Machine Learning Applicability to Ejecta Production

Los Alamos Computational Physics Student Summer Workshop

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Outline

- Introduction
  - Shock physics
  - Experiments and simulation description
- Project setup
- Single shock/supervised learning projects
  - Ejecta binary classification
  - Surface height prediction
  - Total mass ejected prediction
- Double shock/unsupervised learning project
  - Ejecta classification

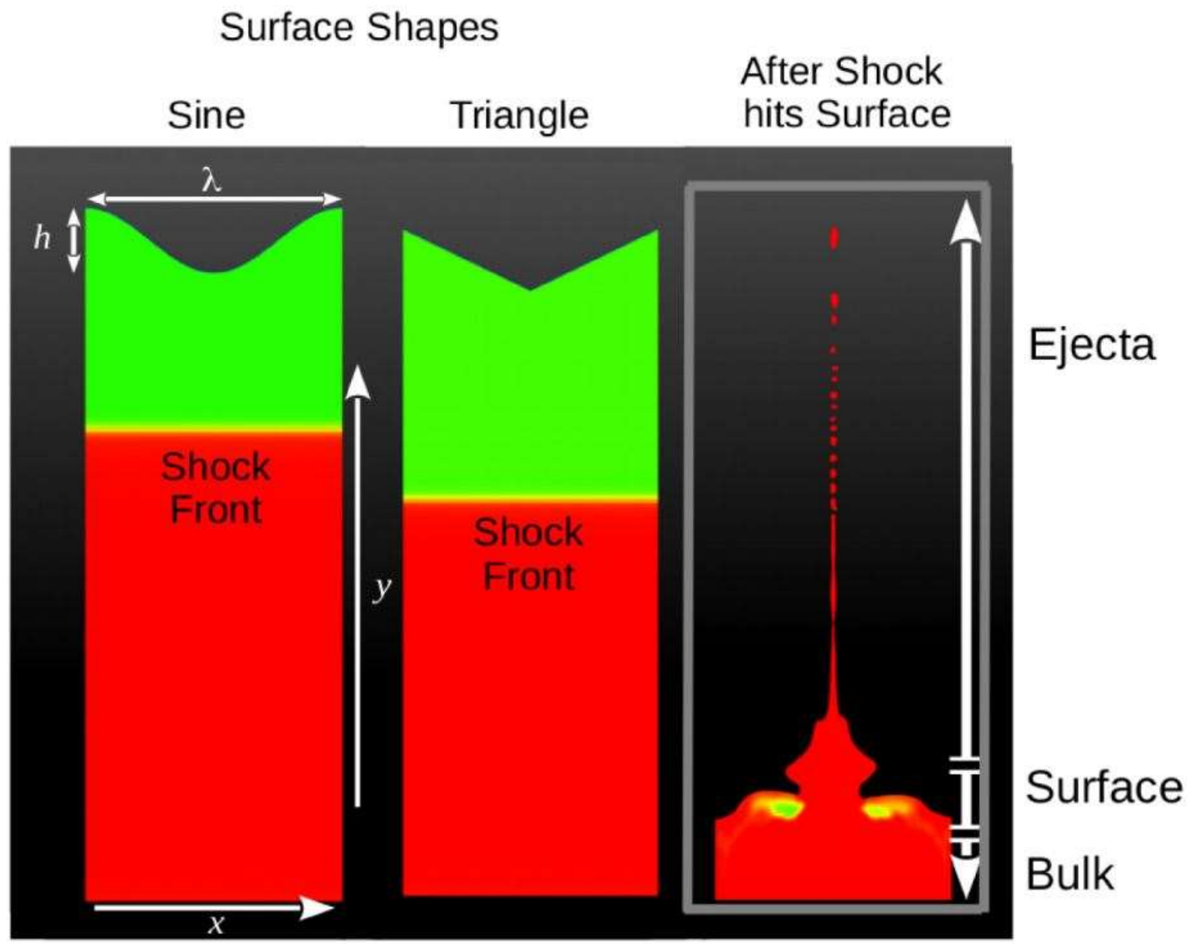
Ejecta Physics

Shock velocity

Particle velocity

$$U_s = c_0 + Su_p$$

Material parameters



Simulation setup

- Tin target and impactor
- Simulations are training data
- Single and double shock simulations

