This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

SAND2022-6025C

Sandia National Laboratories

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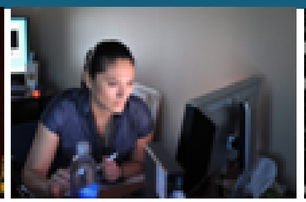
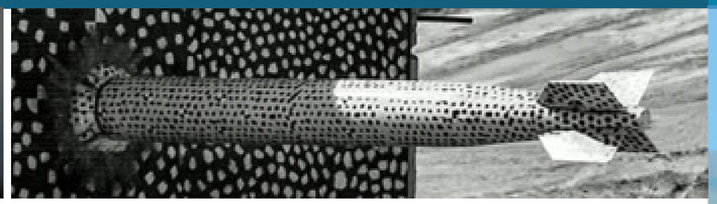
IMPROVING CHEMISTRY TABULATION WITH PARTITION OF UNITY NETWORKS





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U.S. DEPARTMENT OF ENERGY

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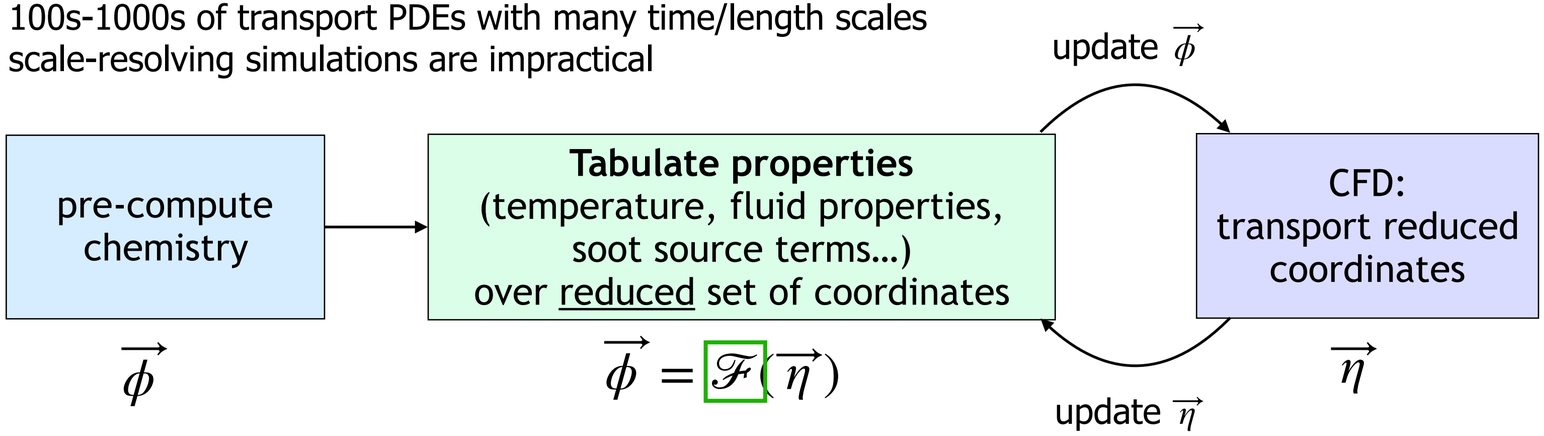
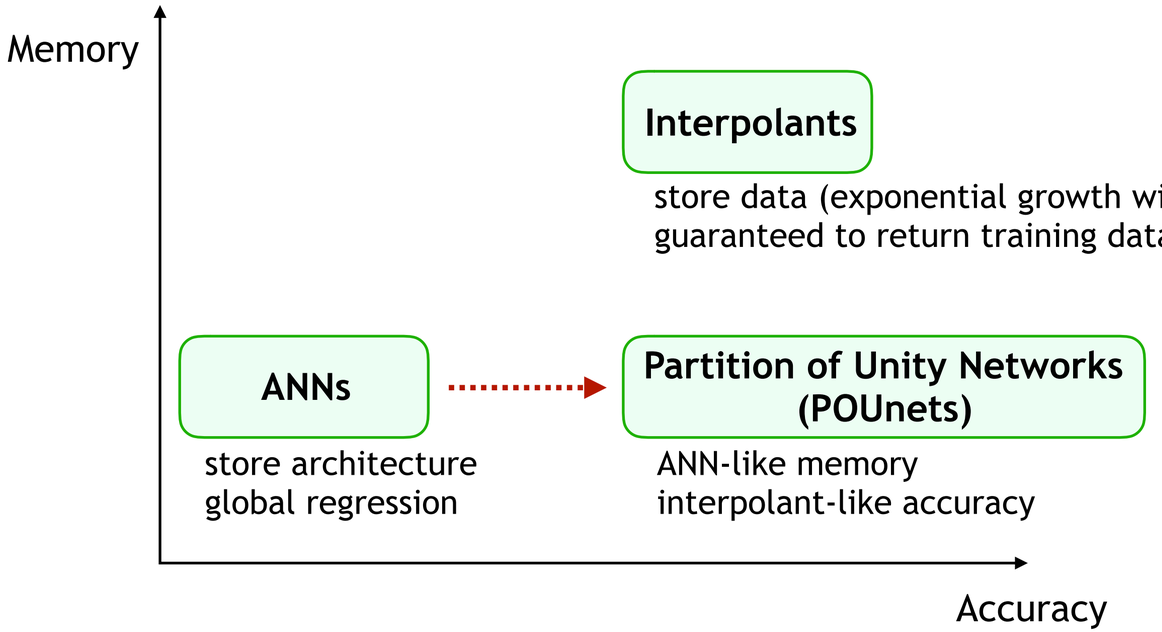
Chemistry tabulation facilitates practical simulation of combustion at engineering scales

100s-1000s of transport PDEs with many time/length scales
scale-resolving simulations are impractical



Example simulation
SIERRA/Fuego



Recent methods localize regression to increase accuracy of ANNs

1. **Classification**
2. **Regression**

Classification can be done using
- physical intuition
- machine learning
  (e.g., mixture of experts)

We propose using POUnets to achieve this desired accuracy

Partition of Unity Networks (POUnets) provide localized polynomial approximations

Classification

provides a mesh-free partition of space

Regression

approximates property data

Inputs → single-layer RBF network with normalized neuron outputs creates a POU → polynomial basis multiplied by each neuron creates local approximations → Sum to compute output

Hyper parameters: number of partitions | polynomial degree

Trainable parameters:

RBF parameters
partition locations & shapes

basis parameters
polynomial coefficients

Example:
5-partitions, degree 1
→ 20 trainable parameters

Training Algorithm:

