A Neural Network Surrogate Model for Nonlocal Thermal Flux Calculations

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Strategic Deterrence
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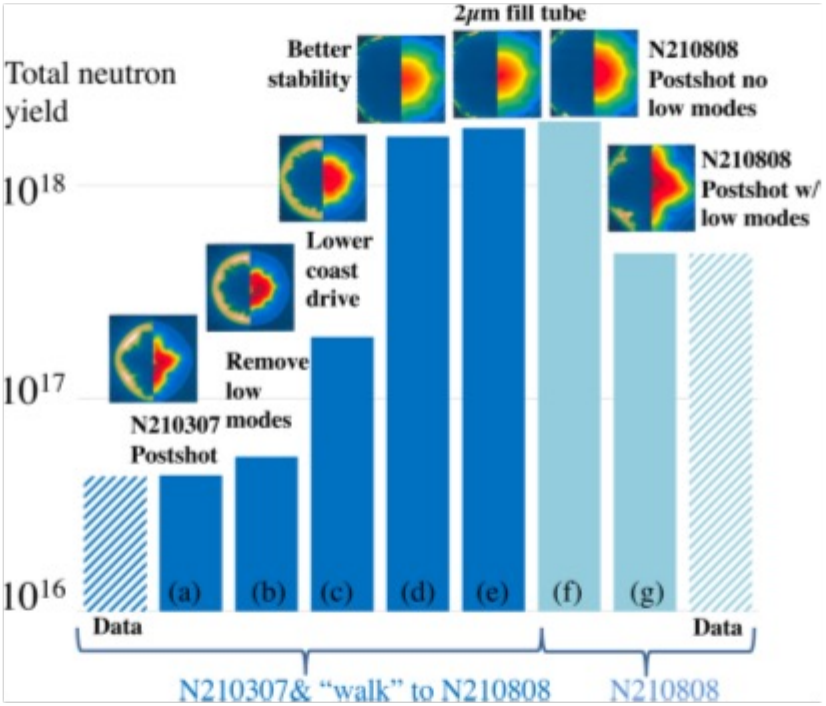
MFEM Community Workshop

26 Oct 2023

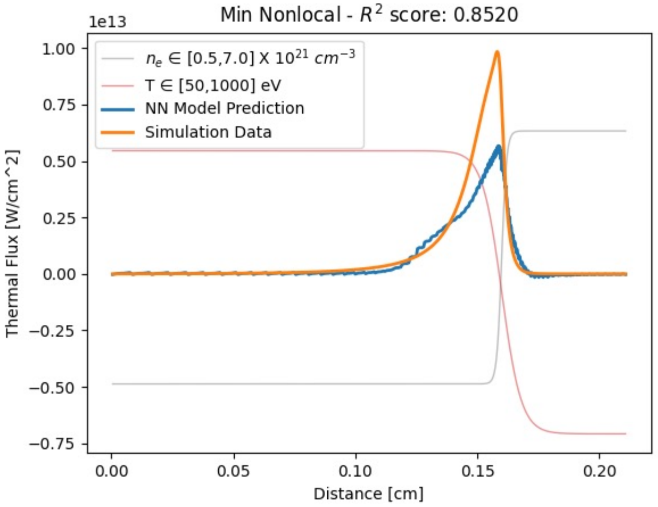
Physics Motivation

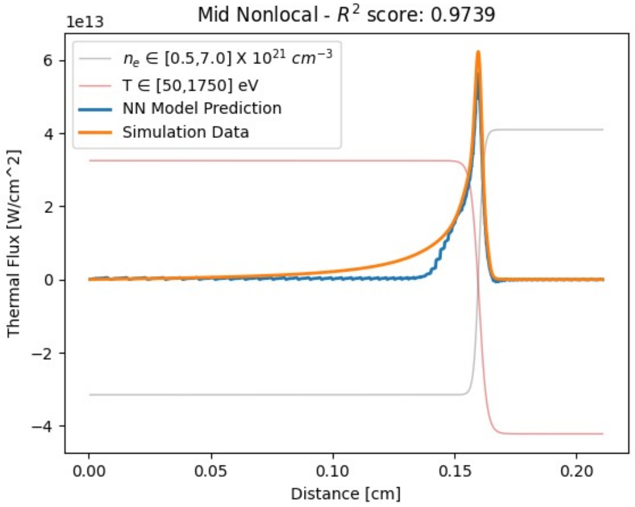
- NIF's "break-even" fusion reaction in December consumed only 4% of its fuel
  - How do we achieve 5, 10, 20%?
- Higher-fidelity simulations allow for more accurate experimental modeling
  - Unfortunately, higher-fidelity calculations are a great deal more computationally expensive
- Nonlocal rad-hydro equations with closure can more accurately calculate thermal flux
  - Kinetic solver: 10^{12} operations
  - Neural network: 10^{6} operations
- **A neural network could approximate thermal flux in ICF simulations up to 1,000,000 times faster!**

