconstructed with transfer learning

Reconstructed without transfer learning

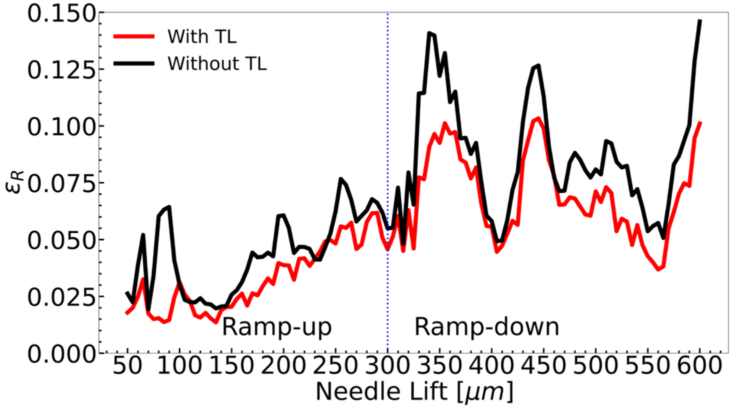


δ_{RU}
Needle lift during ramp-up phase

δ_{RD}
Needle lift during ramp-down phase

Reconstruction error

$$\varepsilon_R \triangleq \frac{||\mathbf{x} - \tilde{\mathbf{x}}||_2}{||\mathbf{x}||_2}$$

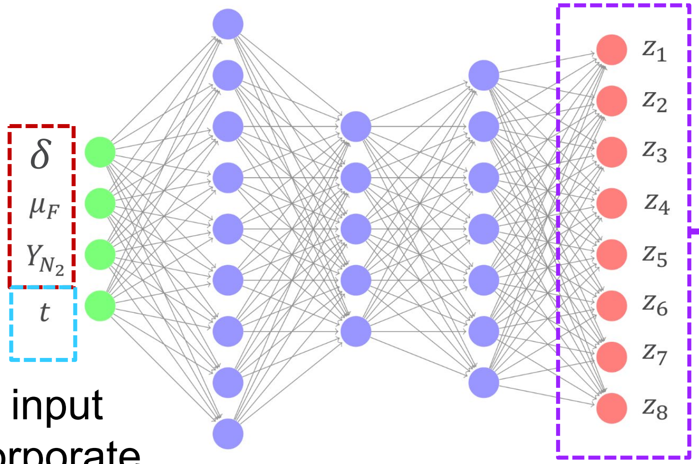


- Transfer Learning results in better reconstruction performance
- ~5% reduction in ε_R when transfer learning was employed

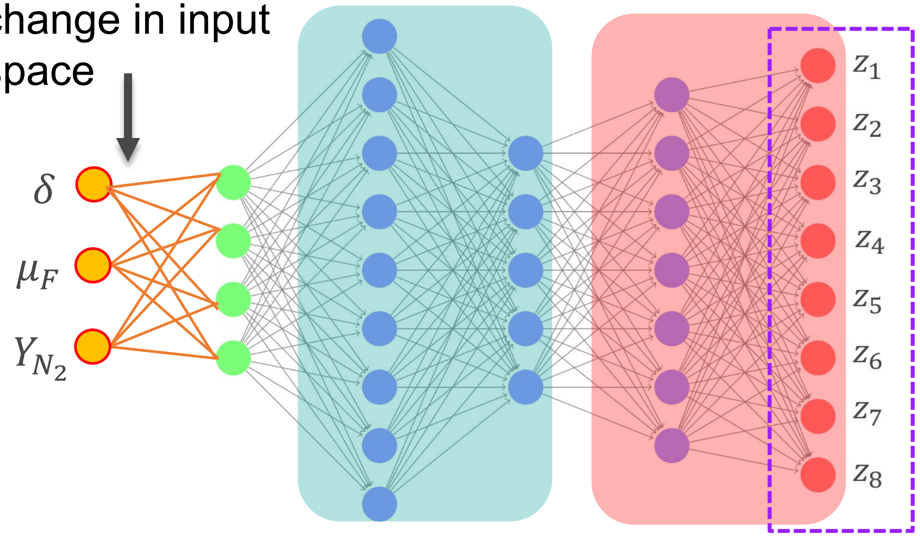
IMPROVING TRANSIENT INJECTION PREDICTIONS

Building upon the static needle regression framework

The regression model is another deep neural network that maps the design variables and time to the reduced dimensional latent space

