Physically Consistent Neural Network Models for Equations of State

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WCI WEAPONS AND COMPLEX INTEGRATION

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MOTIVATION

The National Ignition Facility (NIF) performs inertial confinement fusion experiments. To better understand the process, we run intricate simulations of the experiment. Equations of state (EOS) provide key information to simulate the hydrodynamic processes in the fuel capsule.

GOAL: Use neural networks to improve equation of state models for NIF simulations

Improve Equations of State

- Currently, EOS data is stored in memory intensive tables and requires interpolation between data points
- Neural networks take minimal time and memory to evaluate and can be queried at any point

Incorporate Physics into Machine Learning

- Typical neural networks may not obey physics; it is unclear how well these tools learn the physical laws from data
- We can force the model to obey phase transitions and create thermodynamically consistent outputs by structuring the model accordingly

DATA AND METHODS

Data:

- LEOS 1018 Equation of state tables for Deuterium and Tritium mixture
- Input: density (0 – 12500 g/cm^3), temperature (5 – 2e9 K)
- Output: energy (-2e10 – 2e17 erg/g), entropy (0 – 1.5e12 erg/K)
- Irregularly spaced grid (8800 points)

Methods:

- Shift and normalize data, transform to log space
- Deep Jointly Informed Neural Networks (DJINN) use decision tree models to guide neural network structure[(1)]
- Ensemble method, the results of 10 tree models are used to select the best prediction

Model 1:

- Feed data directly into single DJINN model

Model 2:

- Incorporate phase transitions into the model, hopefully to reduce error around phase transitions
- K-Means clustering algorithm to identify 3 phases in the data
- Train 3 separate DJINN models, one on each phase

- Results are evaluated using mean squared error (MSE) and mean absolute error (MAE) metrics:

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(X_i - \hat{X}_i)^2 \qquad \mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}\left|X_i - \hat{X}_i\right|$$

(1): Humbird, Kelli D., J. Luc Peterson, and Ryan G. McClarren. "Deep neural network initialization with decision trees." *IEEE transactions on neural networks and learning systems* 30.5 (2018): 1286-1295.

MODEL 1: SIMPLE NEURAL NETWORK

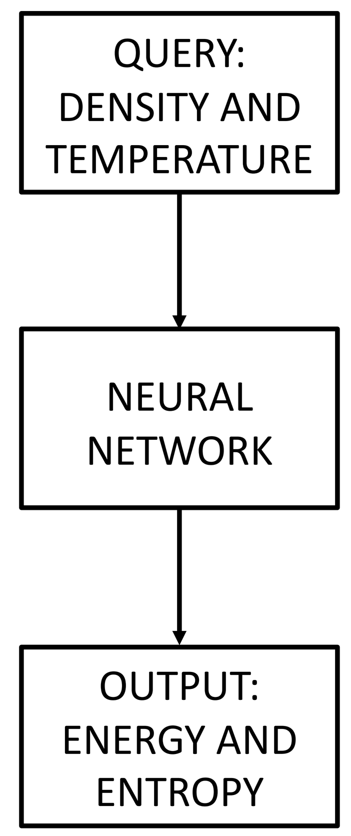
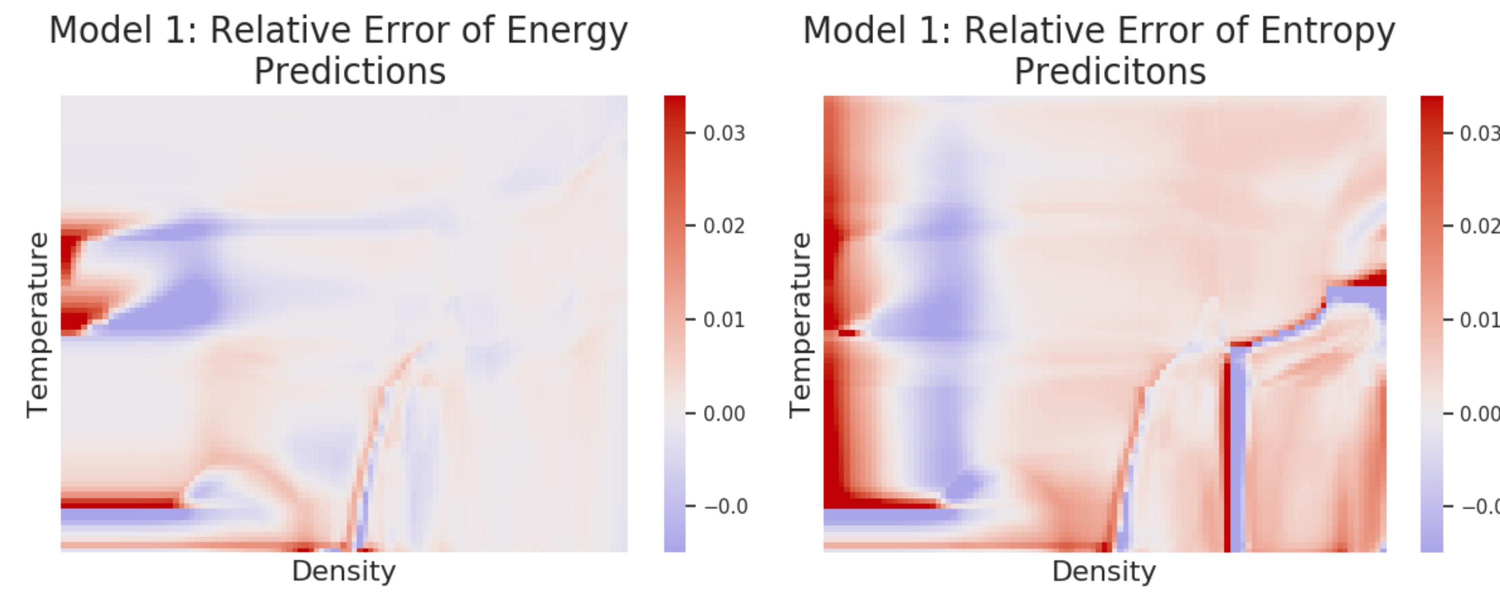