1. **Initialize trainable parameters**
2. **Single Gradient Descent Step**
   Update RBF parameters
   (Hold basis parameters constant)
3. **Least Squares Regression**
   Update basis parameters
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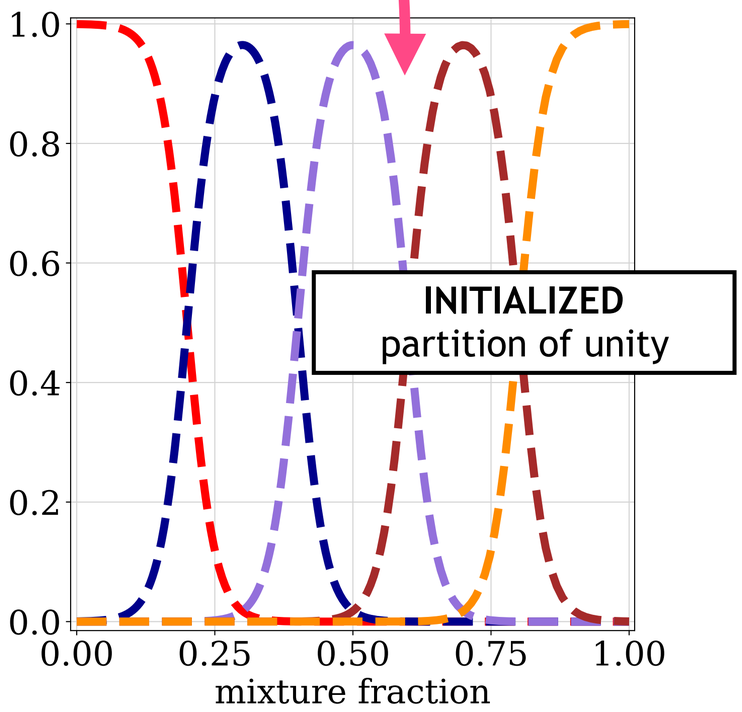
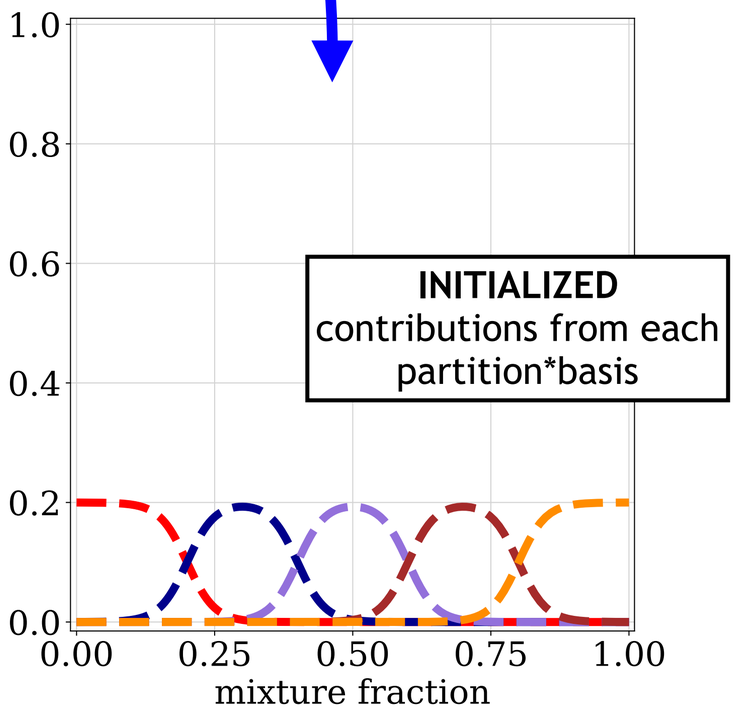
4. **Repeat 2-3 until converged**





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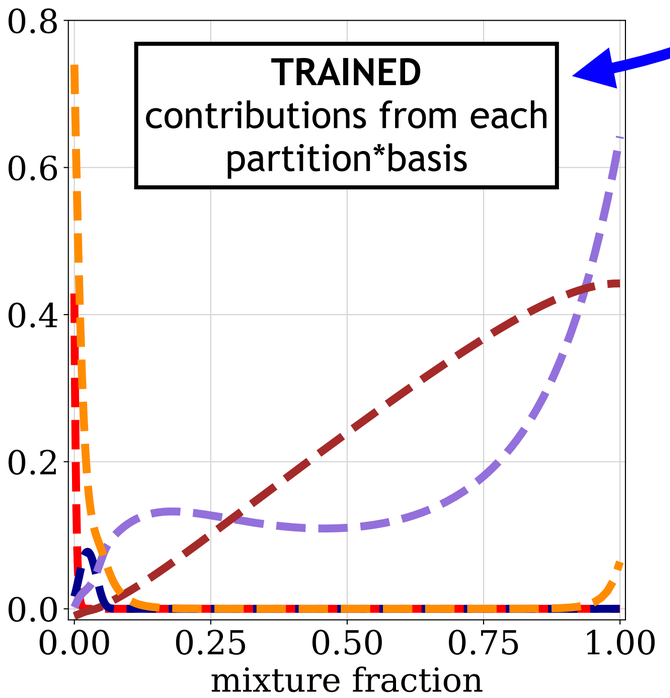
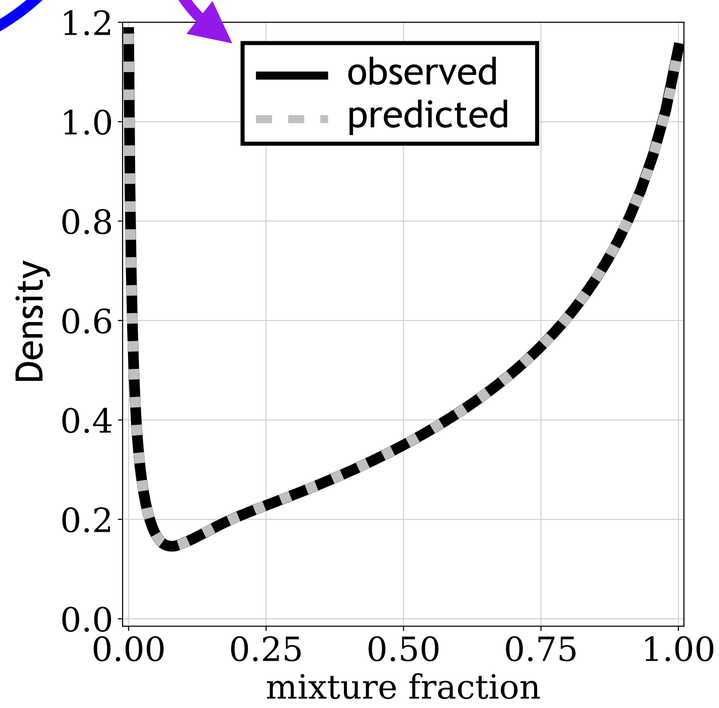
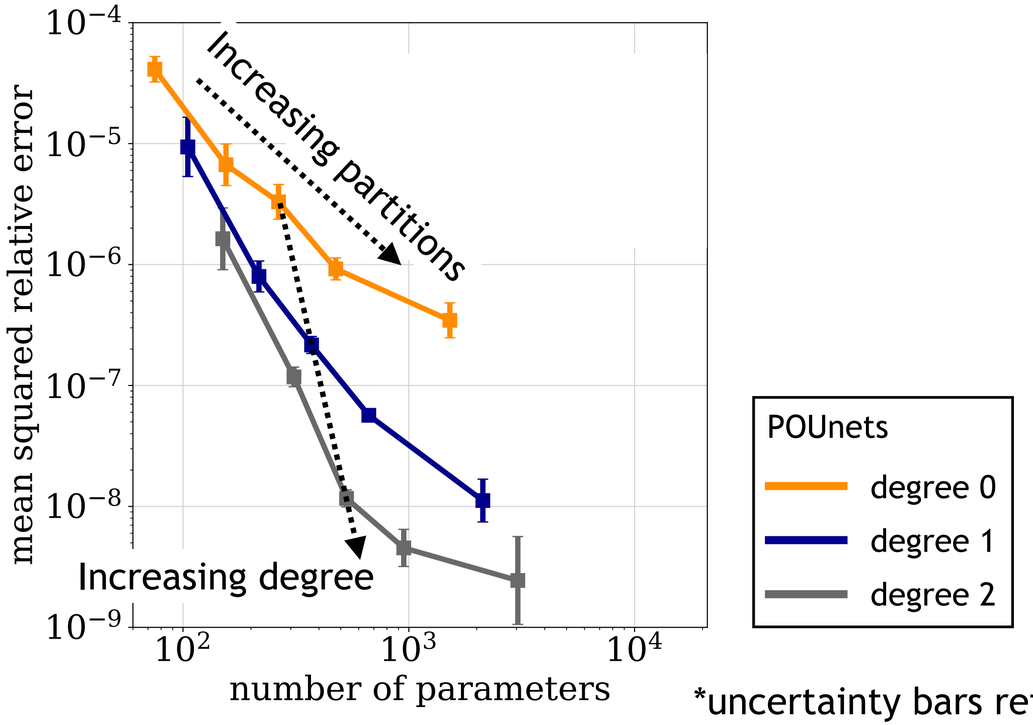




