Development of Neural Thermal Scattering (NeTS) Modules For Data Representation and Applications

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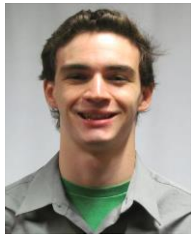
Acknowledgement

- NNSA Nuclear Criticality Safety Program (NCSP)
  - collaboration with LLNL
- Naval Nuclear Propulsion Program (NNPP)
- DOE NE through the NEUP program
- The LEIP Team







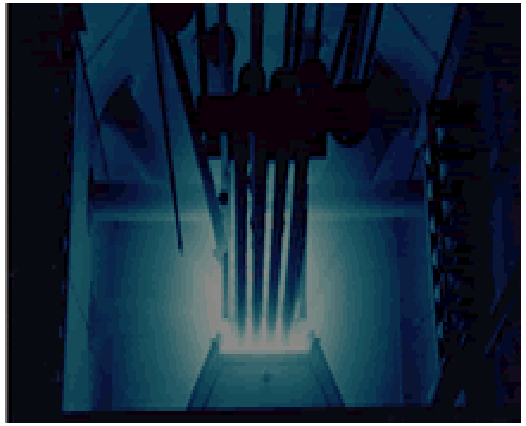
Outline

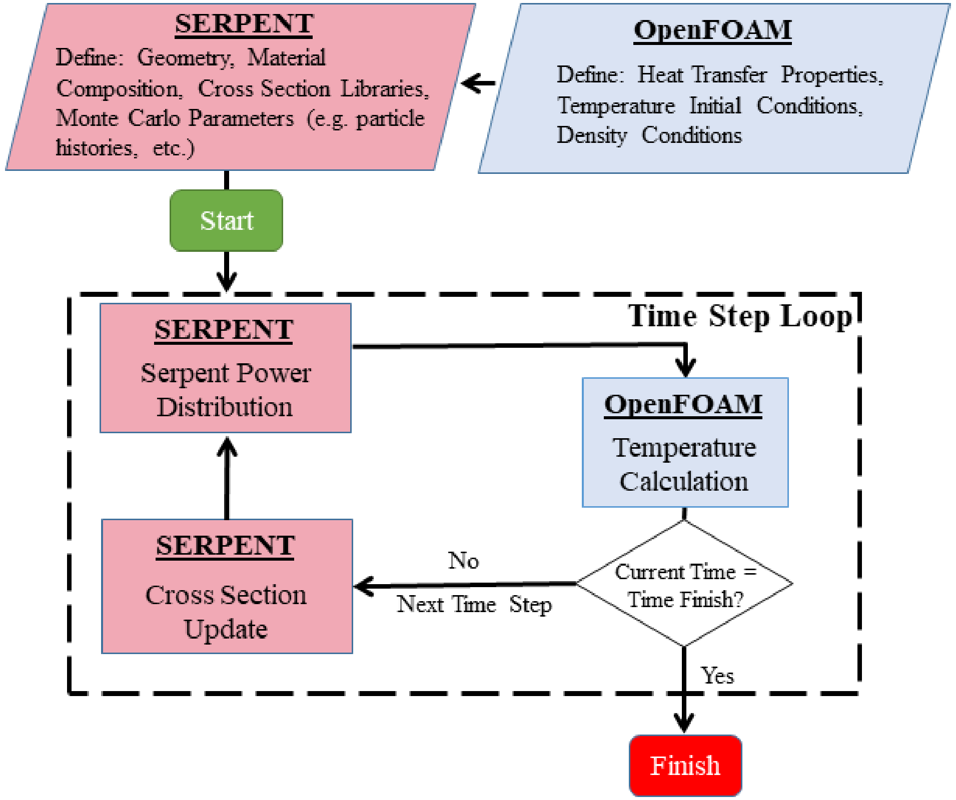
- Motivation
  - Advanced reactors
  - Multi-physics analysis
  - Neutron interactions
- Introduction
  - The thermal scattering law (TSL)
- TSL Evaluation in *FLASSH*
  - Nuclear data ENDF/B files
- Artificial Neural Networks
  - NeTS development
- Progress & Summary

Motivation

- Develop a thermal neutron scattering, continuous and accurate, data representation that supports the needs of advanced modeling and simulations
  - Multi-physics analysis
  - Real time, on the fly, data generation

PULSTAR Reactor
NCSU





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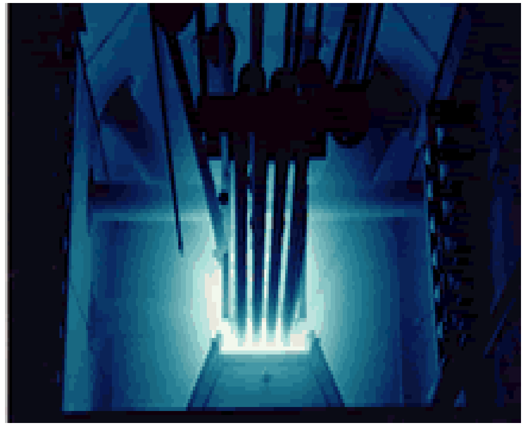
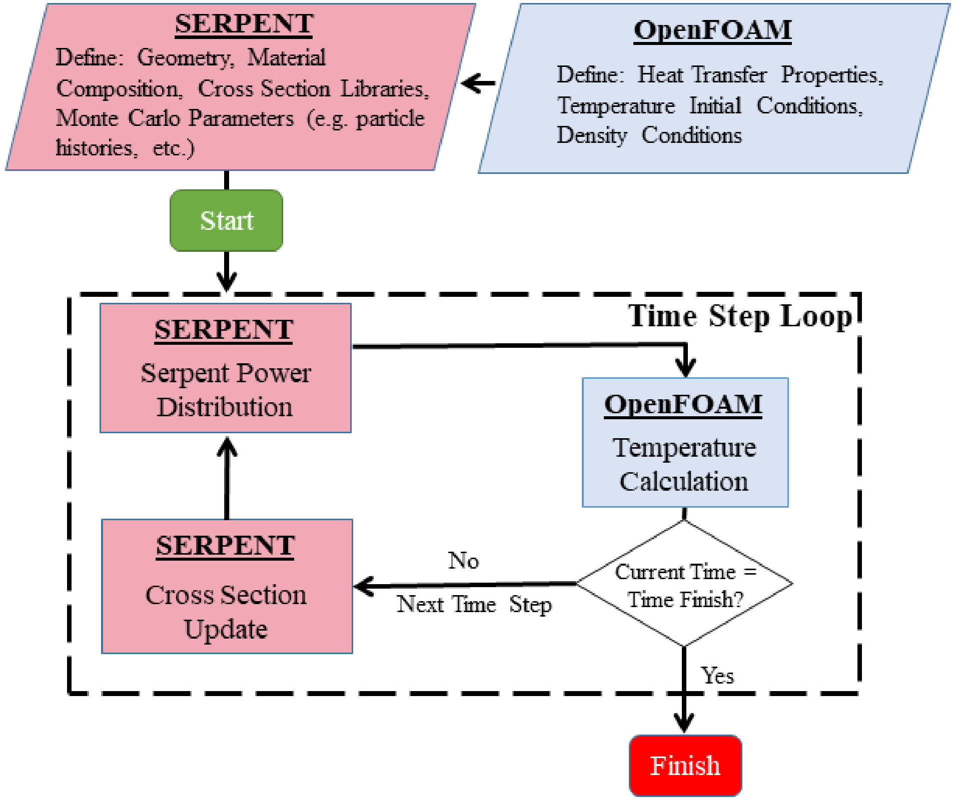
PULSTAR Reactor NCSU





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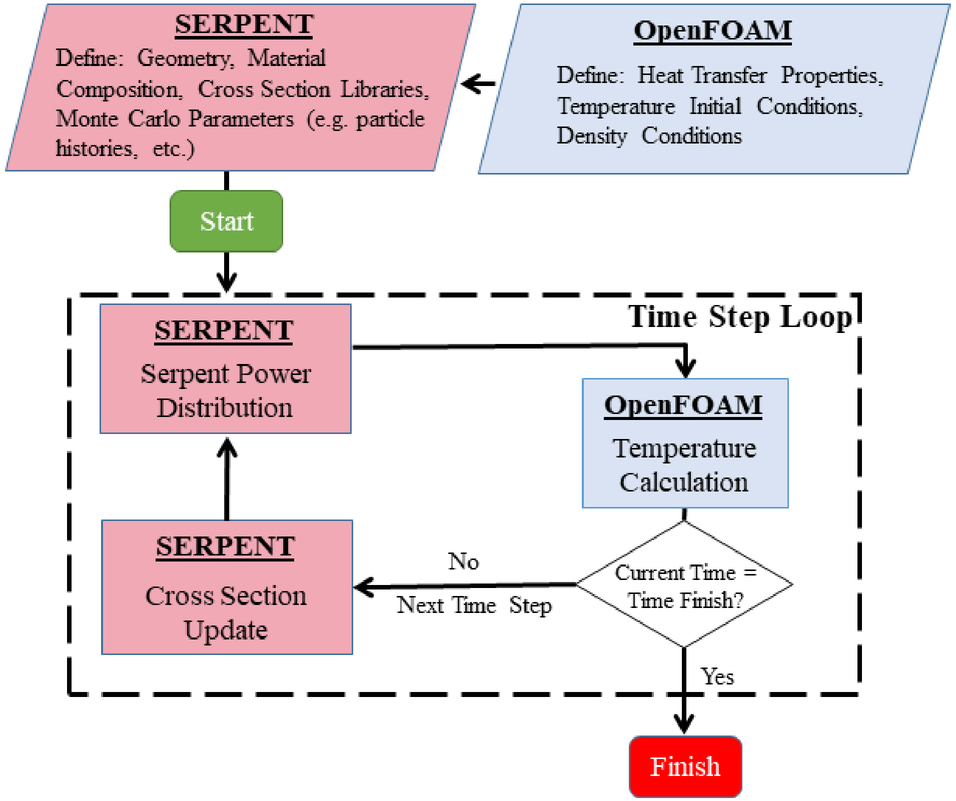
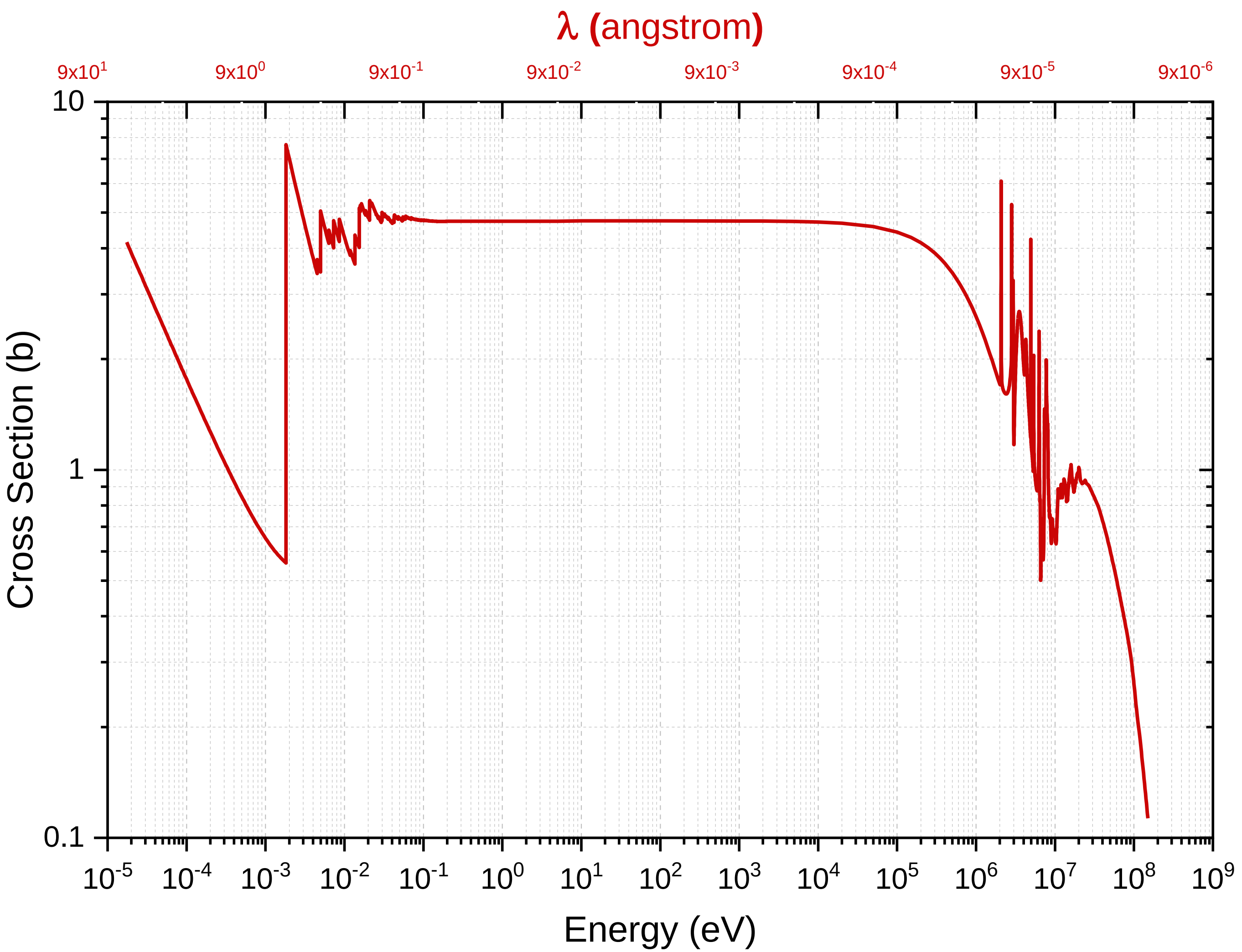
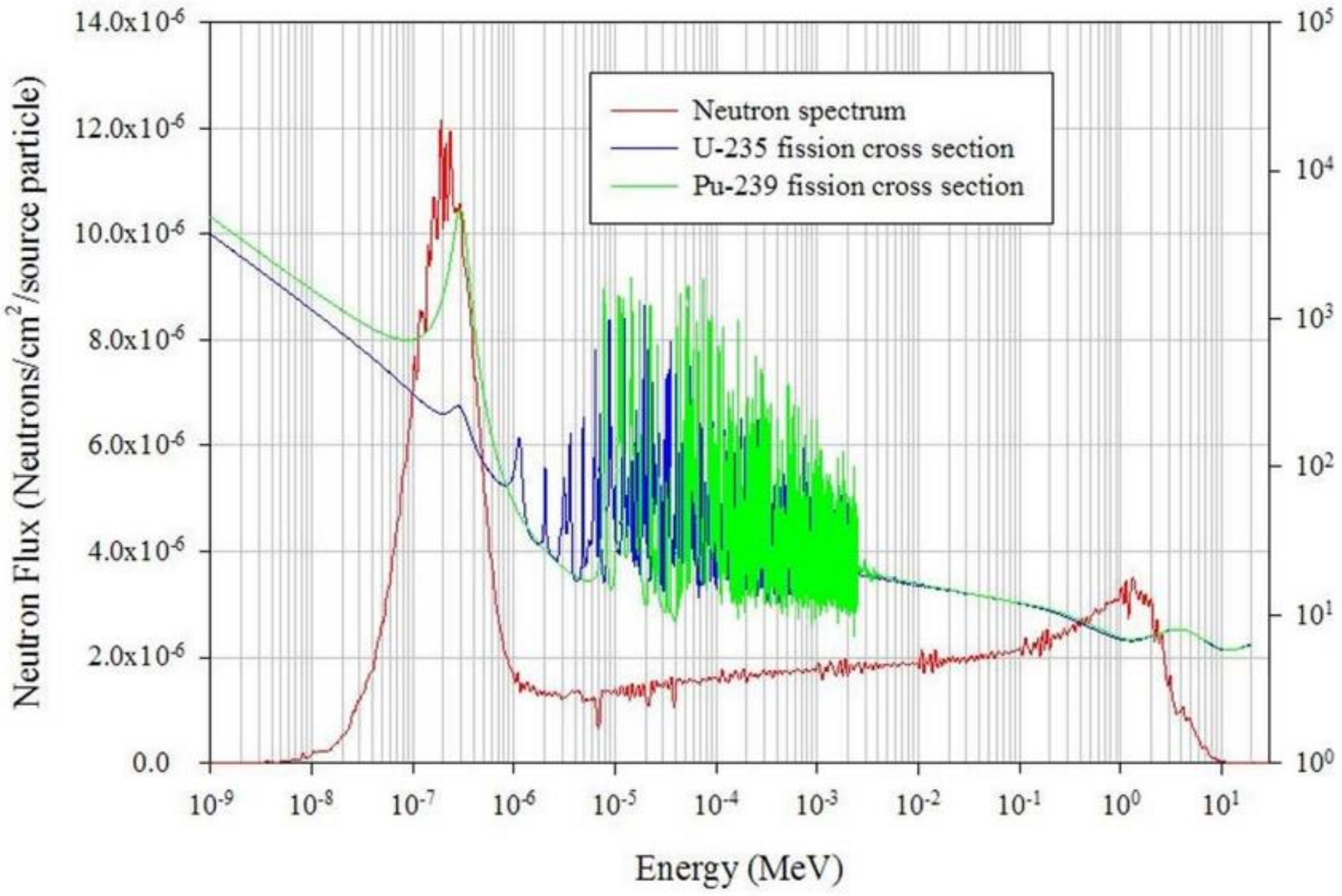


