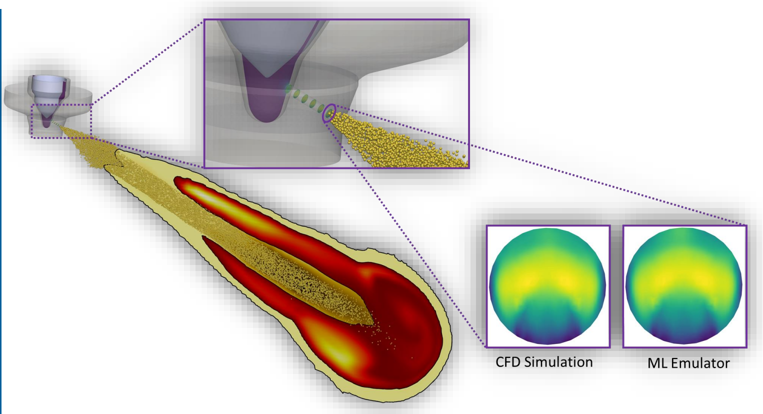
LES4ECE CONFERENCE

June 18th, 2021 Virtual Meeting

Using machine learning to overcome the computational bottleneck of coupling injector and spray simulations



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Argonne National Laboratory

DISCLAIMER / ACKNOWLEDGMENTS

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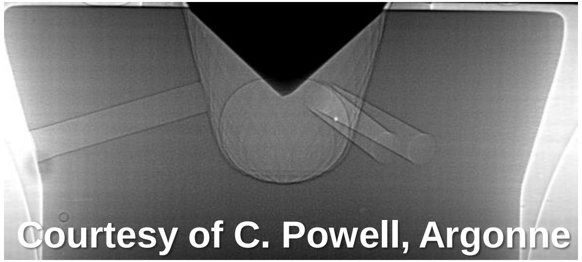
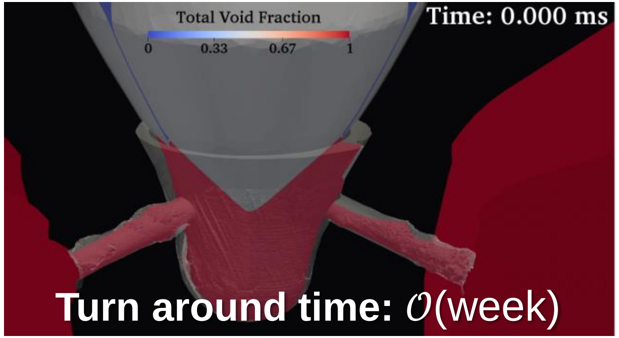
- **Convergent Science, Inc.** for providing software licenses and technical support
- **LCRC and ALCF computing resources** at Argonne National Laboratory
- Petro Junior Milan (Georgia Institute of Technology)
- Romit Maulik (Argonne National Laboratory)

Industry has voiced their need for accurate simulation tools that can link fuel injector and engine performance with efficiency and emissions

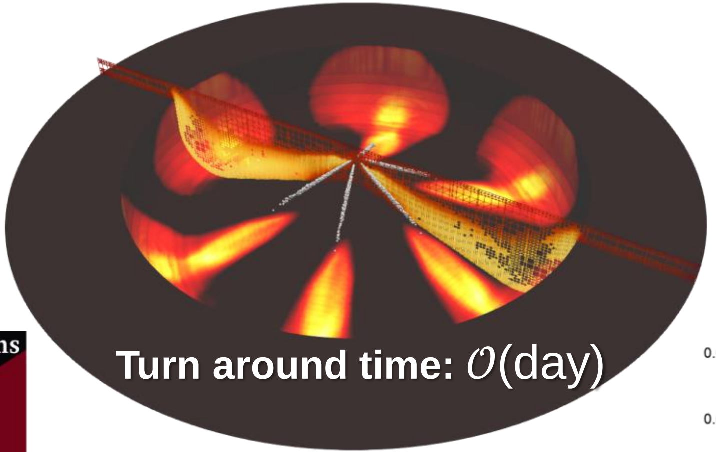
Informed boundary conditions using <u>x-ray measured quantities</u>



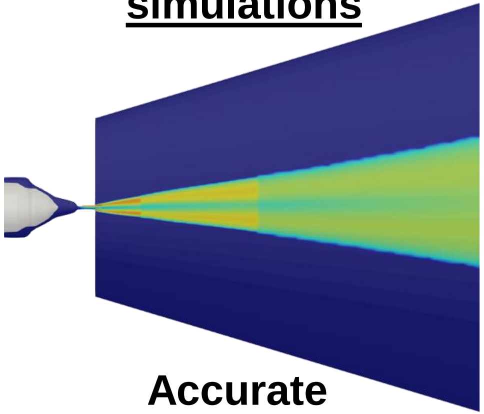
Detailed <u>injector simulations</u>



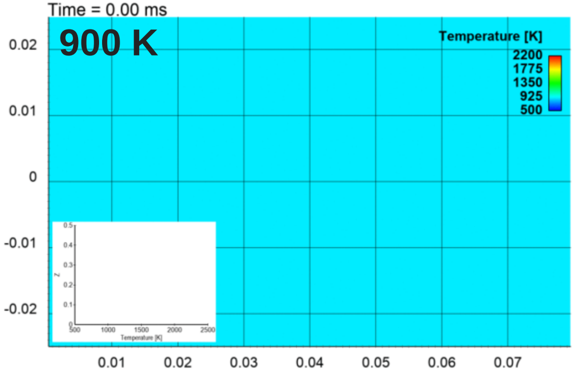
<u>Engine CFD Simulations</u>



Predictive spray <u>simulations</u>

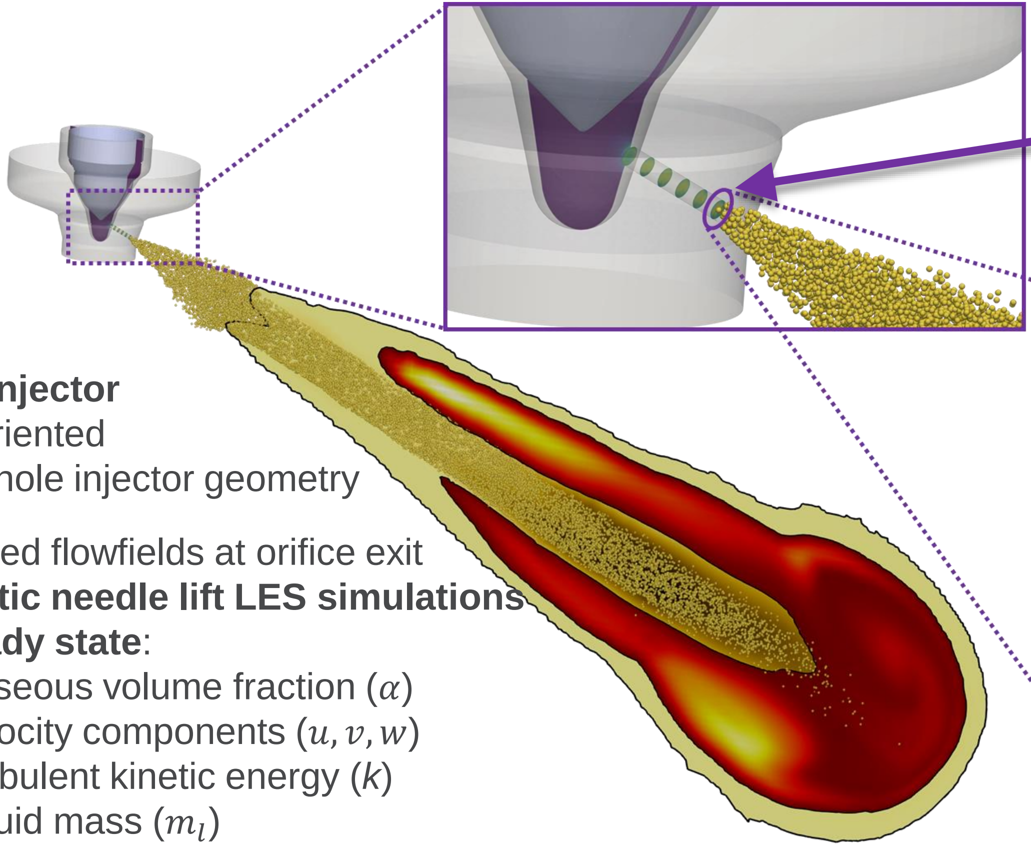


Accurate <u>combustion model</u>



To address the expense of injector simulations, a data-driven emulator is used to predict the spatiotemporal injection profile