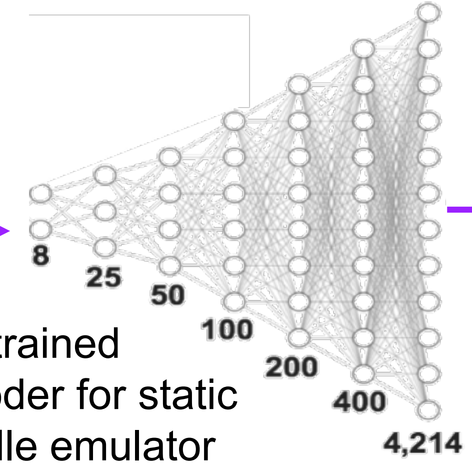


Adding new input layer to incorporate change in input space

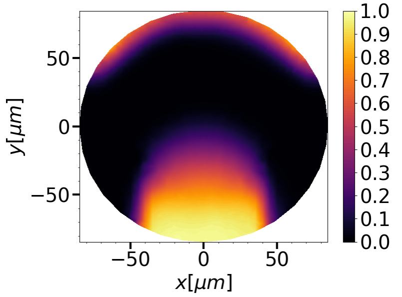


Freeze a few initial hidden layers

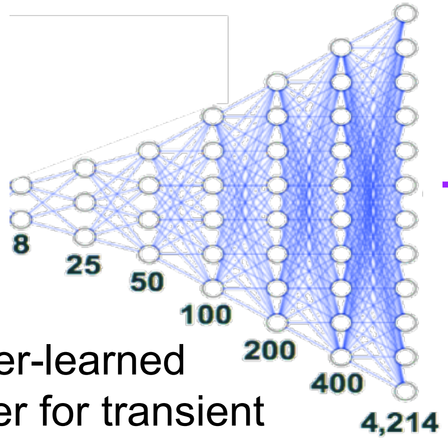
Retrain last few hidden layers with transient simulation data



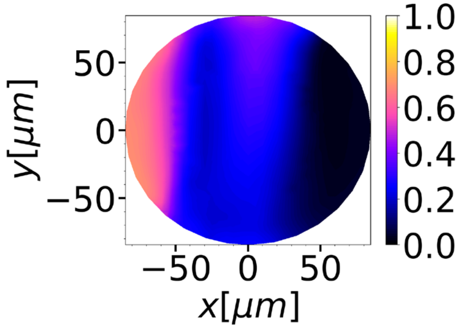
Pre-trained decoder for static needle emulator



Emulated static needle flowfield



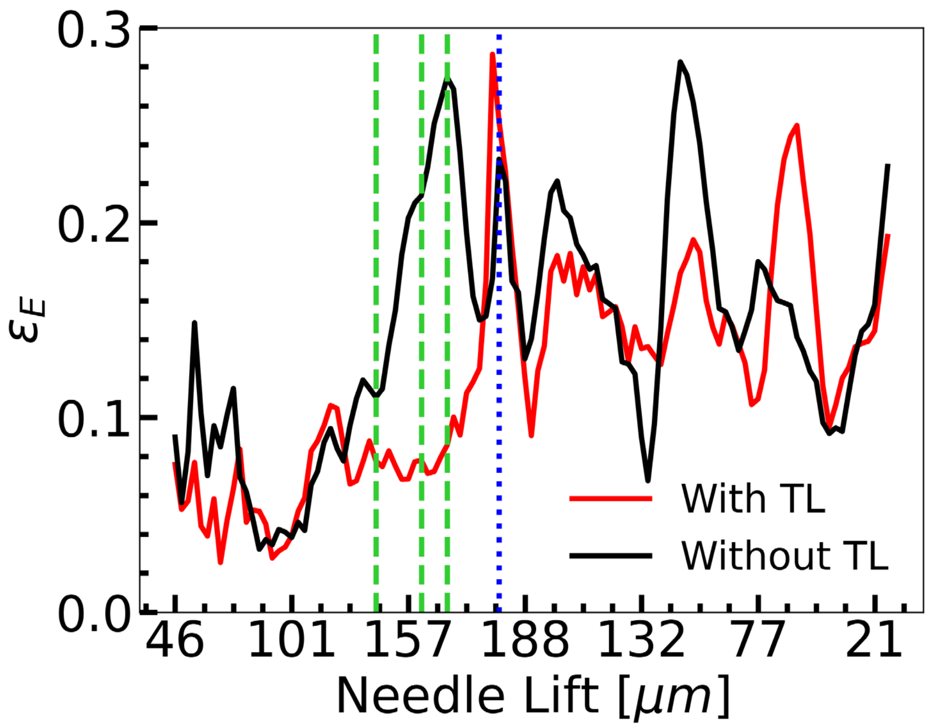
Transfer-learned decoder for transient needle emulator