A = Perturbation amplitude
λ = Perturbation wavelength

$$kh = \frac{4\pi A}{\lambda}$$

Motivation

- System is difficult to model mathematically
- Simulations are computationally expensive
- Accurate models of single shock systems can help analysis of double shock systems
- Ejecta from double shocked systems are complex
- Applications include fusion research

Simulation data

- Lagrange hydrodynamics code
- Two dimensional
- 1300 single shock simulations
  - Single period sine wave
  - 1.5 microseconds
- 146 double shock simulations
  - Two periods of sine wave
  - 10 microseconds

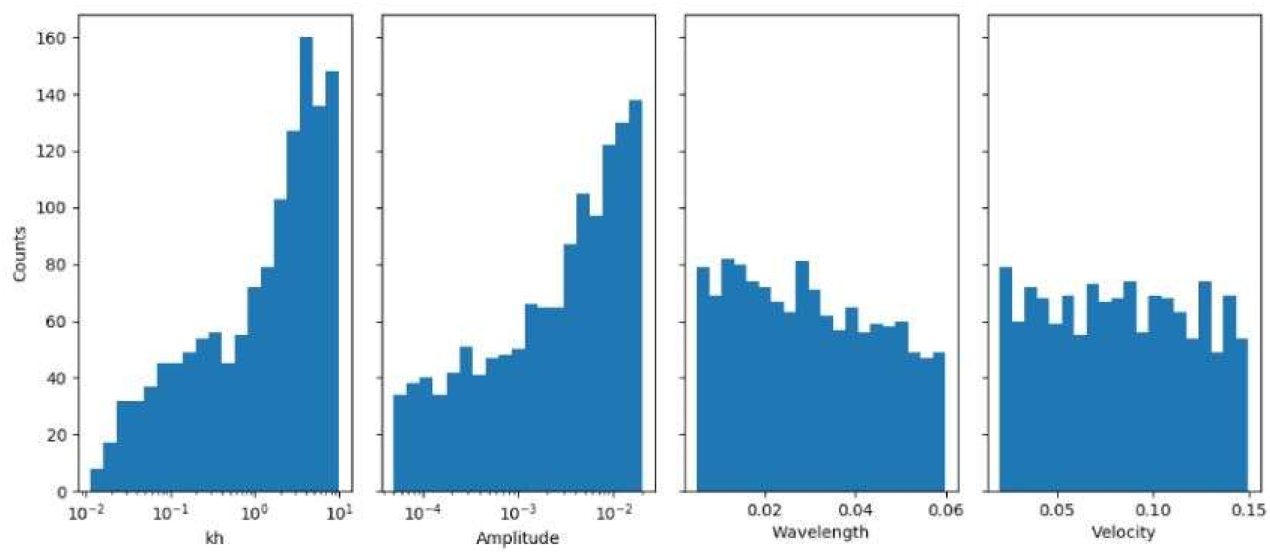
Machine learning

- Single shock data (Supervised training data)
  - Used deep neural network for each model
  - Binary classifier for ejecta production
  - Predict surface kh at given time
  - Predict total mass ejected at given time

- Double shock data (Unsupervised training data)
  - Extract ejecta from simulation
  - Categorize ejecta in simulations with k-means algorithm