Neutron Interactions
Moderation & Thermalization



Neutron Interactions



Neutron Thermalization

Using first Born approximation combined with Fermi pseudopotential, it can be shown that the double differential scattering cross section has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{4\pi}\sqrt{\frac{E'}{E}}\left\{\sigma_{coh} S(\vec{\kappa},\omega) + \sigma_{incoh} S_s(\vec{\kappa},\omega)\right\}$$

The scattering law $S(\vec{\kappa},\omega)$ is composed of two parts

$$S(\vec{\kappa},\omega) = S_s(\vec{\kappa},\omega) + S_d(\vec{\kappa},\omega)$$

Van Hove's space-time formulation

$$I(\vec{\kappa},t) = \int G(\vec{r},t)\exp(i\vec{\kappa}\cdot\vec{r})d\vec{r}$$

$$S(\vec{\kappa},\omega) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\vec{r},t)e^{i(\vec{\kappa}\cdot\vec{r}-\omega t)}d\vec{r}dt$$

where $G(\vec{r},t)$ is the *dynamic pair correlation function* and can be expressed in terms of time dependent atomic positions.

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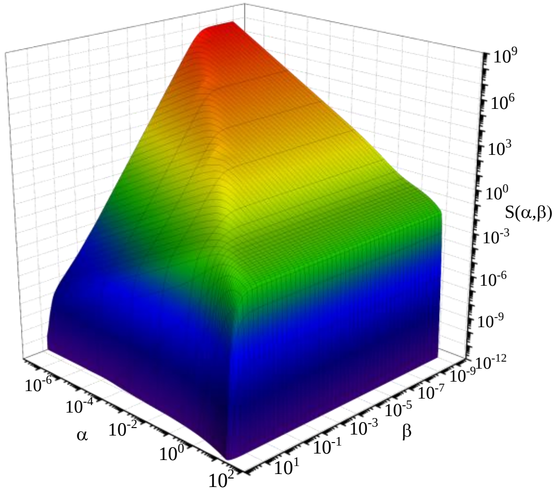

$$S_s(\alpha,\beta) = k_B T \cdot S_s(\vec{\kappa},\omega)$$

$$\left.\frac{d^2\sigma}{d\Omega dE'}\right|_{inelastic} = \frac{\sigma}{2k_B T}\sqrt{\frac{E'}{E}}\,S_s(\alpha,\beta)$$

$\beta = \frac{E - E'}{k_B T}$ Energy transfer

$\alpha = \frac{(E + E' - 2\sqrt{EE'}\cos\theta)}{k_B T}$ Momentum transfer

The scattering law (TSL) is the Fourier transform of a Gaussian correlation function

$$S_s(\alpha,\beta) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\beta t} e^{-\gamma(t)}\,dt$$

$$\gamma(t) = \frac{\alpha}{2}\int_{-\infty}^{\infty} \frac{\rho(\beta)}{\beta \sinh(\beta/2)}\left[1 - e^{-i\beta t}\right] e^{\beta/2}\,d\beta$$

$\rho(\beta)$ – density of states (e.g., phonon frequency distribution)

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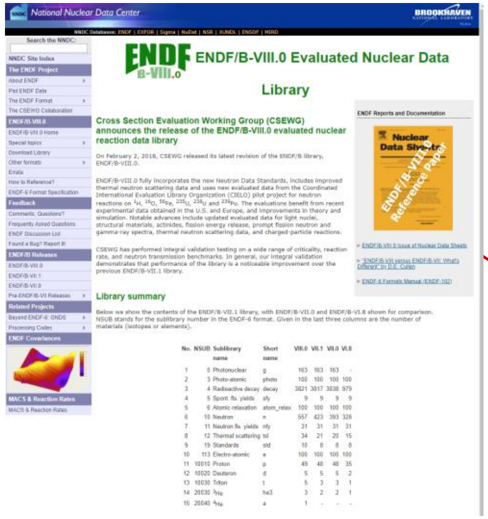
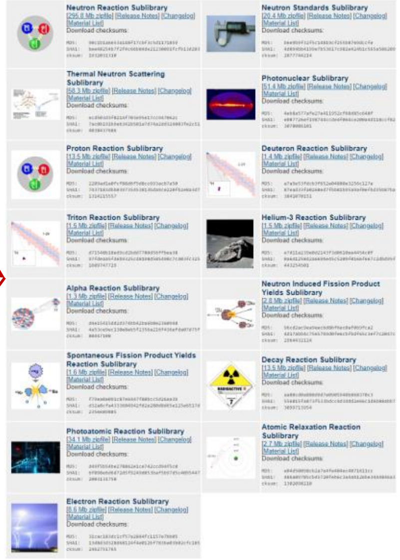
Nuclear Data – ENDF/B

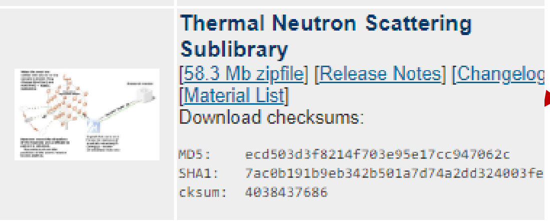
- **Current format**
  - Dated
  - Limited
- **Move to the Generalized Nuclear Database Structure (GNDS)**



Navigate to NNDC website



Open list of reactions

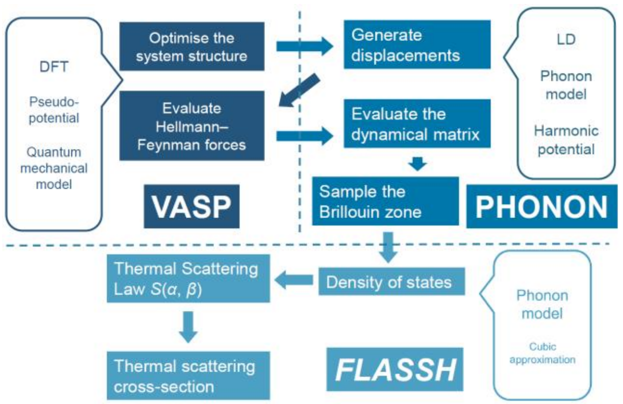


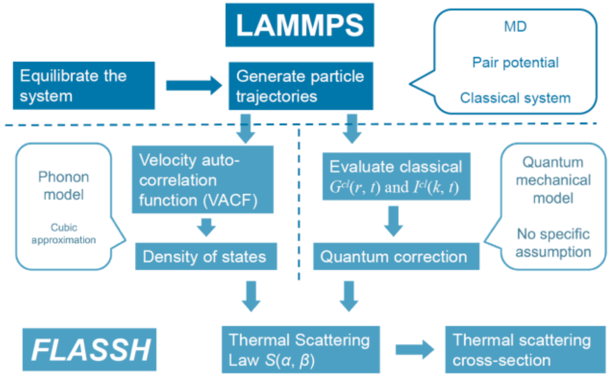
Select thermal neutron scattering

```
1.420000+2 6.955732+0         -1          0          0          0  42 1451
0.000000+0 0.000000+0          0          0          0          6  42 1451
1.000000+0 5.000000+0          0          0         12          8  42 1451
0.000000+0 0.000000+0          0          0         31          3  42 1451
Li(FLiBe) LEIP LABS  EVAL-MAR20 C.A. Manring, Y. Zhu, A.I. Hawari  42 1451
                     DIST-                                         42 1451
----ENDF/B-VIII      MATERIAL  42                                  42 1451
-----THERMAL NEUTRON SCATTERING DATA                               42 1451
------ENDF-6 FORMAT                                                42 1451
                                                                   42 1451
Temperatures = 773 873 923 973 1073 1173 1273 1473 1673 K          42 1451
                                                                   42 1451
BACKGROUND                                                         42 1451
----------                                                         42 1451
The inelastic thermal scattering law data for FLiBe was            42 1451
developed by the Low Energy Interaction Physics (LEIP) group at    42 1451
NC State University using molecular dynamics methods [1,2].        42 1451
This material is a liquid salt mixture, such that the diffusive    42 1451
contribution to the TSL is expected to be consequential. The       42 1451
FLASSH (Beta 3) code was used with a Schofield diffusion model     42 1451
to produce File 7 for Li in FLiBe.                                 42 1451
                                                                   42 1451
REFERENCES                                                         42 1451
----------                                                         42 1451
1. A.I. Hawari, "Modern Techniques in Inelastic Thermal Neutron    42 1451
   Scattering Analysis," Nuclear Data Sheets 118 (2014) 172.       42 1451
2. Y. Zhu, A.I. Hawari, "Thermal Neutron Scattering Cross          42 1451
   Section of Liquid FLiBe," Progress in Nuclear Energy 101        42 1451
   (2017) 468.                                                     42 1451
                                                                   42 1451
-----------------------------------------------------------------  42 1451
                                 1        451         34          0  42 1451
                                 7          4     244757          0  42 1451
                                                                   42 1  0
                                                                   42 0  0
1.420000+2 6.955732+0          0          1          0          0  42 7  4
0.000000+0 0.000000+0          0          0          6          0  42 7  4
9.700000-1 1.000000+2 6.955732+0 2.530000+0 0.000000+0 1.000000+0  42 7  4
0.000000+0 0.000000+0          0          0          1        275  42 7  4
       275          4                                              42 7  4
7.730000+2 0.000000+0          8          0          1        528  42 7  4
       528          4                                              42 7  4
1.177477-8 7.842352+7 4.709910-8 1.960586+7 1.059730-7 8.713706+6  42 7  4
1.883964-7 4.901454+6 2.943694-7 3.136925+6 4.238919-7 2.178416+6  42 7  4
5.769640-7 1.600465+6 7.535856-7 1.225352+6 9.537568-7 9.681764+5  42 7  4
```