POUnets offer interpolant-like accuracy with ANN-like memory

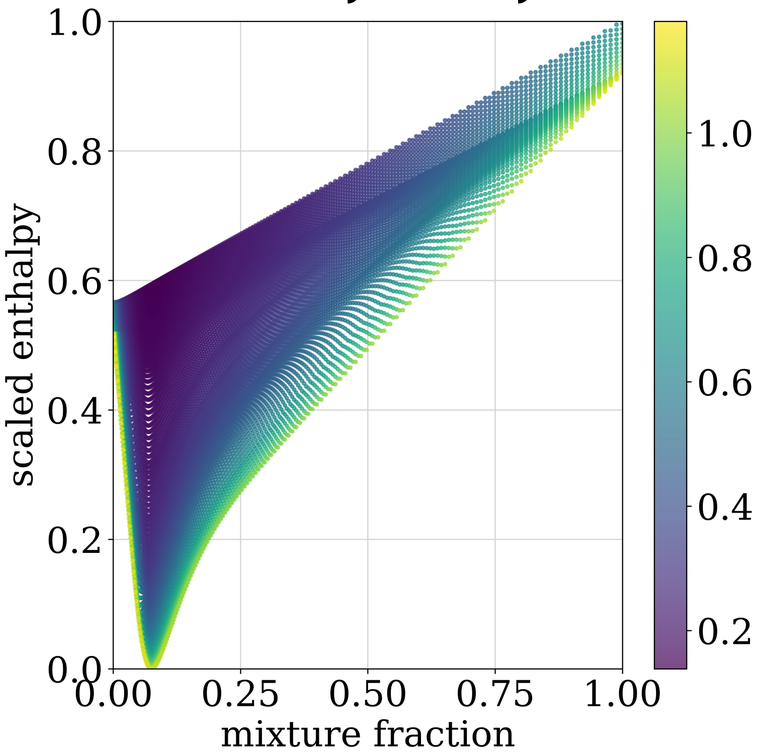
POUnets… offer flexibility in reaching high accuracy (number of partitions, basis degree)

2D model errors



*uncertainty bars reflect random perturbations to initialization

2D unstructured data colored by density



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show interpolant-levels of accuracy with significant memory compression: 40-50X fewer parameters in 2D

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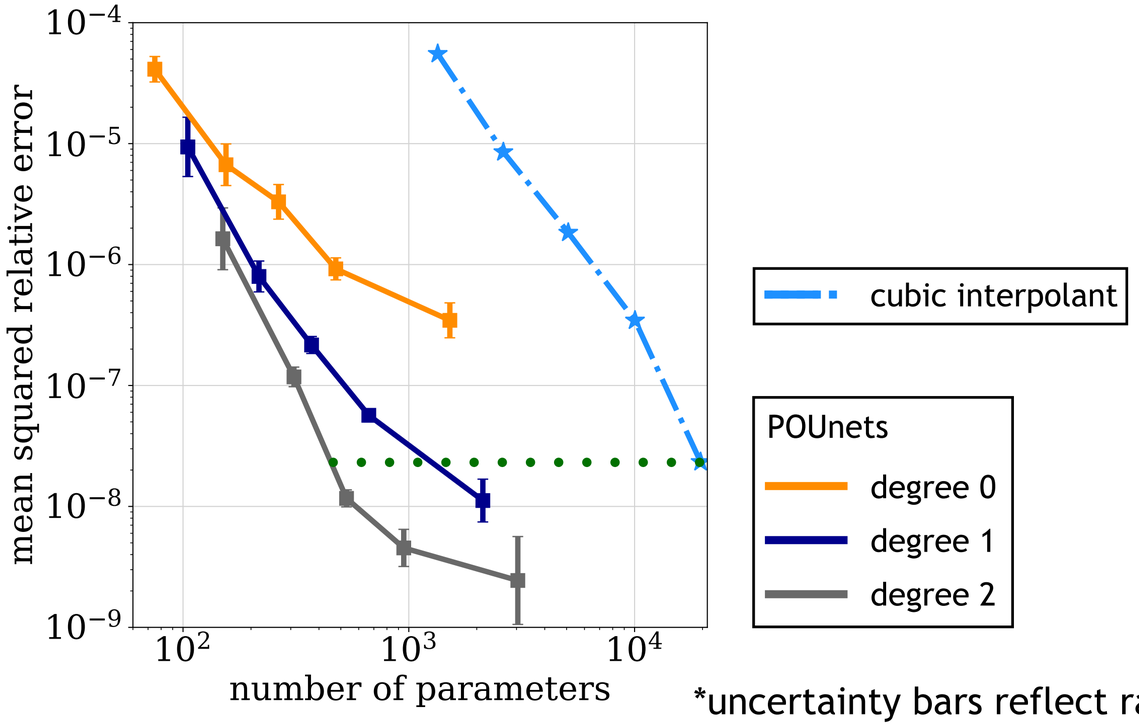

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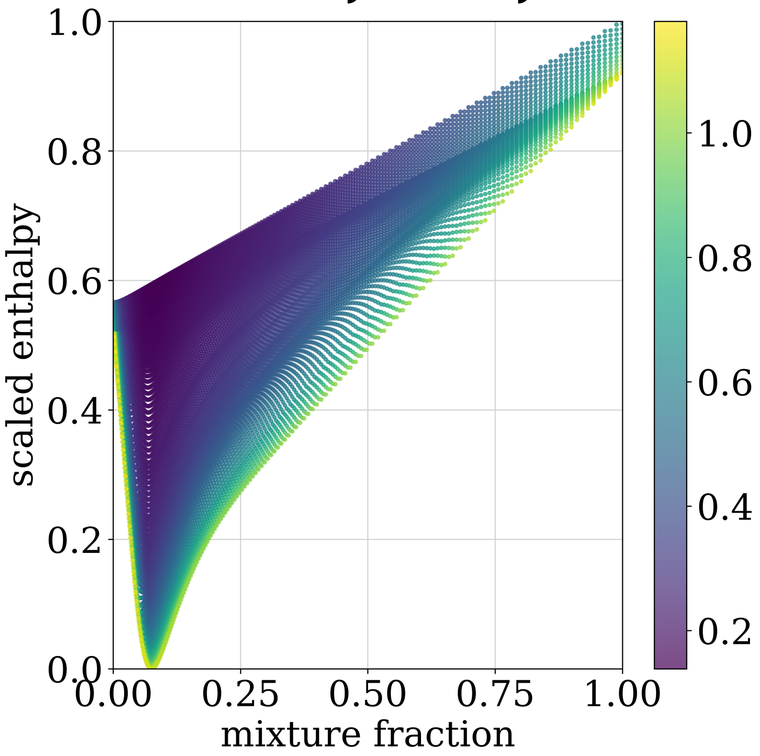