Single shock Data

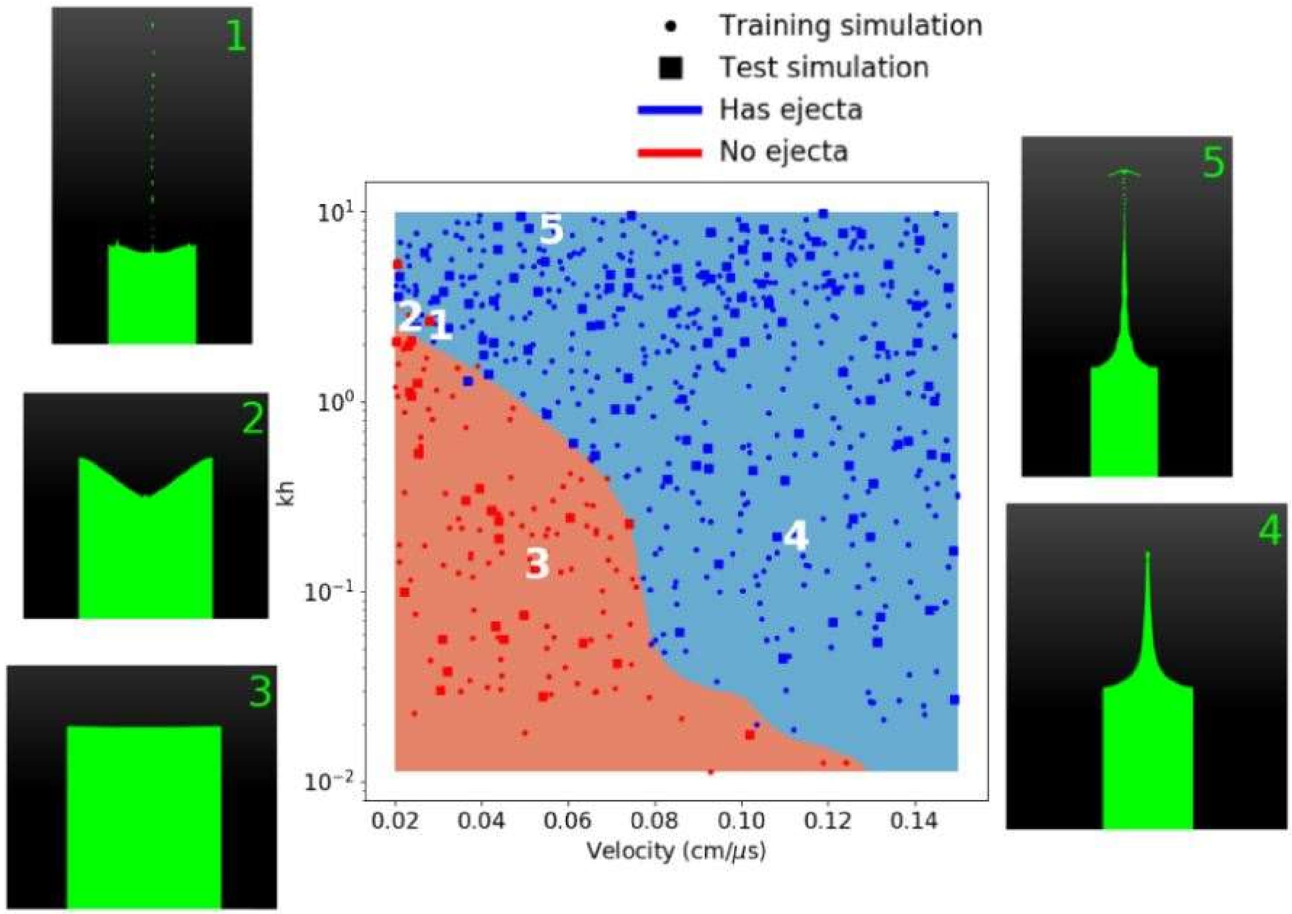
Single Shock Simulations' Parameter Ranges			
Parameter	Minimum Value	Maximum Value	Suggested Sampling Distribution
kh	0.01	10	
Amplitude (cm)	0.00005	0.02	Log Uniform
Wavelength (cm)	0.005	0.06	Uniform
Velocity (cm/μsec)	0.02	0.15	Uniform



Ejecta binary classifier methodology

- Simulation labeling
  - Check final timestep of simulation for leading clusters of mass separate from bulk material
- Model training
  - Randomly select training simulations and test simulations
  - Particle velocity, wavelength, and amplitude as input
  - Scale feature input by training data mean and standard deviation
  - Used Keras library in python with Tensorflow
  - Dense neural network with one hidden layer