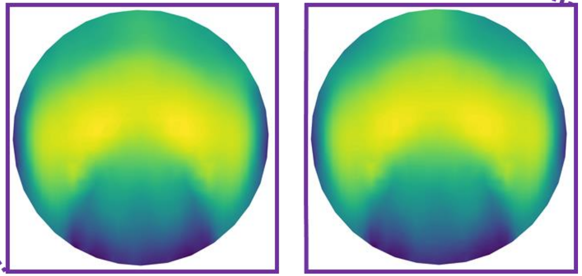
- Machine Learning models emulate internal flow fields at orifice exit
- Emulated flowfields coupled with:
  - Lagrangian spray model[1]
  - Eulerian-Lagrangian Spray Atomization (ELSA) model



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

Emulated flowfields at orifice exit **for static needle lift LES simulations at steady state**:

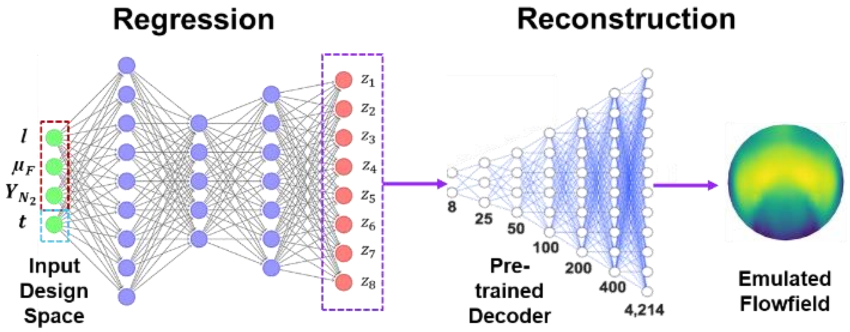
- Gaseous volume fraction (α)
- Velocity components (u, v, w)
- Turbulent kinetic energy (k)
- Liquid mass (m_l)



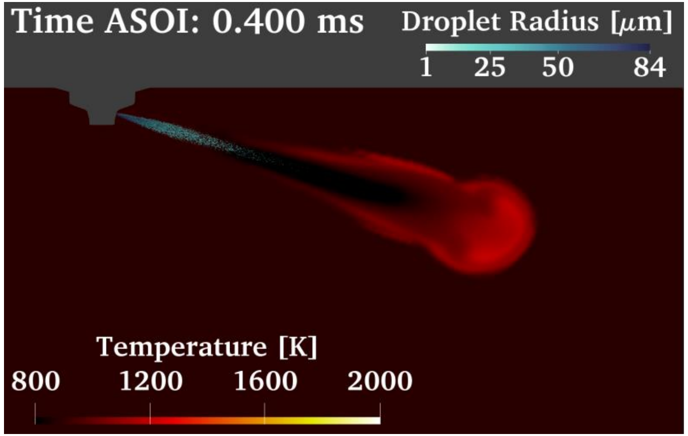
[1] Mondal, Torelli, Lusch, Milan, Magnotti, SAE International, 2021.

Our recent work has focused on developing and coupling the spatiotemporal emulator with different spray models

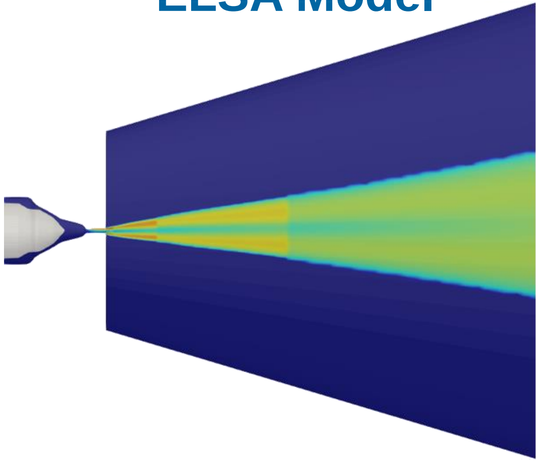
Development of Emulator Framework



Coupling of Emulator with Lagrangian Spray Model

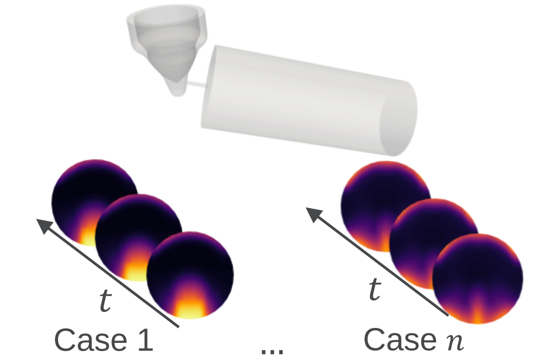


Coupling of Emulator with ELSA Model

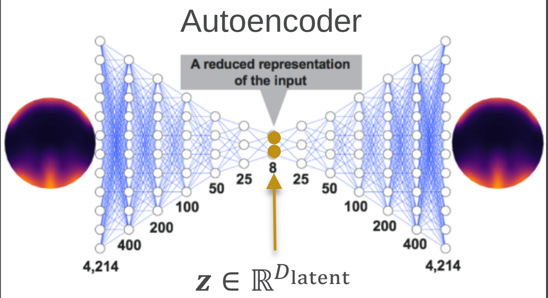


The construction of an emulator is organized into three phases:

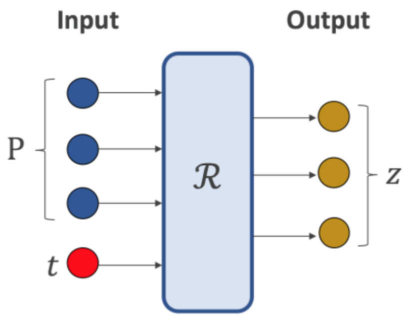
1. Training Data Generation



Reduced-Order Modeling[1]