Figure 1 (left)**:** Diagram of model 1, a simple neural network design to model equations of state.

Figure 2 (right)**:** Relative error of energy and entropy predictions from Model 1. Structure within the heat maps suggests there are patterns in the data that the neural network has trouble capturing.



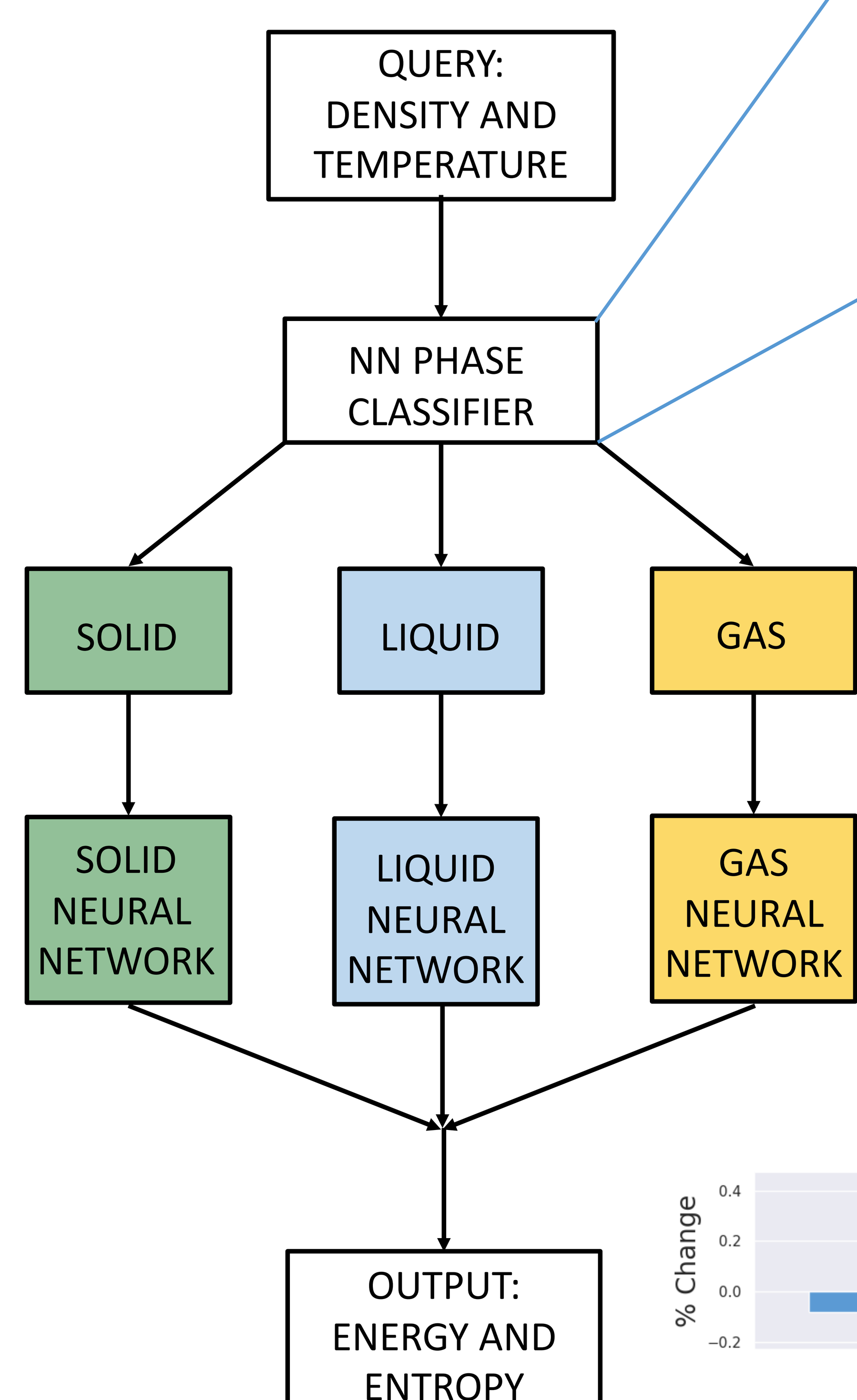
Mean Squared Error: 0.025257
Mean Absolute Error: 0.073088
Explained Variance: 0.999080

