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Title: Bridging Scales for Materials Modeling using Machine Learning

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Bridging Scales for Materials Modeling using Machine Learning

Using ML to rapidly provide upscaled crack statistics for more accurate damage modeling

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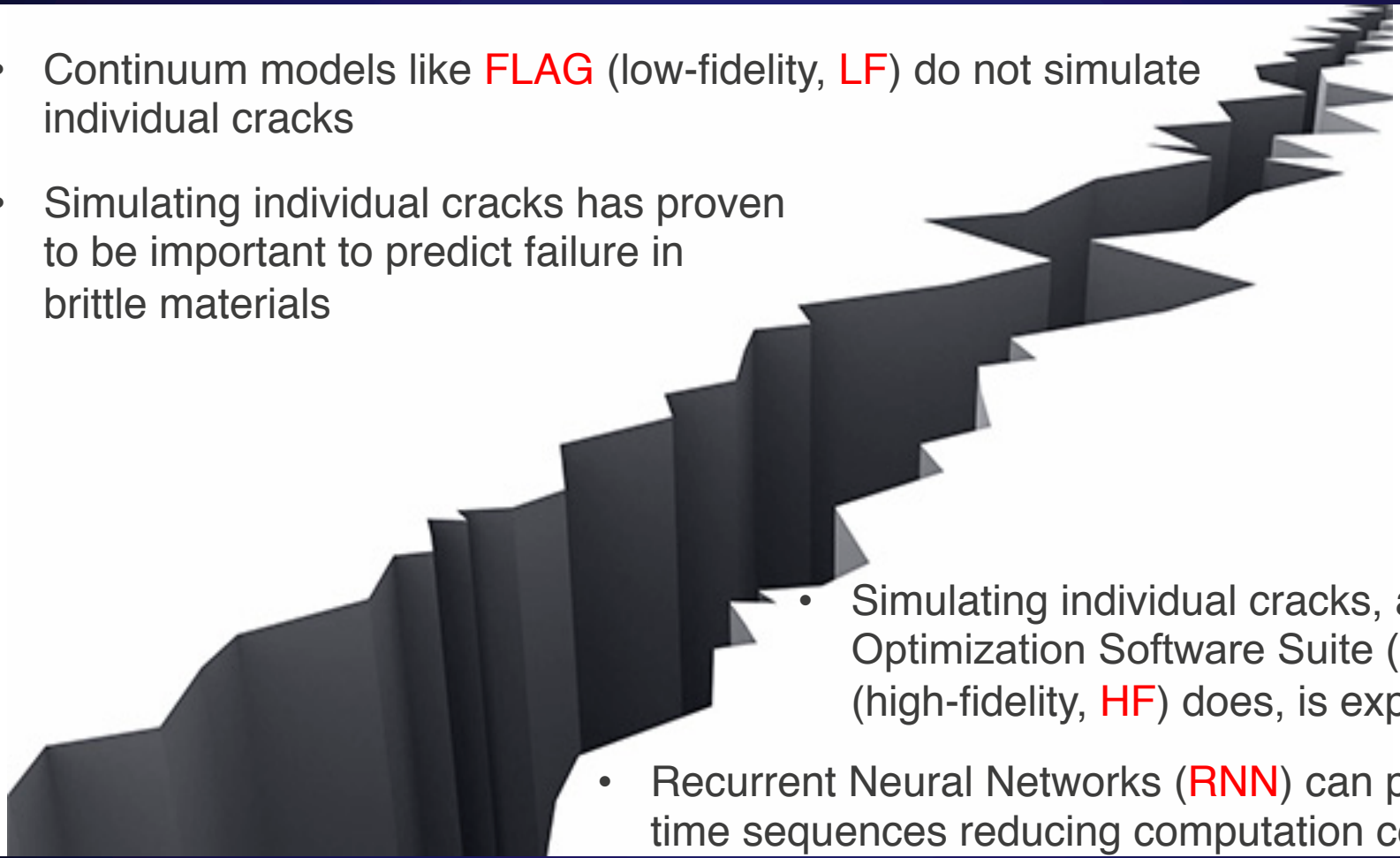
Motivation

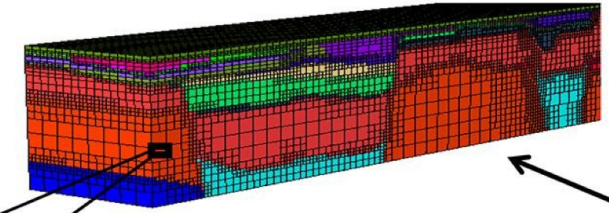
- Continuum models like FLAG (low-fidelity, LF) do not simulate individual cracks
- Simulating individual cracks has proven to be important to predict failure in brittle materials



- Simulating individual cracks, as Hybrid Optimization Software Suite (HOSS) (high-fidelity, HF) does, is expensive
- Recurrent Neural Networks (RNN) can predict time sequences reducing computation cost

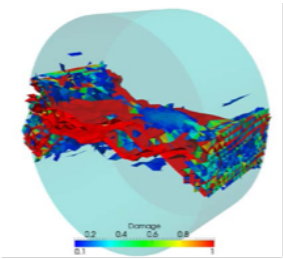
Workflow

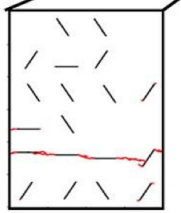
FLAG (LF)



Micro-cracks in one cell (HOSS)

HOSS (HF)