Open TSL (File 7) of choice

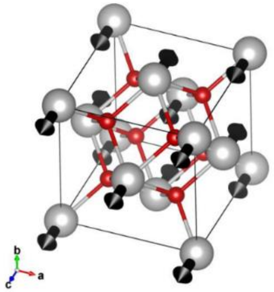
Methodology

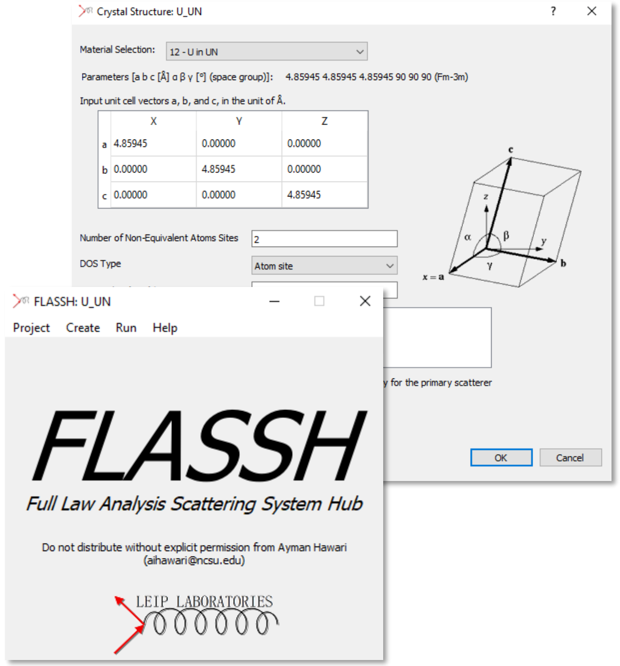


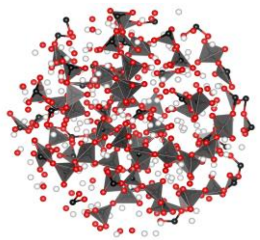


DFT/LD approach

MD approach

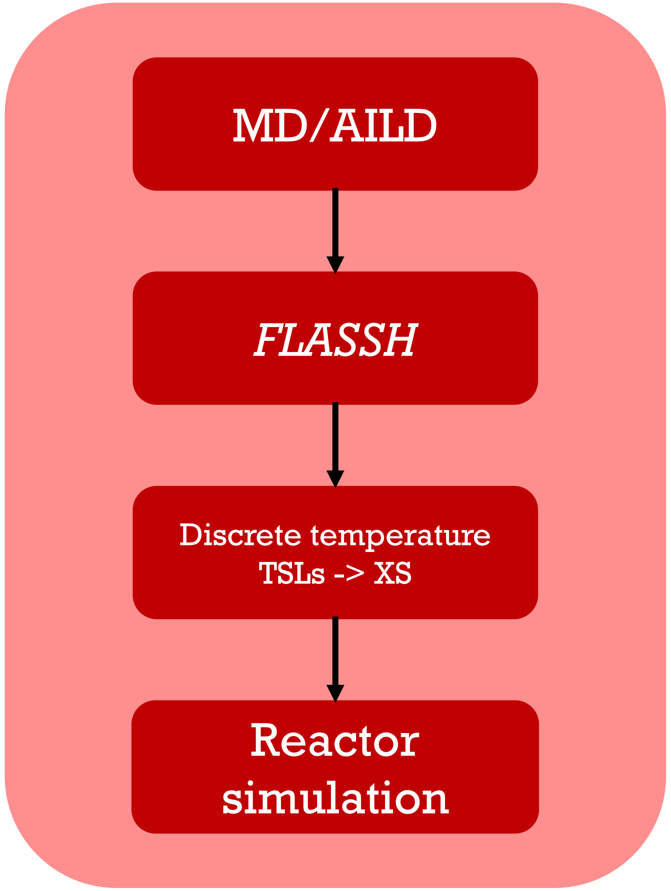






TSL Implementation

- **General task**
  - Provide the most accurate multivariate TSL representation
- **Current capabilities**
  - Discrete temperature grids
  - Interpolation
  - Basis functions
  - Higher max percent deviations
  - Higher memory consumption
- **What is missing?**
  - Continuous temperature (interpolation free)
  - Improve memory footprint
  - Improve accuracy
  - Maintain or Improve computation speed
    - Context dependent



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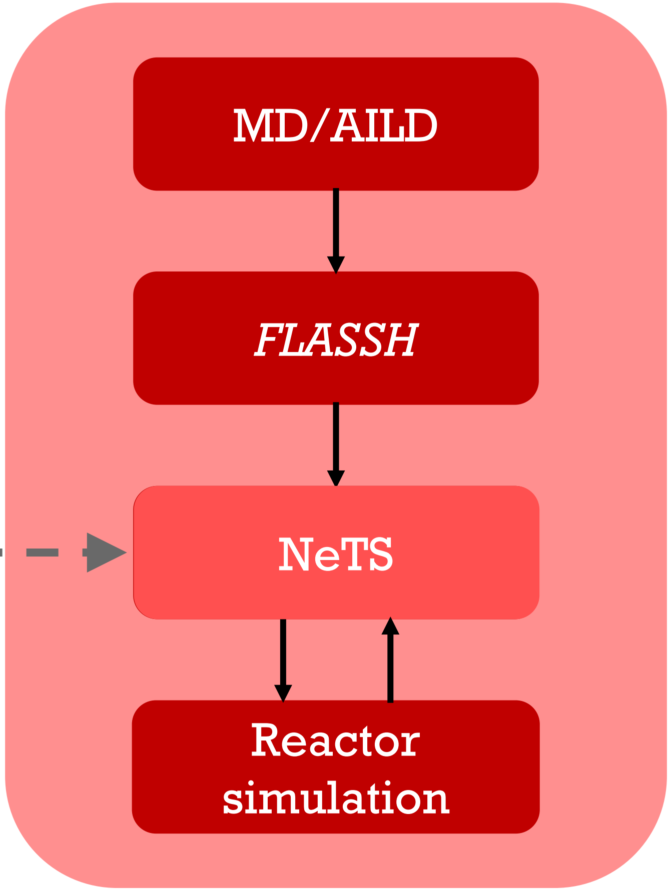
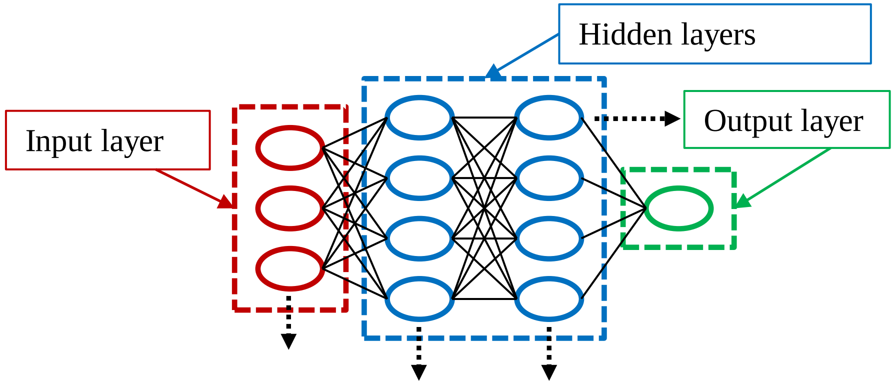
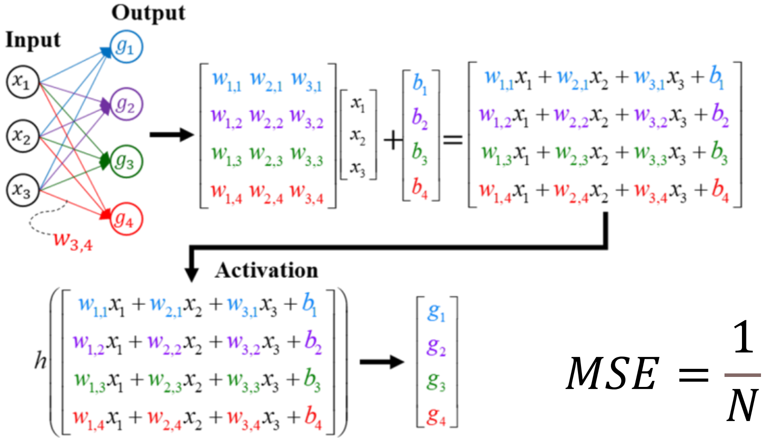


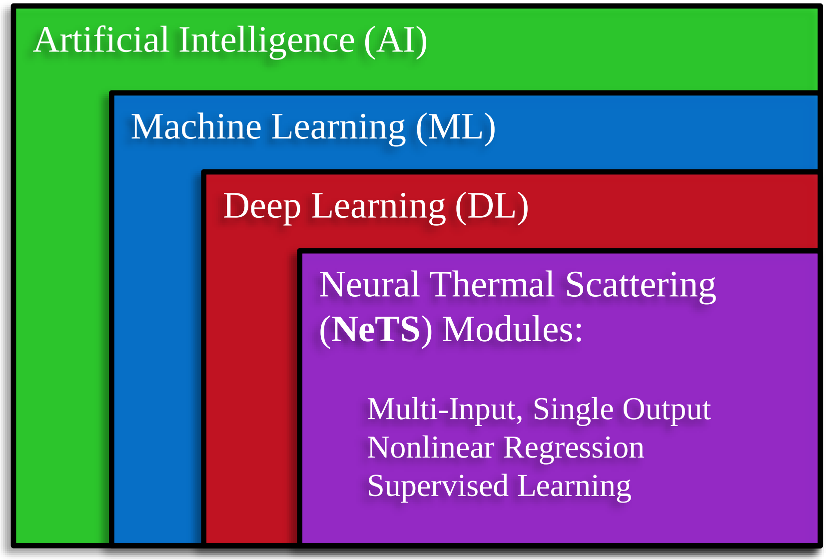
Artificial Neural Networks

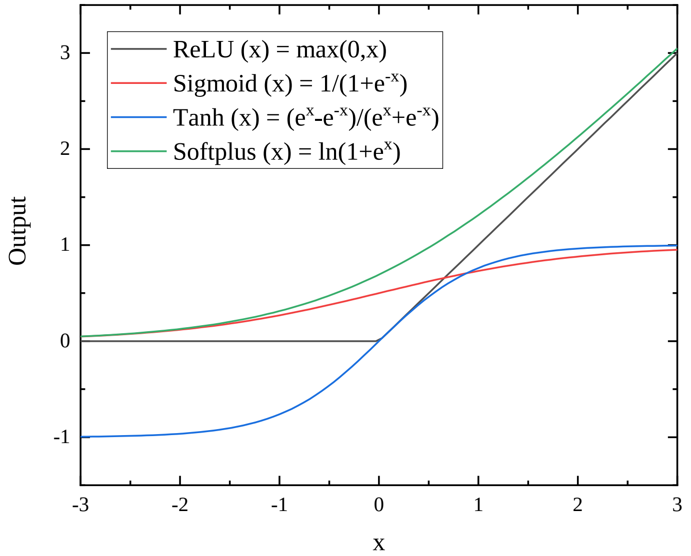
A data representation originally inspired by the abstraction of biological neurons





$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$





Neural Thermal Scattering (NeTS) Flow Chart

0. DOS: Calculate/verify *ab initio* phonon density of states

1. *FLASSH:* Produce training data and aggregate S(α,β)