Mean Squared Error: 0.049740
Mean Absolute Error: 0.128513
Explained Variance: 0.997258

➢ Even the naive model achieves high accuracy – on average, energy prediction is within 1.5% of the true value, while entropy prediction is within 3%

MODEL 2: NEURAL NETWORK WITH PHASES

Figure 3 (below)**:** Diagram of model 2, a neural network design incorporating phase changes. Ideally, structuring the neural network to incorporate phase changes will alleviate some of the structured error seen in Model 1.



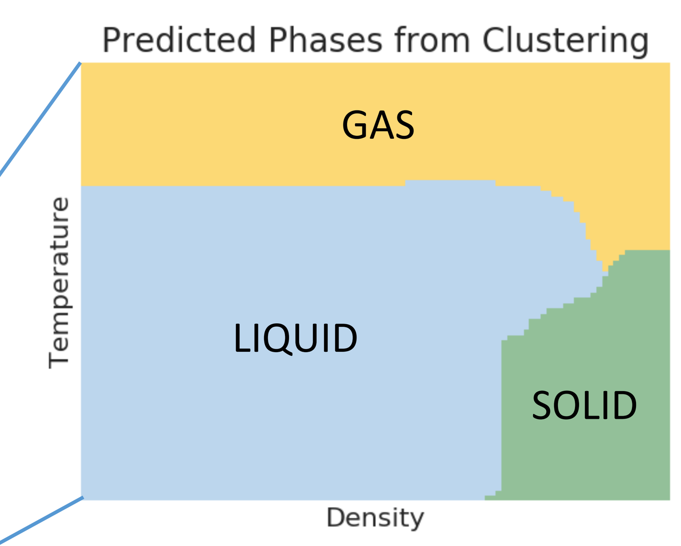
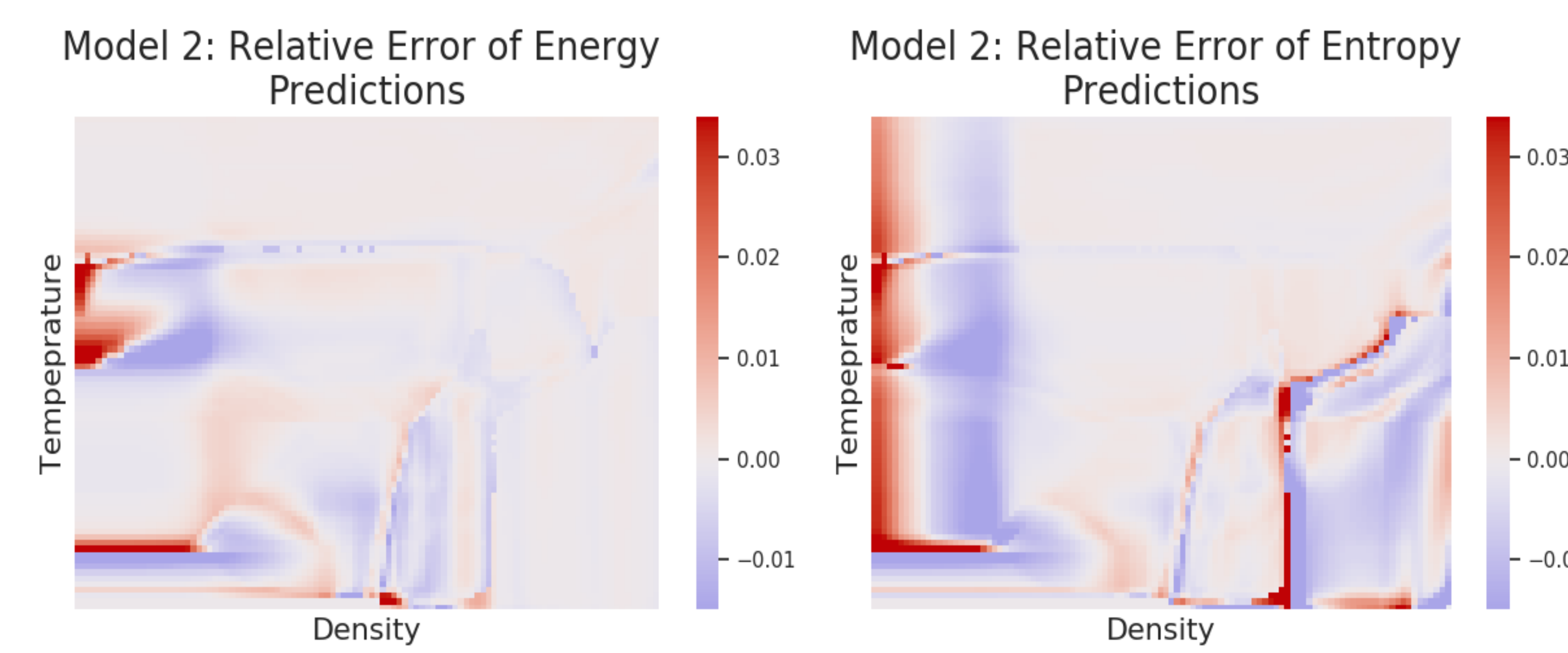


Figure 4 (left)**:** Diagram of 3 phases identified by K-Means algorithm. The phase boundaries seem to largely align with the error structures in the heat plots.

Figure 5 (below)**:** Relative error for energy and entropy predictions from Model 2. Overall, results appear to be slightly improved. The entropy predictions see the greatest benefit from incorporating phase information.



Mean Squared Error: 0.020873
Mean Absolute Error: 0.067006
Explained Variance: 0.999240

Mean Squared Error: 0.047914
Mean Absolute Error: 0.094997
Explained Variance: 0.997116