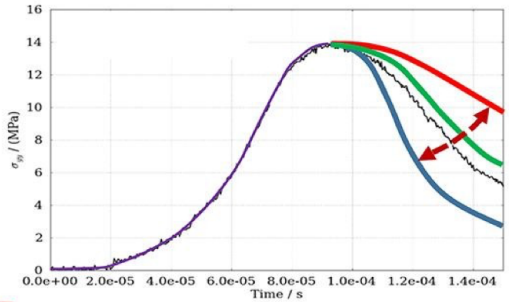




Constitutive model for effective moduli

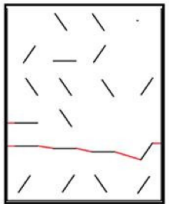
Computationally intensive

Damage evolution accounts for crack interactions



Computationally efficient

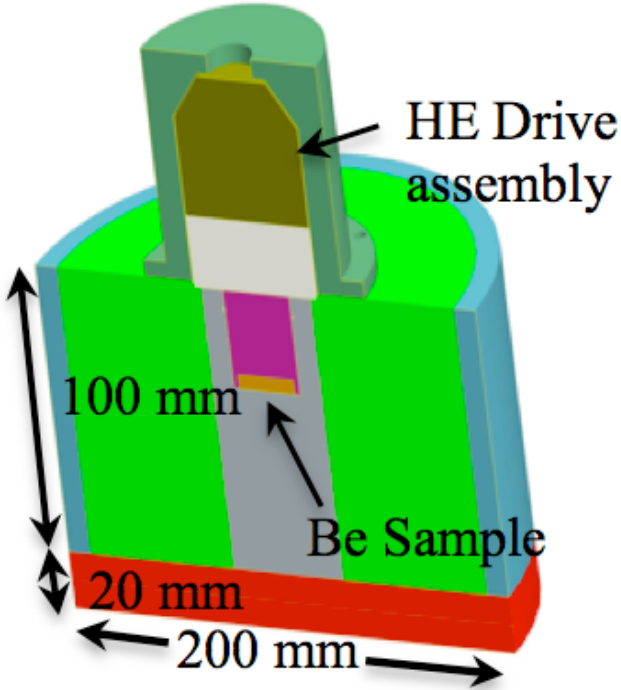
Machine Learning



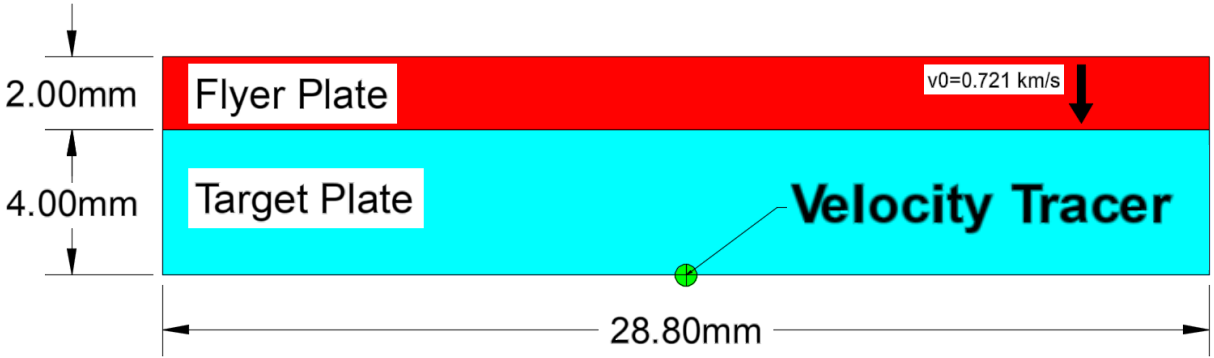
Constitutive model for effective moduli

Our goals is to bridge between meso and continuum scales in an efficient ML-driven workflow.

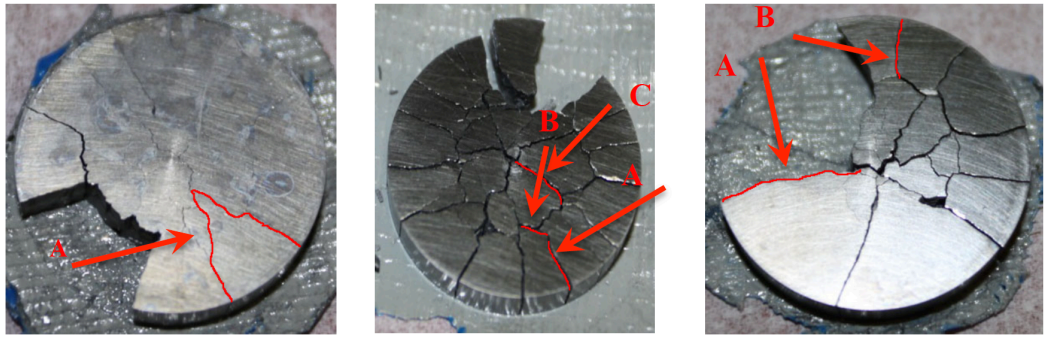
Validation Data



Shock recovery assembly for the arrested beryllium experiments. Ref. Cady et al. 2011 LANL Report No. LA-UR-11-06976



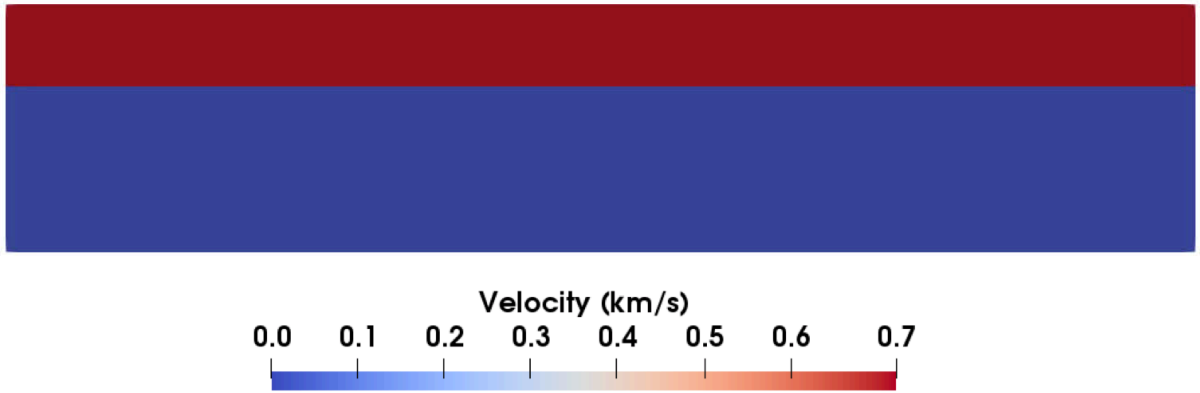
Experimental setup, dimensions and velocity tracer (VISAR probe) location