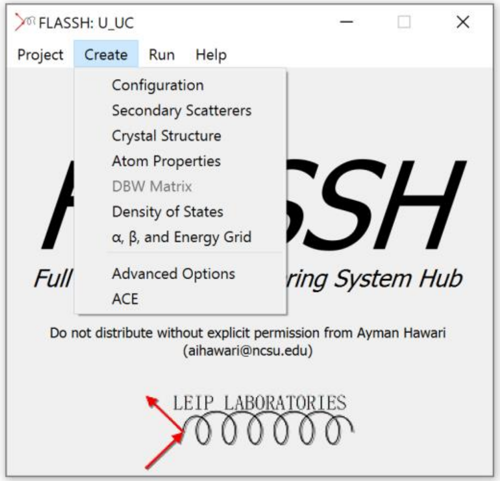
2. Data-preprocess: Scale alpha, beta, temperature, S(α,β) data and split between training/validation/test datasets

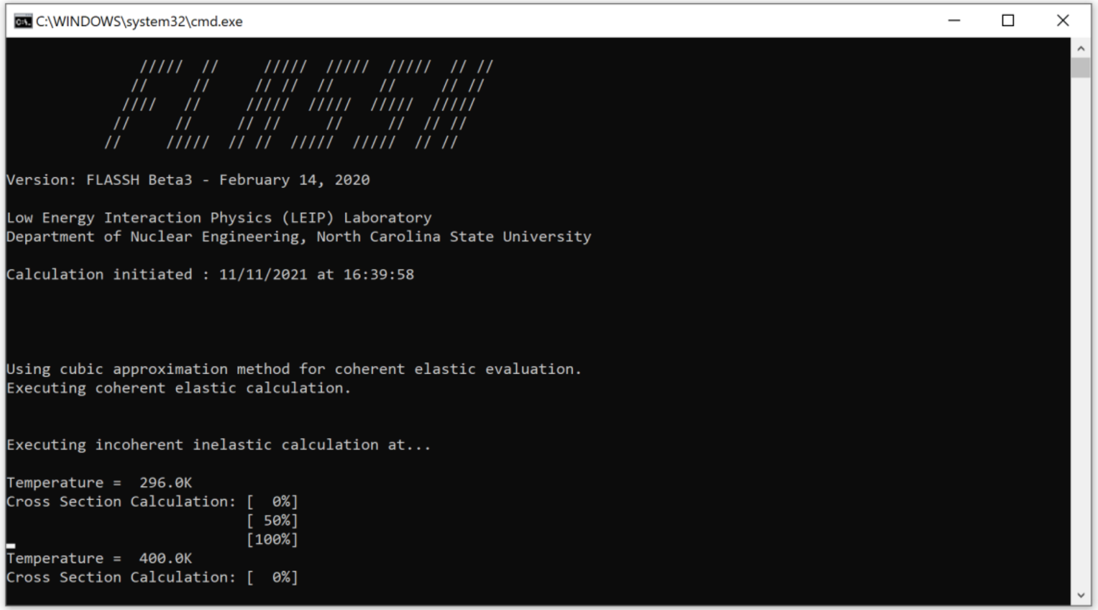
3. Network training: Train Artificial Neural Network (ANN)

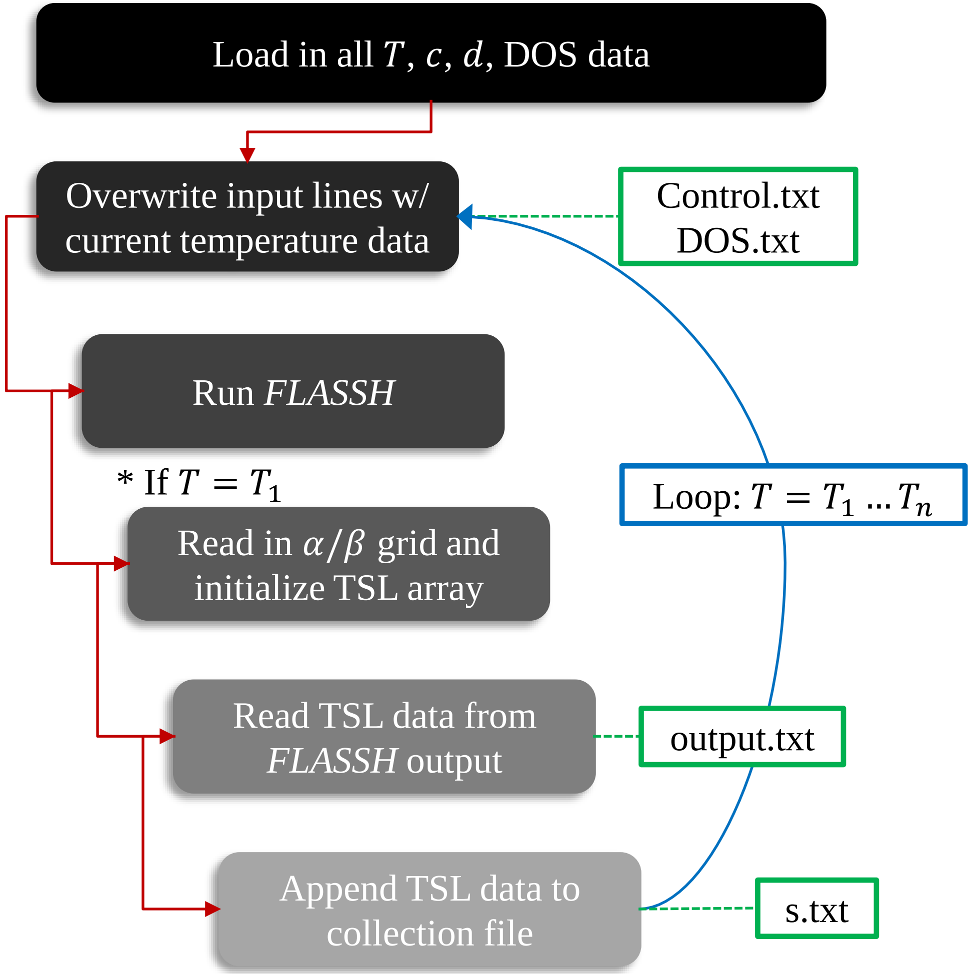
4. Evaluate network: Produce deviation metrics for train, validation, test datasets