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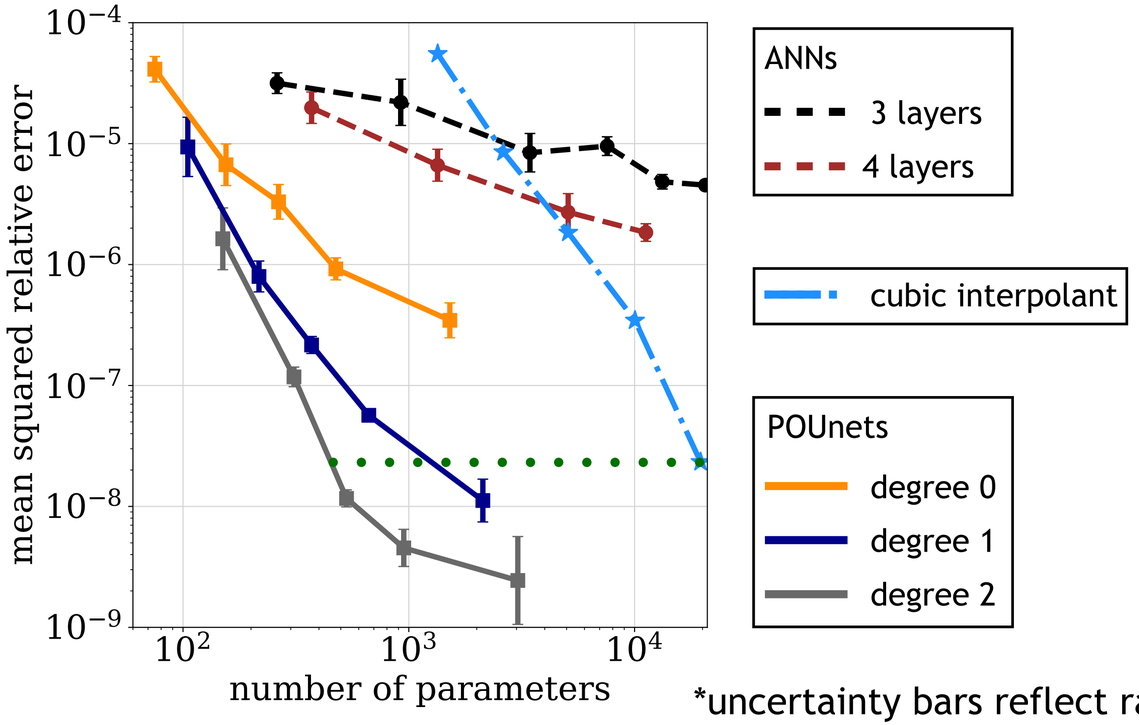

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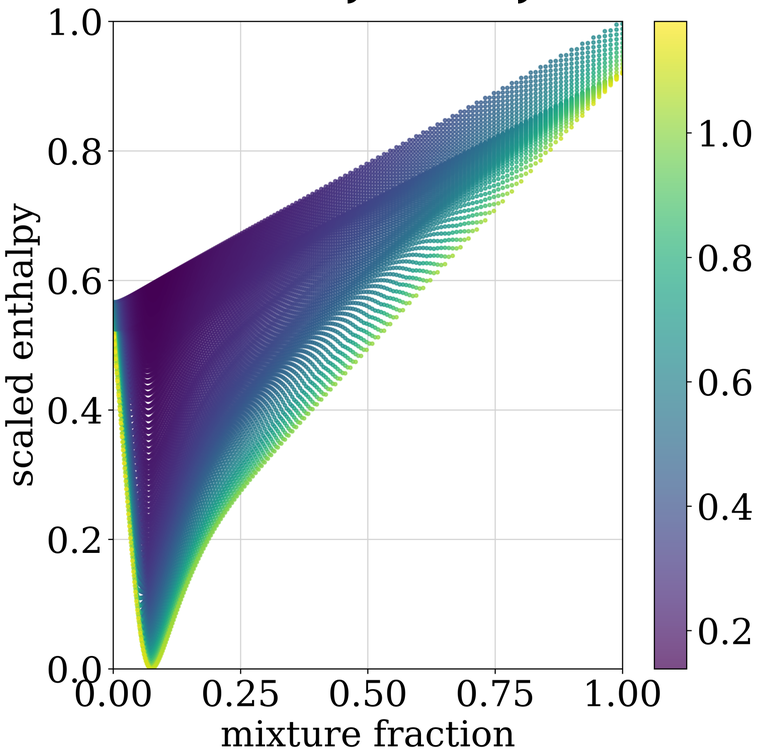

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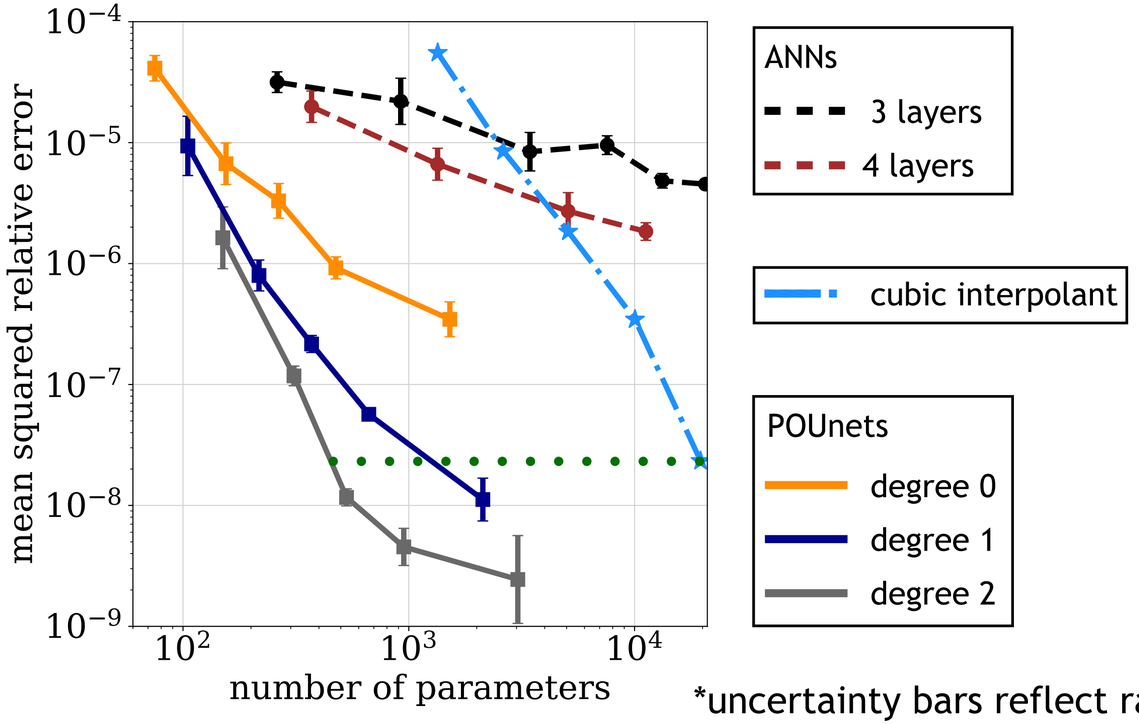