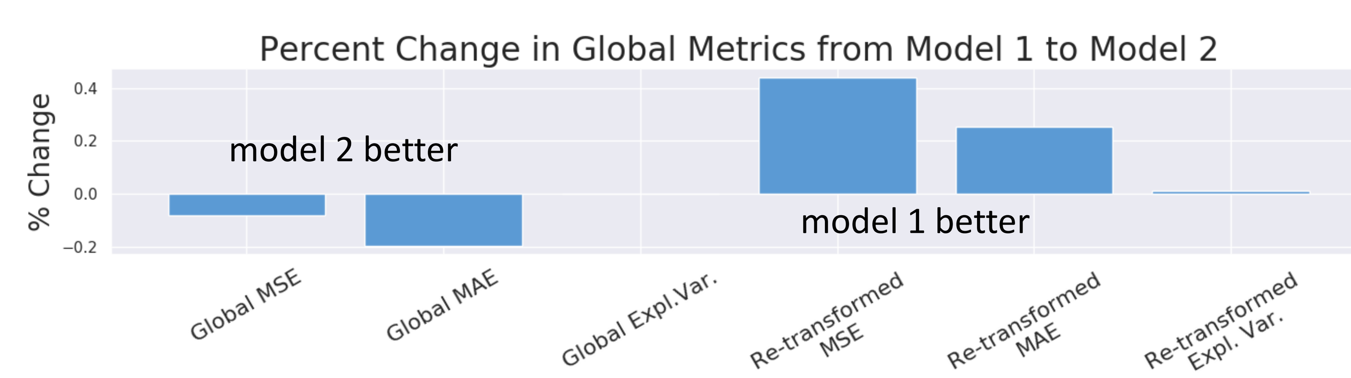


Figure 6 (left)**:** Chart of percent improvement of error metrics. Global metrics and re-transformed explained variance are all improved. The re-transformed MSE and MAE show somewhat worse results.

DISCUSSION

Integrating phase changes into equations of state neural network models improves localized error and includes physical behavior.

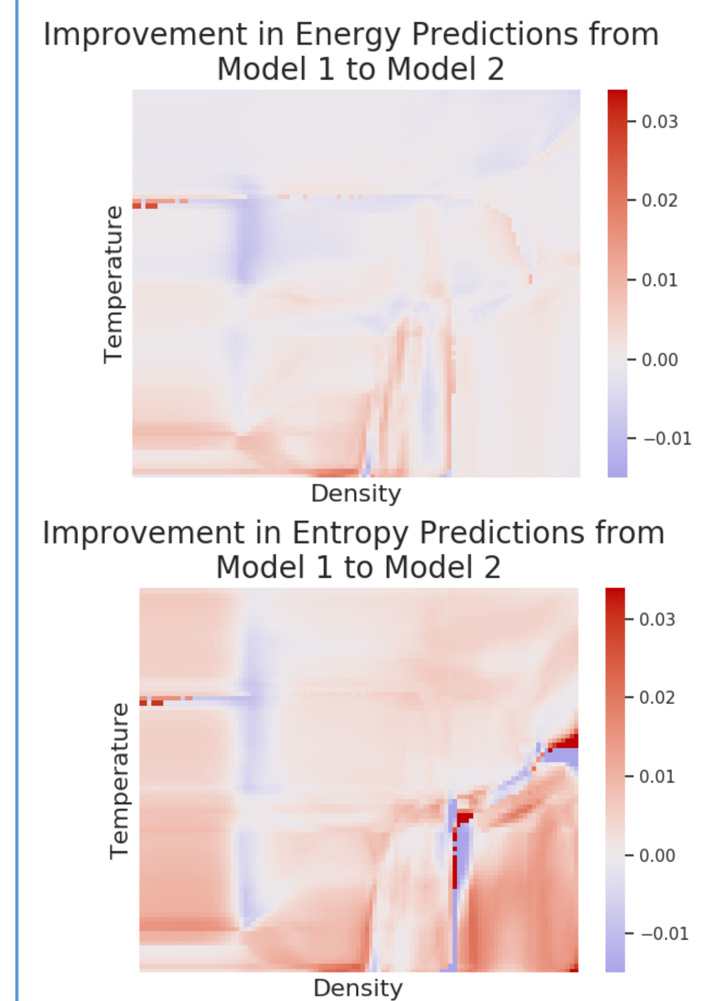


Figure 7: Relative improvement in energy and entropy prediction by incorporating phase changes into neural network model.

- Neural networks are effective at predicting equation of state values, mostly within 1%.
- Model 2 is guaranteed to contain phase information.
- Metrics and heat maps of error show general improvement by incorporating phase transitions.
- Entropy predictions are improved the most from including phase information.
- Although some global metrics are slightly worsened in Model 2, the model still is an excellent predictor.

CONCLUSIONS AND FUTURE DIRECTIONS

Phase transition incorporation suggests promising results for manually integrating physical knowledge into data science models.

- Global error metrics are not necessarily indicative of localized model quality
- Neural networks can create accurate models for DT equations of state, within 1% of true values in most cases
- Structuring neural networks to include phase transitions improves localized prediction outcomes

Next: Thermodynamically Consistent Output to Embed in Hydrocodes

- From energy and entropy predictions, we can calculate free energy
- Other desired quantities, such as pressure and sound speed, can be obtained by differentiating free energy. Differentiation is easy for neural networks.
- Such calculations ensure thermodynamic consistency, allowing use in hydrocodes and incorporating additional physics

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