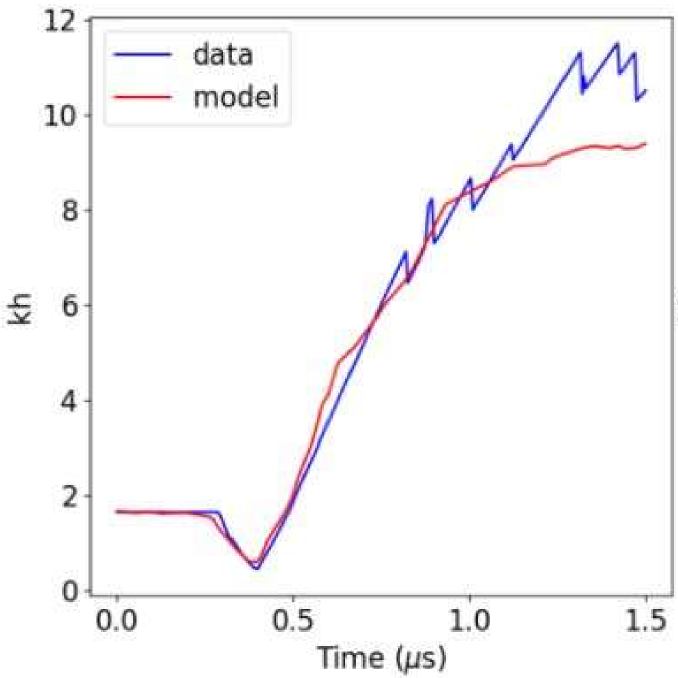
Ejecta binary classifier results

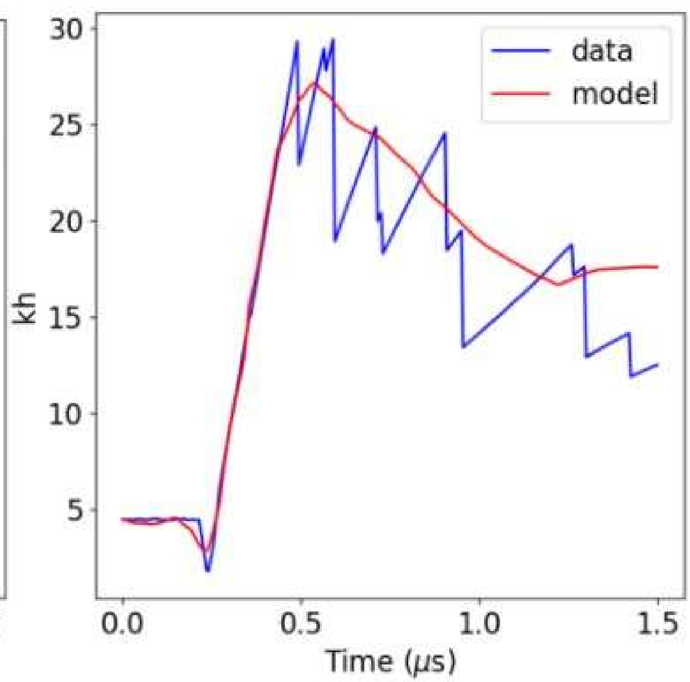


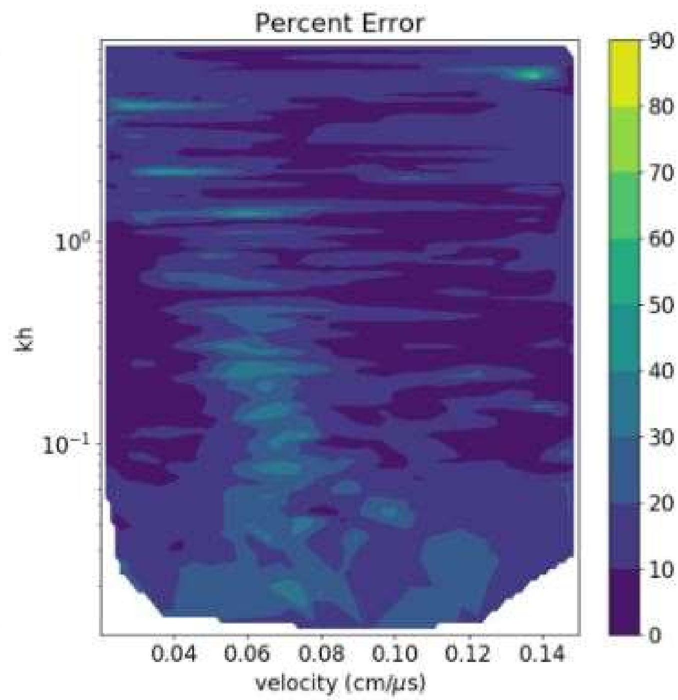
Surface height prediction methodology

- Finding height at each timestep
  - Find lowest and highest points on surface and the distance between them in the direction of the shock
- Model training
  - Particle velocity, wavelength, amplitude, and simulation time as input
  - Train regression model on log of height to prevent prediction of negative height
  - Scale feature input by training data mean and standard deviation

