ACCELERATING PHASE FIELD SIMULATIONS USING MACHINE LEARNING
SURGE -2023

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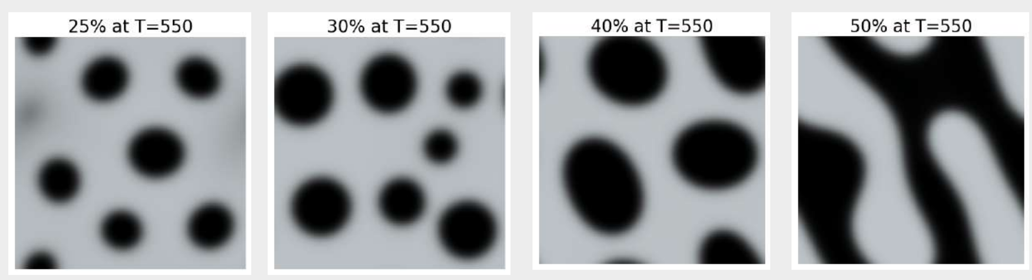
INTRODUCTION

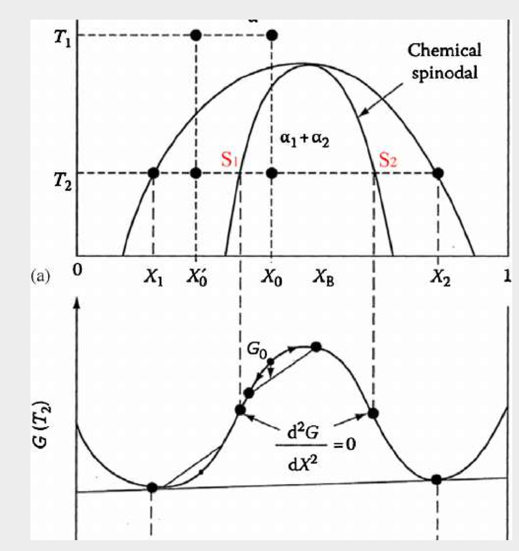
- Phase-field modelling is done by making use of the Cahn-Hiliard equation and it is an effective tool to study the microstructure evolution of a particular alloy.
- However, even though taking into account its highly accurate predictions, phase-field modelling itself is a computationally expensive tool.
- We focus on building an ML model, which consists of an auto-encoder along with a ConvLSTM for microstructure evolution prediction based on already generated frames from the phase-field modelling.
- This ML model will help us skip 'n' phase-field steps and save computation time.

SPINODAL DECOMPOSITION

- "*Spinodal decomposition*" is a mechanism by which a single thermodynamic phase spontaneously separates into two phases without nucleation.
- The Cahn-Hilliard equation is used for the simulation of microstructures.
- Using this technique, 1000 images of 10 different compositions between the 2 points of inflection of the G vs X curve are generated.