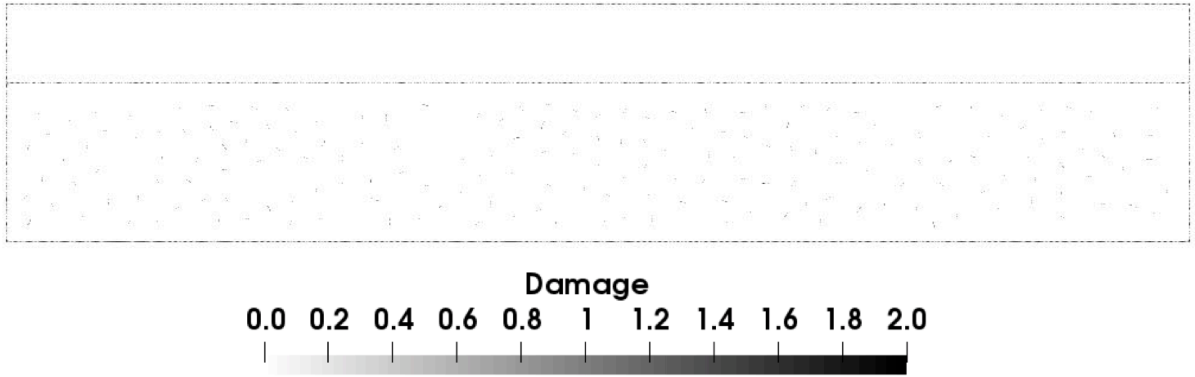
Disc fragments selected for fracture surface characterization for three tested samples. Ref. Cady et al. 2011 LANL Report No. LA-UR-11-06976

HOSS Data – 2D HF model

Evolution of the shock wave velocity

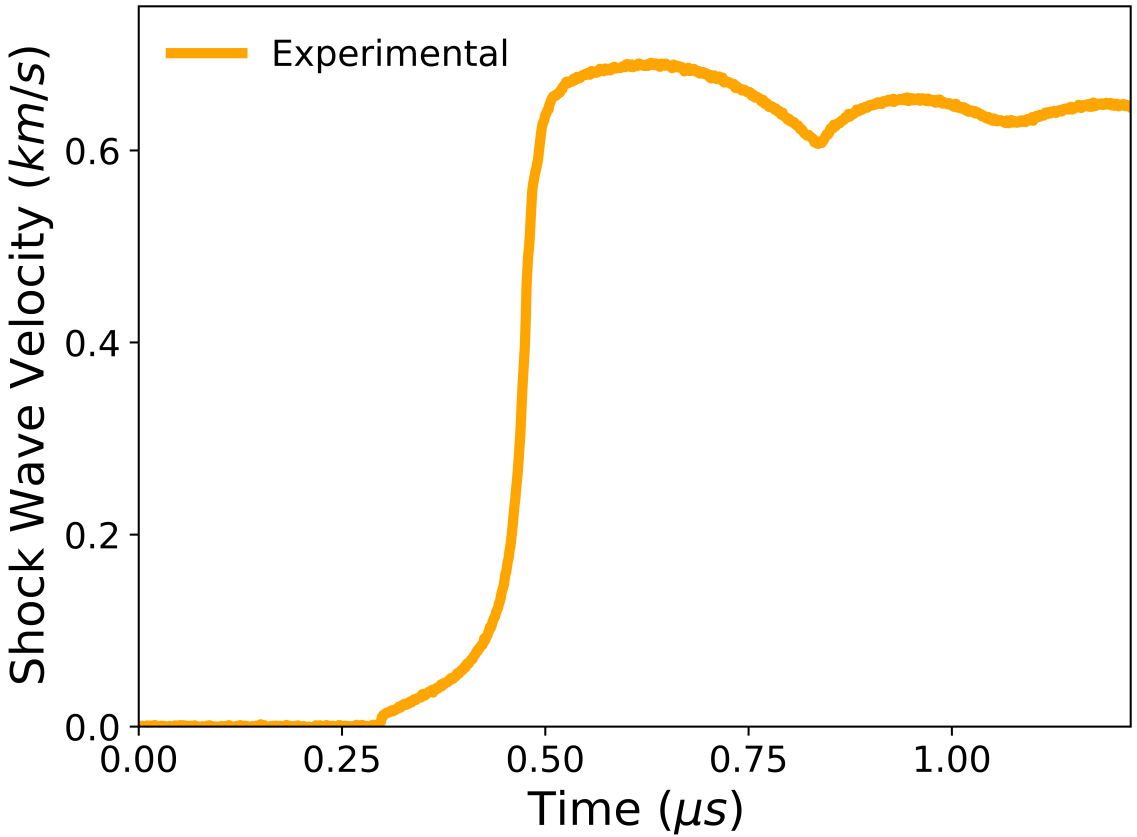


Evolution of damage



- **Number of HF simulations available** = 100
- **Cost** = hundreds of processors hours
- **Variable** = initial crack location, length and orientation

