Machine learning for physics simulation anomaly detection

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Introduction

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Hydrodynamics

- Hydrodynamics is the subsection of Fluid Dynamics that studies the flow of liquids
- Used in many areas of study and application
  - Ocean Currents
  - Blood Flow
  - Rocket Engines
  - More
- These problems often not have known analytical solutions…
- Example: Navier-Stokes Equations

Direct Numerical Simulation (DNS)

- DNS is used to find solutions to hydrodynamic (and other) problems with no known analytical solutions
- Uses numerical methods to compute accurate approximations of the solutions
- Often is computationally intensive and requires extensive computational resources
  - Requires High Performance Computing (HPC)

HPC, Faults, and Anomalies

- HPC Clusters tend to have large amounts of computational resources such as CPUs, Memory, and more
- There is a significant probability of memory faults at the high scales found in HPC
- Some faults could simply cause job failure, but others may cause silent data corruption (SDC) anomalies
  - Costly
- It's also possible for anomalies to come from other sources

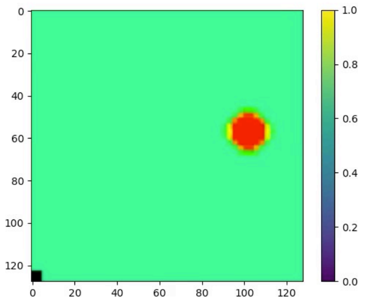
Anomaly Detection

- Computer-Vision techniques have been used to detect anomalies in images
  - Concrete Deficiencies
  - Skin Diseases
  - More
- One approach is reconstruction loss
  - Train an autoencoder to recreate nominal images
  - If the autoencoder is unable to recreate an image, it is likely anomalous
- We applied this idea to hydrodynamic simulations

Methodology

Dataset

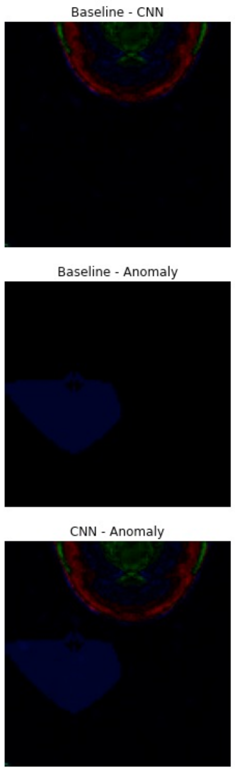
- We created a dataset of simulations using a tool called CLAMR
  - Simulations of the shallow water equation
- Consists of 459 pairs of simulations
  - Nominal and anomalous
  - 100 frames each
  - Varies on mesh size, domain size, and initial state
- Each of the 100 frames was turned into an image
  - 128x128 pixels



One simulation from the dataset

Method

- Reconstruction Loss Anomaly Detection
  - Train a model to reconstruct nominal data
    - Usually using an autoencoder
  - If an input is anomalous, the autoencoder should fail to create an accurate reconstruction
  - Train a classifier to determine if the error between the input and reconstruction implies anomalous input



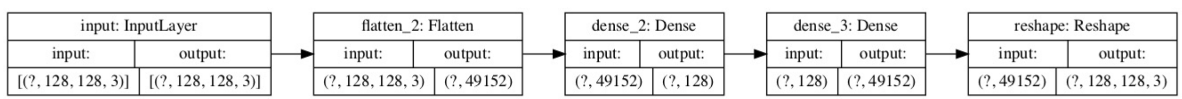
A comparison of differences
Baseline – CNN
Baseline – Anomaly
CNN – Anomaly

Methods (cont.)

