A Physically informed Surrogate Approach to Causal System Modeling

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Abstract

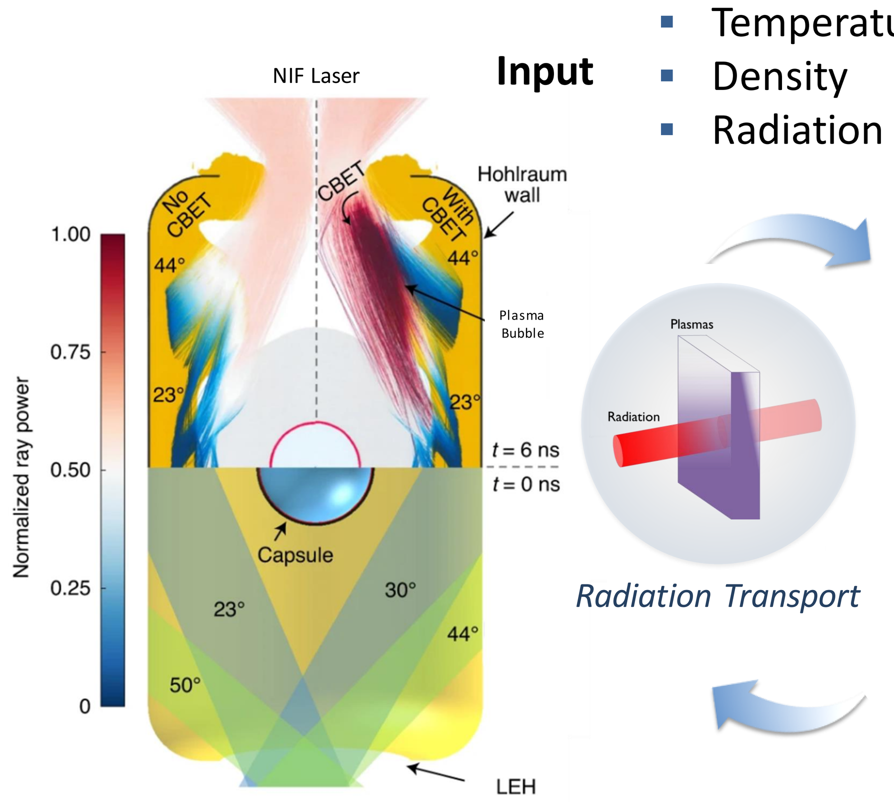
For complex systems in basic scientific research, surrogate models promise great speedups over traditional methods. However, traditional surrogates are hampered during training by non-physical error formulations. Here we develop a new Physics Informed Loss function (PIL) that targets important physics by reformulating a surrogate's output representation. Our PIL reformulation introduces two transformations of opacity and emissivity, which emphasize energy and radiation transport. PIL networks can reduce the necessary data by focusing the learning task on key attributes of non-Local Thermodynamic Equilibrium (NLTE) physics via a tunable hyperparameter. Future work will explore integrating PIL surrogates into a complete multiscale Inertial Confinement Fusion (ICF) model.

Multiscale Physical Models of Inertial Confinement Simulations Are Compute Bound By "NLTE" models

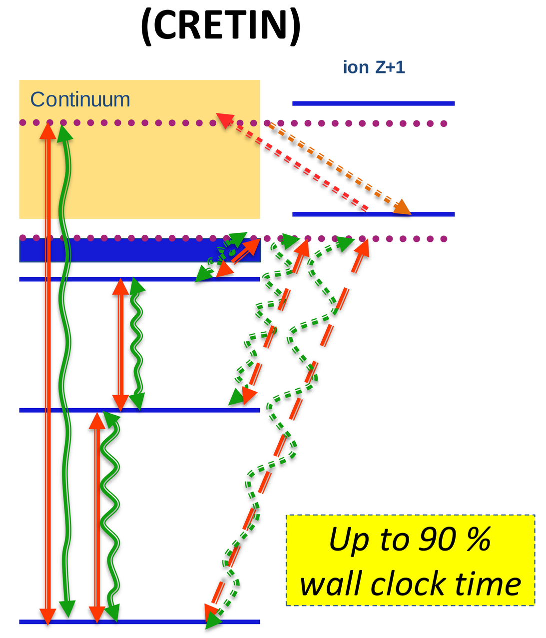
On December 5 2022, LLNL achieved the first and historic controlled fusion ignition experiment, producing more fusion energy than the driving laser energy[1]