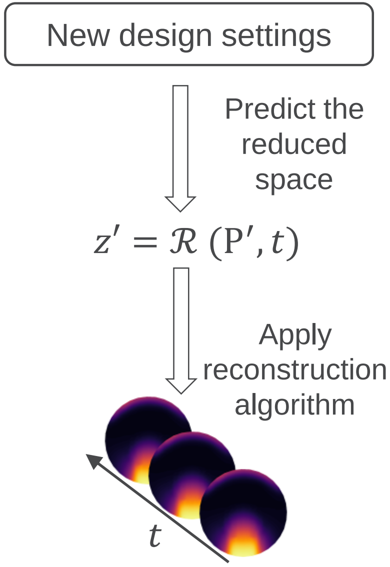


2. Regression Modeling



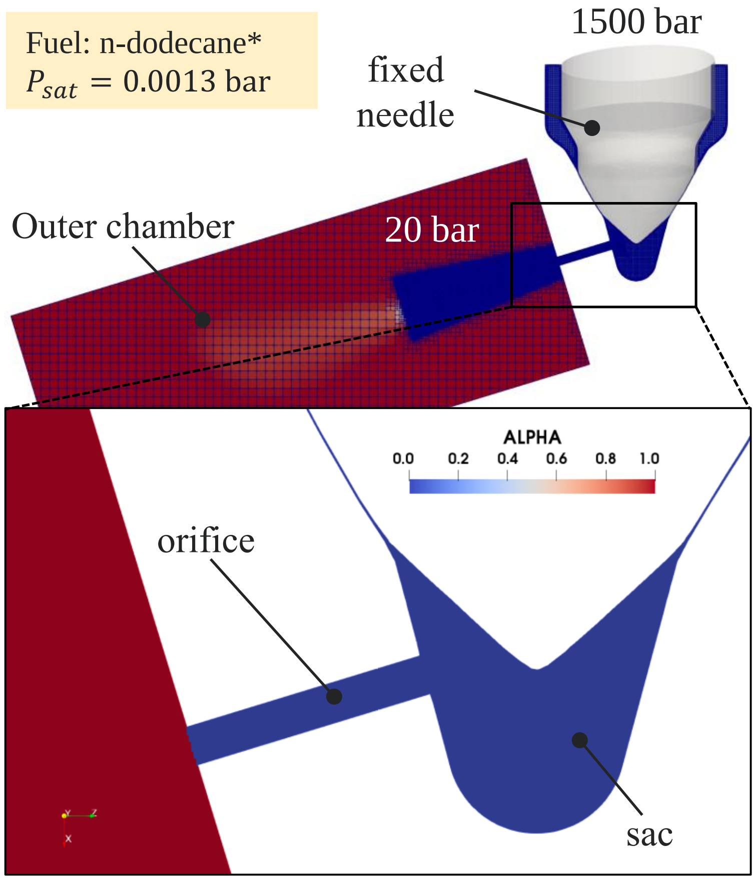
Learn the relationship between the design parameters (P) and reduced space (z):
$\mathcal{R}: (\mathrm{P}, t) \longmapsto z$

3. Emulator Formulation



- Demonstration case for single-hole injector with fixed needle lift
- DoE approach explores 3 design parameters: needle lift, fuel viscosity, and level of dissolved gas

Simplified injector simulations are performed that capture the salient physics of internal flow development



Model Set-up [2,3]	
Software	CONVERGE
Eqs. & Turbulence	Navier-Stokes LES, Dynamic Structure Model
Two-phase flow	Multiphase single mixture model w/ Homogeneous Relaxation Model (HRM) [4] Gas: compressible, RK EOS Liquid: compressible, barotropic fluid
Mesh spacing	160 μm base grid size 5 μm min grid size in embedded regions Peak cell count: 5.4M to 6.6M cells
Run time	1400 – 2000 CPU-hours per 10μs of simulated time. Max CFL = 0.25, dt< 1e-09 s

[1] Milan et al., AIAA SciTech, 2021
[2] Milan et al., Atomization and Sprays, Vol. 30, 2020
[3] Torelli, Magnotti et al., SAE International, 2019
[4] Bilicki & Kestin, Proc. Royal Society London A, Vol. 428, 1990

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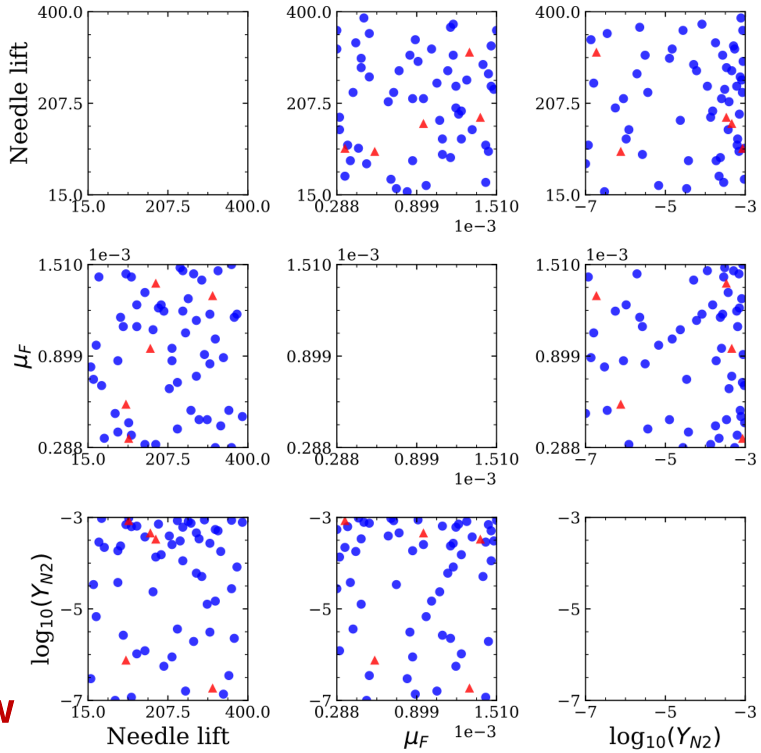
A design of experiments approach is used to efficiently explore the set of parameters that are known to affect cavitation

Design Parameters	Range		
Static 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} [-]	1×10^{-7}	1×10^{-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)

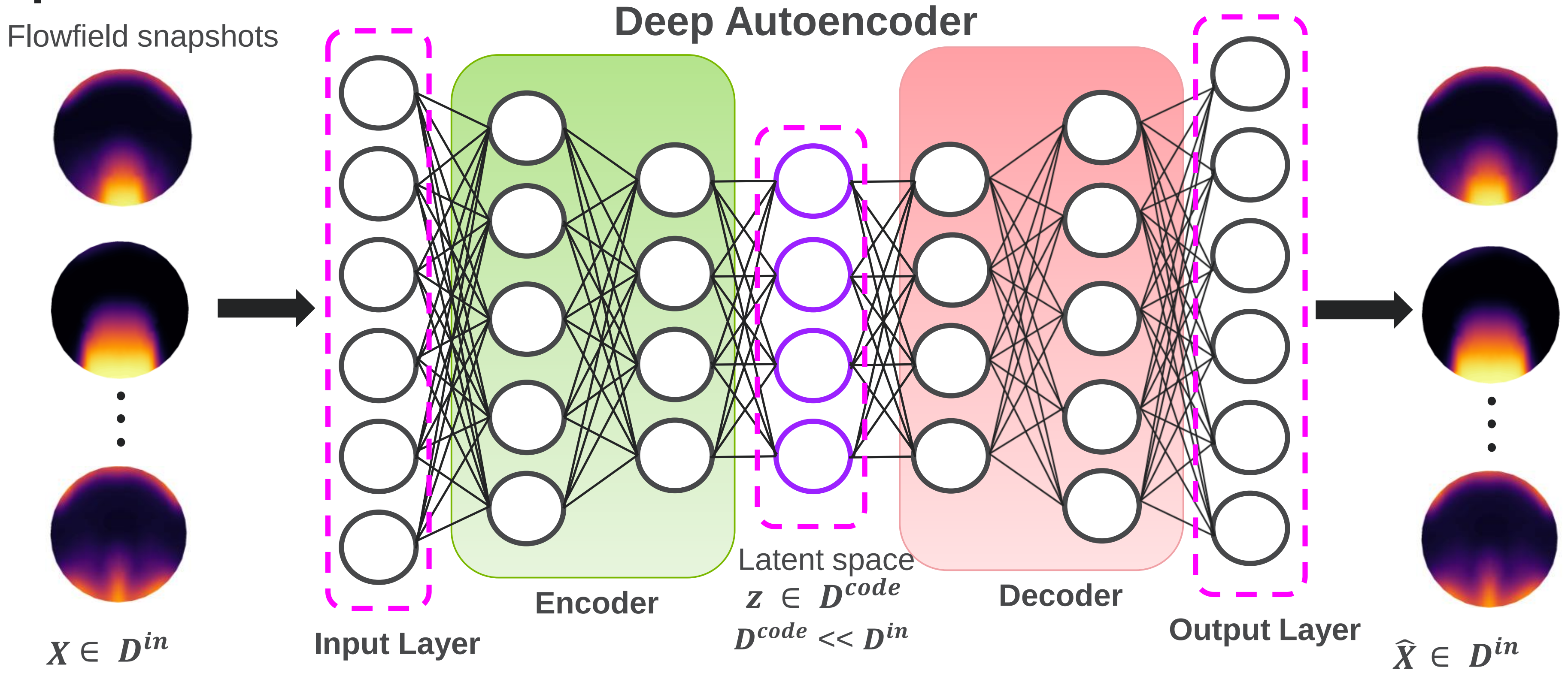
The test cases are chosen using input sensitivity analysis to encompass the different gas phase flow structures of the gas phase in the design space[4]



Reproduced with permission from Mondal et al., SAE Int. J. Adv. & Curr. Prac. in Mobility 3(3):1408-1424, 2021.