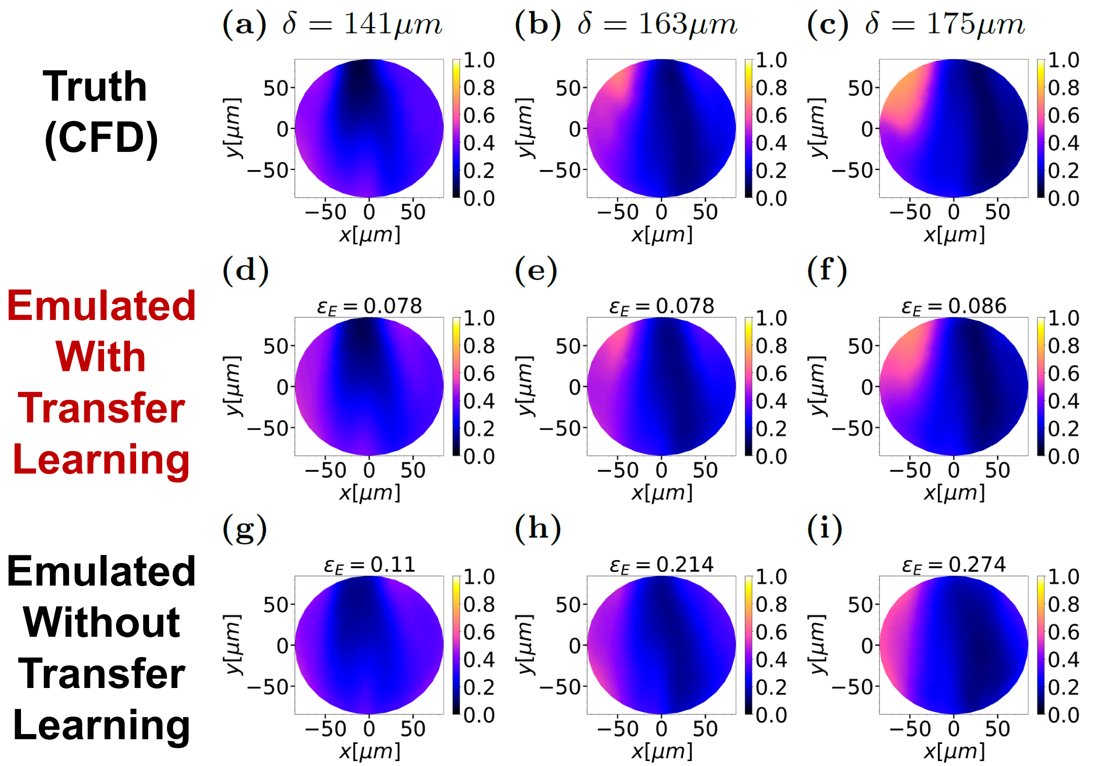


Emulated transient needle flowfield

IMPROVING TRANSIENT INJECTION PREDICTIONS

Performance evaluated on reconstruction error for total void fraction





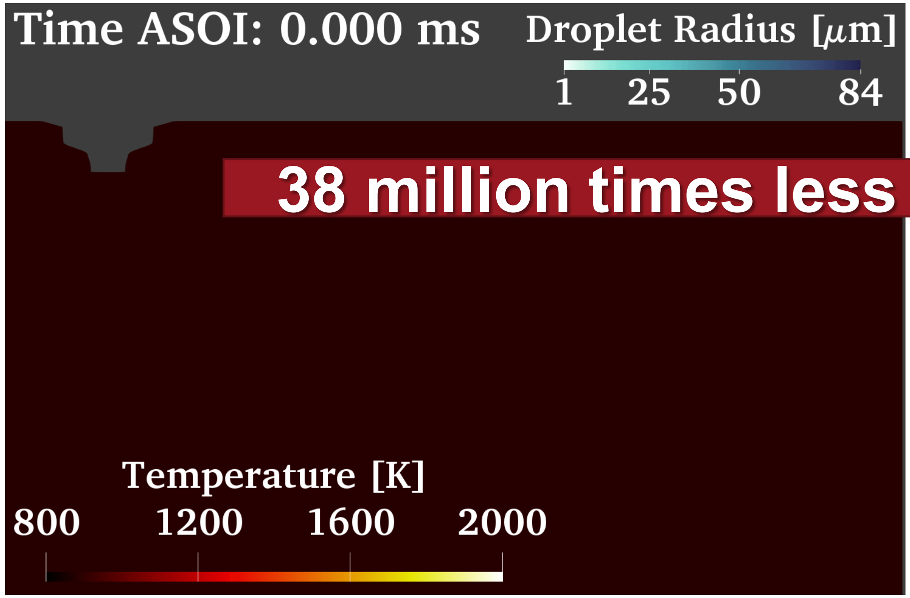
- 3% reduction in average emulation error over time
- A peak reduction of 20% in emulation error before the end of ramp-up phase

