A Supervised Learning Framework for Arbitrary Lagrangian-Eulerian Simulations

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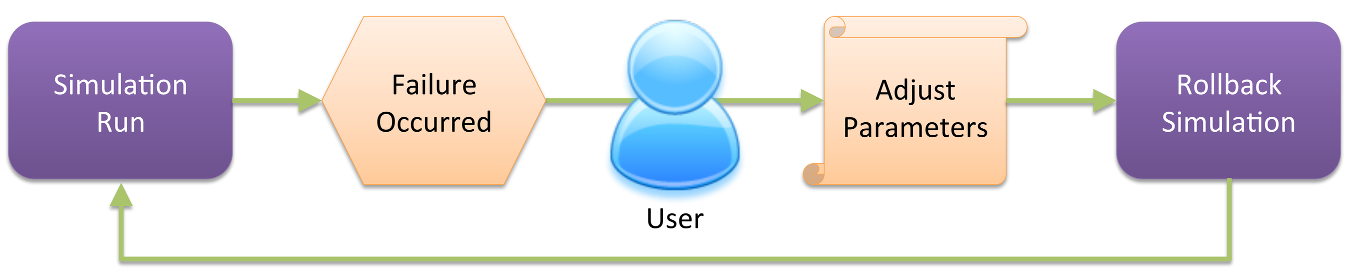
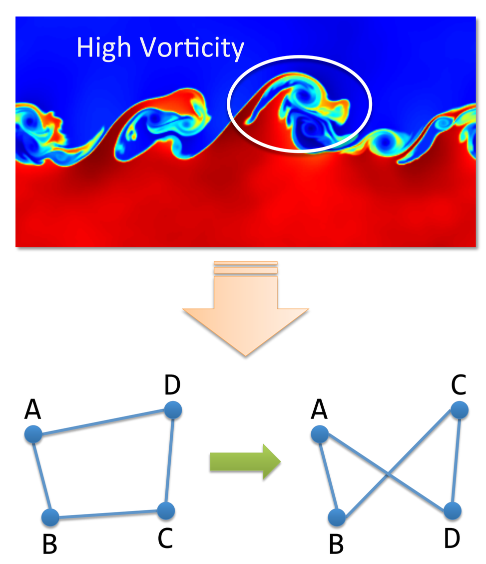
Introduction

- The **Arbitrary Lagrangian-Eulerian (ALE)** method is used in a variety of engineering and scientific applications for enabling multi-physics simulations.
- Unfortunately, the ALE method can suffer from **simulation failures** that require users to adjust parameters manually in order to complete a simulation.
- Finding the right **ALE strategy** (which parameters to adjust, when and by how much) is a trial-and-error process that can be disruptive and time consuming.