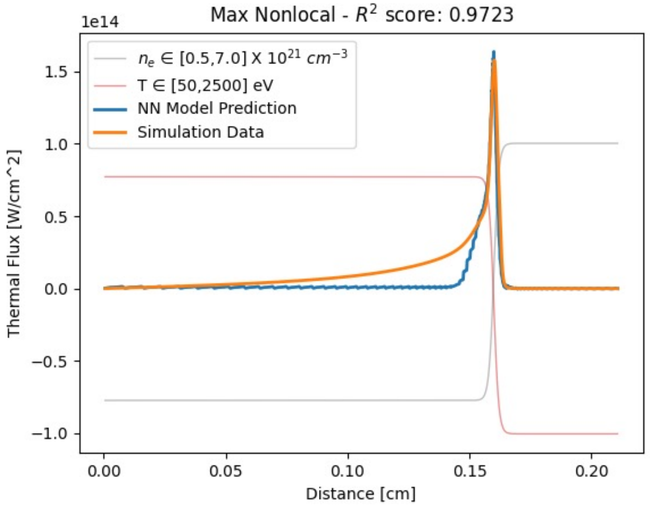


Initial Model and Results

- Constructed a dataset of 300 MFEM Simulations
  - Kinetic solver, 1D2V Phasespace, General-SN, 3rd-order
  - Swept over a range of temperature parameters
- Designed a feed-forward neural network
  - "Shifting window" used multiple neighboring input elements for each output prediction
- **Model reports 99.3% accuracy across entire testing set**

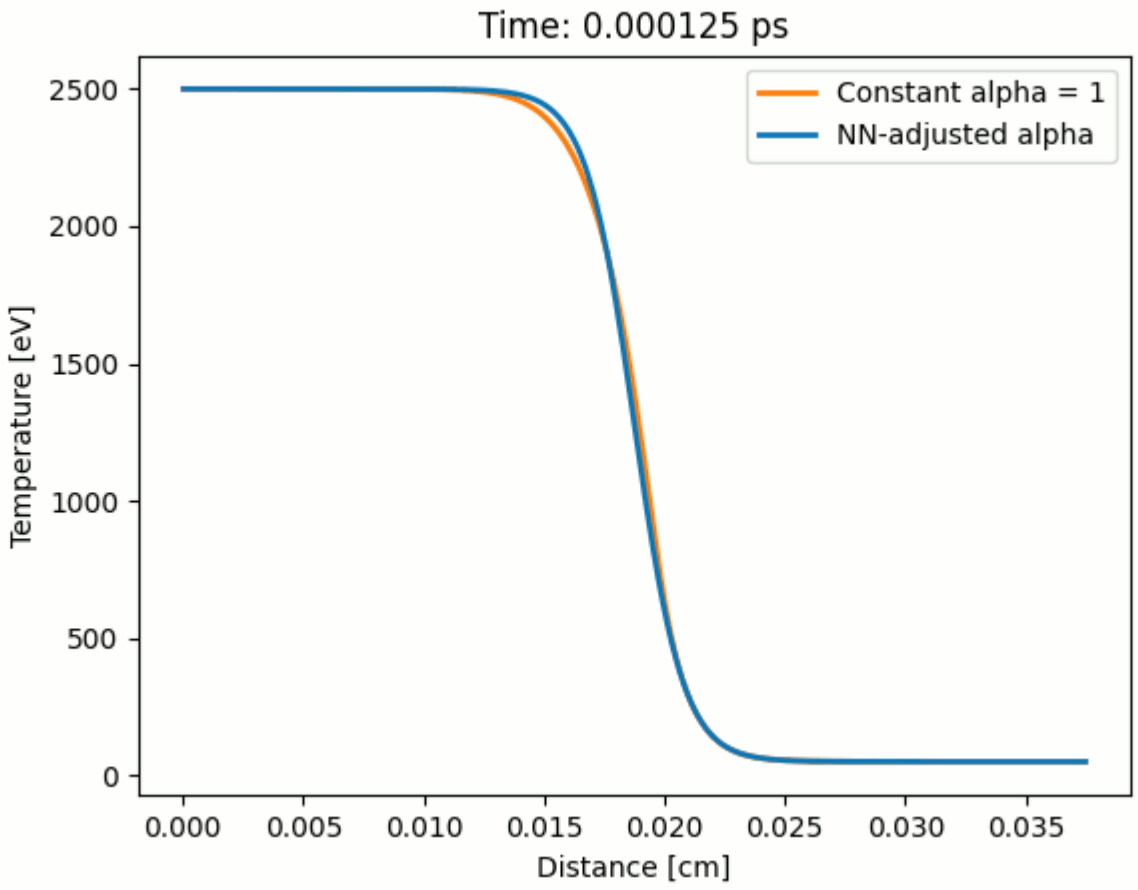






Time Evolution of Temperature

- Existing simulations use a linear formula to evaluate temperature change:
  - $\frac{du}{dt} = \nabla \cdot (\kappa + \alpha u)\nabla u$
- Experimenters want the more accurate (but complex) version of this formula:
  - $\frac{du}{dt} = \nabla \cdot (\alpha u^{\beta})\nabla u$
- Using the NN predictions, we can more quickly approximate α
  - Retrained NN on 500 simulations
  - 5x spatial elements, improved mesh scaling
- **NN-adjusted α demonstrates improved temperature smoothing expected with nonlocal thermal flux values**



Future Development

- Modeling software could “take it from here”
  - Use NN output as a springboard in simulations to reduce number of iterations until convergence
- More Data is Always More Better
  - Expand time evolution dataset to include changes in ionization/electron density
  - Change more simulation parameters and include their effects on temperature
- Expand Model Domain
  - Incorporate temperature shift as hohlraum material is heated
  - Expand model to predict other moments of distribution function
  - Higher spatial dimensions, building up to full 7-dimensional phase space
- More Advanced Deep Learning Architectures
  - Convolutional Neural Networks (allows for “shifting windows” in 2D/3D)
  - Graph Neural Networks (add mean free path information into dataset)