- Transfer Learning from static needle simulations helps in improving the predictions of total void fraction field for transient injection conditions.
- **Maximum achievable speedup ~ 38 million**

APPLICATION OF EMULATED FLOWFIELDS

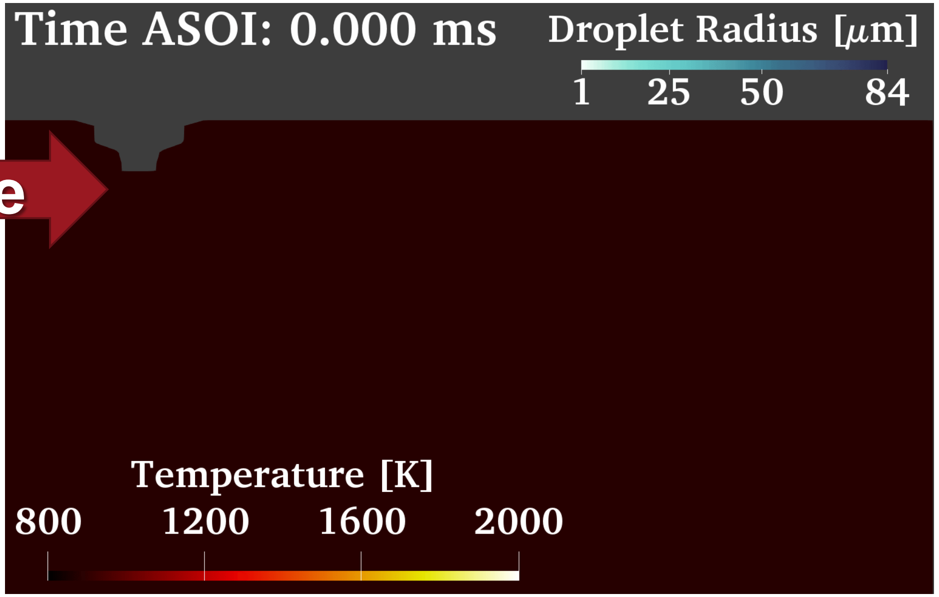
Use of emulated transient injection maps

Injection Map from CFD (“Truth”)

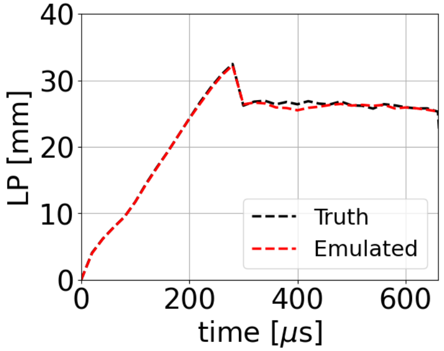


38 million times less expensive

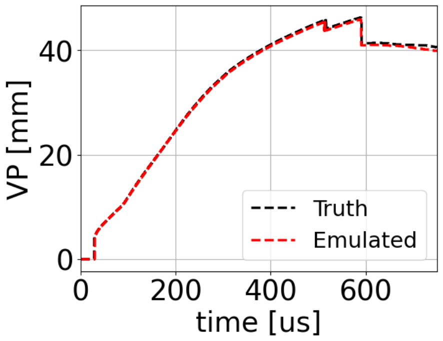
Injection Map from GP-based Emulator



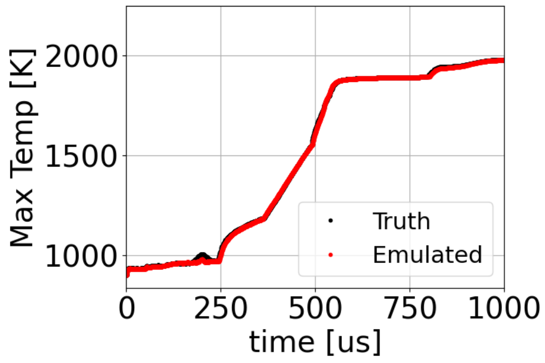
Liquid Penetration [mm]
Error < 1%



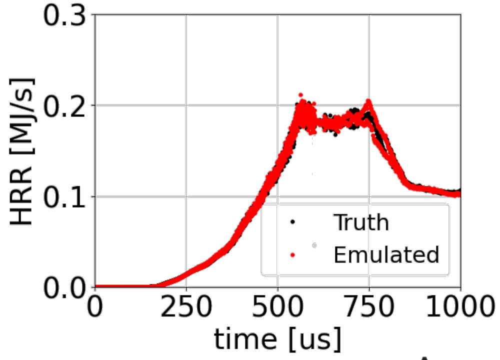
Vapor Penetration [mm]
Error < 1%



Max Temperature [K]
Error < 1%



Heat Release Rate [MJ/s]
Error < 1%



THANK YOU

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