Surface height prediction results

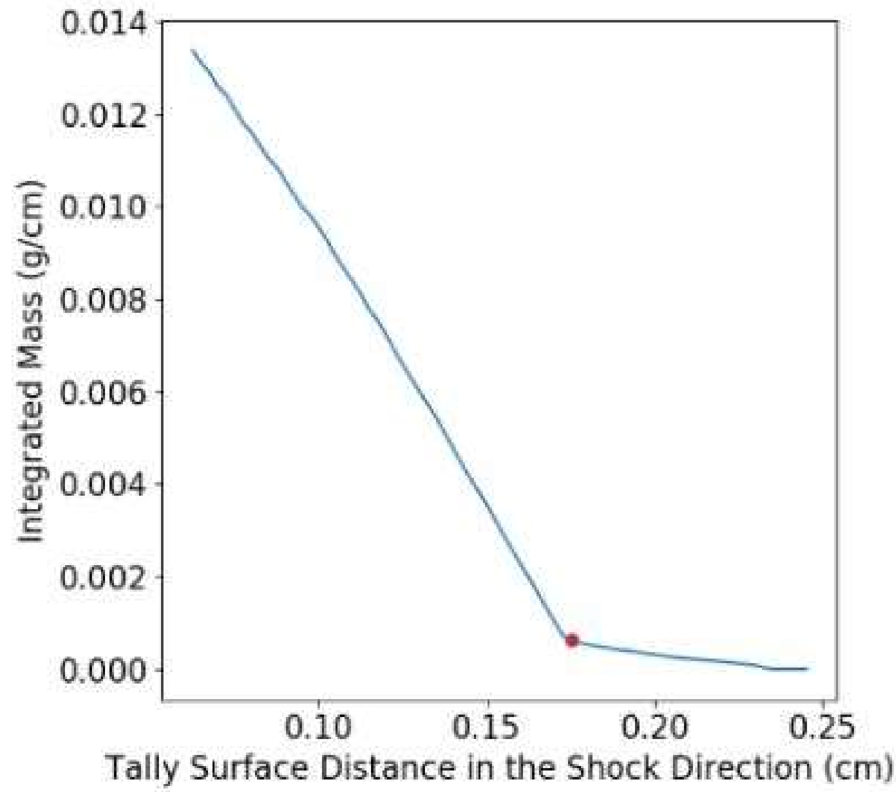




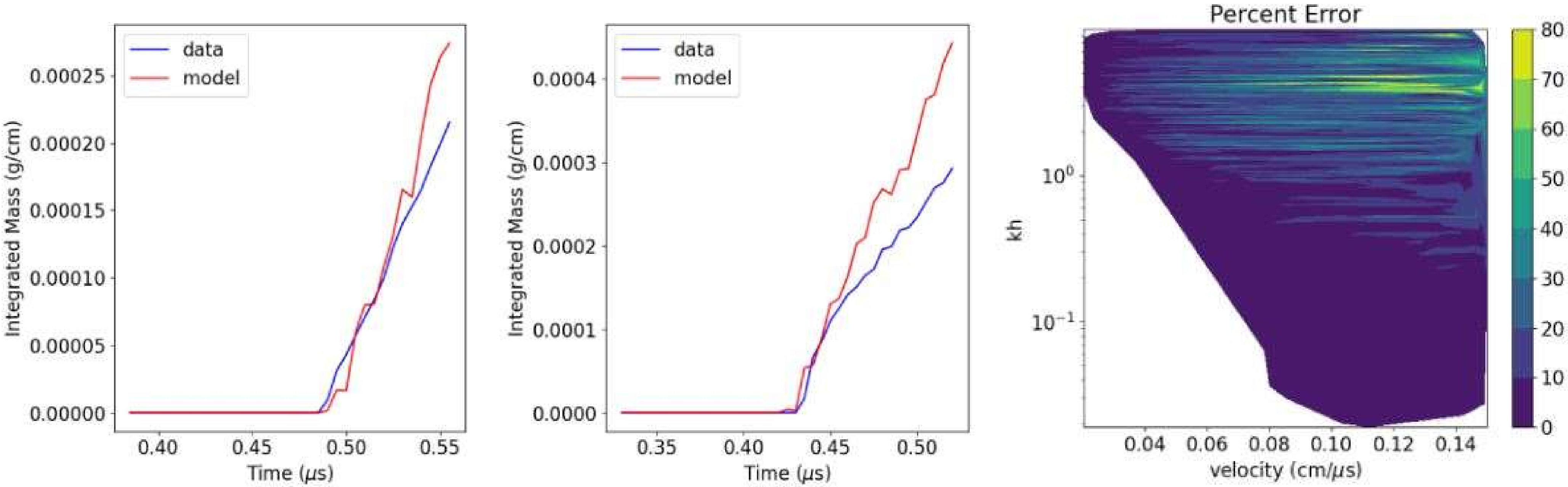


Total mass ejected methodology

- Finding total mass ejected
  - Find boundary between ejecta and bulk
  - Note total mass past given set of points ahead of bulk for each timestep
- Model training
  - Particle velocity, wavelength, amplitude, simulation time, and tally distance as input
  - Train regression model on log of integrated to prevent prediction of negative mass