Input
- Temperature
- Density
- Radiation Field

NLTE model (CRETIN)



Radiation Transport



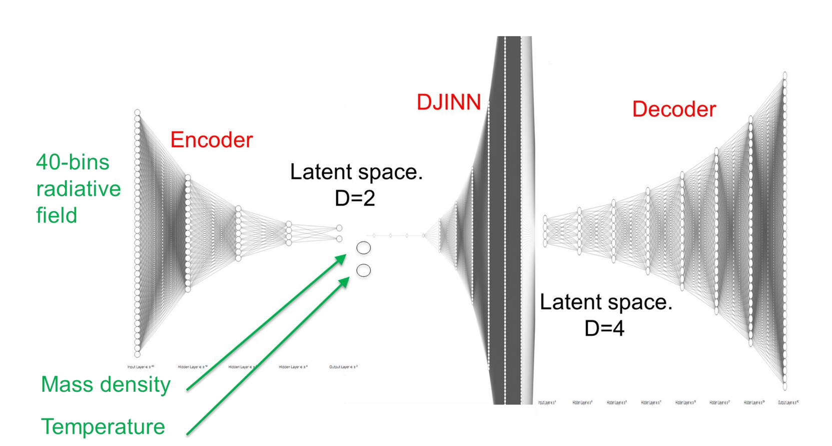
ICF Radiation Hydrodynamic (RH) Simulation [2]

output
- Emissivity ($\vec{\epsilon}$): Radiation power emitted
- Absorption ($\vec{\alpha}$): Radiation attenuation

- **The traditional NLTE surrogate successfully speeds up ICF Hohlraum simulations but can be prohibitively expensive to train due to impractically large data volumes needed. We aim to more efficiently train by emphasizing physically relevant regimes during model fitting.**

Autoencoder (Encoder + Decoder)
determines a low-dimensional representation of high-dimensional data

Deep Jointly Informed Neural Networks (DJINNS)
maps from low dimension inputs to low dimension outputs



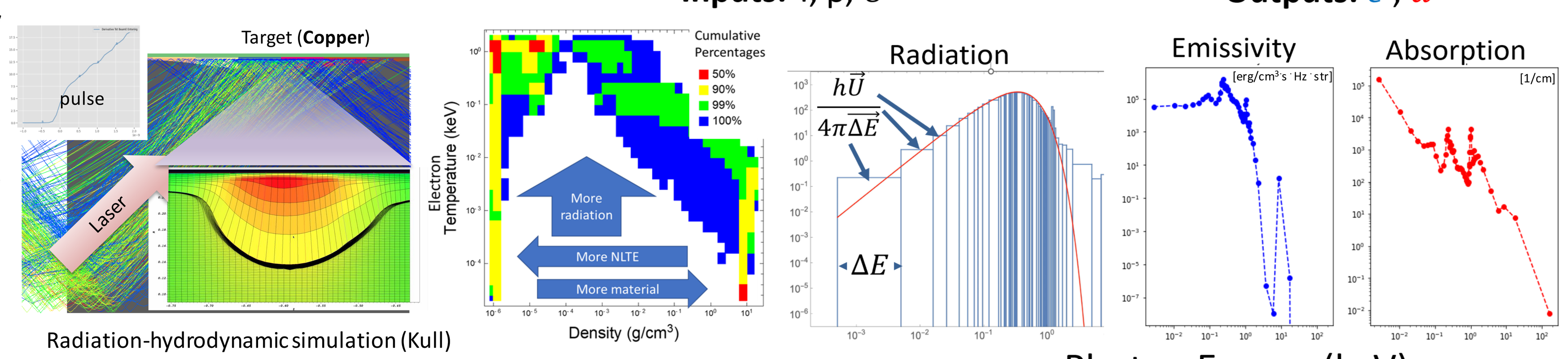
Network Architecture of CRETIN Surrogate [3]