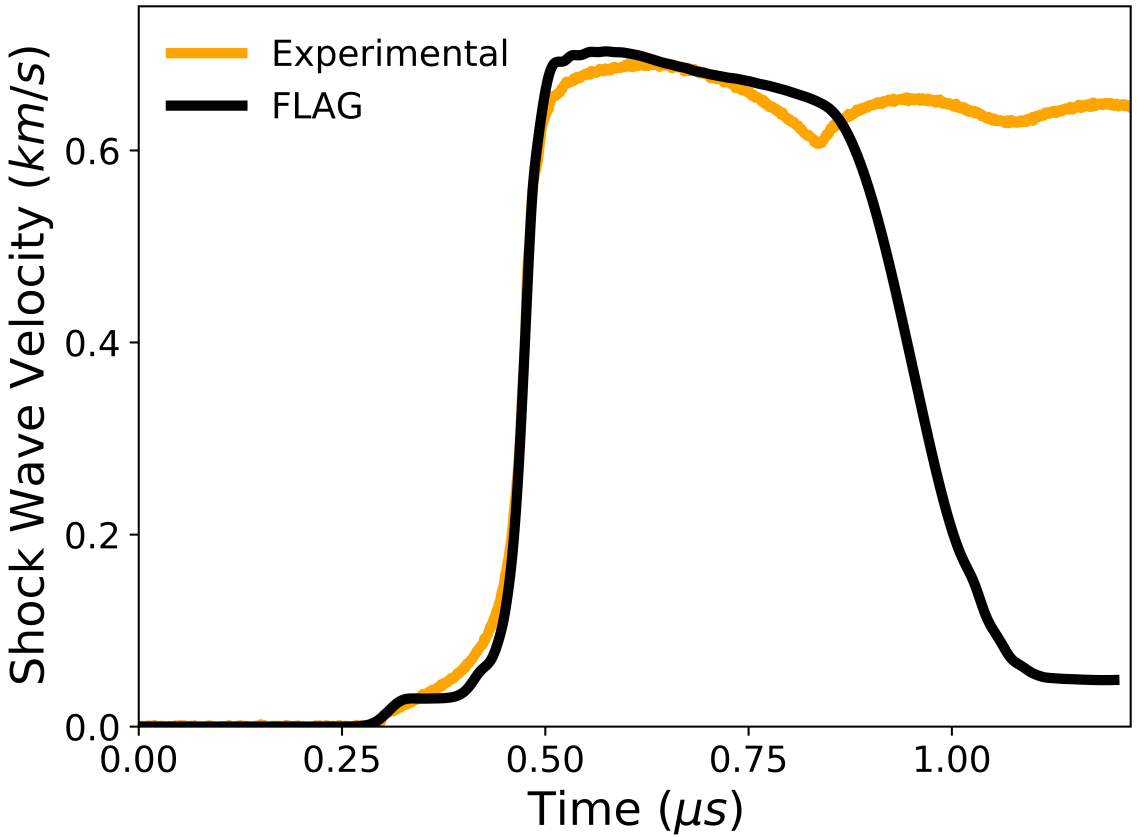
Experimental Results



Temporal evolution of shock wave profiles

- Results extracted from experiments using a VISAR probe centered on the rear of the target
- The figure shows the temporal evolution of the shock wave profile.
- Velocity roughly constant between 0.5μs to 2.5μs
- Oscillations are due to the reflection of the shock wave

Challenge



Temporal evolution of shock wave profiles

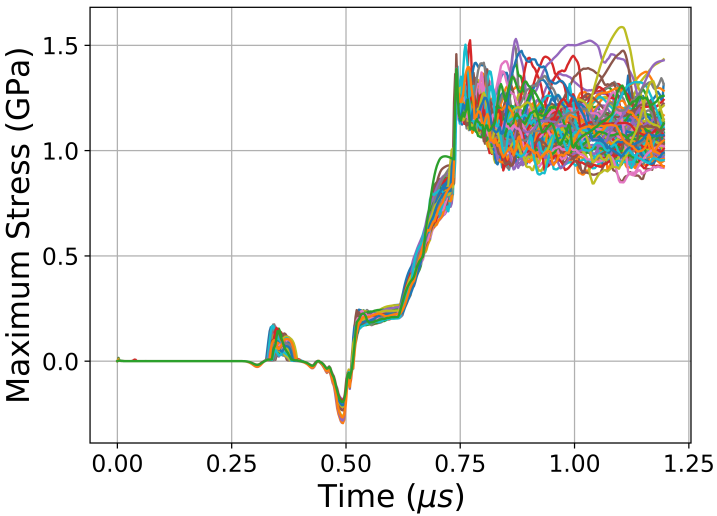
- In black results using FLAG LF model
- PTW (Preston-Tonks-Wallace) model specifies stress as a function of strain, strain rate, and temperature
- PTW does not model cracks
- FLAG model needs to be improved to validated