[1] Guo et al., SAE International, 2020. [2] Magnotti and Som, ASME ICEF, 2019.
[3] Battistoni et al., Atomization and Sprays, Vol.25, 2015. [4] Mondal et al., SAE International, 2021.

The autoencoder structure allows for a compressed representation and reconstruction of the flow to be learned

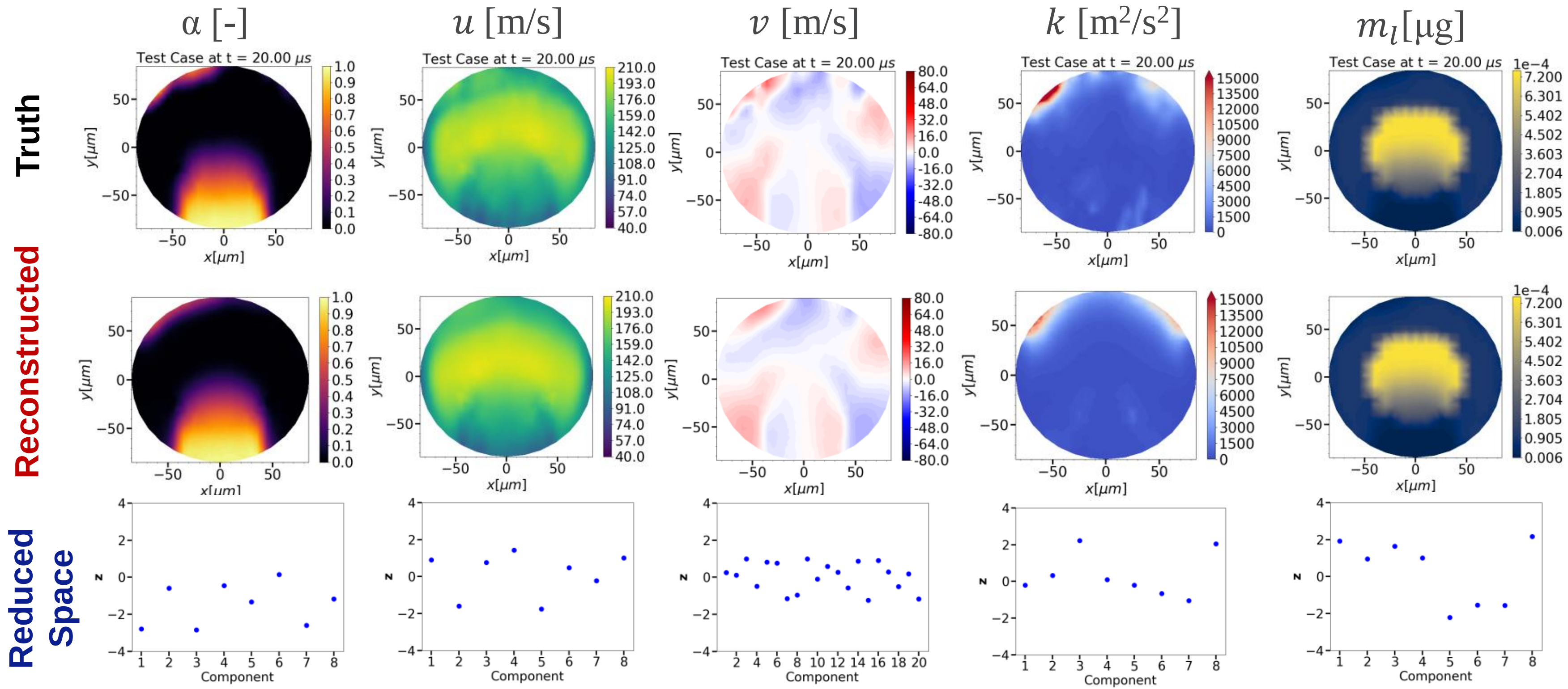


For our case, D^{in} = 4214, which is the # of grid points in the 2D snapshots

Ideally we want: $X = \hat{X}$

Autoencoder: $minimize_{\theta}\ ||X - \hat{X}\ ||$

The autoencoder allows for faithful reconstruction of flowfields



Reconstruction error of time-averaged flowfields

Errors averaged over 5 test cases

Flowfield	α	u	v	tke	m_l
Error	2%	1%	8%	15%	1%

Demonstrations shown for Case 51

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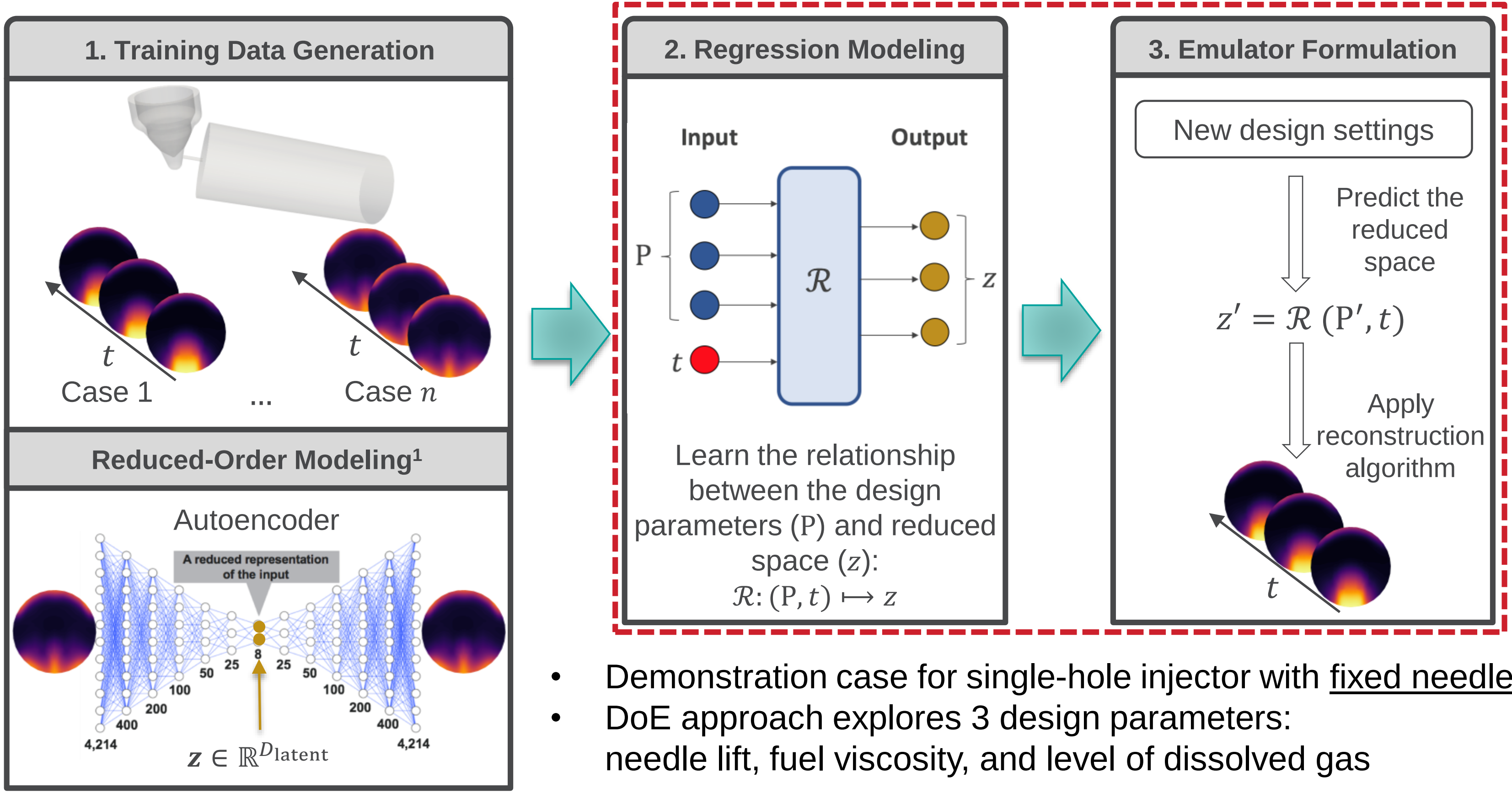
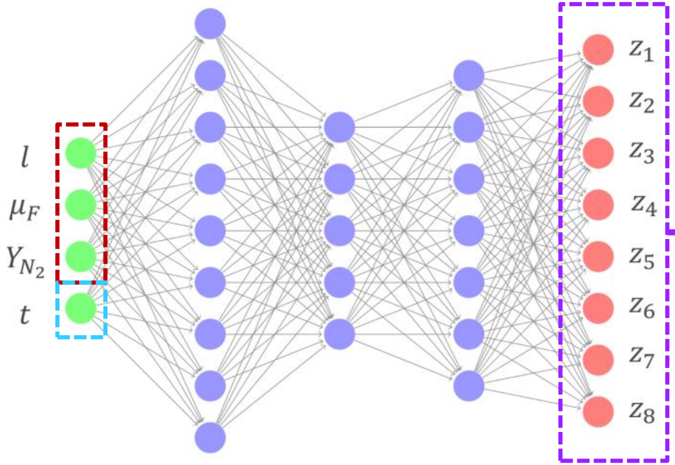
The construction of an emulator is organized into three phases:



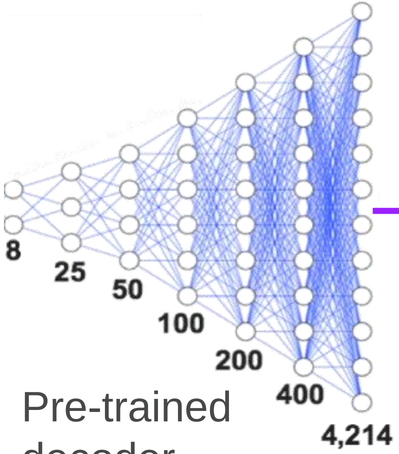
- Demonstration case for single-hole injector with <u>fixed needle lift</u>
- DoE approach explores 3 design parameters:
  needle lift, fuel viscosity, and level of dissolved gas

The emulator is comprised of deep learning-based models to relate design parameters to the predicted spatiotemporal flowfield

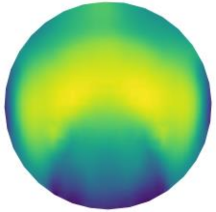


The regression model is another deep neural network that maps the design variables and time to the reduced dimensional latent space

Tuned Hyperparameters	Value
Number of hidden layers	4
$\mathcal{T}_{enc}$	[8, 16, 32, 32]
Optimizer algorithm	Adam
Learning rate of optimization	1×10^{-4}
Number of epochs	500
Batch size	25
L2 Regularization parameter	2×10^{-3}

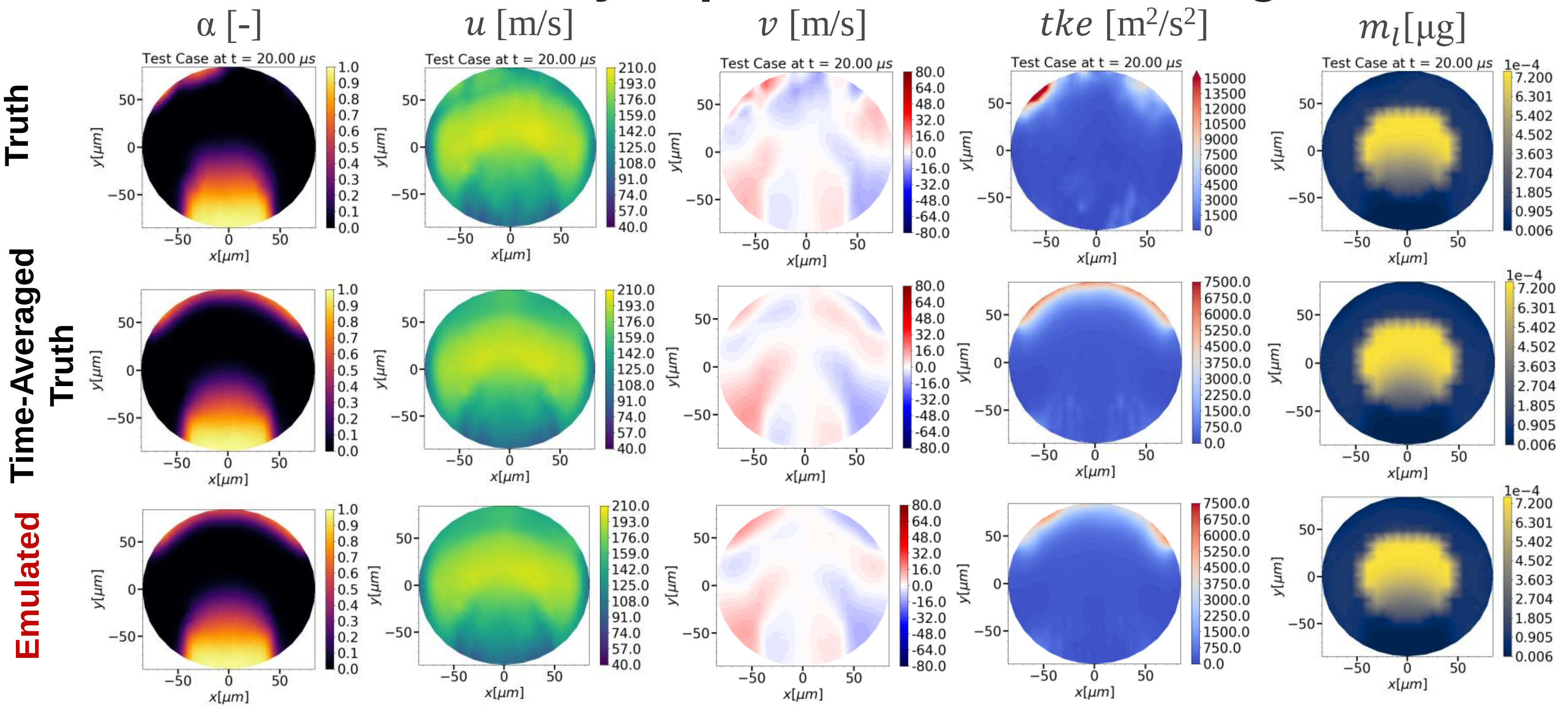


Pre-trained decoder



Emulated flowfield of Interest

The emulator accurately captures the time-averaged flowfield



Emulation error of time-averaged flowfields

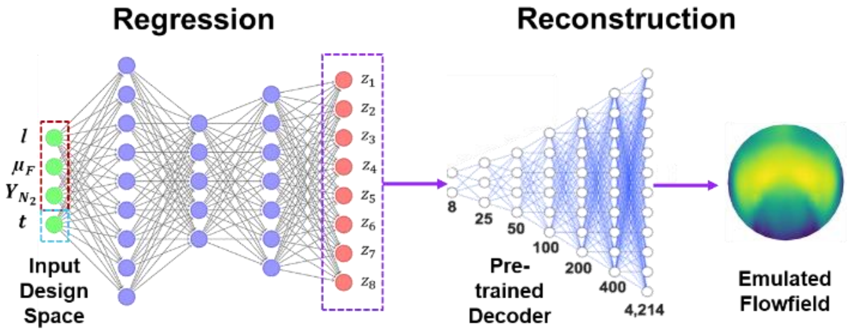
Flowfield	α	u	v	tke	m_l
Error	8%	2%	22%	24%	2%