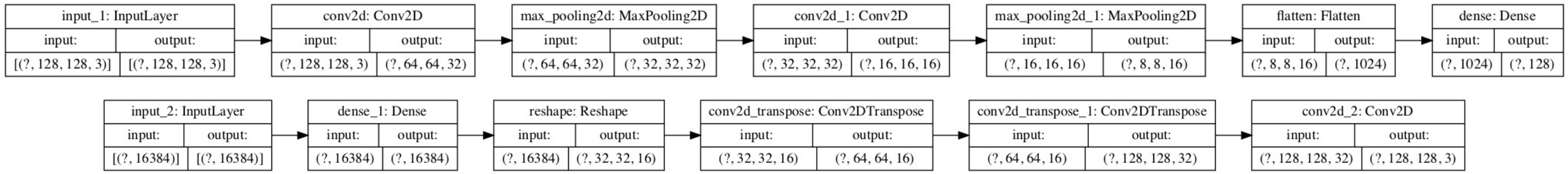
- Predictive Reconstruction
  - Since an anomaly may have the same ”shapes” as nominal data, we modified the technique
- Predict a subsequent frame based off the previous two frames
- Find the difference between the prediction and the same frame from the simulation
- Relies on model learning how to progress the simulation rather than learning nominal reconstructions

Autoencoders

- We tried two traditional autoencoders
  - Baseline feed-forward ANN
  - Convolutional
- Both predict a frame given the frame two timesteps back



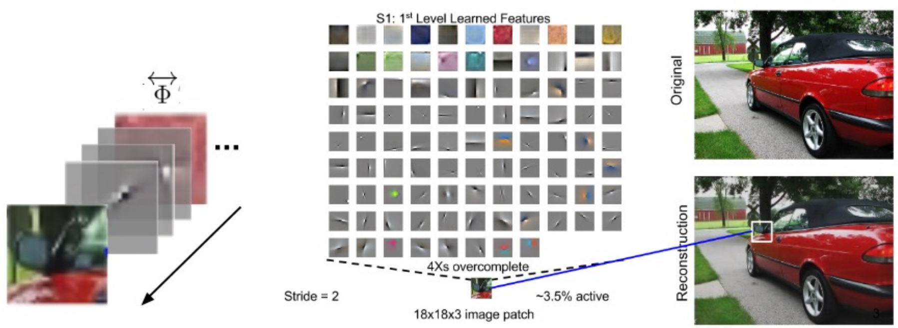
ANN Autoencoder Structure



CNN Autoencoder Structure
Encoder (top) and decoder (bottom)

PetaVision

- We also used PetaVision, a neuromorphic sparse coder
- Has been used for impressive computer vision problems
- Learned a Spatiotemporal Dictionary for predicting a frame given the two previous frames



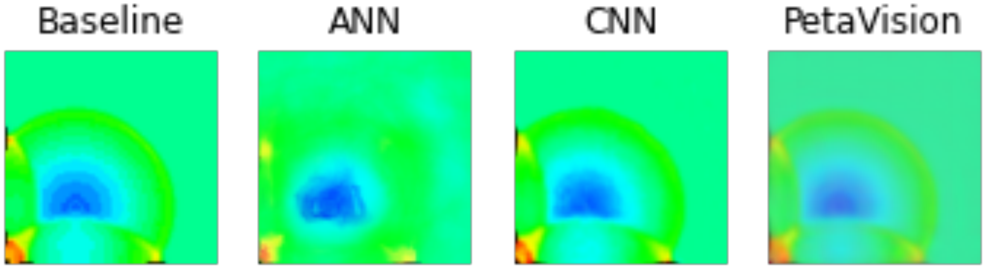
$$\overbrace{\overrightarrow{I}}^{\text{Original}} \approx \overbrace{\overleftrightarrow{\Phi}\, T(\overrightarrow{u})}^{\text{Reconstruction}}$$

$$E = \overbrace{\frac{1}{2}||\overrightarrow{I} - \{\overleftrightarrow{\Phi}\, T(\overrightarrow{u})\}||_2^2}^{\text{Reconstruction Term}} + \overbrace{\lambda||T(\overrightarrow{u})||_1}^{\text{Sparsity Term}}$$

