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NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

Optimizing TEX-Pu for Testing Thermal Scattering Cross Sections and Maximizing the Intermediate Fission Fraction

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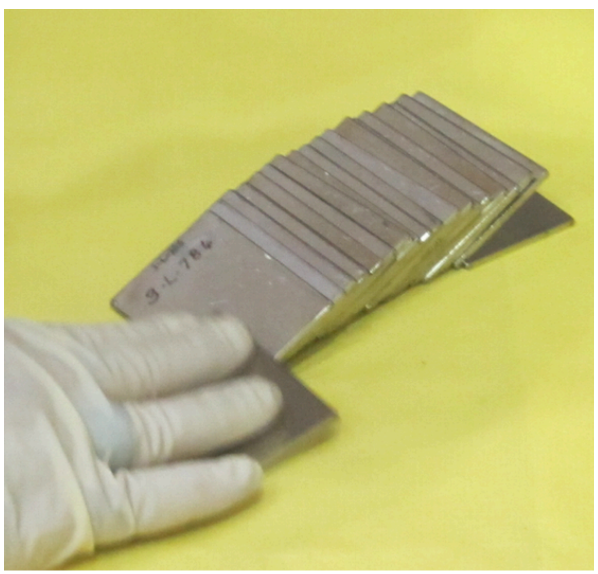
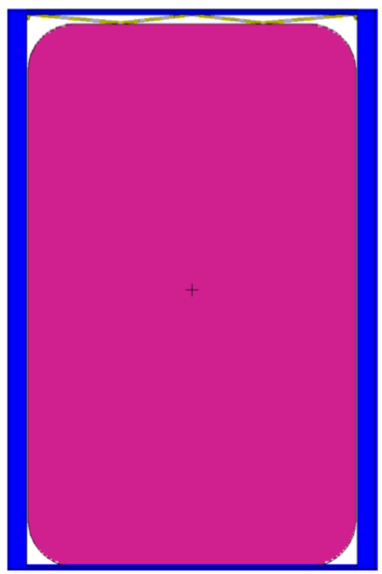
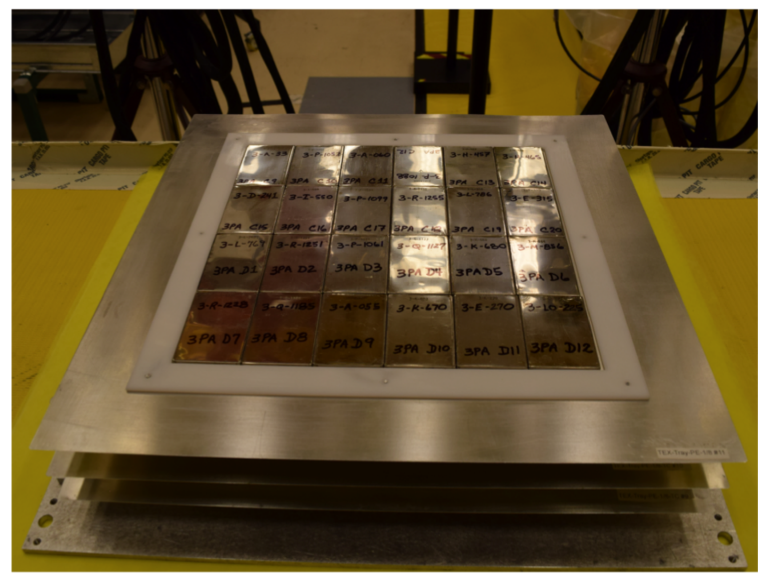
IER 184: Thermal/Epithermal eXperiments (TEX)

- IER 184 created a testbed of five baseline Pu experiments moderated with varying thicknesses of polyethylene using Pu-Al Zero Power Physics Reactor (ZPPR) plates
- FY17 work extended the IER 184 design
  - Optimize TEX configurations to validate new Thermal Scattering Laws generated through molecular dynamics models at NCState
  - Optimize Pu-ZPPR configurations for intermediate and unresolved resonance region using alumina as a reflector/moderator

