Using deep learning to develop a fast, versatile NLTE spectral model for application to HED systems

Marc-Andre Schaeuble, Will Lewis, Stephanie Hansen, and Taisuke Nagayama

Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185, USA

Non-local thermodynamic equilibrium (NLTE) effects significantly influence radiation transport and atomic level populations of high energy density (HED) plasmas. Under optically thin conditions, NLTE effects lead to a deviation of atomic populations from their equilibrium values, which can significantly change plasma emissivities and opacities. Simulations and experimental analyses of HED systems must therefore accurately and efficiently account for these effects. Calculating the needed NLTE data requires substantial computational resources, leading simulations to utilize simplified, low-resolution NLTE spectra and experimental analyses to assume simple plasma structures. Deep learning (DL) has been used to develop efficient and accurate NLTE spectral models, but each is limited to a specific problem [1-3]. Using the published models as inspiration, we outline in this talk, our approach to developing a versatile DL NLTE spectral model that can predict optically thin spectra from 0.01 - 10 keV in electron temperature and $10^{19} - 10^{22}$ cm⁻³ in ion density, a 4x/7x increase in each parameter over the largest published model [1]. Multiple DL models, each of which captures a charge state, are needed to achieve the desired accuracy over the entire parameter space. The resulting DL model predicts an optically thin, high-resolution (20x higher than other work) NLTE spectrum in ~160 ms with 99.5% accuracy, making it ~10⁵ times faster than its source model, the NLTE code SCRAM. Our approach works equally well for Ar and Kr spectra, demonstrating the robustness of our approach (see Fig. 1). We also discuss our progress for including arbitrary radiation fields in our existing model. If successful, the model with arbitrary radiation fields could address many existing NLTE challenges encountered in HED physics simulations and analyses.

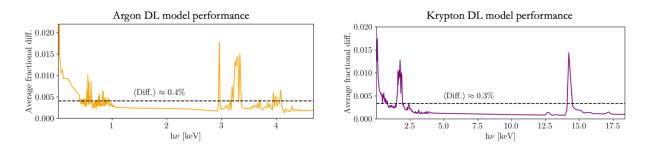


Figure 1: Left – Photon energy $(h\nu)$ resolved average difference between DL model and independent validation set for Ar. Right – same as left, but for Kr. Model architecture is consistent for both elements, and performance surpasses expectations for each case.

References

[1] Kluth, G. et al., Phys. Of Plasmas, 27, 052707 (2020)

- [2] Mariscal, D. A. et al., Phys. Of Plasmas, 29, 093901 (2022)
- [3] Vander Wal, M. D. et al., IEEE Trans. on Plasma Science, 51, 1 (2023)

Sandia is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.