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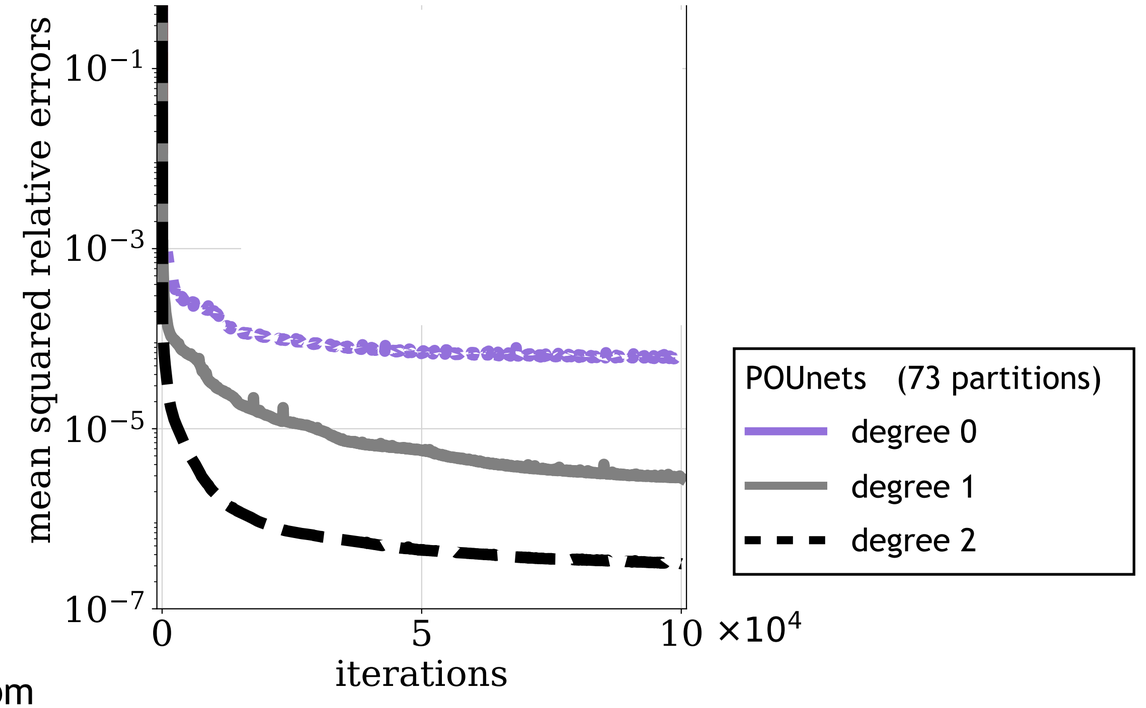
3D model errors



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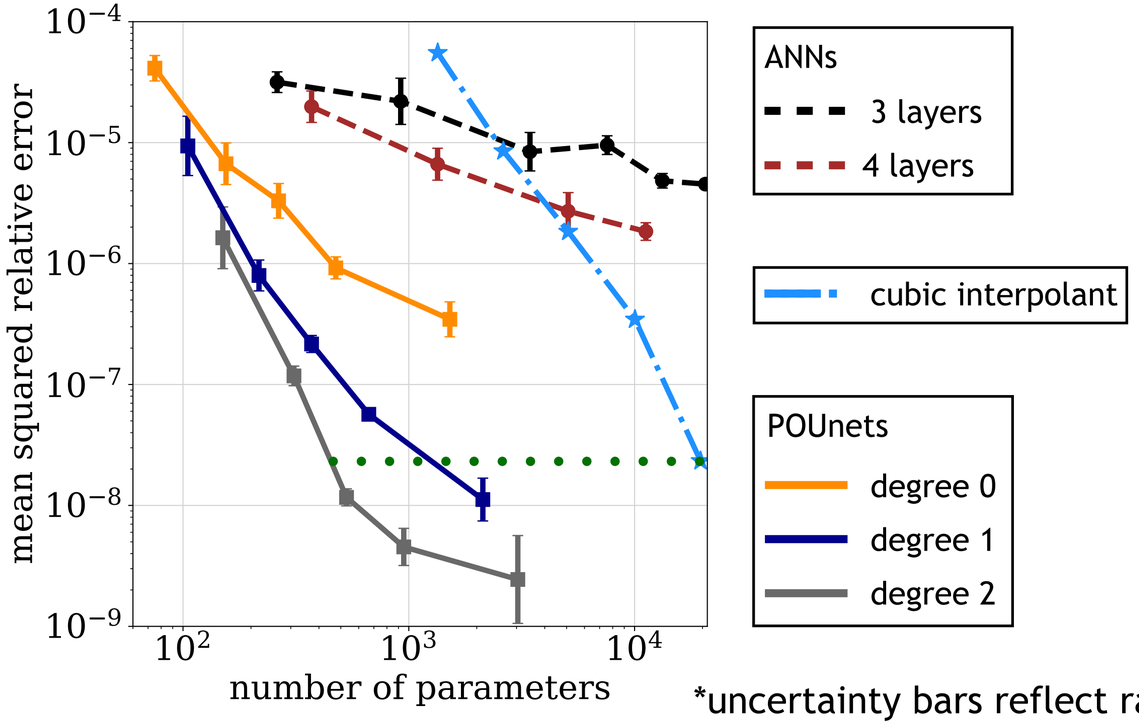
40-50X fewer parameters in 2D

100X fewer parameters in 3D

→POUnets grow with dimensionality **slower** than interpolants

2D model errors



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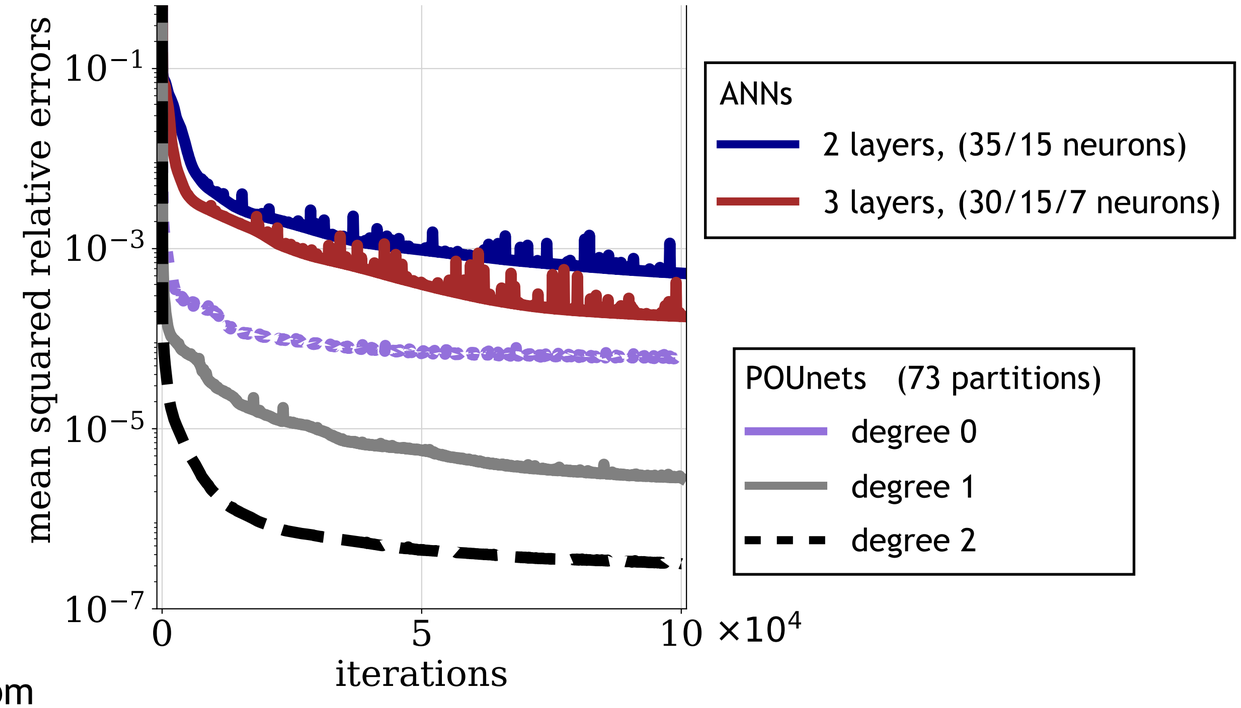