5. Produce S(α,β) data: Use optimized network weights with neural architecture

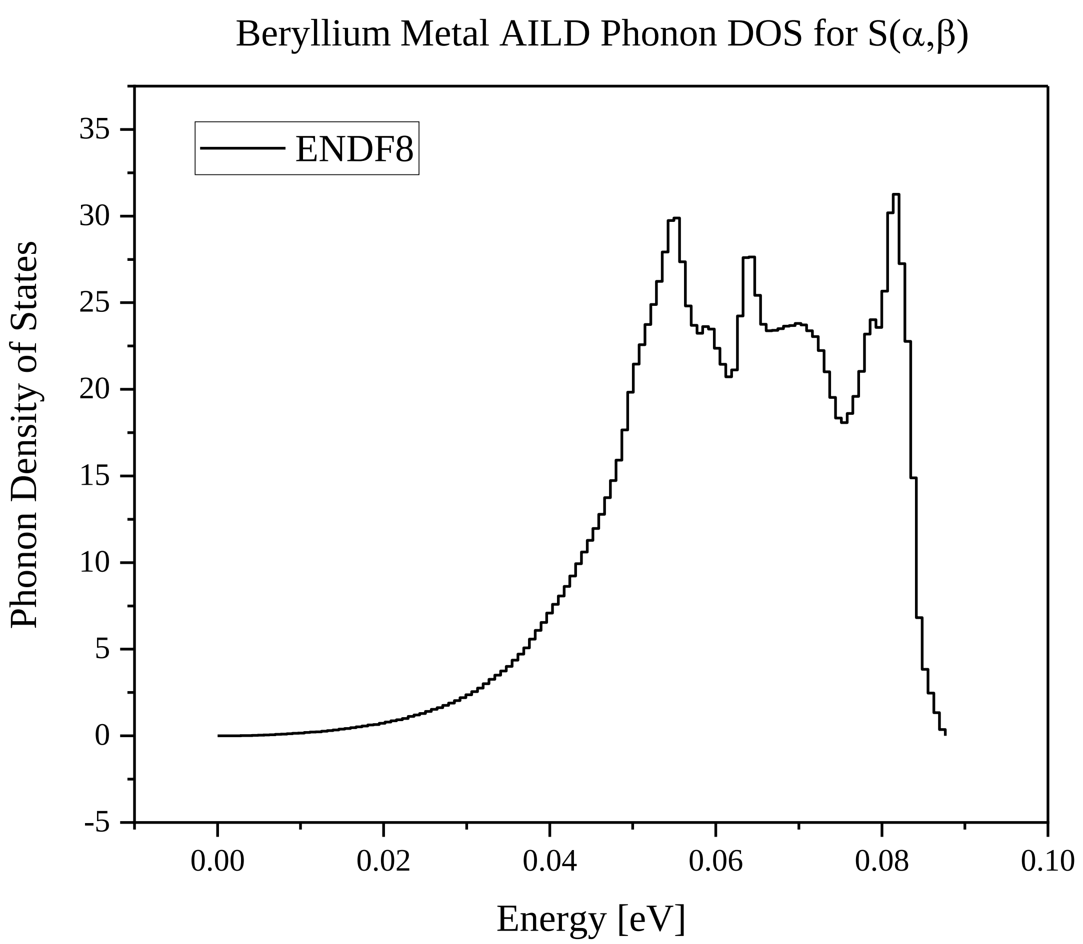
1. Training Data: *FLASSH* Loop

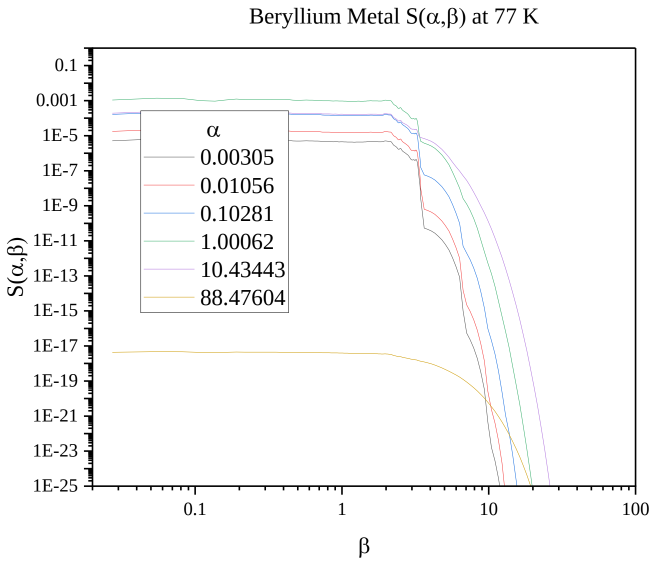


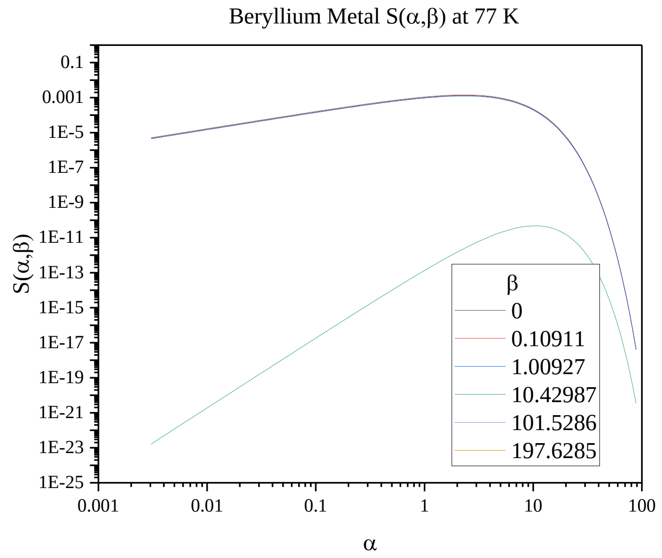




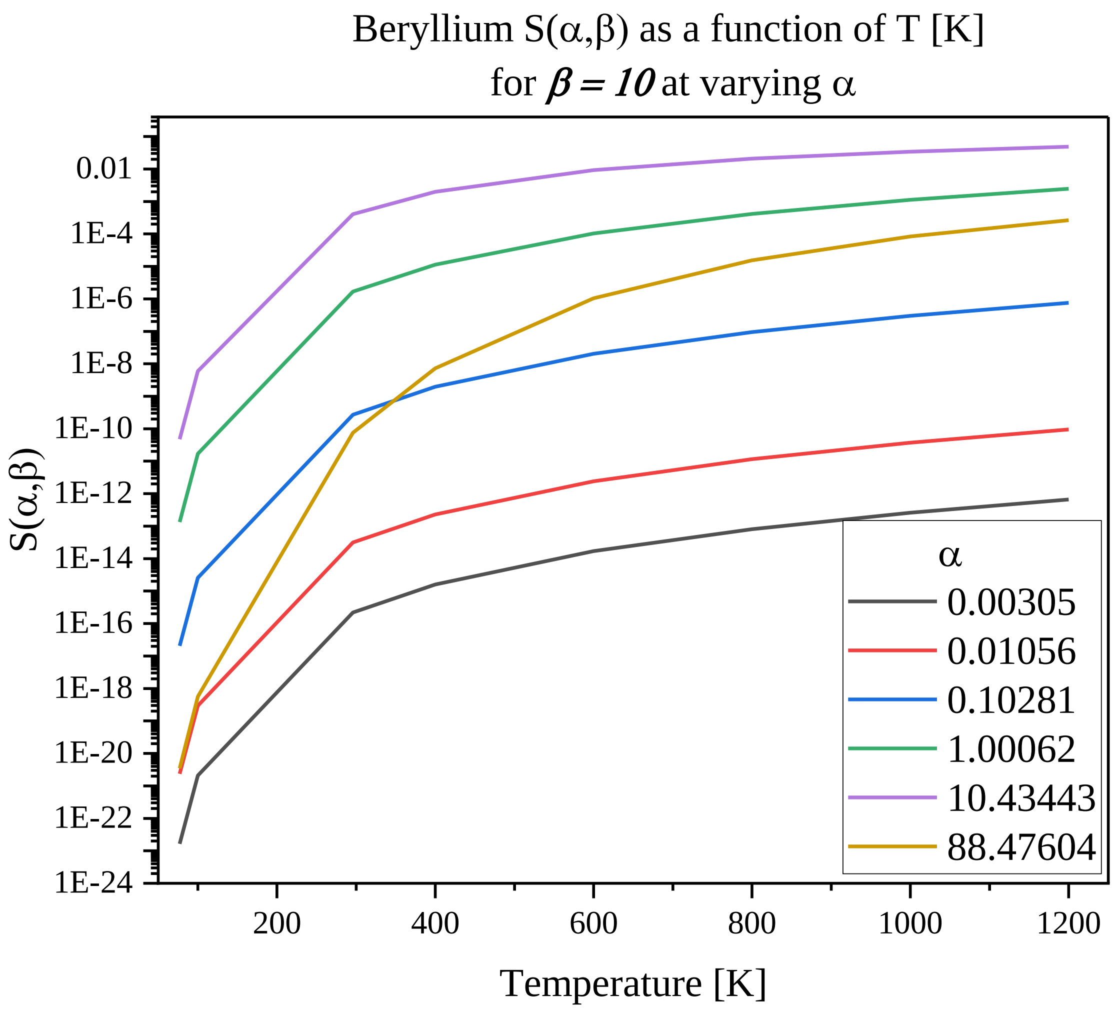
1. Beryllium Metal Evaluation at 77 K

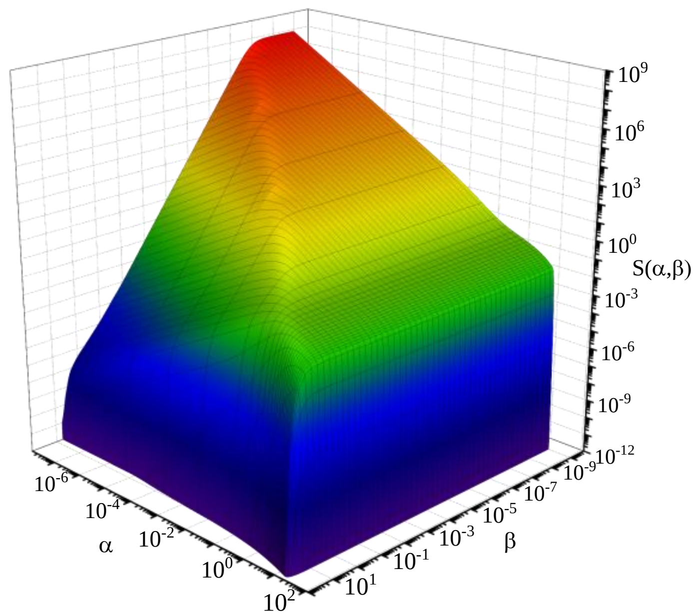






1. Beryllium Metal Temperature Dependence





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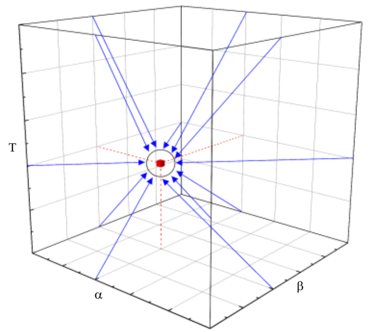
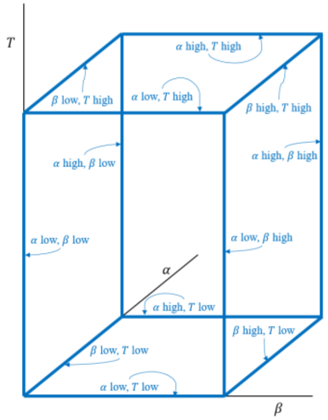
2. *FLASSH* Data Preprocessing

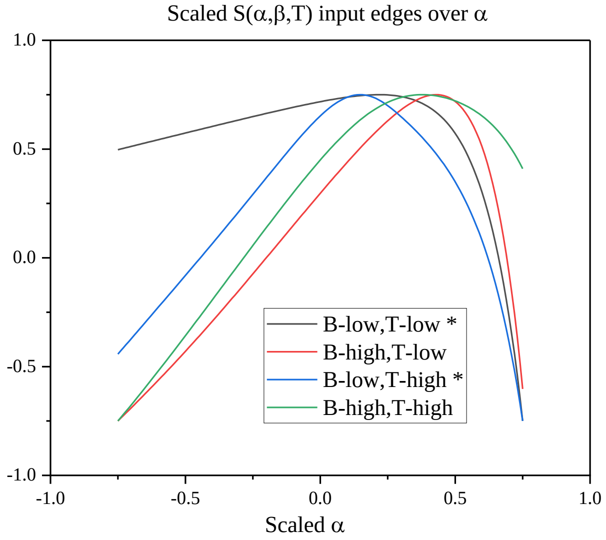
1. Linearize alpha (log10), beta (log10) , temperature grids (1/T) to [-.75 , .75]

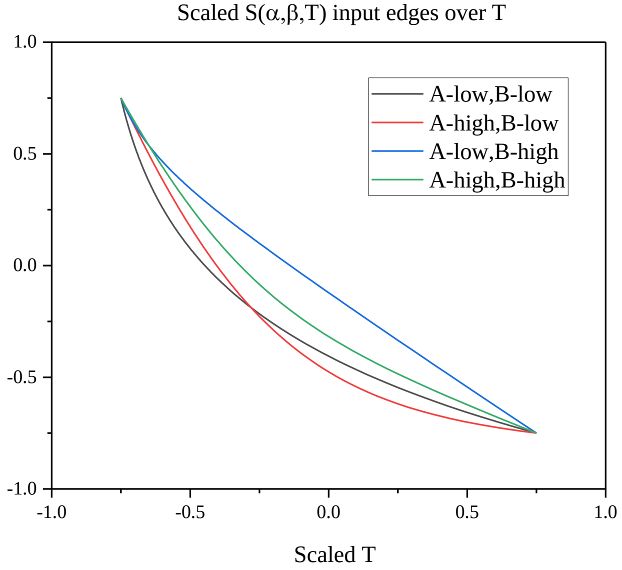
2. Transform Thermal Scattering Law Data (log10)

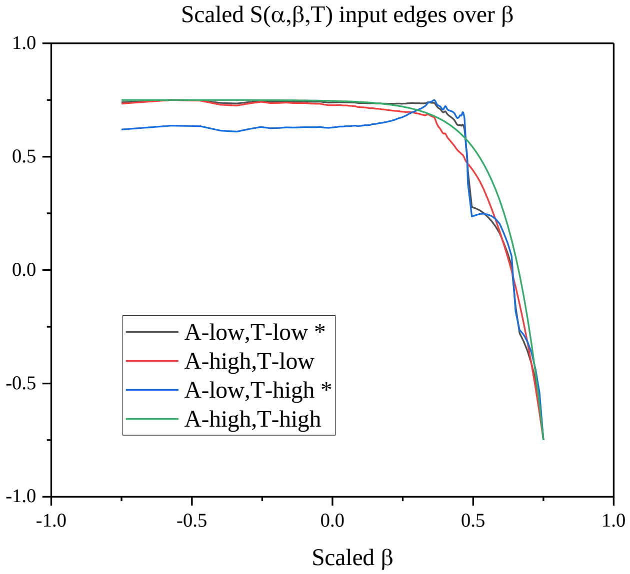
3. Generate input “edges” to assist training (feature engineering)











4. Divide dataset into training (99%), validation (.5%), and test (.5%)

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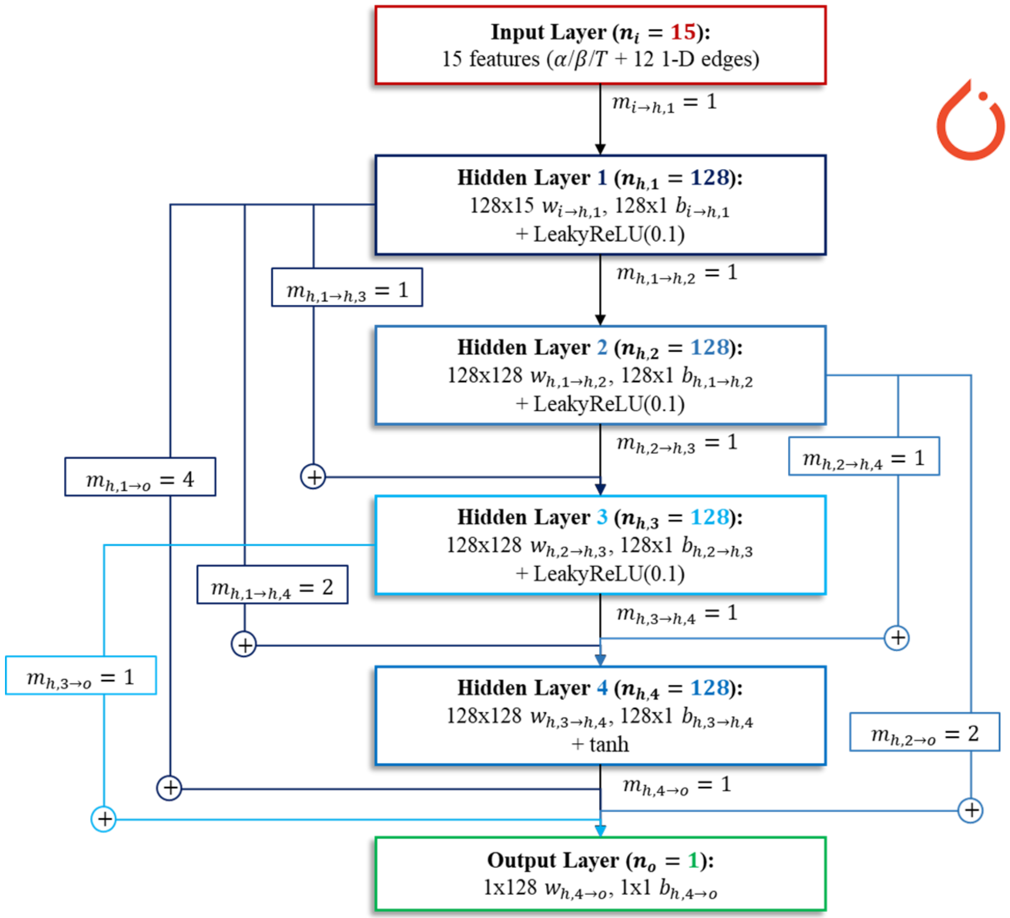
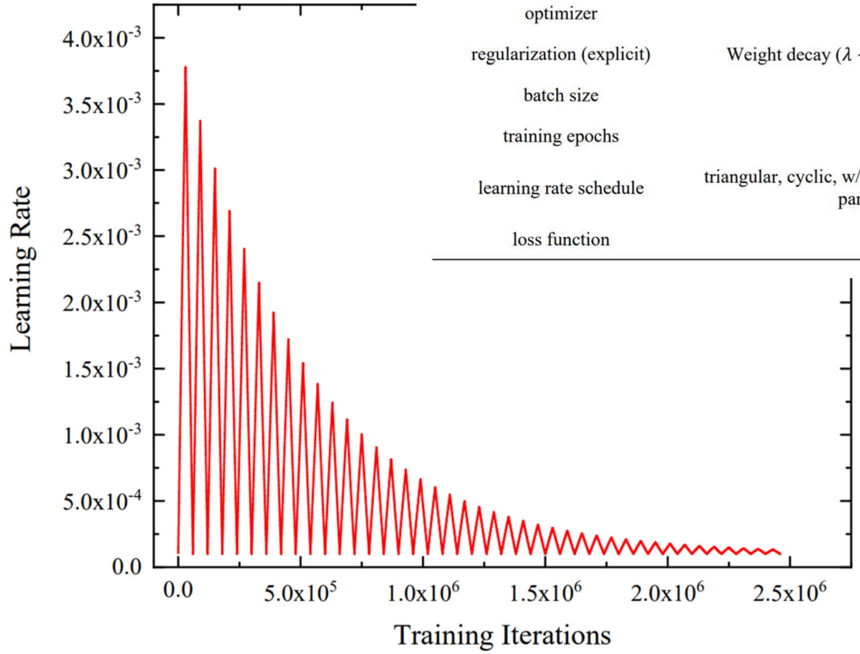
3. Network Architecture and Hyperparameters