Total mass ejected results

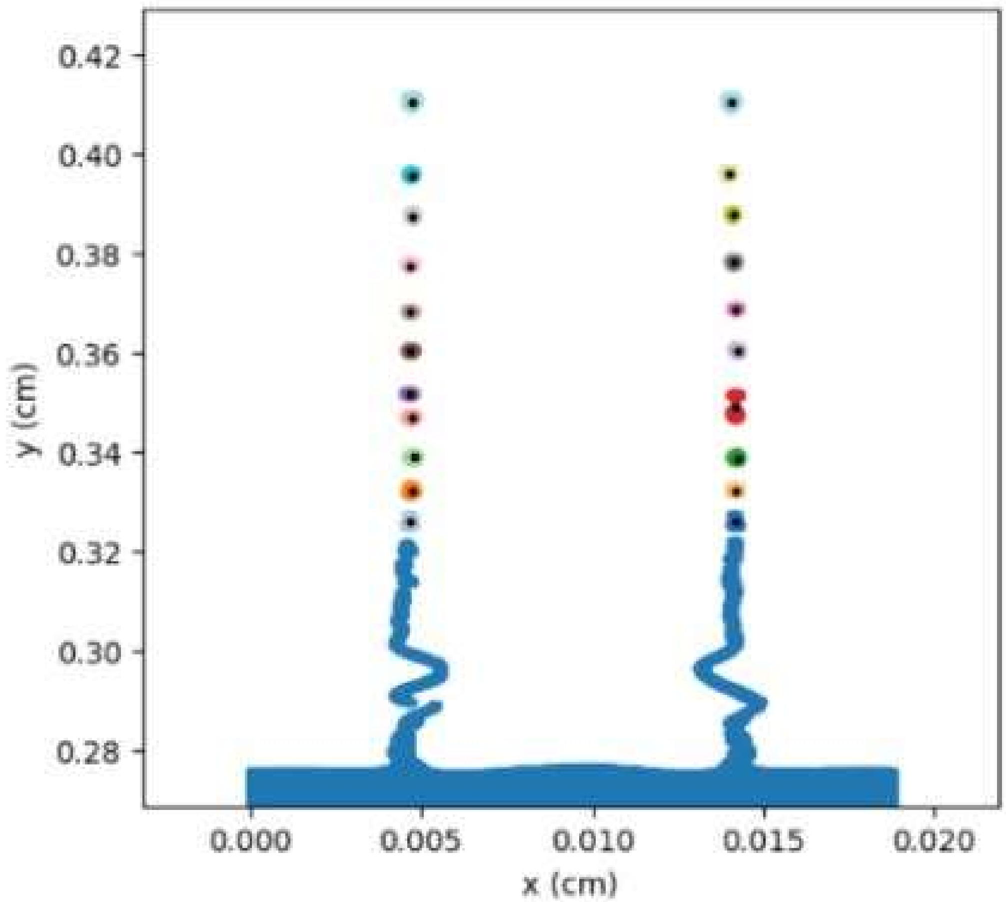


Double shock data

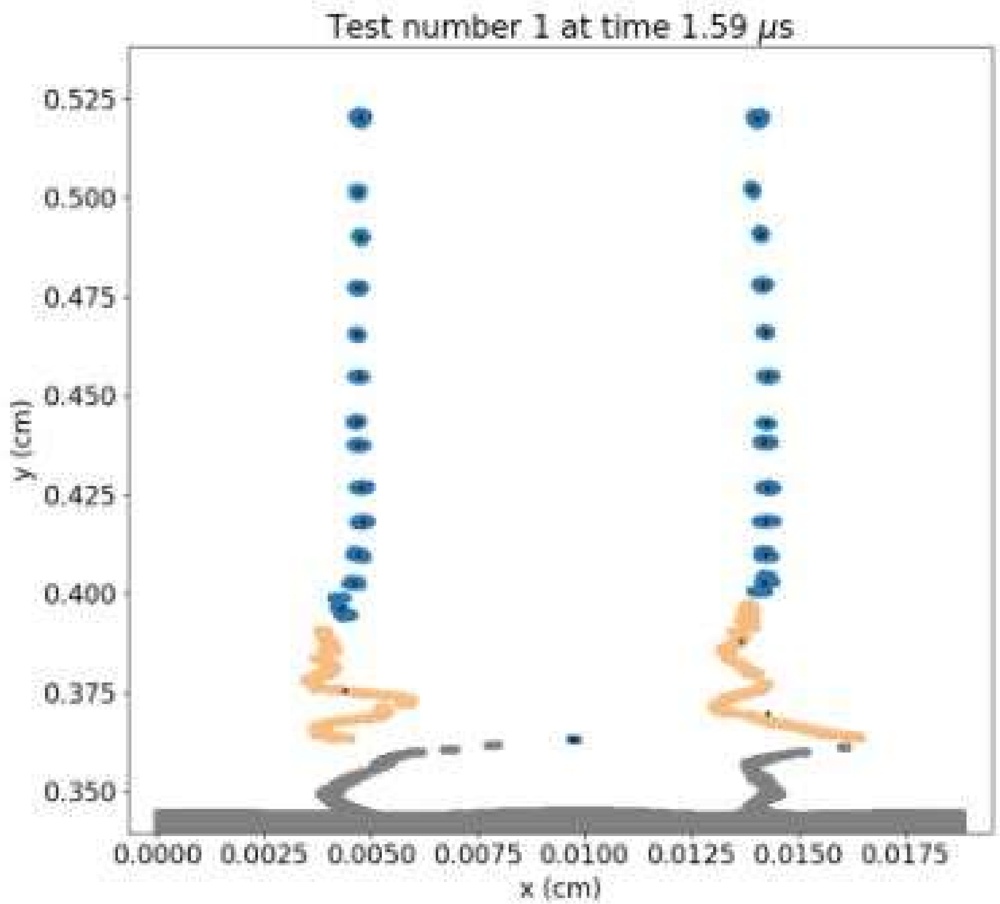
Double Shock Simulations' Parameter Ranges			
Parameter	Minimum Value	Maximum Value	Sampling Distribution
kh	0.3	4.0	
Amplitude (cm)	0.0005	0.002	Uniform
Wavelength (cm)	0.005	0.02	Uniform
Velocity 1 (cm/μsec)	0.02	0.15	Uniform
Velocity 2 (cm/μsec)	0.022	0.24	
Time between Shocks (μsec)	0.5	3.5	Uniform

Double shock ejecta classification methodology

- Separating ejecta
  - Remove bulk material
  - Cluster simulation node points
  - Ignore largest cluster (bulk material)
- Determining features for ejecta classification
  - Create feature vectors from node point data within each ejecta
- Scale features
- Principal component analysis



Double shock ejecta classification results



Conclusions

- Simple supervised methods can reproduce known facts correctly
  - Ejecta binary classifier was able to find velocity where free surface melts
  - Surface height predictor can find
- Supervised methods can be used to bypass simulations
- Simple supervised methods for single shock experiments can be used as analysis aids for double shock experiments
- Unsupervised methods have the potential to reveal non-obvious interpretations of ejecta data

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