Conclusions

Chemistry tabulation facilitates practical simulation of combustion at engineering scales

We present POUnets as a tabulation strategy with interpolant-like accuracy and ANN-like memory

POUnets create localized polynomial approximations through combining classification and regression techniques

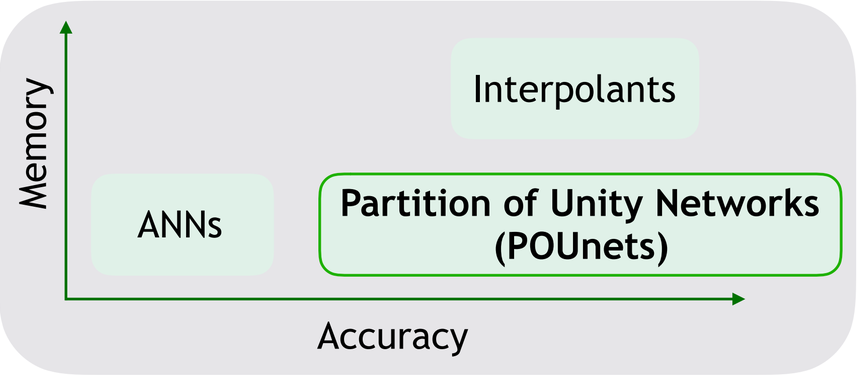
POUnets offer flexibility (number of partitions, basis degree, data structure) for reliably reaching high accuracy

POUnets show promise in application to higher dimensional tabulation

Future Work

Continue studying POUnet application to higher dimensions / more complex physics

Potential improvements to training (regularization, parameters, etc.)



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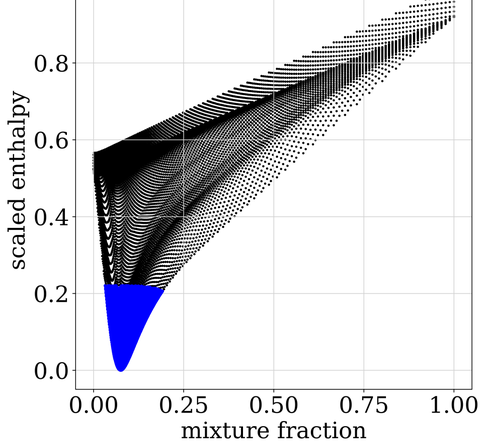
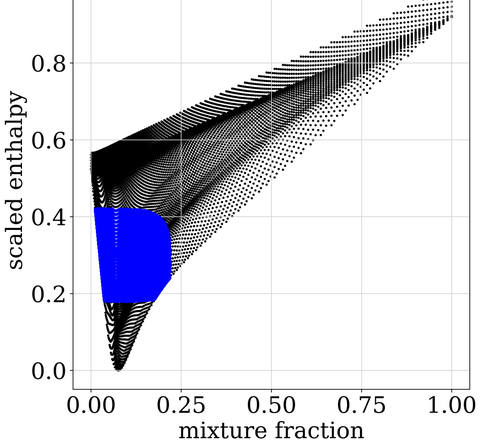
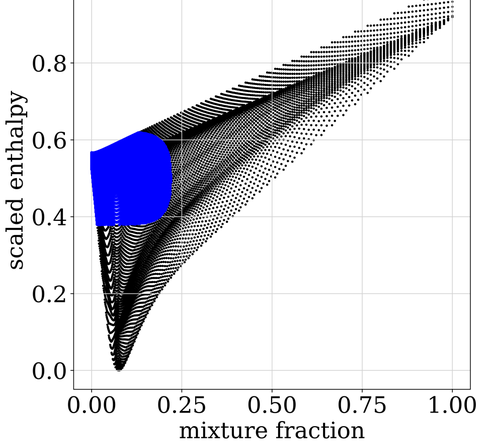
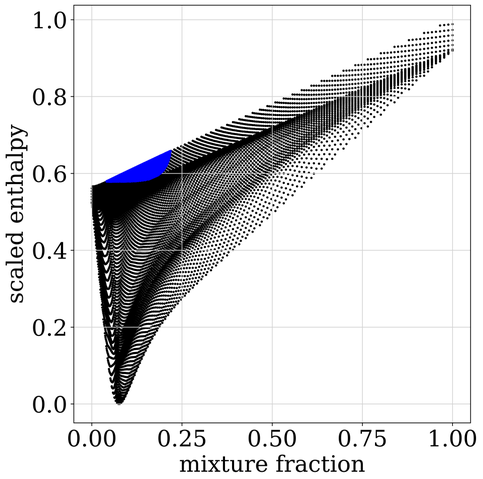
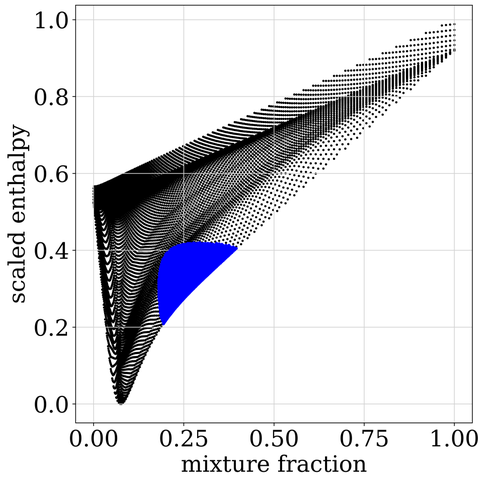
2D contributions **before** training