PyTorch

Setting	Selection
n_{hidden_layers}	4
n_h	128
cascading	none
skip connections	dense, weighted
skip weight scheme	multiplicative, 1:2:4
activation function	LeakyReLU(0.1) in hidden layers 1-3, tanh in hidden layer 4
weight initialization	Xavier uniform
optimizer	AdamW
regularization (explicit)	Weight decay ($\lambda \to$ 1e-6, as implemented in AdamW)
batch size	1024
training epochs	400
learning rate schedule	triangular, cyclic, w/ exponentially decaying amplitude (see parameters in Table 4.3)
loss function	MSE



3 LEIP Cluster NVIDIA V100 GPUs, 32 GB onboard memory each
Intel Xeon E5-2690v4 CPUs (sharing 128 GB RAM)

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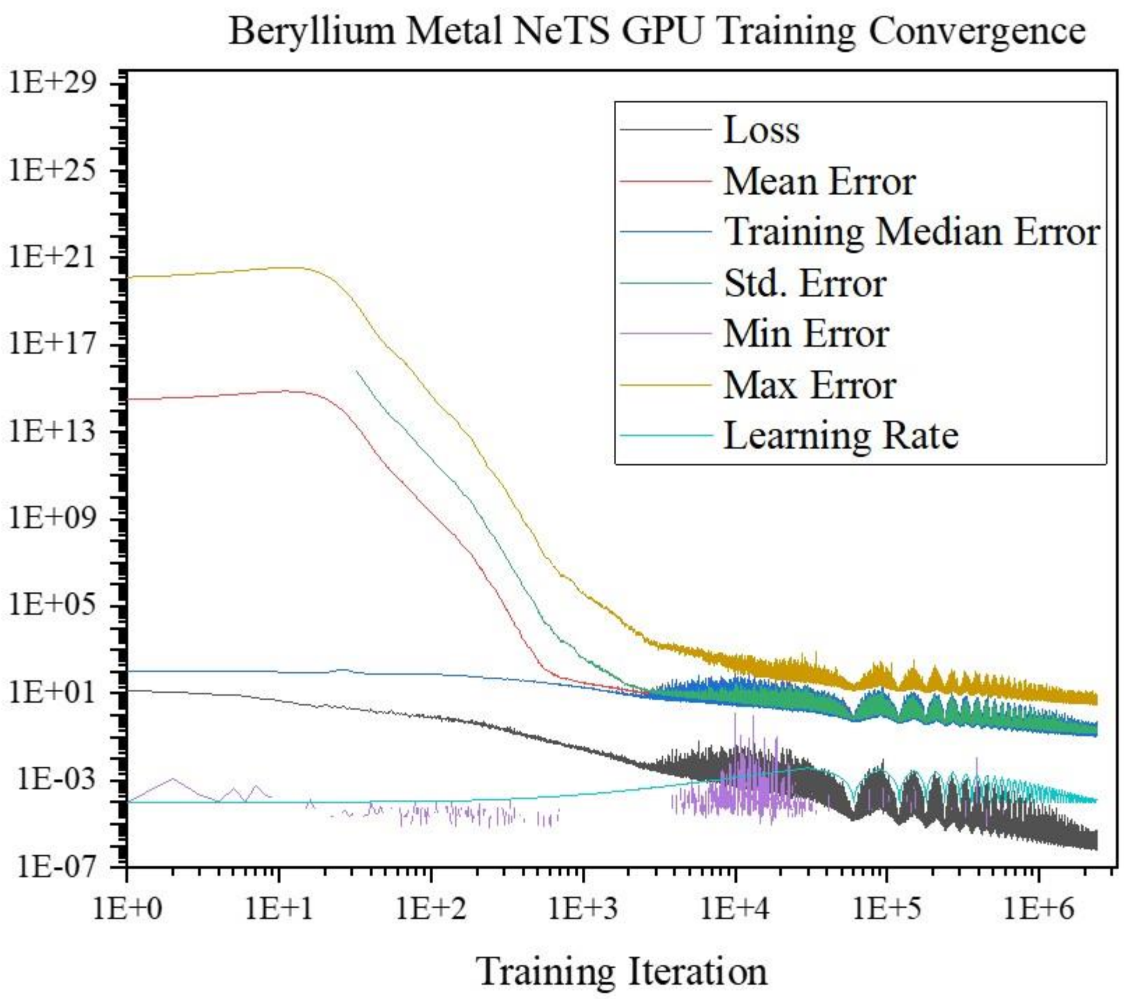
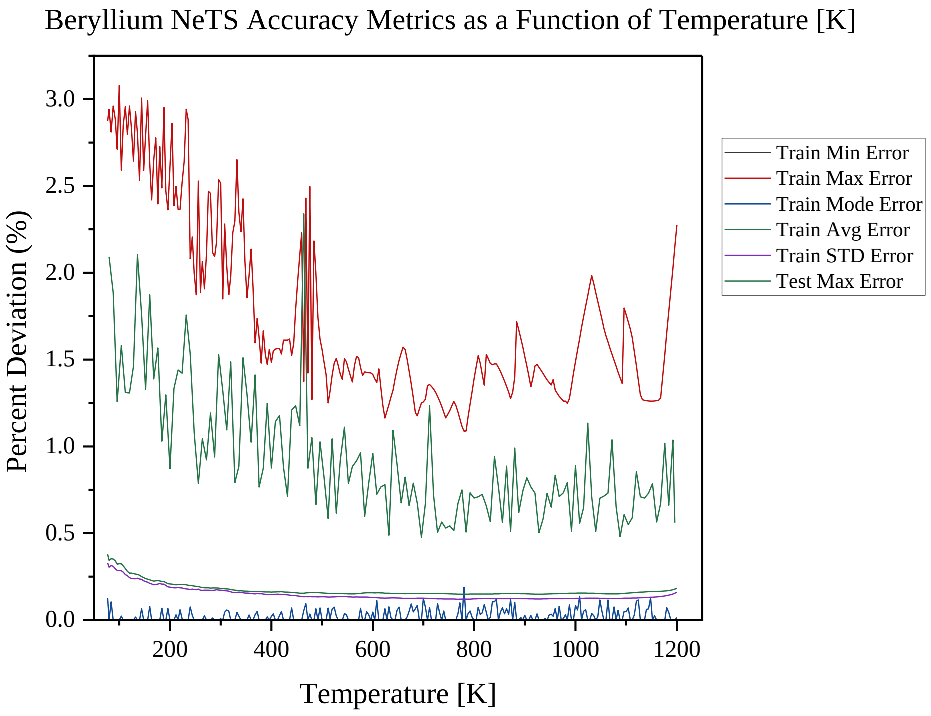
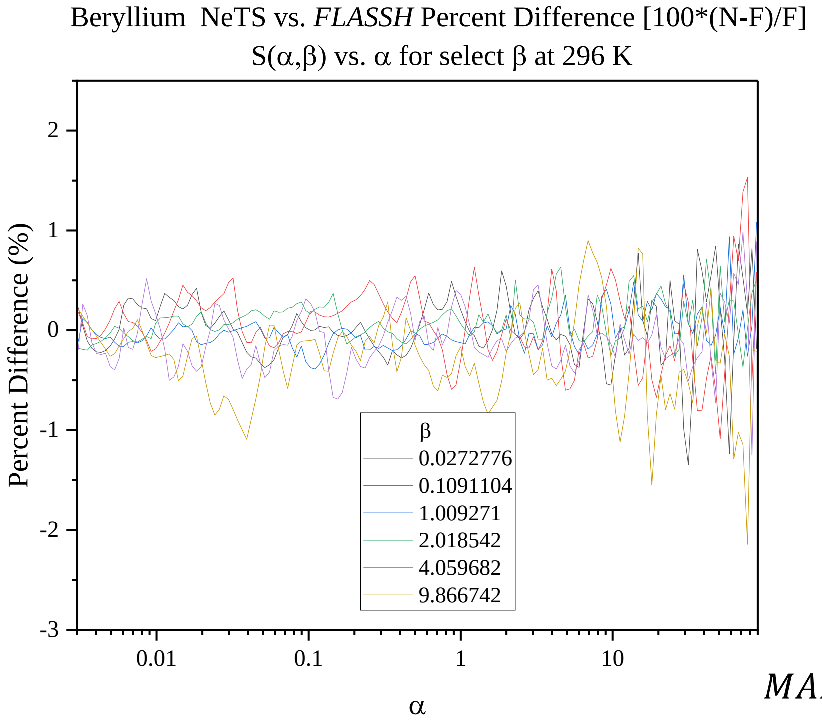
3. ANN convergence