Our Physically Informed Loss (PIL) Transforms the Output to Isolate Key Physics

Training Data Set

Inputs: T, ρ, $\vec{U}$

(from CRETIN and Minikin) [4),5)]
Outputs: $\vec{\epsilon}$, $\vec{\alpha}$



Radiation-hydrodynamic simulation (Kull)
Each zone and time yields input/output

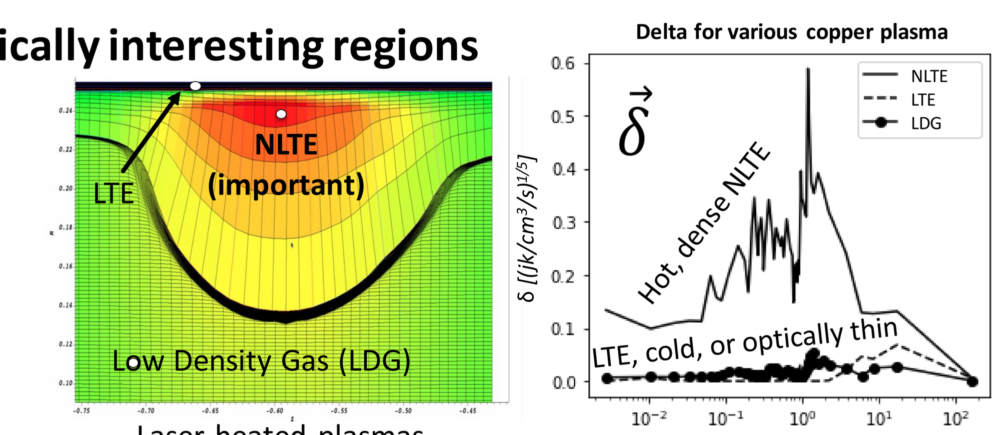
Photon Energy (keV)

- **δ: Net change in radiation energy - couples radiation to matter**
  - **δ emphasizes data of physically interesting regions**

$$\vec{\delta} = \frac{4\pi}{h}\overrightarrow{\Delta E} \circ \vec{\epsilon} - c\vec{U} \circ \vec{\alpha}$$

Emitted — Absorbed

$$\|\vec{U}\|_1 \propto T_r^4$$



Laser-heated plasmas

  - **δ is the actual parameter used in radiation hydrodynamics simulations**

Matter

$$c_p\rho\frac{\partial T_e}{\partial t} + \nabla\cdot\boldsymbol{q} = -\|\vec{\delta}(\vec{\epsilon},\vec{\alpha})\|_1 + \textit{other terms}$$

Temperature equation

Emission
$\vec{\delta} = net$
Absorption
Energy exchange

Radiation

$$\frac{\partial\vec{U}}{\partial t} + \nabla\cdot\vec{F}(\vec{\alpha}) = \vec{\delta}(\vec{\epsilon},\vec{\alpha})$$

Radiation Transport equation

- **We focus on learning radiation transport, only for physically important length scales**

$$\vec{\tau} = \frac{2}{\pi}\tan^{-1}[\log(\vec{l}^*)]$$

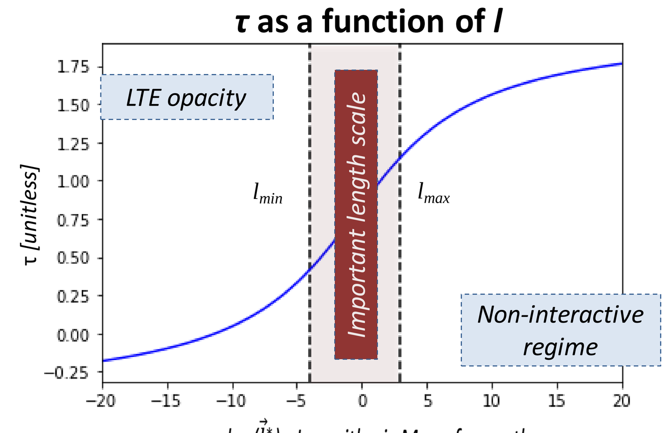
$$\vec{F} \sim -\nabla\cdot\frac{cl}{3}\nabla\vec{U}$$