Errors averaged over 5 test cases

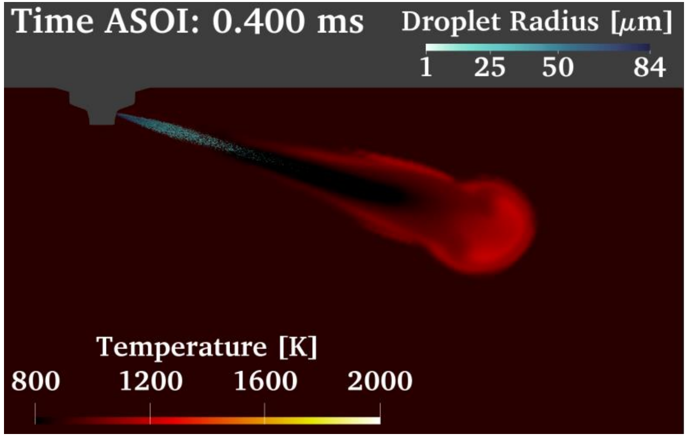
Demonstrations shown for Case 51

Our recent work has focused on developing and coupling the spatiotemporal emulator with different spray models

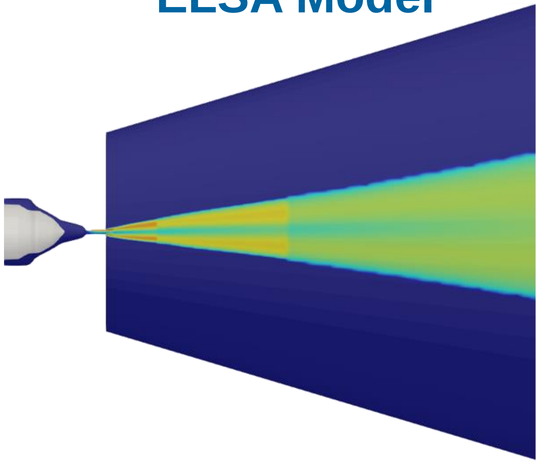
Development of Emulator Framework



Coupling of Emulator with Lagrangian Spray Model



Coupling of Emulator with ELSA Model



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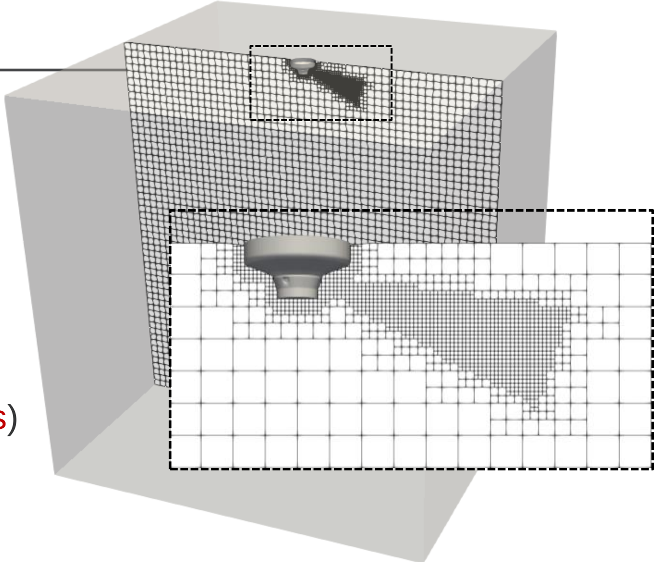
The emulator is tested by comparing the spray development using the CFD- and emulator-predicted injection profiles

Liquid 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 v2.4
Parcel Initialization	Static coupling, LVF threshold = 0.1
Spray breakup	KH-RT, NTC collision model
Turbulence	RANS, RNG κ-ε
Combustion	UFPV – 4D tabulation $(\chi, c, \widetilde{Z''^2}, \tilde{Z})$ 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: 300,000 cells
Run time	~20 core-hours per 10 μs simulated time Max convective-based CFL = 1.0, dt ~ 1e-07 s



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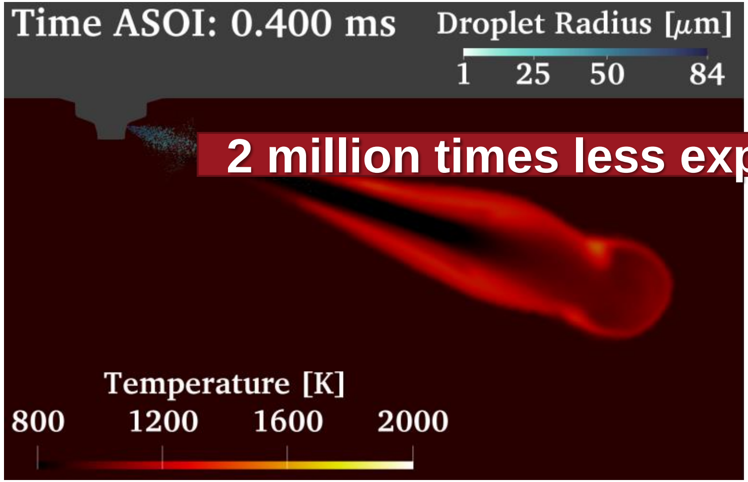
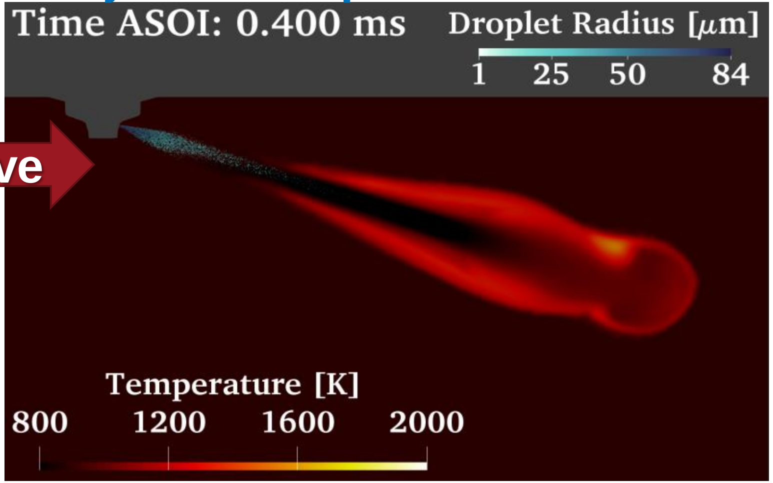
The emulator provides accurate spray combustion predictions at a fraction of the cost of simulating the next design point of interest

Injection Map from CFD (“Truth”)

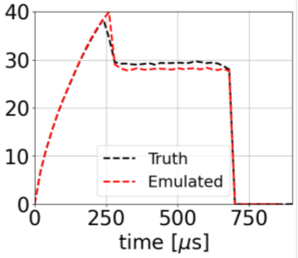


2 million times less expensive

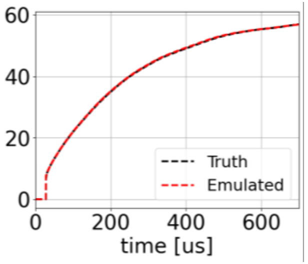
Injection Map from Emulator



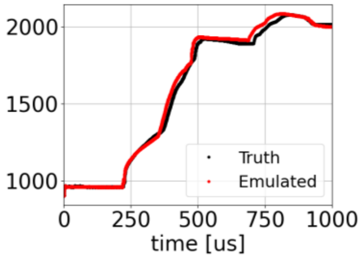
Liquid Penetration [mm]
Error < 3%



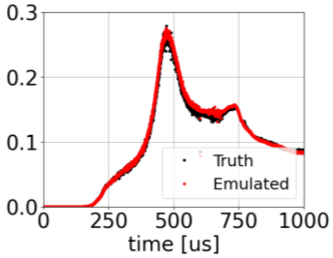
Vapor Penetration [mm]
Error < 1%



Max Temperature [K]
Error < 2%

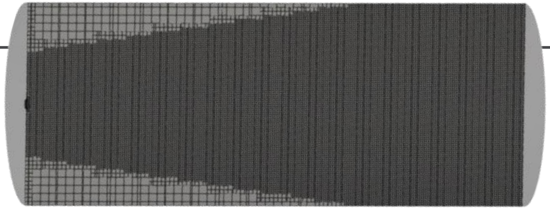


Heat Release Rate [MJ/s]
Error < 1%



The emulator has also been extended to provide the injection profile for the Eulerian Lagrangian Spray Atomization model