Images generated from phase-field

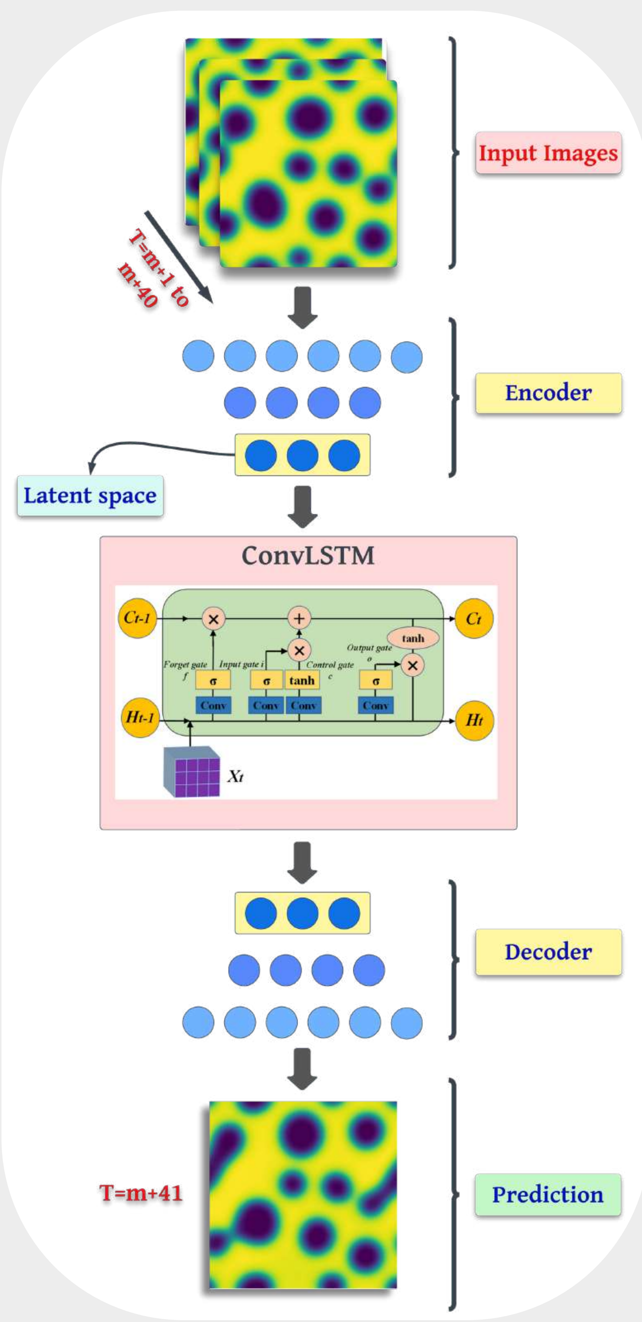




OBJECTIVES

- Generate a dataset of 10,000 images consisting of 1000 images for 10 different compositions of a binary alloy.
- Develop an Autoencoder for encoding the images into smaller dimensions so that ConvLSTM will be fast.
- Next, pass the encoded images into a ConvLSTM model as input and train this network, which will take the previous 'm' previous frames and predict the next frame.
- Test the model on a different composition to predict the microstructure evolution.

WORKFLOW



Phase-field generated images sent to an encoder to reduce the dimensional complexity to a smaller "*latent space*".

For example - an RGB image of dimensions (256 x 256 x3) reduced to (32 x 32 x8)

Images are sent into a "ConvLSTM" (Long-Short term Memory) Network where the next image in the series is predicted

Images are decoded

We get our final predicted image

Test Case:

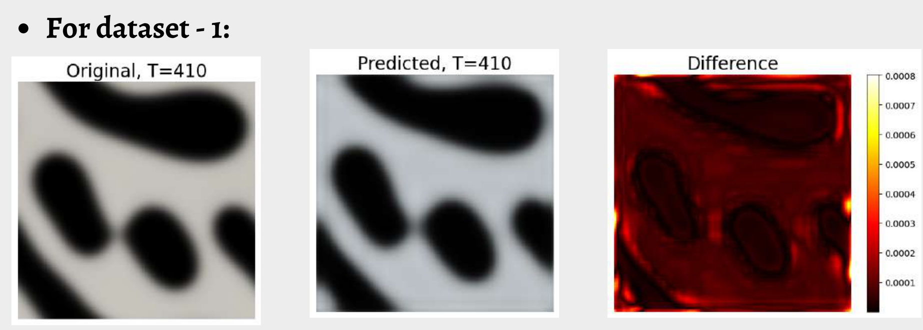
We consider a case where we now take 3 types of datasets each with 10 different compositions and 1k images each:

Dataset	Performance:
Time step=1, Time step=2 . . . . Time step=1000 — Dataset 1, 1k images	Prediction accuracy - 99.26%
Time step=5, Time step=10 . . . . Time step=5000 — Dataset 2, 1k images	Prediction accuracy - 98.36%
Time step=10, Time step=20 . . . . Time step=10,000 — Dataset 3, 1k images	Prediction accuracy - 98.69%

Now, we test our models on a different composition (46%) and compare the *1st, 10th*, and *100th* common predictions.