- $\vec{l}^*$: *mean free path* $(\vec{\alpha})^{-1}$ *normalized with* l_{min} *and* l_{max}
- l_{max} *~ hohlraum size*
- l_{min} *~ mesh size in the RH simulation*

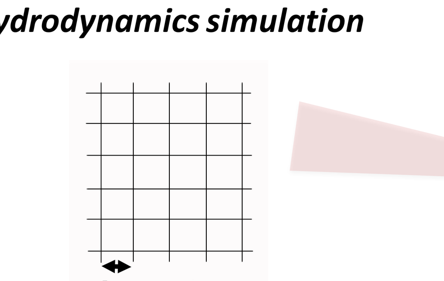
The path length sets the diffusion constant

- **τ stretches out the information of interest and suppresses others**

τ as a function of *l*



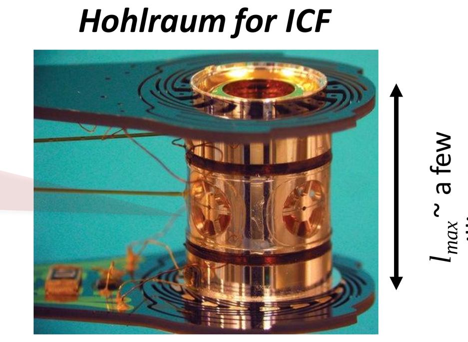
Mesh for radiation hydrodynamics simulation



l_{min} ~ a few nanometers

Radiation absorbed within zone ($l < l_{min}$)

Hohlraum for ICF

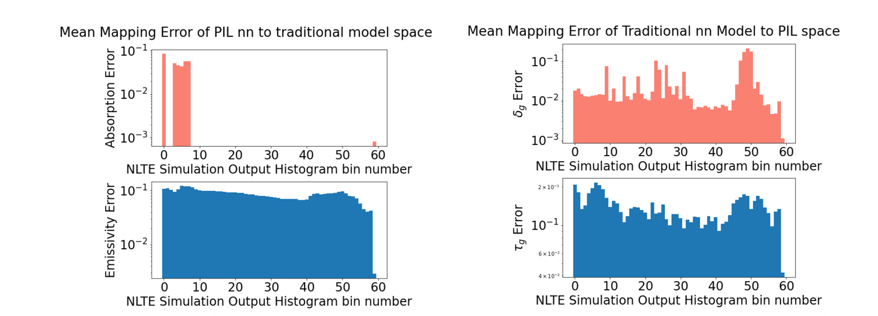


l_{max} ~ a few millimeters

Radiation goes through without any interaction of matter ($l > l_{max}$)

PIL can be leveraged to Design A Surrogate NLTE model

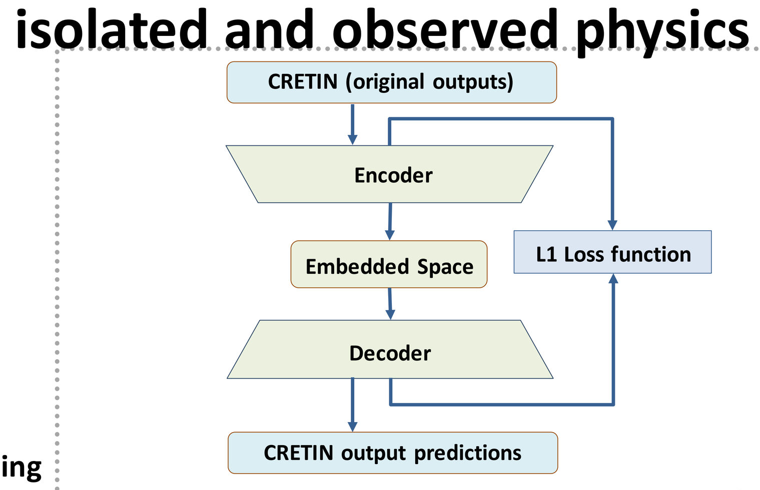
NLTE Surrogates trade off between isolated and observed physics