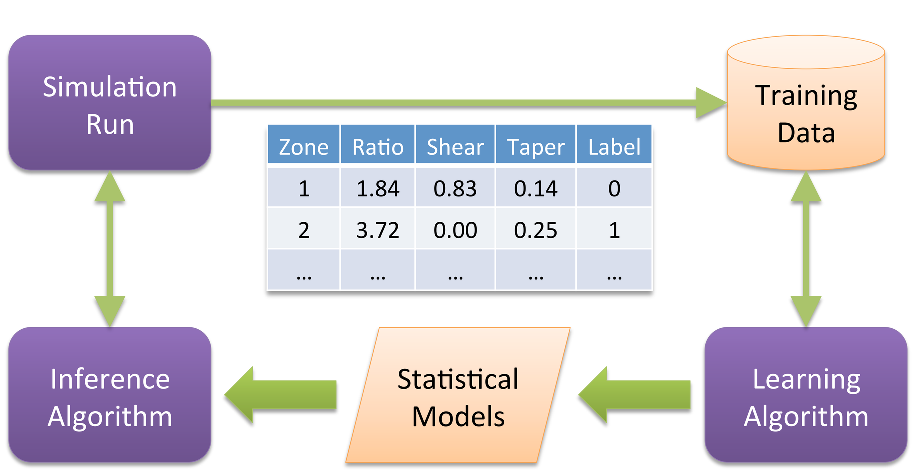


- In general, the ALE method consists of two phases:
  1. An arbitrary number of Lagrangian steps
  2. An advective remap phase to relax the mesh
- There are numerous parameters that control how the mesh moves during the remap phase.
- There are two general ways that failures can occur:
  - Mesh geometry distortions: **mesh zone tangling**
  - Physical quantity distortions: **anomalous hot spots**



Goal: Semi-automate the manual process for developing ALE strategies, by applying machine learning to predict ALE simulation failures.

Supervised Learning Framework



Zone	Ratio	Shear	Taper	Label
1	1.84	0.83	0.14	0
2	3.72	0.00	0.25	1
…	…	…	…	…

- Novel workflow for **ALE + ML**:
  - Collect labeled training data from ALE simulation run
  - Apply learning algorithm to derive statistical models for predicting failures
  - Use models in inference algorithm for ALE strategy in future simulation runs

Learning Representation

- Map ALE simulation domain onto supervised learning formulation
- Given zone z at time t:
  - A learning instance i is a pair (z,t)
  - Features $X(i)$ are metrics of (z,t)
  - Class of i is the failure state of z at t
- **Features**: 16 mesh quality metrics for 2D quadrilateral zones

Generating Labeled Data

+ Positive class examples:
  - Failed zones: negative side or corner

− Negative class examples:
  - Non-failed zones: everything else

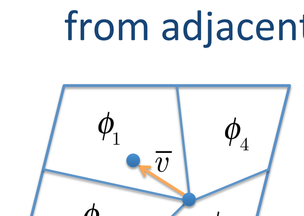
Predicting Failures

- Need to predict failures before they occur to apply mesh relaxation
- **Our approach**: train a regression model using time history of failures
- Given failure instance (z_f, t_f), we define labels for **soon-to-fail** zones:

$$\phi(z_f,t) = 1 - \frac{(t_f - t)}{T},\ s.t.\ \phi : [t_f - T, t_f] \rightarrow [0,1]$$

ALE Code Integration

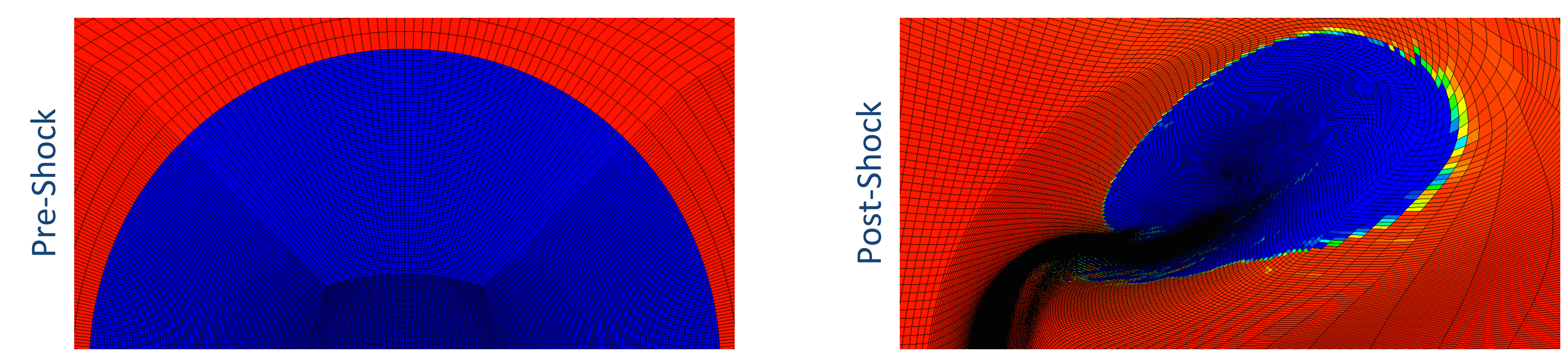
- Learning algorithm: **random forest**
- We developed LAGER library:
  - Integrates KULL with scikit-learn
  - Nodal relaxation: average predicted ϕ from adjacent zones z_a of node n