Quantities of Interest for training ML

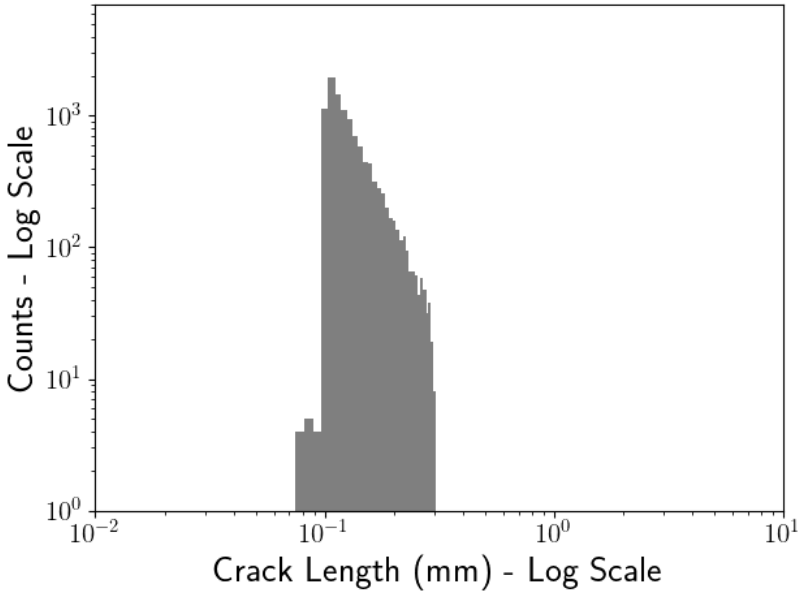
Compliance Tensor Correction

Number of cracks →

Length of each crack →



Maximum tensile stress as a function of time

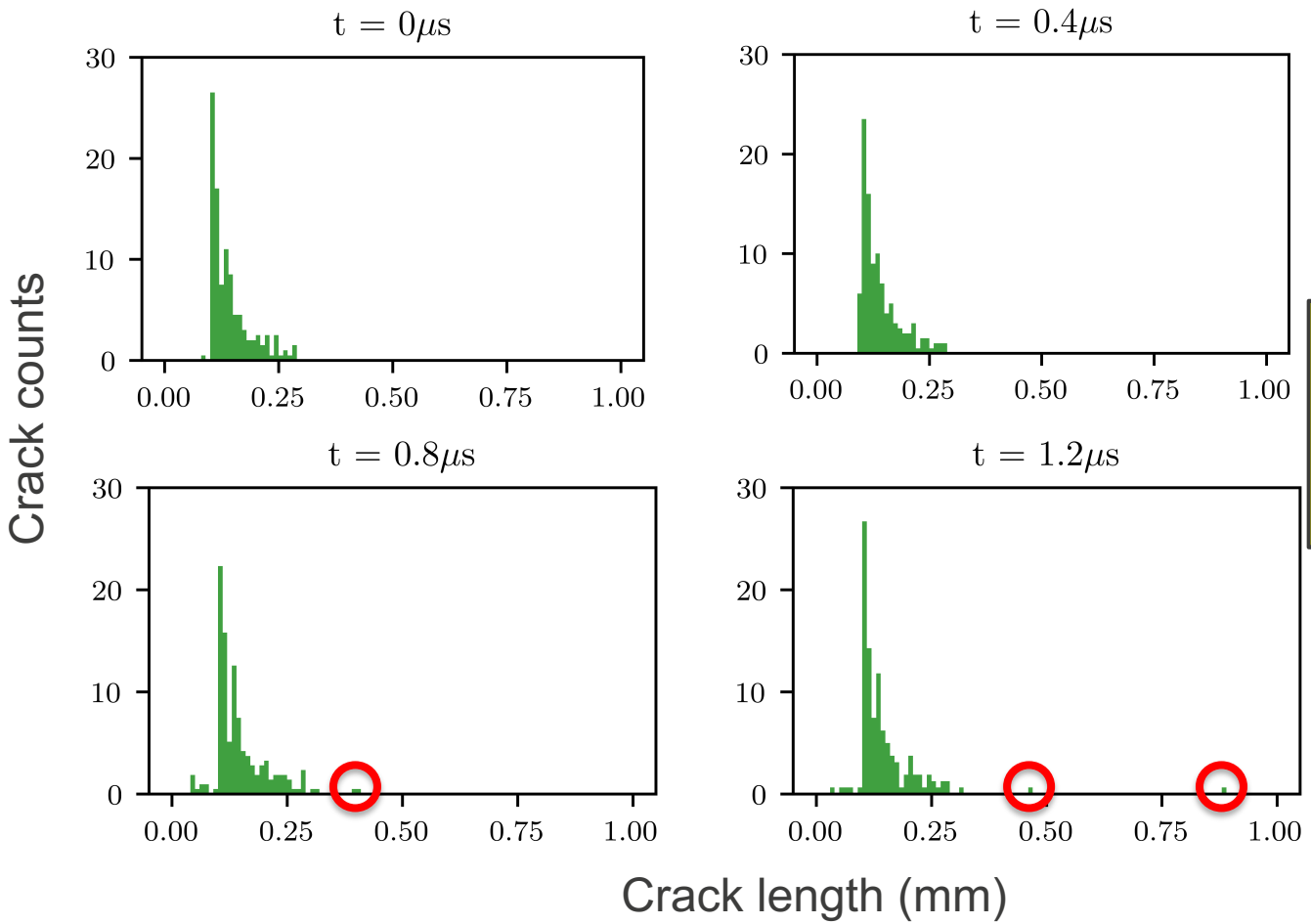


Temporal evolution of number of cracks as a function of crack length

Maximum tensile stress

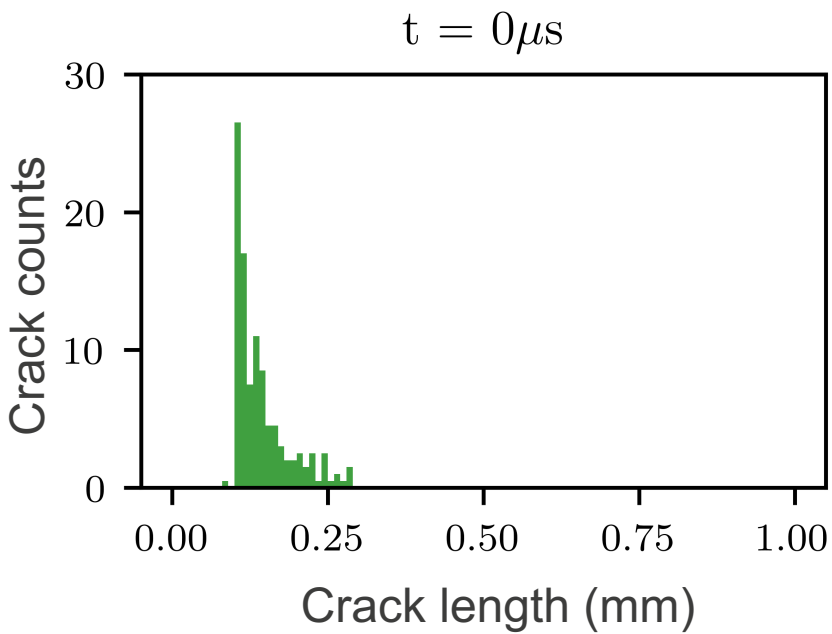
At each time step!

