Abstract ---

When a neutron born in fission thermalizes to the order of kT, it's de-Broglie wavelength and energy approach the order of interatomic spacing and elementary lattice oscillations, respectively. $S(\alpha, \beta, T)$, or the scattering law, quantify these temperature-dependent crystallographic contributions to total cross section (or reaction rate). In a Monte Carlo analysis, cumulative distribution functions (CDFs) of $S(\alpha, \beta, T)$ are loaded to memory from "A Compact ENDF" (ACE) files for stochastically selecting thermal scattered neutron trajectories. In this work, novel neural thermal scattering (NeTS) modules for $S(\alpha, \beta, T)$ CDFs are designed, trained, serialized and embedded within SERPENT using Python's limited C-API for on-the-fly deployment of crystalline graphite $S(\alpha, \beta, T)$ sampling. Torchscript tracing and Numba just-in-time (JIT) compilation streamline neural inference on NVIDIA GPUs with CUDA libraries.

Demonstrations of bare sphere thermalization of fast and thermal sources show excellent agreement between embedded NeTS in SERPENT and MCNP. With an explicit model of the reactor, NeTS can predict on-the-fly changes in TREAT neutron spectra as a function of local temperature, which can serve to improve transient and accident predictions in a multiphysics analysis framework. This framework can be further extended to account on-the-fly for changes in local graphitic microstructure to scattering cross sections, and outlines a novel coupling of modern machine learning with state-of-the-art reactor physics methods.