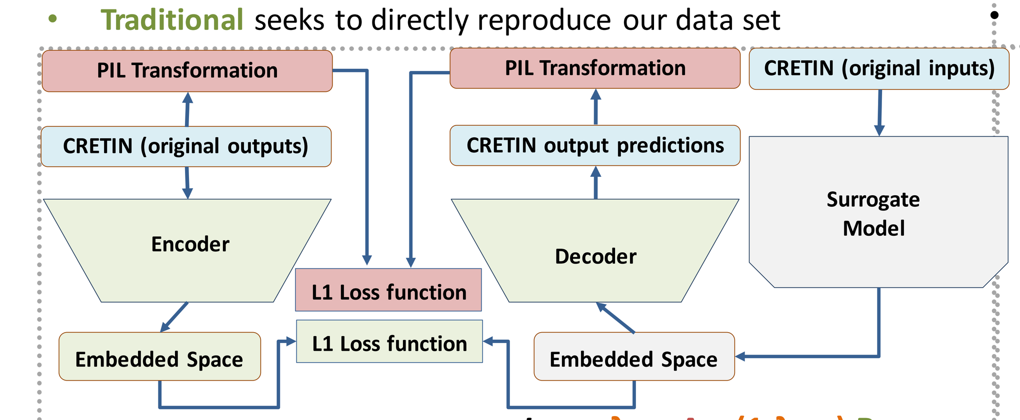
PIL models neglect certain dataset features

Traditional models neglect key physics in the dataset

PIL and traditional learning target different aspects of data modeling
- PIL targets important radiation transport values
- PIL seeks to conserve energy
- Traditional seeks to directly reproduce our data set

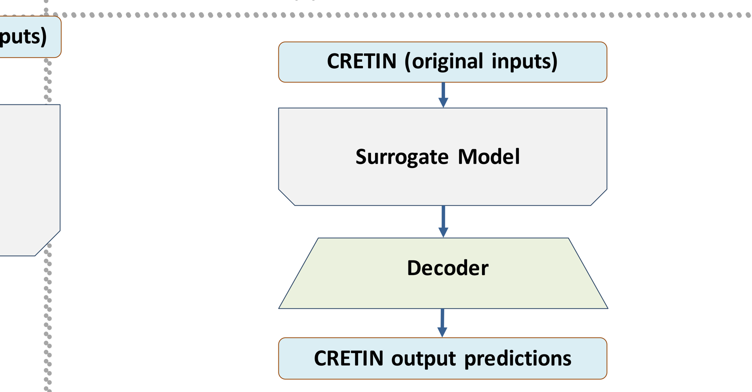


Step 1, CRETIN output Traditional Autoencoder trained
- Non-physical output correlation is learned
- Correlation mapped to low dimensional embedding



Loss $=\lambda_{Emb}$ A + $(1-\lambda_{Emb})$ B

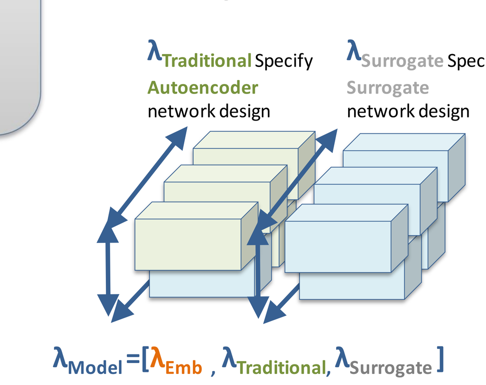
Step 2, Surrogate is trained
- Surrogate learns output correlation informed by physically important PIL loss term and a traditional loss on embedded space
- λ_{Emb} hyper parameter controls weight ratio of PIL/Traditional