A Closer Look at the Crack Density Evolution

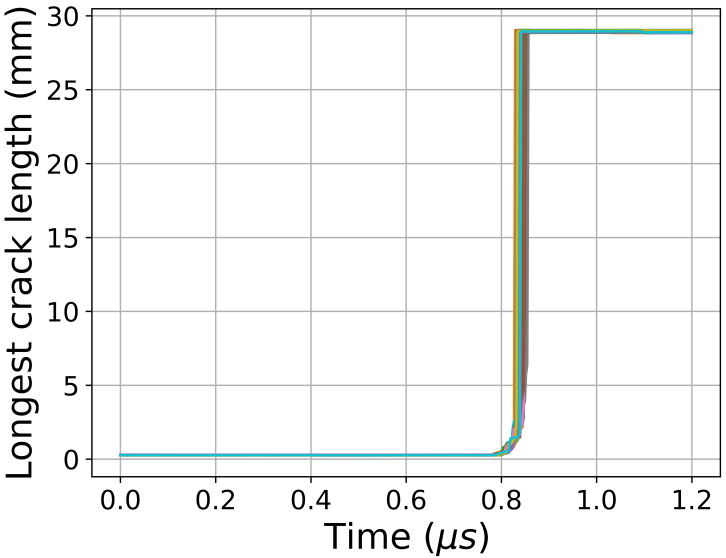


Initial distribution does not change substantially as a function of time

Updated Damage for Training ML



Initial crack length distribution



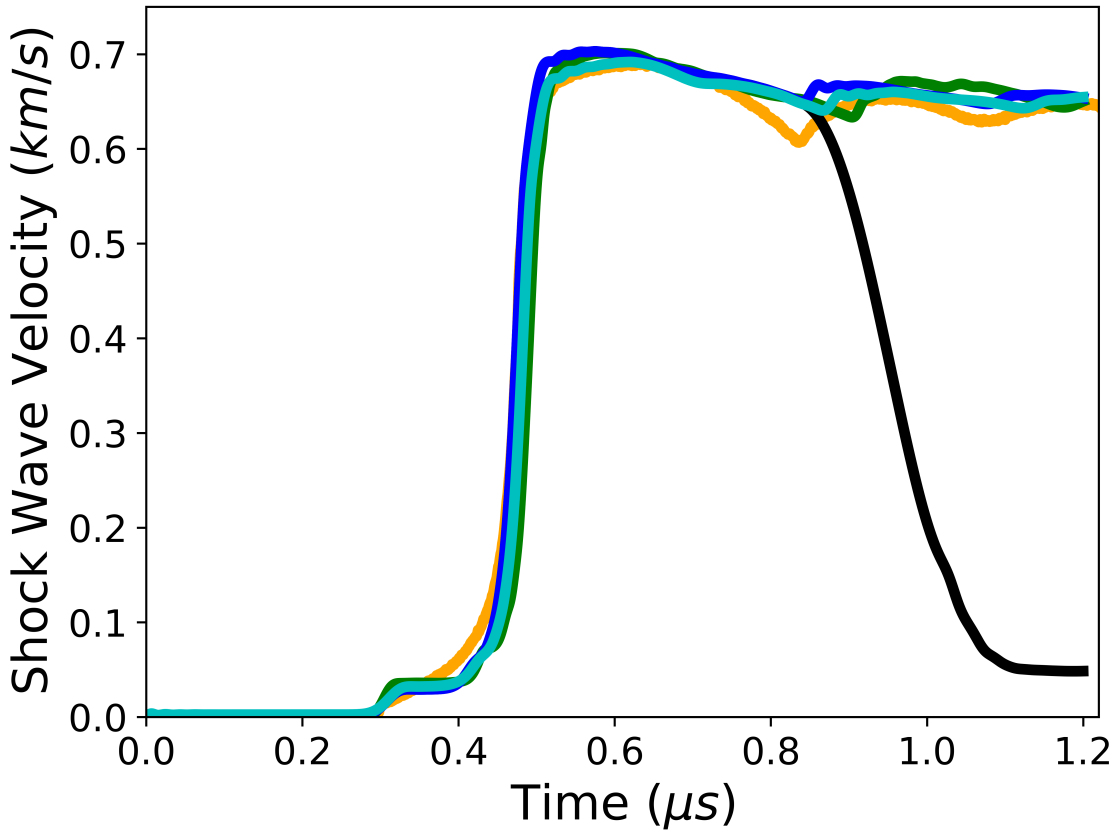
Length of the longest crack as a function of time (100 simulations)

Our approach: Use the initial distribution for all times evolving only the longest crack

Results using HF HOSS

- Experimental
- FLAG (No Corrections)
- HOSS
- FLAG + HOSS (all cracks)
- FLAG + HOSS (longest crack)

- HOSS performs similar to the experiments
- FLAG with corrected compliance evolving all cracks compare with HOSS performance
- FLAG with corrected compliance with only the longest crack shows also a good performance