$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

4. Network Evaluation (Train/Valid/Test)

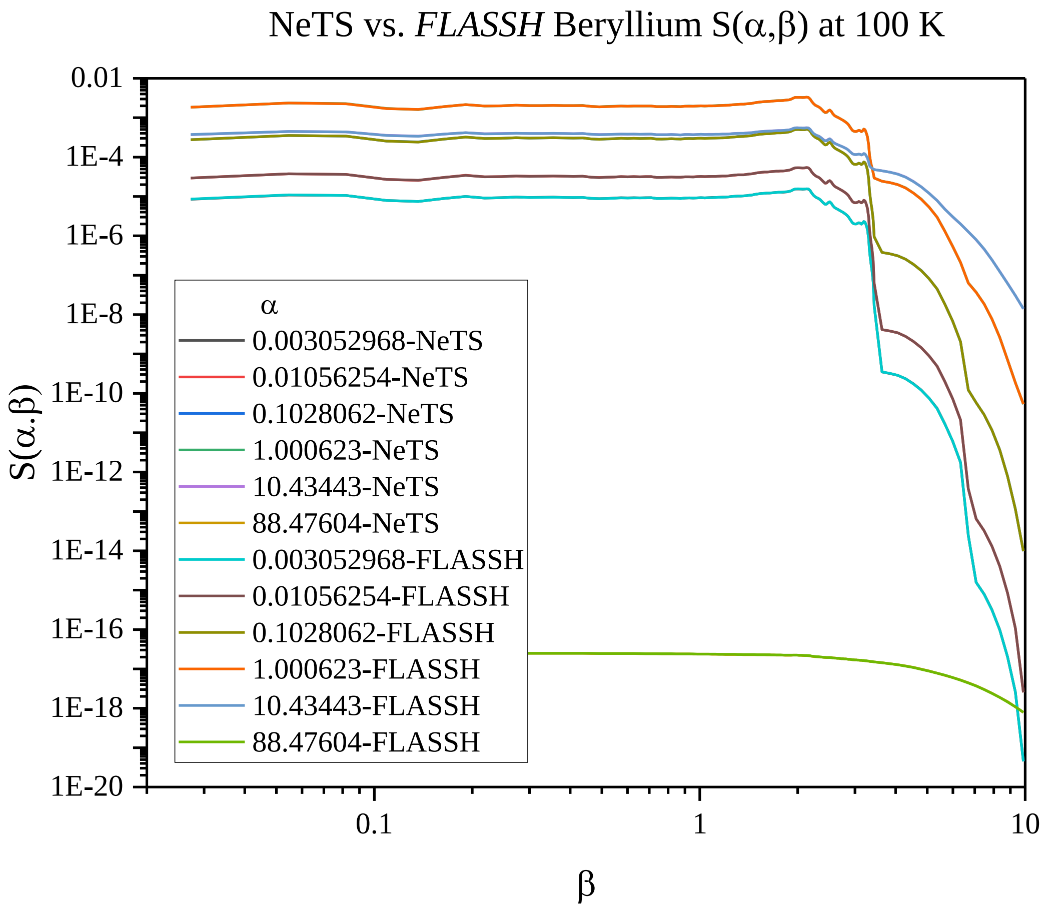


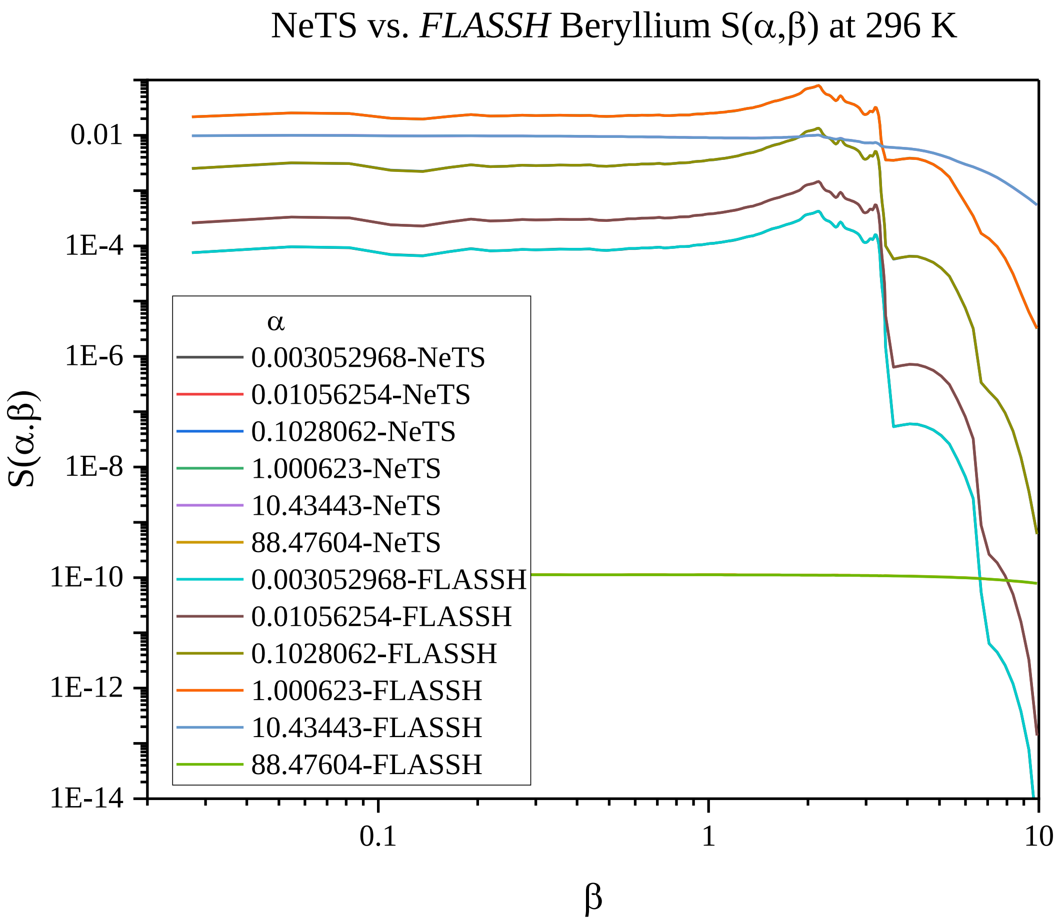


$$MAPE = \frac{100}{N}\sum_{i=1}^{N}\left|\frac{y_i - \hat{y}_i}{y_i}\right|$$

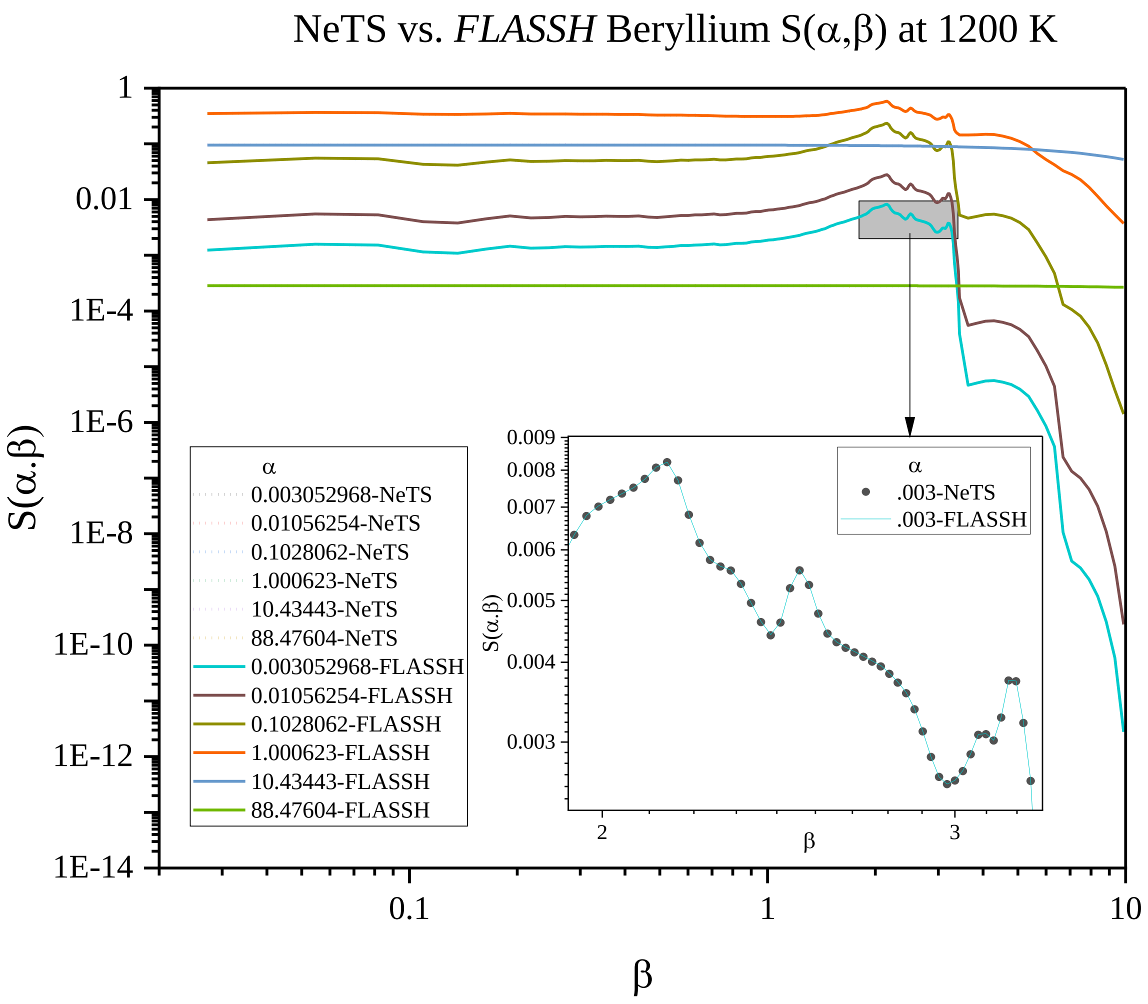
Dataset	Mean APD [%]	Med. APD [%]	Max APD [%]	< 2% [%]	< 1% [%]
Train	0.1755	0.1574	3.0190	99.9959	99.8477
Validation	0.1775	0.1579	2.7552	99.9955	99.8139
Test	0.1770	0.1574	1.6474	100.000	99.7913

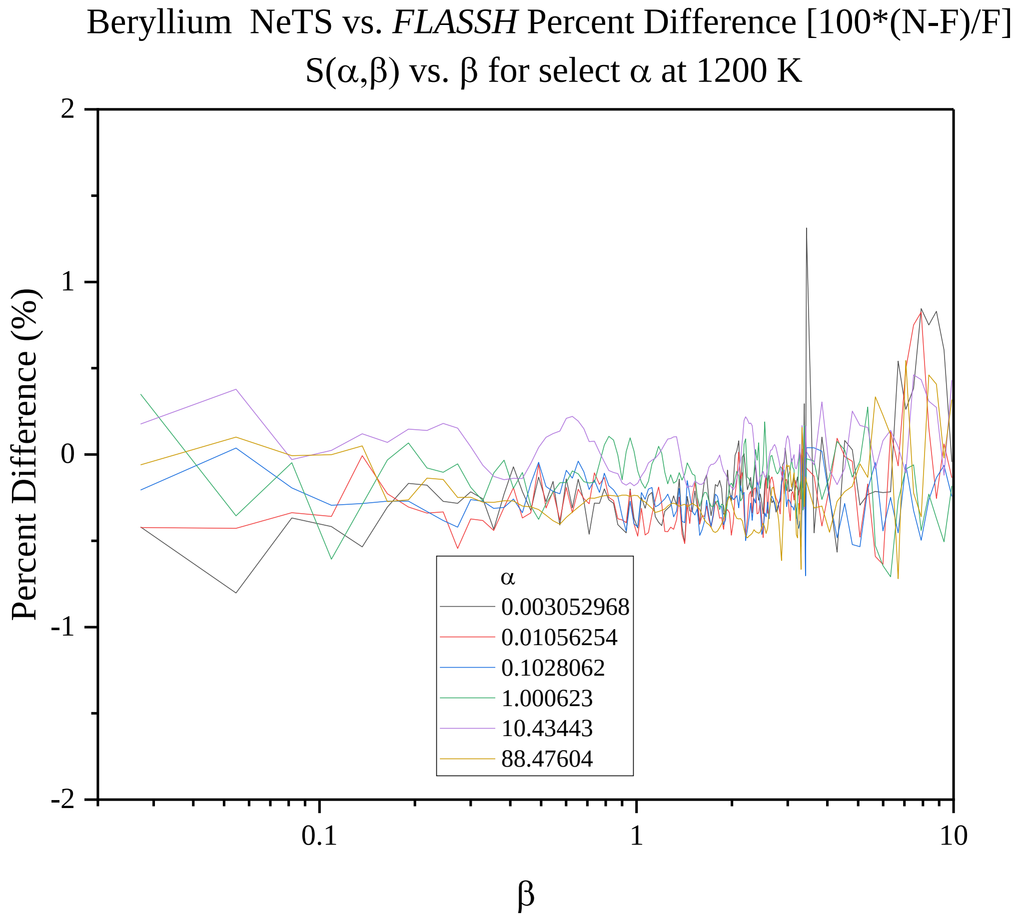
5. ANN S(α,β,T) Prediction at 100 K , 296 K





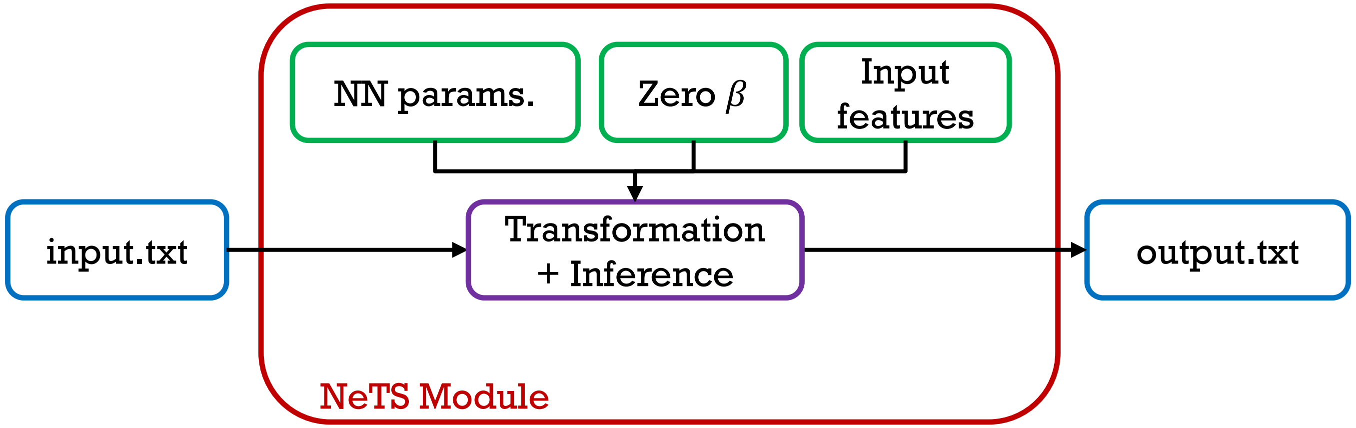
5. ANN S(α,β,T) Prediction at 1200 K





Finally … What's a NeTS Module

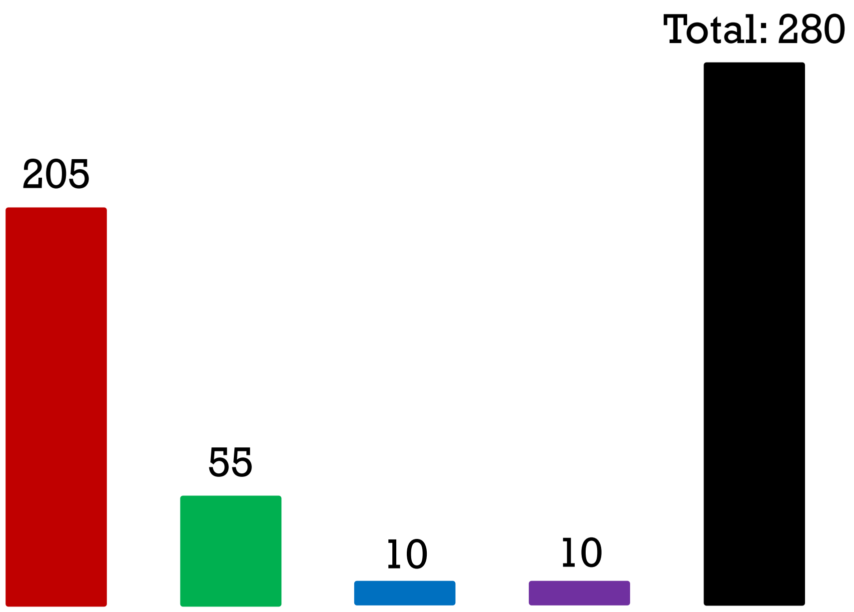
- **Compact, accurate functional representations of TSL data for a specific material over a given range of input conditions**
  - α/β
  - Temperature
  - Porosity
  - Burnup
  - Alloy %
  - Pressure