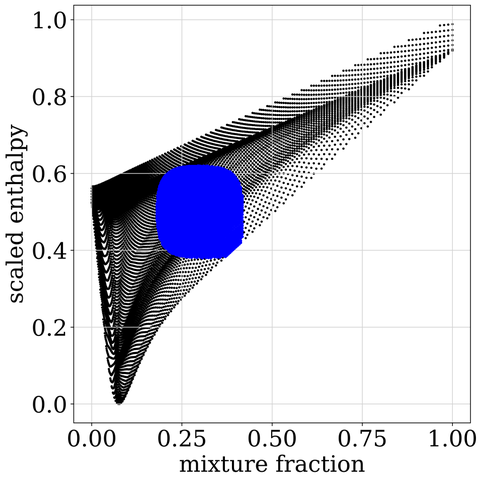


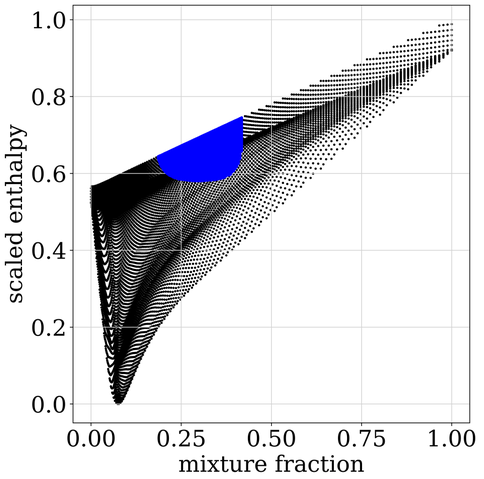


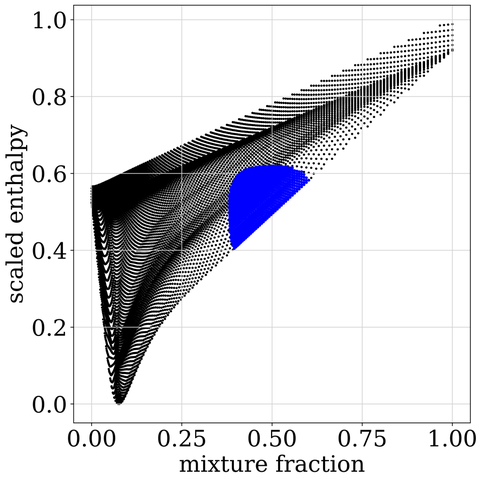


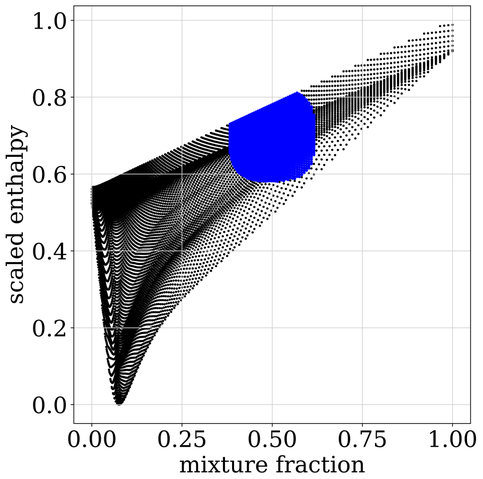


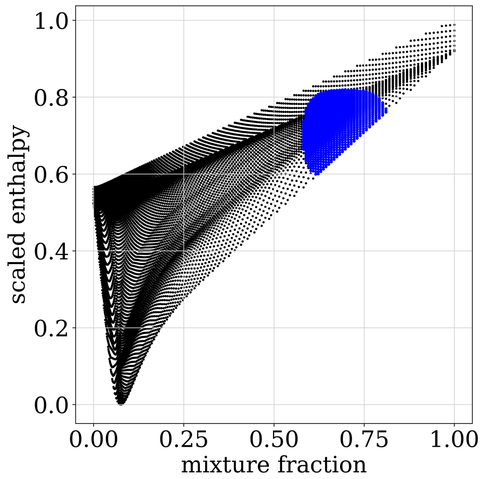


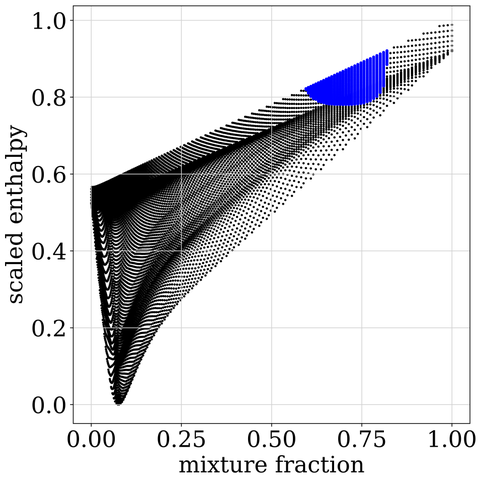


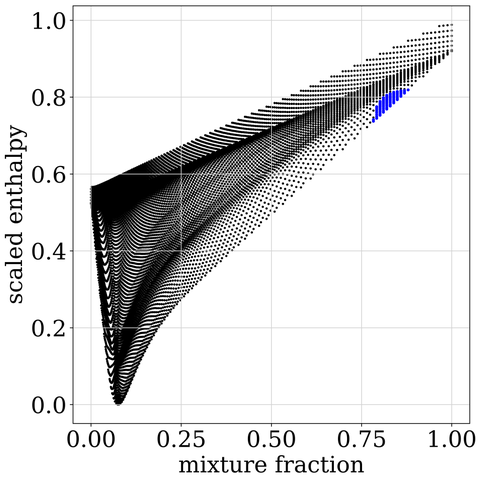


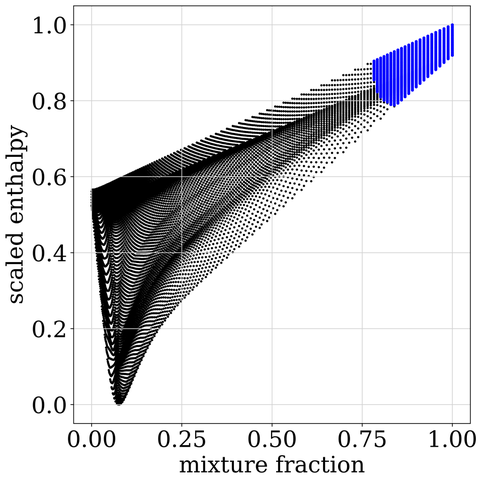


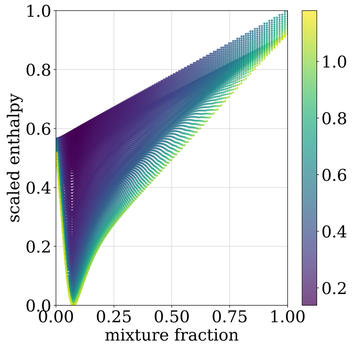
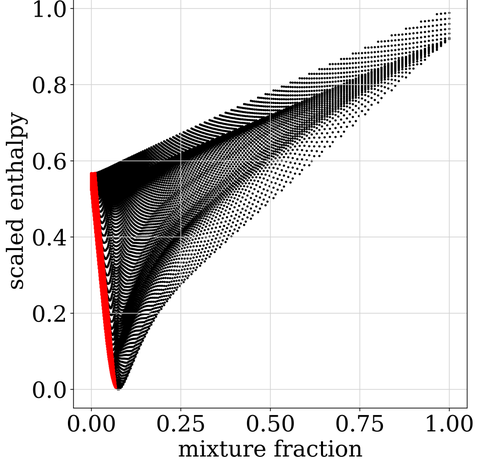
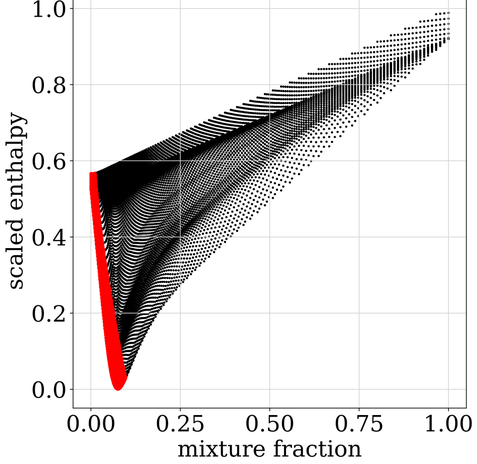
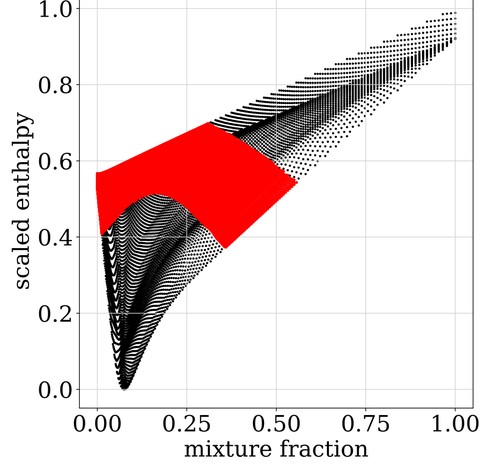