Temporal evolution of shock wave profiles

One-to-Many Machine Learning Model

Training data shape= # simulations (N), # timesteps, # features = N x 480 x 2

Input Layer
Input=Nx1x2
Output= Nx1x2

LSTM Layer
Input=Nx1x2
Output=Nx10

Repeat Vector Layer
Input=Nx10
Output=Nx100x10

LSTM Layer
Input=Nx100x10
Output=Nx100x10

Time Distributed (Dense(100)) Layer
Input=Nx100x10
Output=Nx100x100

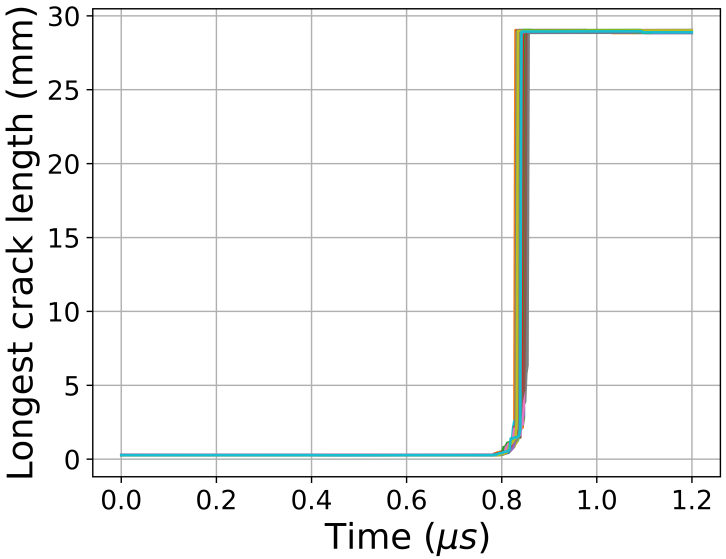
Time Distributed (Dense(2)) Layer
Input=Nx100x100
Output=100x2

Model input = Nx1x2
Model output = Nx100x2

#Training data = 70 → 70,000 (augmented)
#Test data = 30

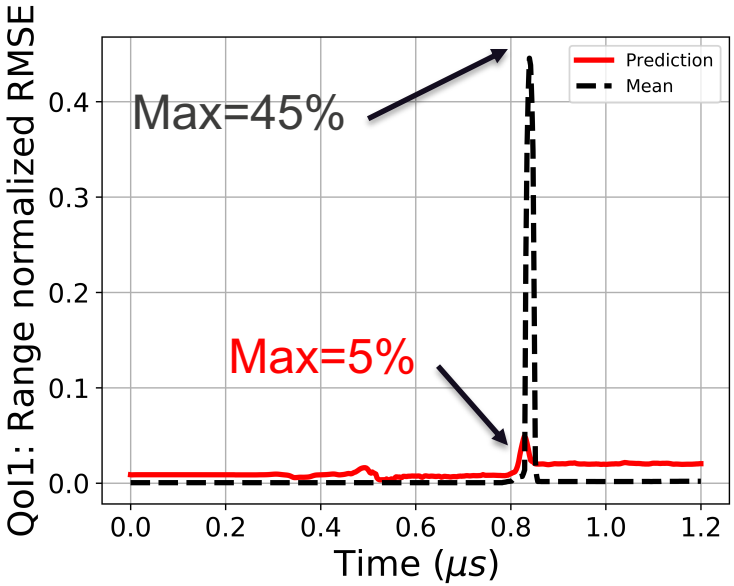
Length of the Longest Crack Predictions

Training Data



Length of the longest crack as a function of time.

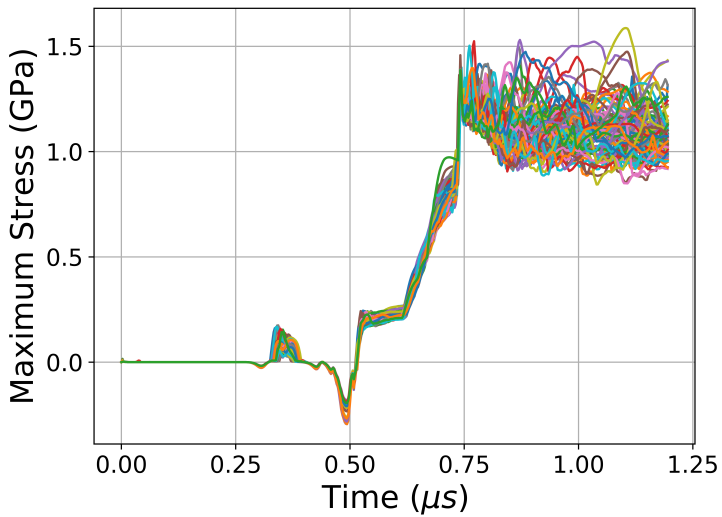
Error



Mean range normalized RMSE using 30 test data points.

Maximum Stress Predictions

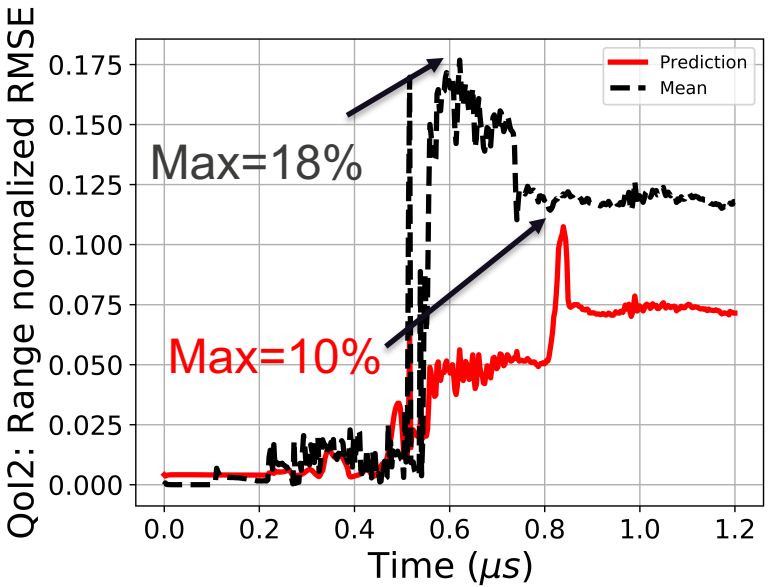
Training Data



Maximum tensile stress as a function of time

Maximum stress as a function of time.