Illustration of how PetaVision reconstructs images

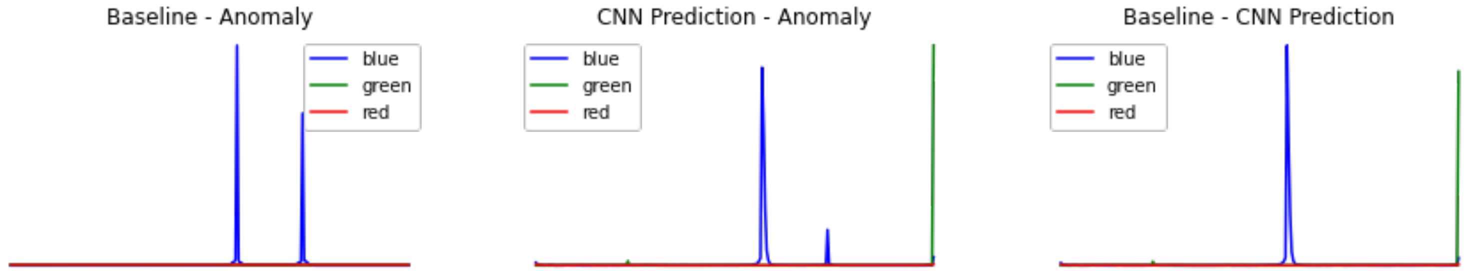
Predictions

- Each autoencoder achieved different levels of reconstruction
  - ANN failed to recreate the proper shapes, colors, and patterns
  - CNN achieved correct colors but the shapes were not sharp
  - PetaVision learned accurate shape reconstructions but the coloring was off



Classification

- In order to classify anomalous frames, we converted the images to feature vectors and computer the difference
- Analysis showed that there were often differences in the blue channel
- We found that one set of blue features in particular were found in the anomalies



Feature Vector Differences Represented as Histograms

Classification (cont)

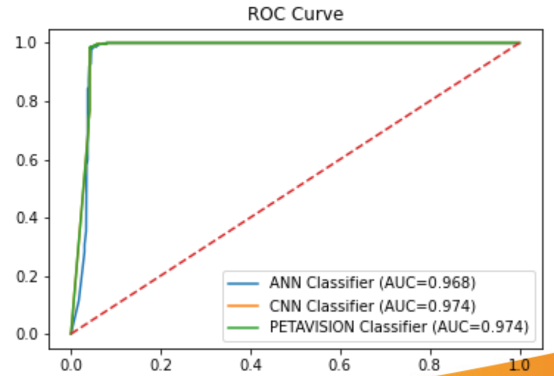
- We trained a Gradient Boosted Decision Tree (GBDT) Classifier
  - Also tried random forest and multi-layer perceptron but they performed worse
- We used the feature vector differences as input
  - 3 channels X 256 color values = 768 features
- Each Autoencoder was paired with its own classifier

Conclusions

Results

- Overall we got very similar classification performance regardless of autoencoder
- The classifier achieved impressive metrics (~0.97 AUC)
- This was surprising considering the difference in frame predictions

Auto-Encoder	Accuracy	Precision	Recall	F1	AUC
ANN	0.966	0.944	0.992	0.967	0.968
CNN	0.969	0.950	0.991	0.970	0.978
PetaVision	0.966	0.942	0.994	0.967	0.974



Conclusions

- Despite differences in predictions, we achieved very good classification results
- Using a random forest we discovered that only a small subset of features seemed to attribute to the classification
  - That blue spike seen in the histograms earlier
- Our dataset may have been too “easy” for the classification, but this is still a good first step

Next Steps

- Generate a new dataset of more complex simulations
- Look at more computer vision techniques
  - PetaVision has potential we did not use here
- Find different types of anomalies that may appear
- Trace an anomaly through timesteps if possible

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Thank You

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