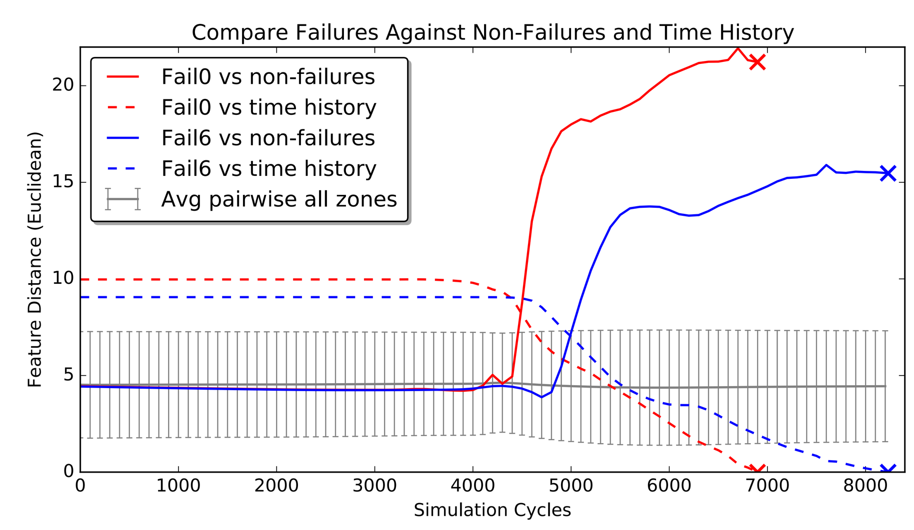


$$\Phi(n,t) = \frac{1}{N}\sum_{a=1}^{N}\phi(z_a,t)$$

Experimental Results

- Bubble Shock: a well-known ALE test problem modeling a planar shock traveling through a spherical helium bubble in air from the right side of the geometry.





$$\delta(i,j) = \left\|\hat{X}(i) - \hat{X}(j)\right\|^2,\ s.t.\ \hat{X}(i) = \frac{(X(i) - \mu_i)}{\sigma_i}$$

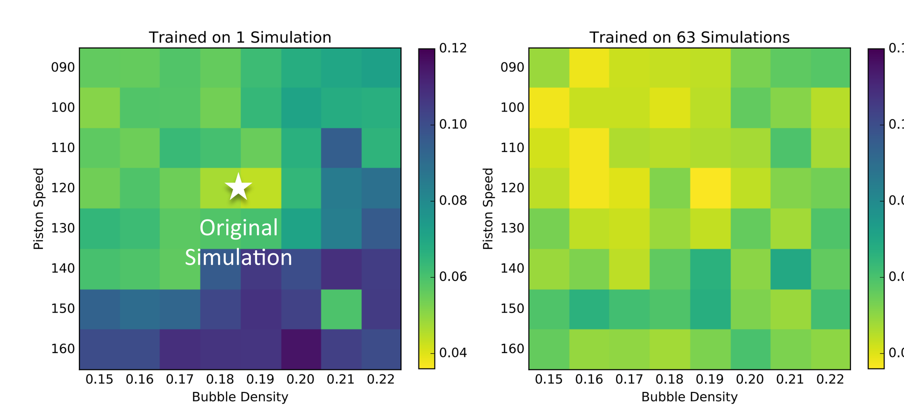
$$\Delta(z,t) = \frac{1}{M}\sum_{m=1}^{M}\delta((z,t),(z_m,t))$$