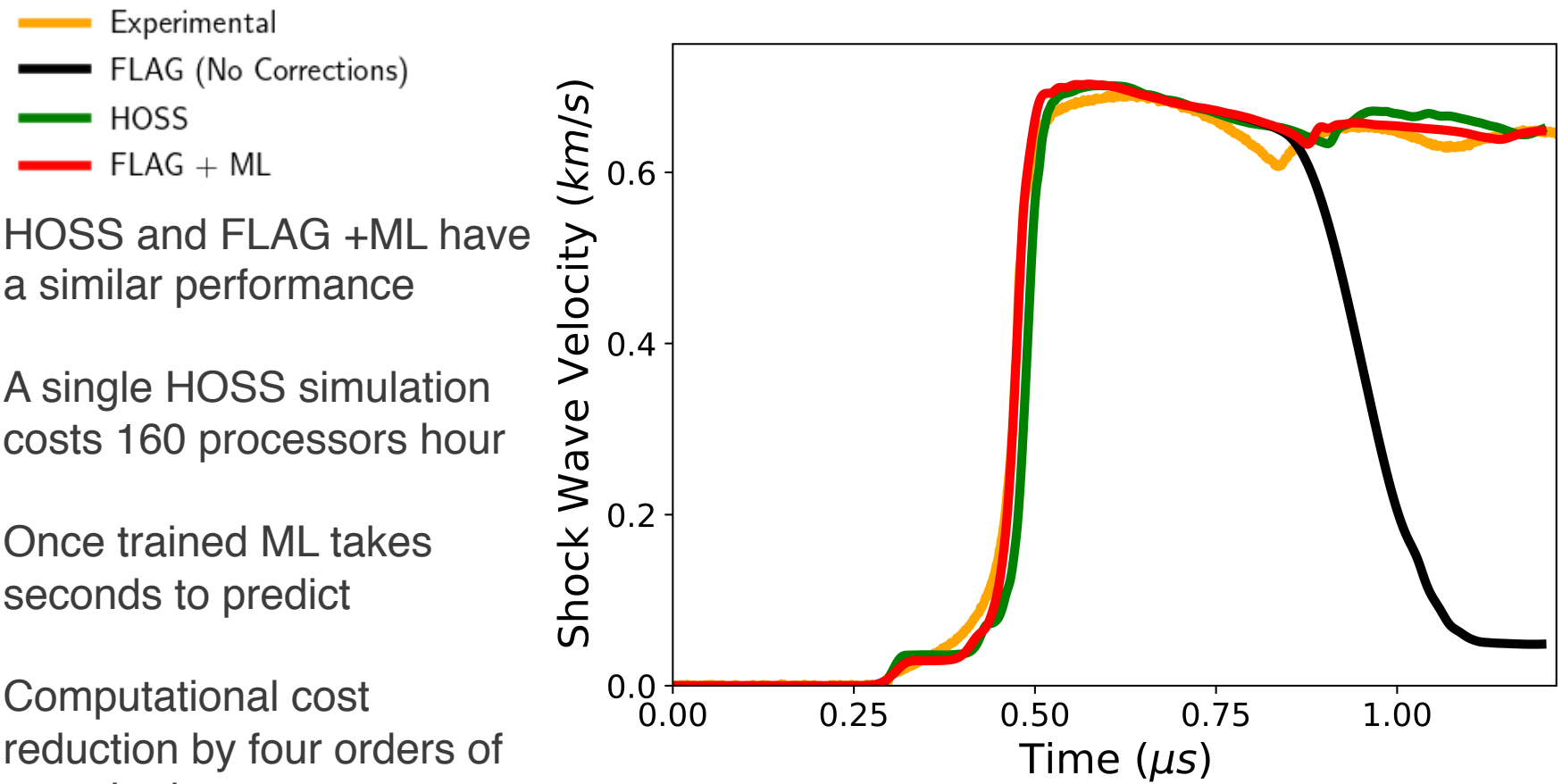
Error



Mean range normalized RMSE using 30 test data points.

Results using HOSS vs. FLAG + ML

- HOSS and FLAG +ML have a similar performance
- A single HOSS simulation costs 160 processors hour
- Once trained ML takes seconds to predict
- Computational cost reduction by four orders of magnitude



Temporal evolution of shock wave profiles

Summary, Conclusions and Future Work

- Reduced dimensionality of the problem
- Developed a fast ML simulator of HOSS (HF)
- Incorporated ML into the FLAG (LF) workflow
- FLAG + ML give us the accuracy of HOSS but 10,000 times faster
- The current model was tested only for this single experimental condition. Our next step is to consider varying loading conditions

Questions?

1. Schwarzer, Max, et al. "Learning to fail: Predicting fracture evolution in brittle material models using recurrent graph convolutional neural networks." *Computational Materials Science* 162 (2019): 322-332.
2. Cady CL, Adams CD, Prime MB, Hull LM, Addessio FL, Bronkhorst CA, Brown EN, Liu C, Sisneros TA, Brown DW, Blumenthal WR. Los Alamos National Laboratory Report. Report No. LA-UR-11-06976; 2011.
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