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

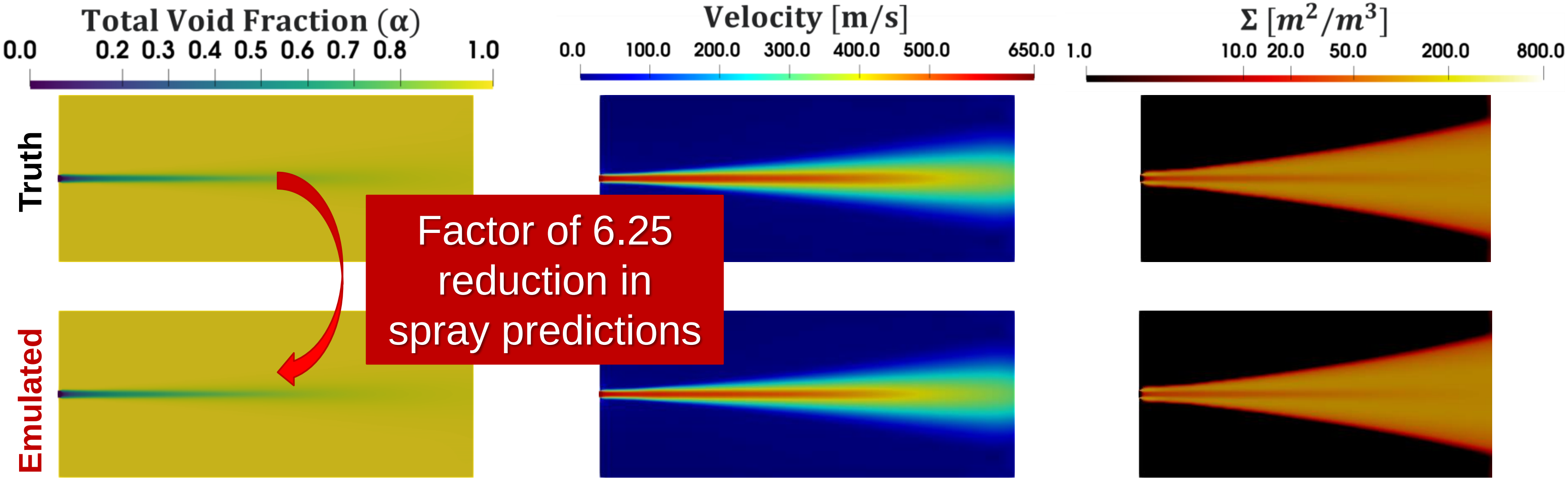


Model Set-up

Software	CONVERGE v3.0
Eulerian Initialization	Static coupling, LVF threshold = 0.1
Turbulence	RANS, RNG κ-ε
Spray structure	$\frac{\partial \Sigma}{\partial t} + \frac{\partial u_i \Sigma}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D_\Sigma\left(\frac{\partial \Sigma}{\partial x_i}\right)\right) + C_\Sigma \Sigma\left(1 - \frac{\Sigma}{\Sigma_{eq}}\right) + S_{init} + S_{evap}$
Mesh spacing	160 µm base grid size 40 µm min grid size (Fixed embedding) Peak cell count: 1.48 million cells
Run time	~120 core-hours per 10 µs simulated time Max convective-based CFL = 1.0, dt ~ 3e-09 s

Compare to internal flow simulation run time: 1400 – 2000 core-hours per 10μs of simulated time (dt < 1e-09 s)

The emulator has been demonstrated to provide accurate spray predictions within the ELSA framework at a fraction of the cost



Error of predicted external flowfields

Field	α	v	w	V_{mag}	Σ
Error	1.5%	8.1%	3.5%	4.0%	6.5%

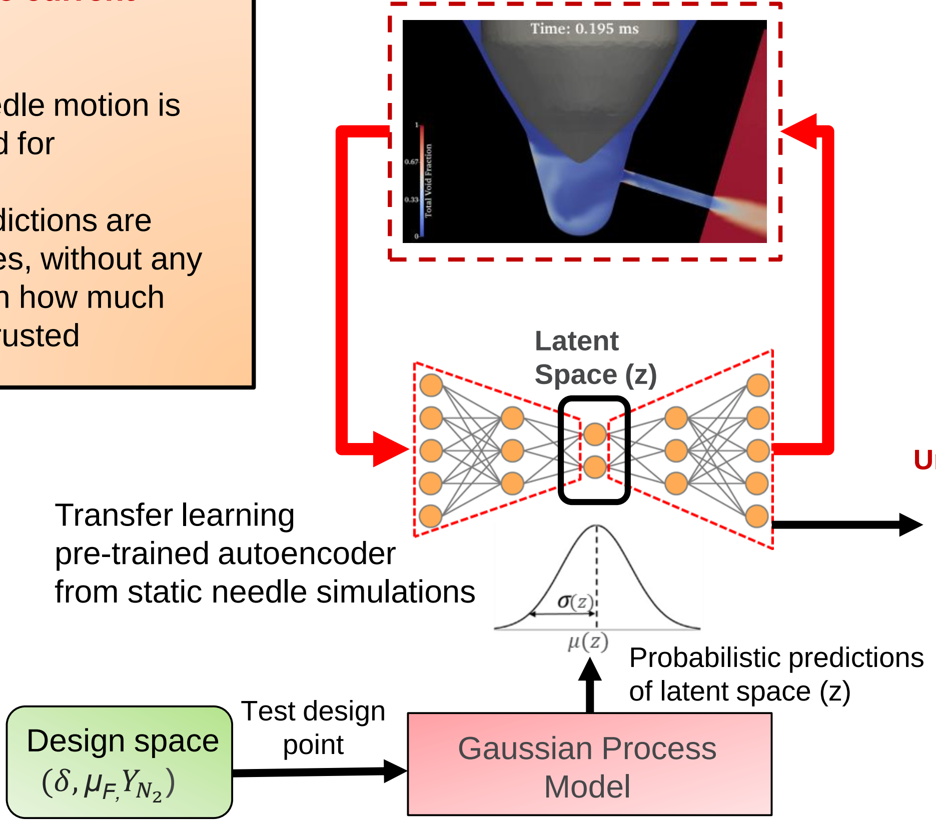
ONGOING RESEARCH AND FUTURE OUTLOOK

Extension of the emulator framework is underway to predict the injection profile for transient injector operation

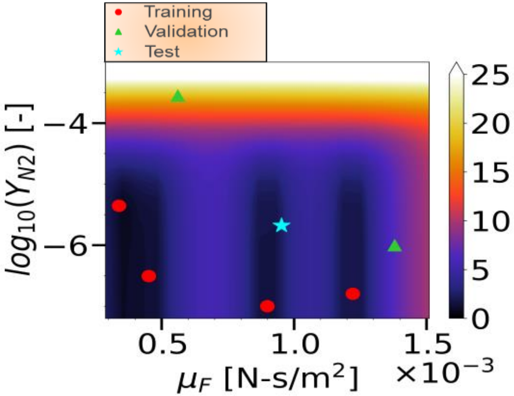
Limitations of the current framework:

- Transient needle motion is not accounted for
- Flowfield predictions are point estimates, without any information on how much they can be trusted

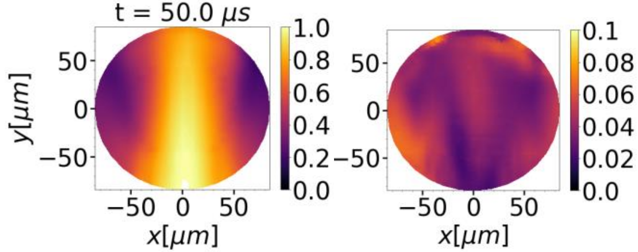
Transient needle simulations



Principled way of adding DoE points to reduce prediction uncertainty



Uncertainty quantification in flowfield predictions



Mean predicted α **Standard deviation in α prediction**

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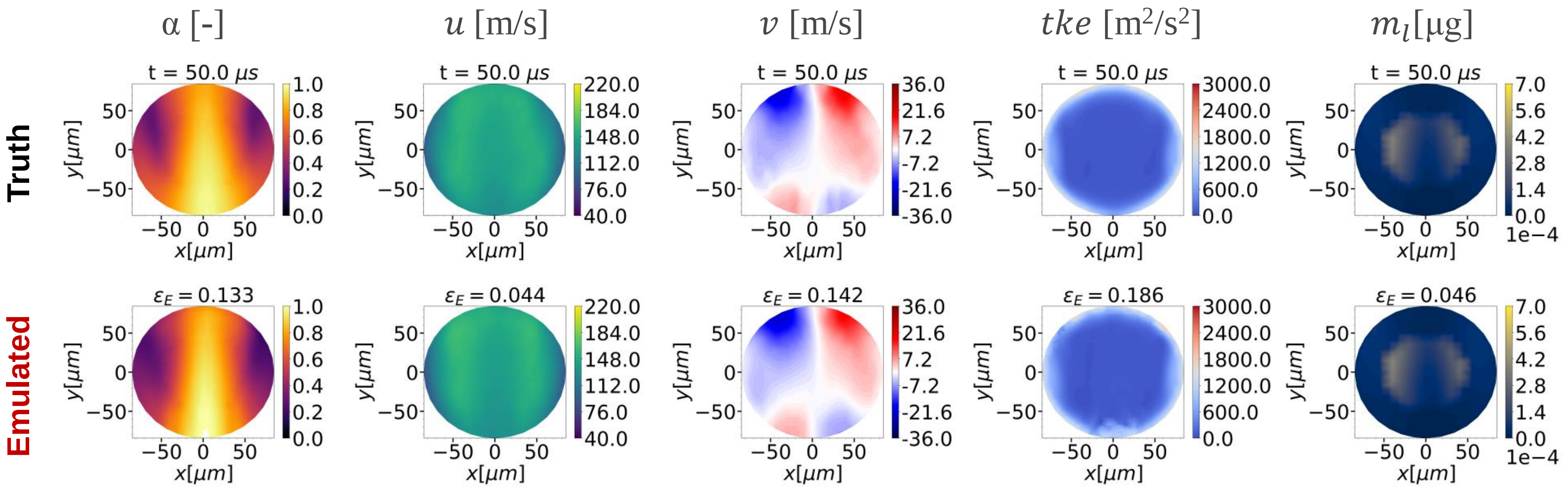
Extension of the emulator framework is underway to predict the injection profile for transient injector operation



Emulation error of flowfields

Flowfield	α	u	v	tke	m_l
Error	10%± 3%	2%± 0.5%	34%± 7%	11%± 2%	3%± 1%

Demonstrations shown for Case 9

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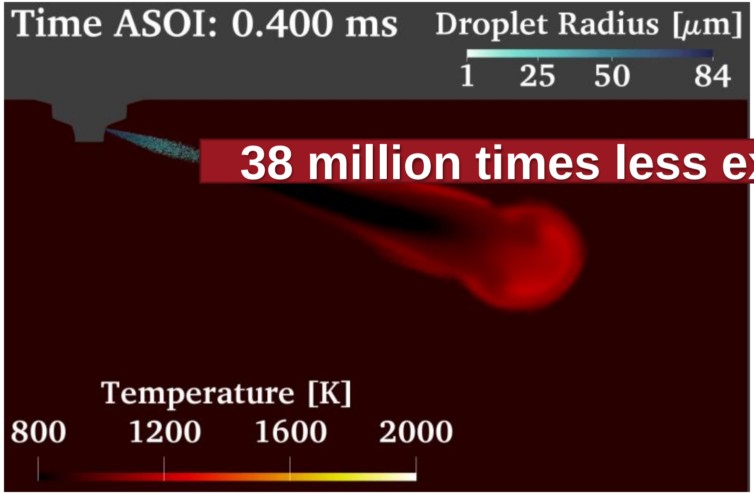
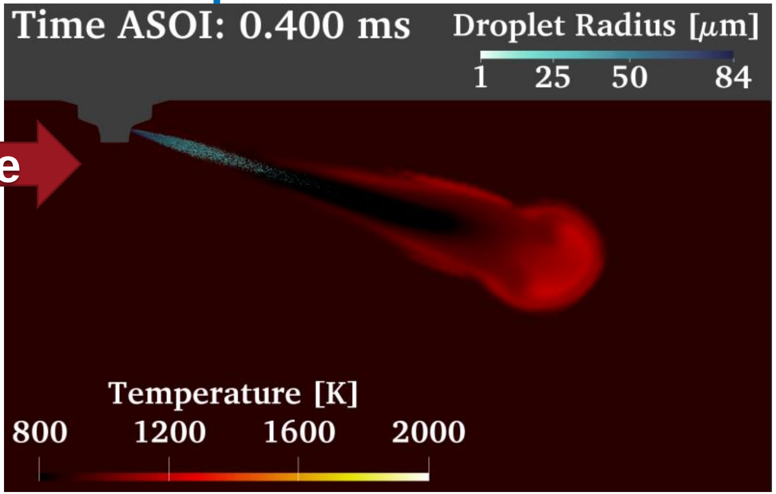
The emulator provides accurate spray combustion predictions at a fraction of the cost of simulating the next design point of interest

Injection Map from CFD ("Truth")

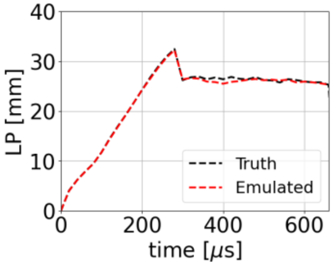


38 million times less expensive

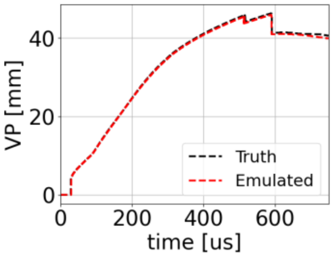
Injection Map from GP-based Emulator



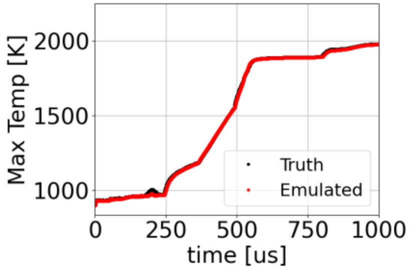
Liquid Penetration [mm]
Error < 1%



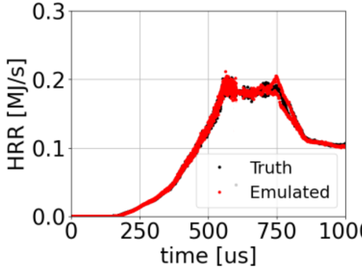
Vapor Penetration [mm]
Error < 1%



Max Temperature [K]
Error < 1%



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



THANK YOU

gmagnotti@anl.gov

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