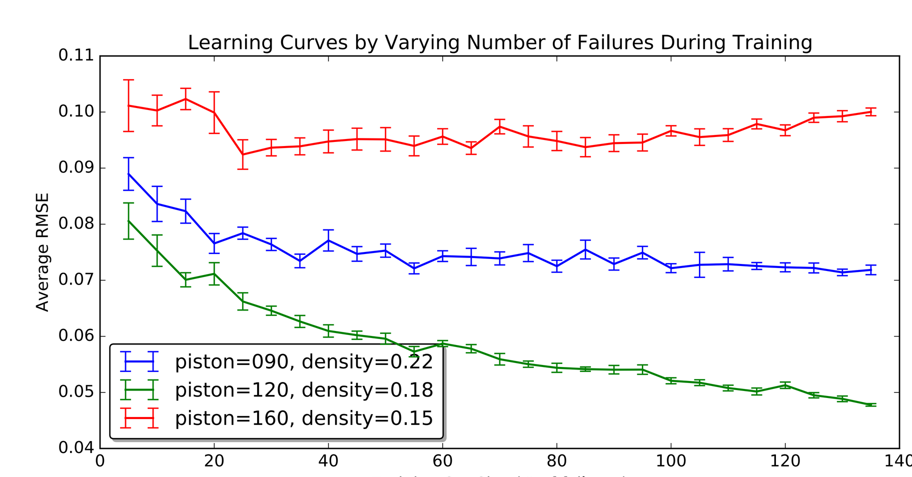
Framework Evaluation

- Evaluate framework design choices:
  - Are features useful for distinguishing failures from non-failures? (*see graph*)
  - How effective is our procedure for generating labeled data? (*see paper*)
  - Is time history of failures suitable for predicting failures? (*see graph*)
- We compare failures against: 1) non-failures, 2) other failures, and 3) time histories, using **feature distance** δ based on mesh quality metrics

Learning Evaluation

- For performance evaluation, we use data from (64) other simulations:
  - Vary piston speed and bubble density
  - Measure RMSE for predicting ϕ values
- Observations from results:
  - Heatmap(left) indicates that **variance** is a significant source of error
  - Graph shows how training data affects performance via **learning curves**
  - Heatmap(right) suggests generalization performance may improve by training on more simulations ($\mu: 0.08 \rightarrow 0.05$ and $\sigma: 0.02 \rightarrow 0.01$)



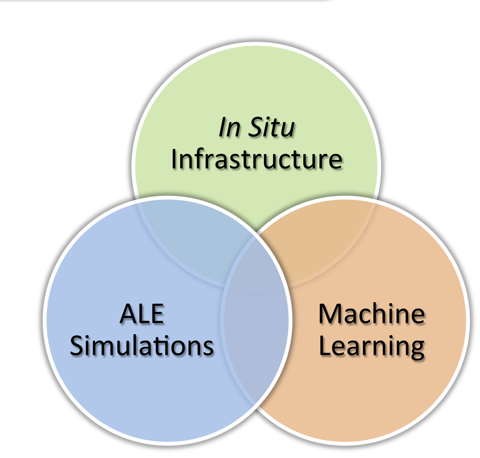


Conclusion and Future Work

- **Key takeaways**:
  - Mesh quality metrics provide early indicators of failure, which are captured by our ML approach (*see time history graph*).
  - Individual simulations differ. Training across multiple simulations improves generalization performance (*see heatmaps*).
  - Our ML approach automatically performs successful ALE on KULL Bubble Shock simulation without human intervention (*see paper*).

We developed a **first-of-a-kind** supervised learning framework for predicting conditions leading to ALE simulation failures.

- **Future research directions**:
  - How much failure time history to consider? Which transition function to use? Can we reduce noise in the negative labels?
  - In terms of physical accuracy, how do we compare simulations produced from different ALE strategies?
  - What is an effective infrastructure for integrating machine learning with ALE simulations?



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