

Step 1: Sample PPS parameters in the parameter space



Step 2: Generate corresponding phonon spectra and input to NJOY



Step 3: Employ NJOY to generate thermal scattering data



Step 6: Test the calibrated results

- Sample over the calibrated parameter sets
- Repeat Step 3 and 4
- Compare the results with “experimental” results



Step 5: Calibrate PPS parameters for the experiment (real or surrogate)



Step 4: Use the data in MCNP simulations and extract the QOIs