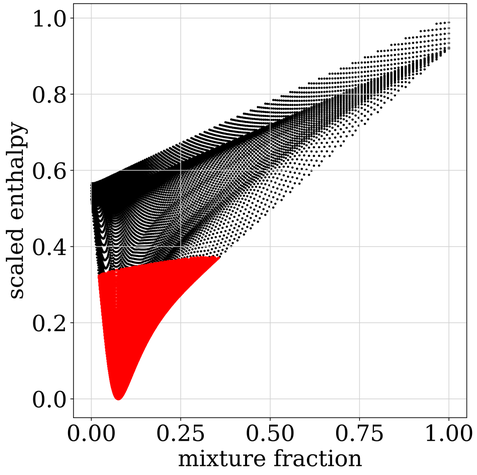
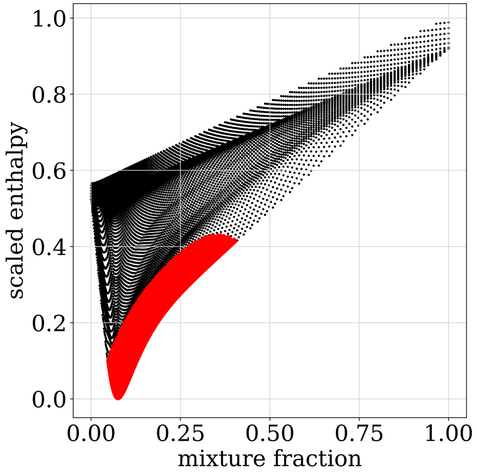
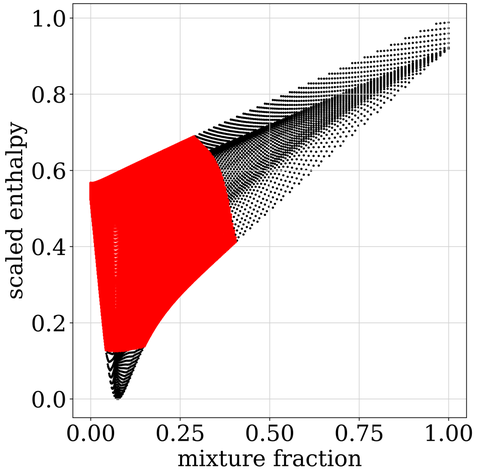
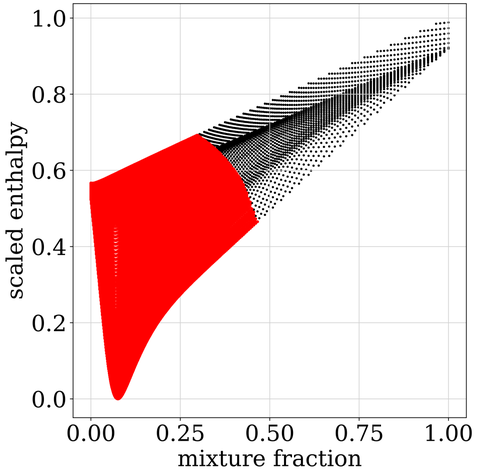
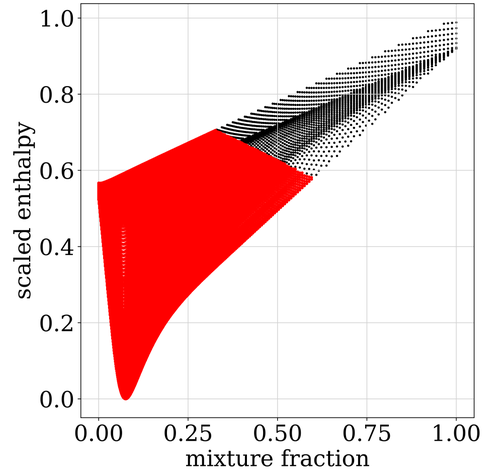
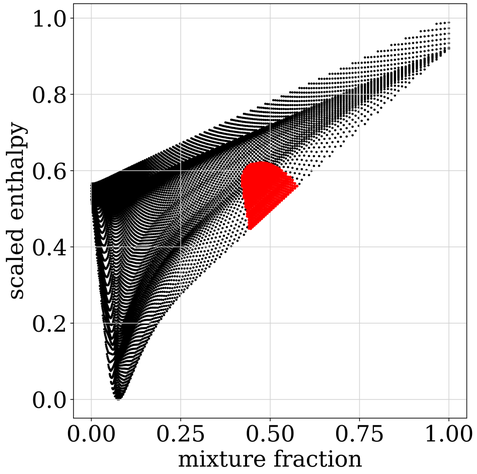
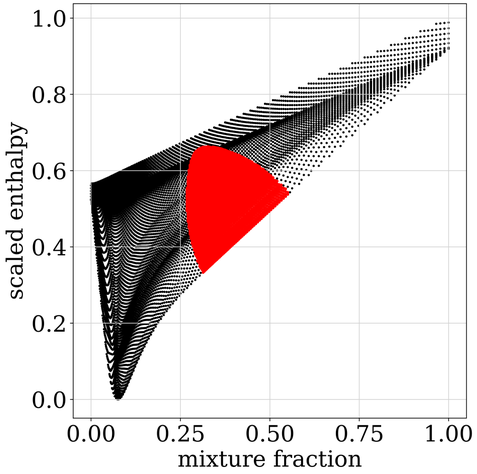
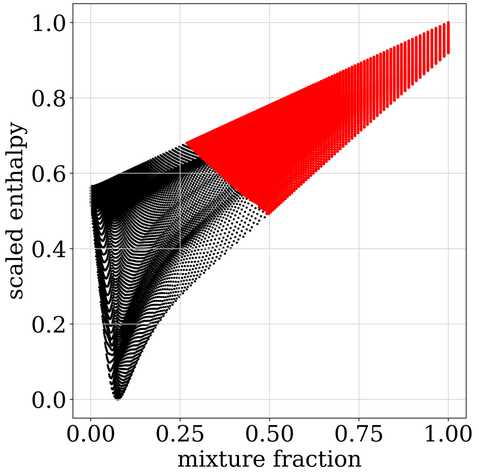
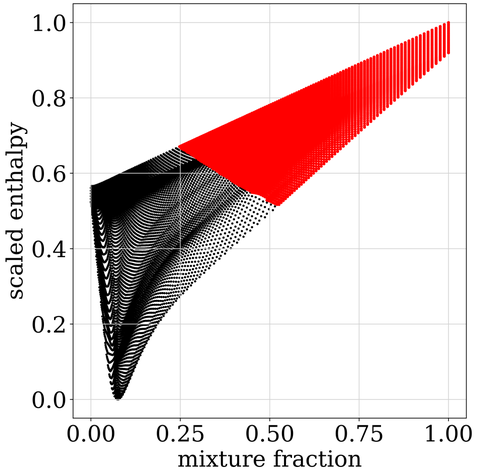
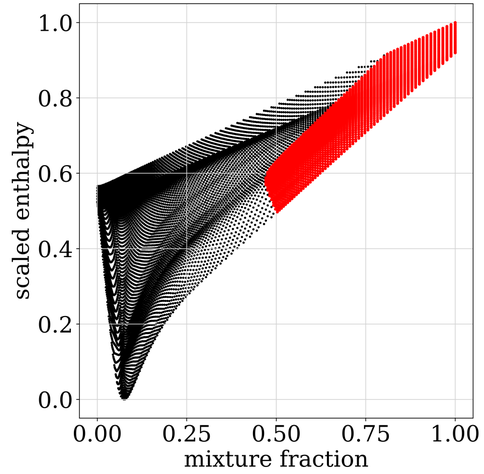










2D contributions **after** training

constant basis