- **Functional**
- **Continuous**
- **Highly accurate**
- **Memory efficient**
  - Explicit vs. representative storage

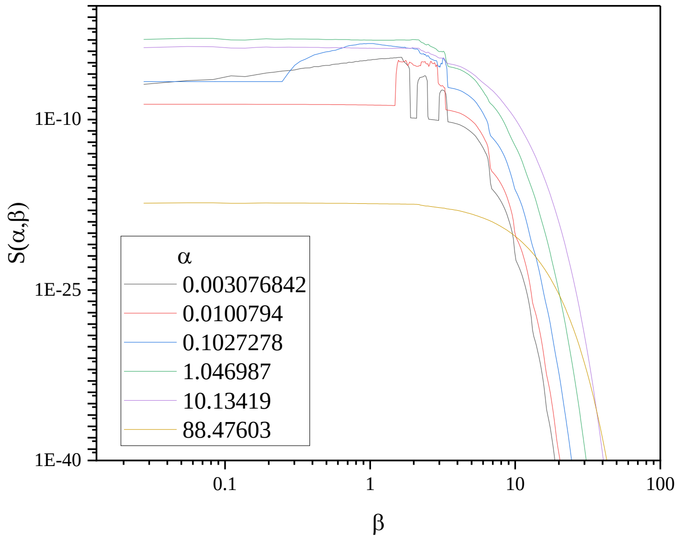
Memory & Speed

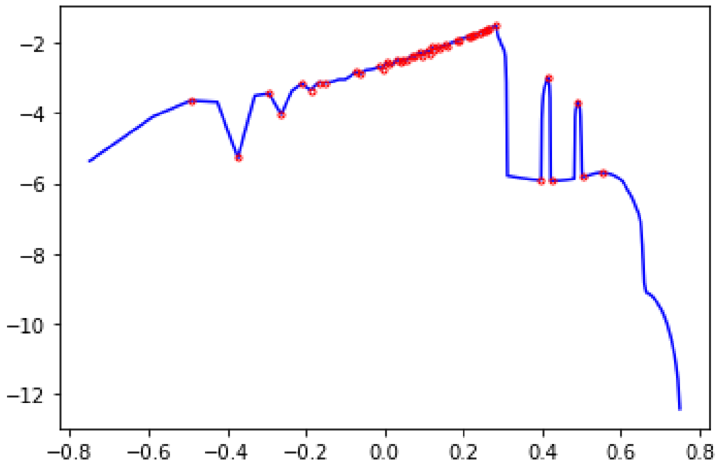
- **Adding it all up…**
  - Big improvements
  - Relative to 10+MB
- **Components**
  - NN parameters
  - Zero β
  - Input features
  - Inference Engine
- **Cache memory utilization**
  - L1, L2

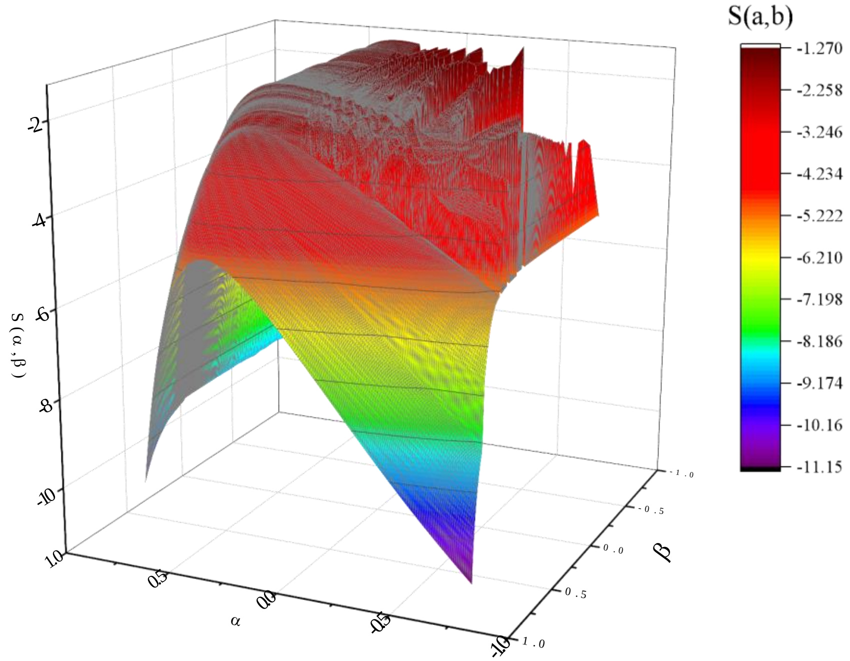


NeTS- Beryllium One-Phonon Correction, $S_d(\alpha,\beta,T)$

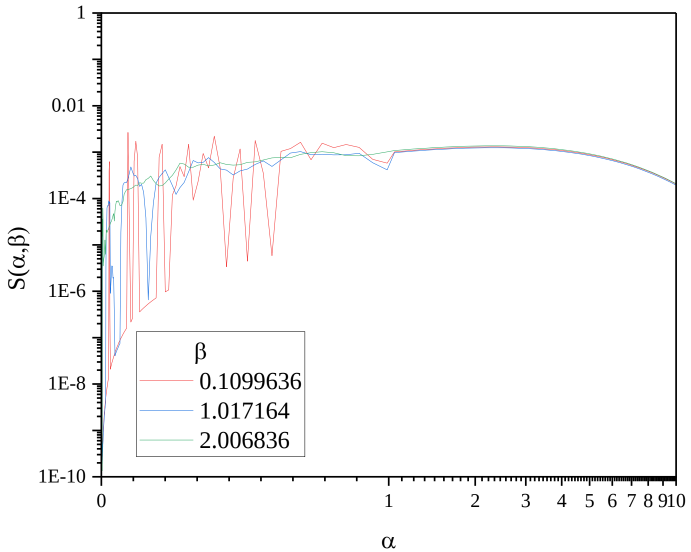
Beryllium Metal $S(\alpha,\beta)+S_D$ at 77 K

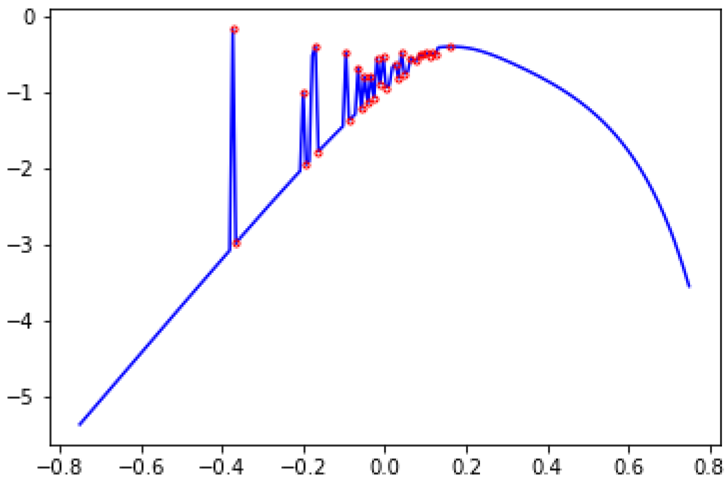






Beryllium Metal $S(\alpha,\beta)+S_D$ at 77 K





LEIP LABORATORIES

Areas for Development and Application

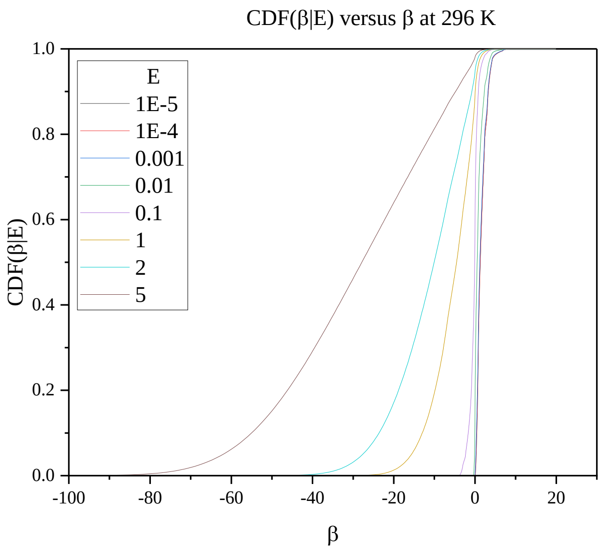
1. Transfer Learning : Warm-start network training from a similar NeTS run (implemented)

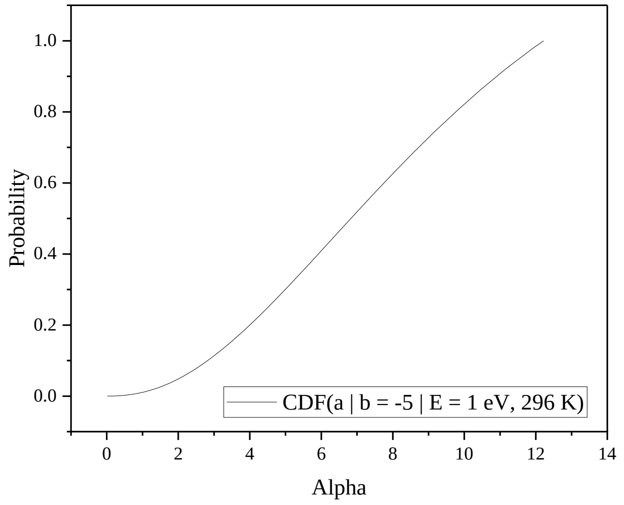
2. Optimal Brain Damage : Reduce final network size, increase network prediction speed by selectively pruning neurons that don't contribute to neural structure (implemented)

3. Include one-phonon correction and train highly structure S(α,β,T) surface (in-progress)

4. Extend dimensionality : additional material properties (i.e., porosity, burnup, pressure), and new materials

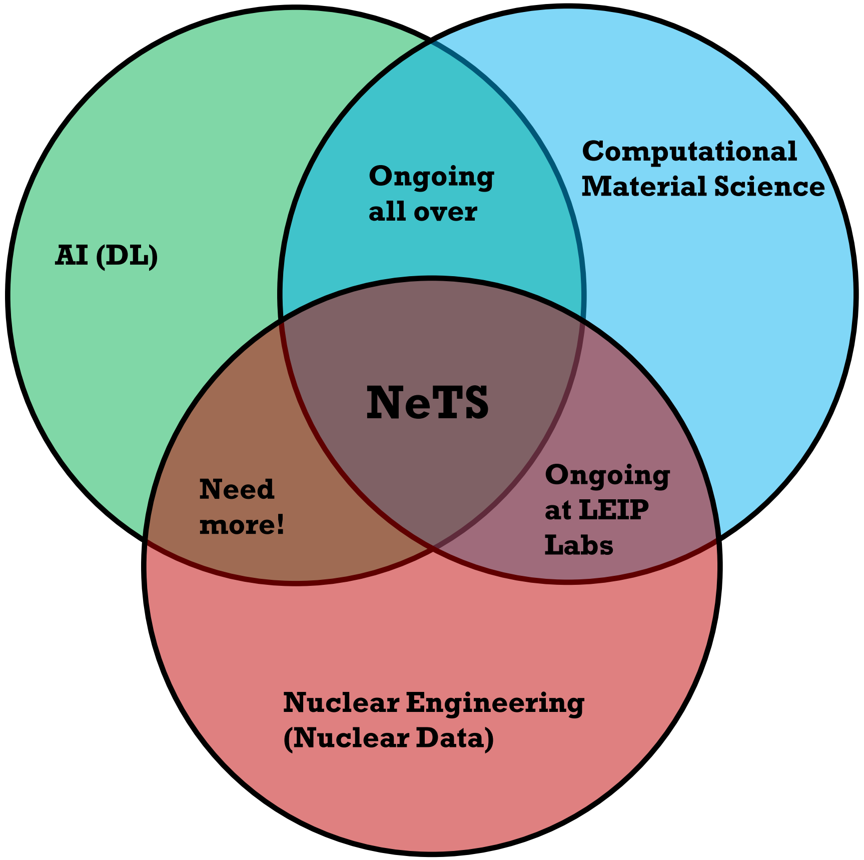
5. Couple NeTS to reactor physics framework (in-progress)





Summary

- **Producing first-of-a-kind NN representations of trivariate TSL data (NeTS)**
- **Improvements**
  - Accuracy
  - Memory consumption
  - Speed implications
- **Many new possibilities**



Thank You