1st common image: T=410

- For dataset - 1:



- For dataset - 2:

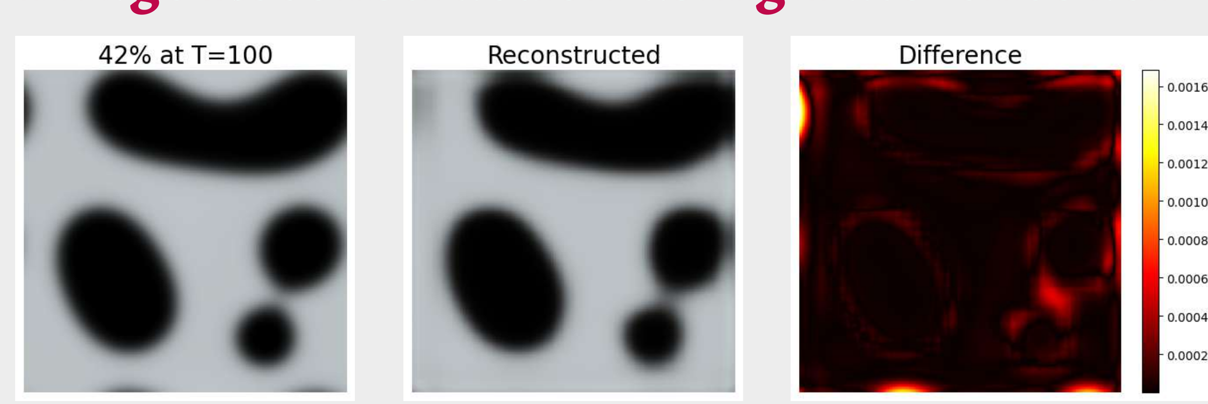
HOW IS THE MICROSTRUCTURE EVOLUTION BEING PREDICTED?

Training Phase:

The 10,000 images were passed into the **Encoder** and the latent space was trained using a ***ConvLSTM*** network with 2 layers with a total of 24 cells. The activation functions used in that layer were - ***tanh*** and ***relu.***

Predicted image was then passed into the decoder to get the final image.

Image Reconstruction using Auto-encoder



Original Image of 42% — Reconstructed Image — Heatmap Difference

Next Frame Predictions using ConvLSTM

Input Encoded Images	Predictions
Frame 1, Frame 2 . . . . Frame 40	Frame 41
Frame 2, Frame 3 . . . . Frame 41	Frame 42
Frame 40, Frame 41 . . . . Frame 79	Frame 80

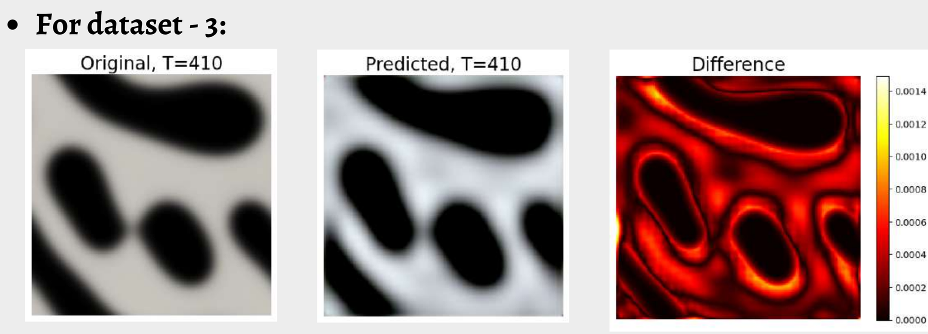
Iteration -1: We take frames 1 to 40 and predict the 41st

Iteration -2: We take frames 2 to 41 and predict the 42nd

Iteration -40: We take frames 40 to 79 and predict the 80th

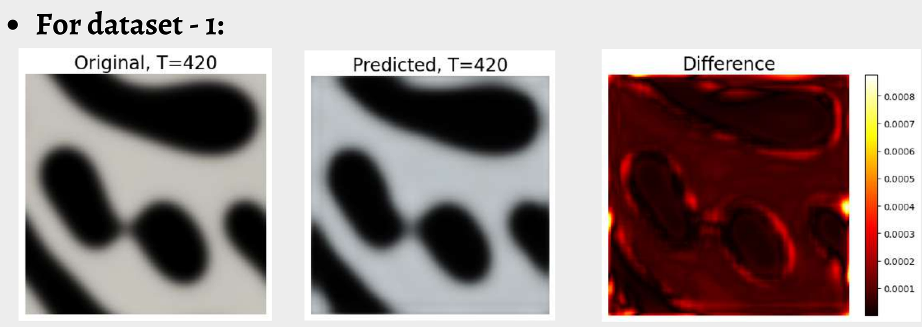
RESULTS & DISCUSSIONS

- For dataset - 3:

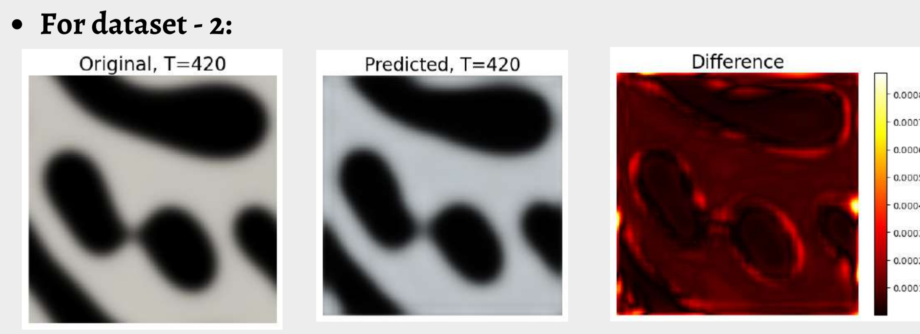


2nd common image: T=420

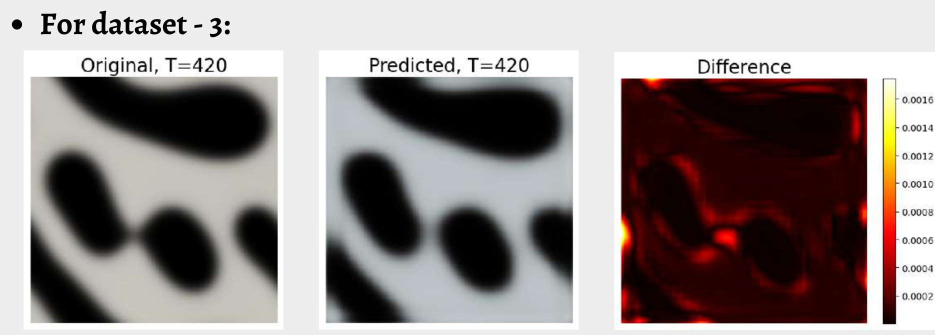
- For dataset - 1:



- For dataset - 2:

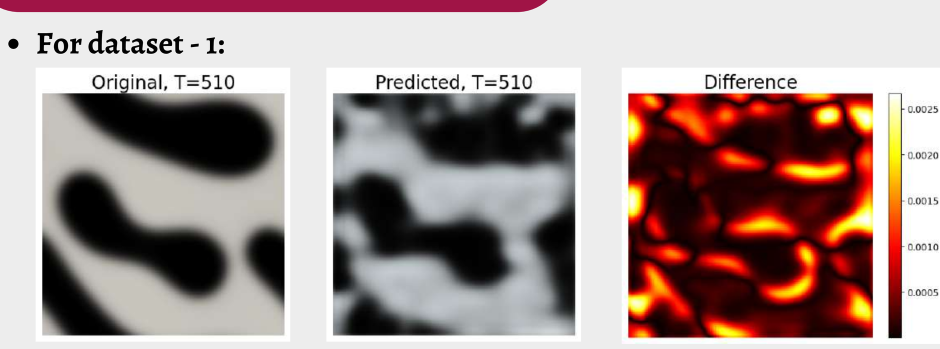


- For dataset - 3:

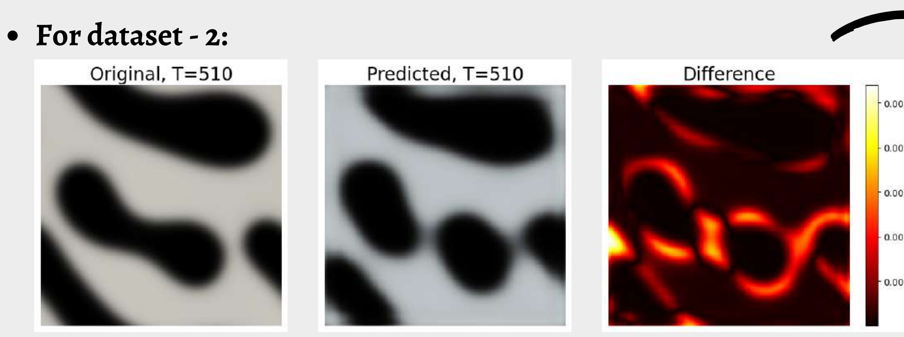


3rd common image: T=510

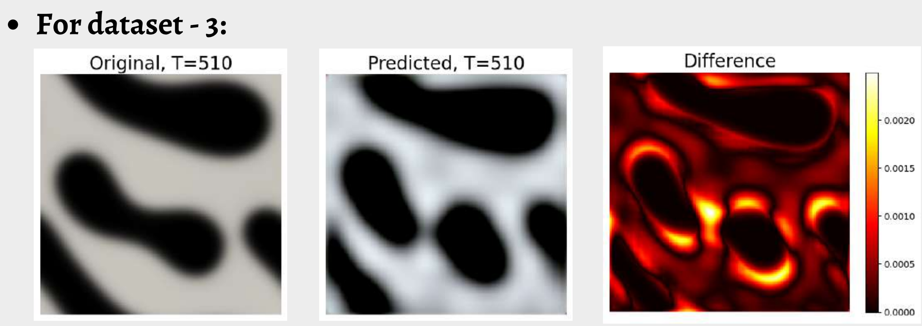
- For dataset - 1:



- For dataset - 2:



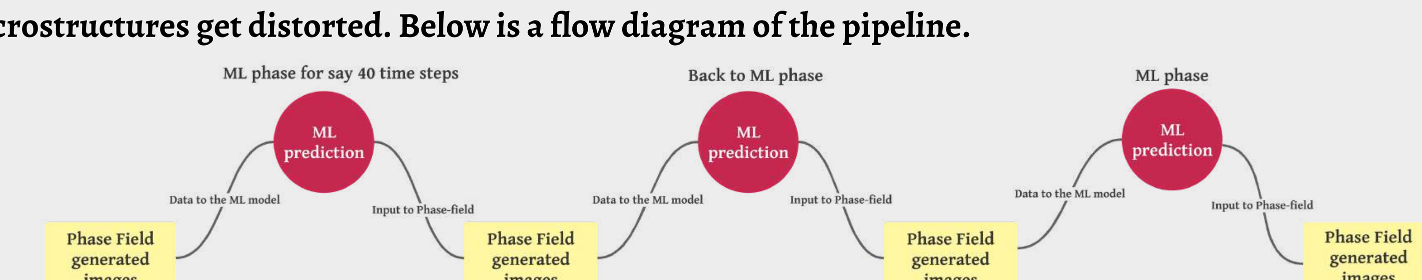
- For dataset - 3:



We see that in datasets 2 and 3, the predictions at long ranges are better than the first, which becomes "*distorted*" at T=510, which is the 100th common time step.

Future Scope of Improvement

- We can use an adaptive dataset for training. For example in the initial changes, where the microstructural changes are significant, we take the images at 1 time step difference. After a certain time, say, 100-time steps, we can take images in 5-time steps and 10-time steps. This will make our dataset contain crucial features, that will help our ML model to learn properly.
- We can take not just 40 frames, but increase to more frames and train the datasets. e.g -80 frames.
- After predicting, let's say 40-time steps through ML, we must switch back to phase-field before the microstructures get distorted. Below is a flow diagram of the pipeline.



Acknowledgement & References

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References: *Owais Ahmad, Naveen Kumar, Rajdip Mukherjee, and Somnath Bhowmick, "Accelerating microstructure modeling via machine learning: a new method combining Autoencoder and ConvLSTM," (2023), arXiv:2305.00938 [cond-mat.mtrl-sci]*


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