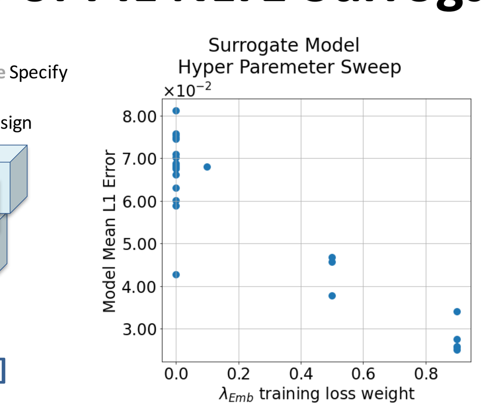
Step 3, Inference
- Encoder from step 1 disregarded
- PIL disregarded
- Output is reconstructed using decoder from step 1

Initial Results

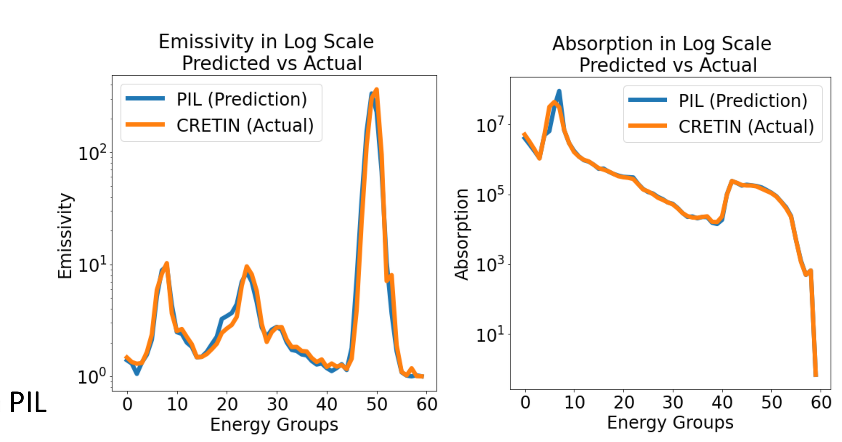
- **The potential of PIL NLTE Surrogates motivates further study**



- We swept multiple PIL network λ hyper parameters
- Target was highest R2 correlation



- Mean model loss decreases with PIL weight in λ_{Emb}
- λ_{Model} can be used to balance PIL learning targets and NLTE prediction artifacts



PIL model predictions are highly correlated in most radiation bins

Summary and Future Work

- PIL reformulation emphasizes physically important quantities to the surrogate model, making PIL networks focus on important physical correlations in non-Local Thermodynamic Equilibrium (NLTE) outputs
- Loss function hyperparameter adjusts surrogate learning to emphasize PIL reformulation or traditional correlations in the original data set
- We are exploring integrating PIL surrogates into a complete multiscale ICF model to explore the tradeoffs of our work in computational efficiency and stability

Association for the Advancement of Artificial Intelligence

1) National Ignition Facility Achieves Fusion Ignition (retrieved Jan 30 2023): https://www.llnl.gov/news/national-ignition-facility-achieves-fusion-ignition
2) A. L. Kritcher, et. al., "Design of inertial fusion implosions reaching the burning plasma regime." Nature Physics 18, 251–258 (2022)
3) G. Kluth, et. al., "Deep learning for NLTE spectral opacities." Physics of Plasmas 27, 052707 (2020)
4) H. A. Scott, "CRETIN – a radiative transfer capability for laboratory plasmas." Journal of Quantitative Spectroscopy and Radiative Transfer 71, 689-701 (2001)
5) H. A. Scott, S. B. Hansen, "Advances in NLTE modeling for integrated simulations." High Energy Density Physics 6, 1, 39-47 (2010)
6) Anirudh Rushil, et al. "Improved surrogates in inertial confinement fusion with manifold and cycle consistencies." Proceedings of the National Academy of Sciences 117.18, 9741-9746 (2020)

National Nuclear Security Administration