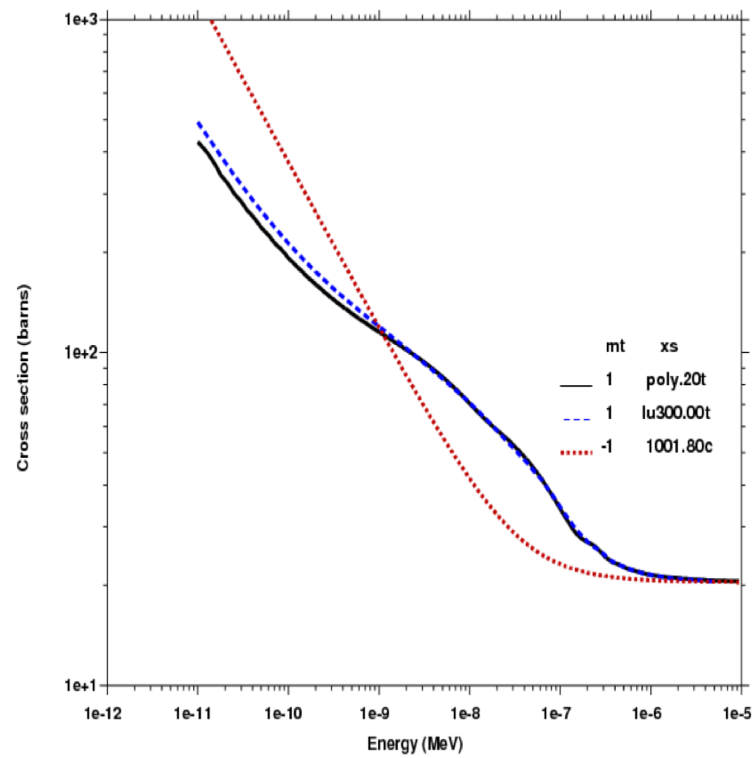






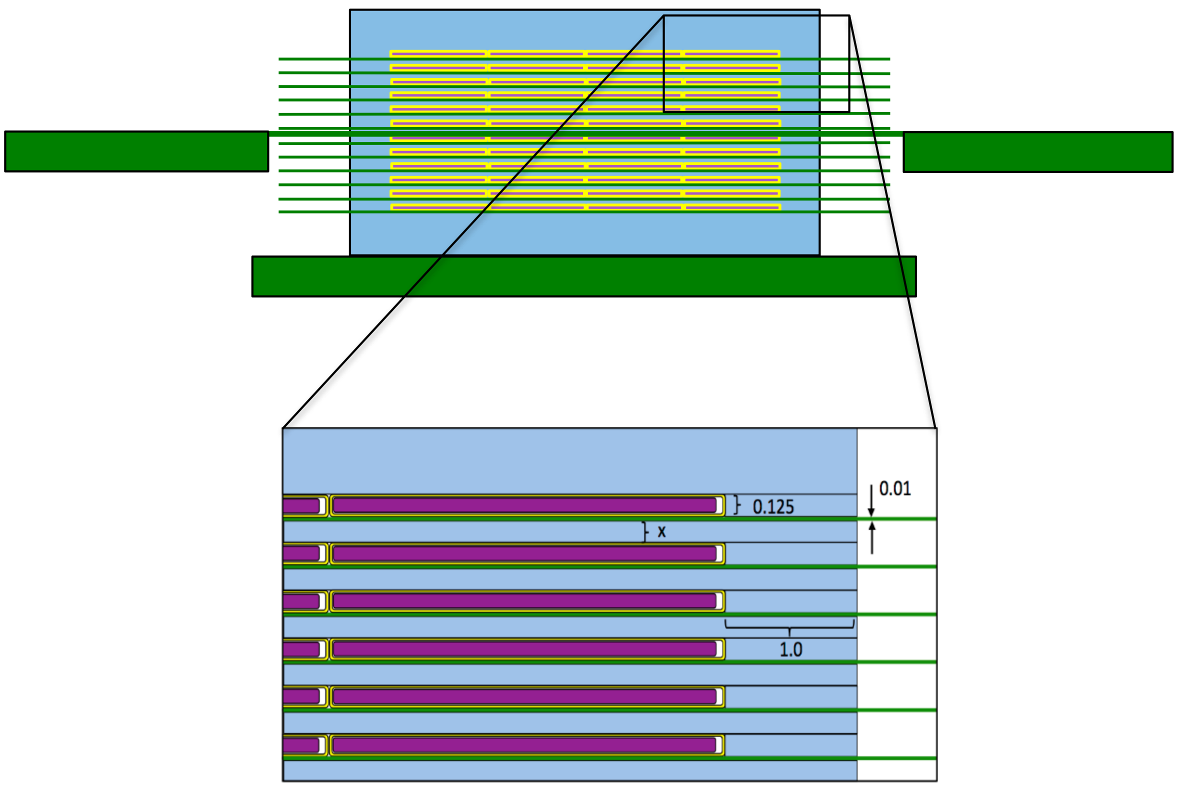
New TSL Data Available, thanks to NCSP

- North Carolina State University has been using first principals molecular dynamics models to generate thermal scattering laws
  - Polyethylene (PE), Lucite (new), graphite, ice (new), many more
- Lucite and PE are ubiquitous moderating structural materials and thus important to criticality safety
- Very few benchmarks in ICSBEP are sensitive to Lucite or PE
  - 142 benchmarks with Lucite or PE
  - Only 15 identified as potentially sensitive to thermal scattering
  - By comparing 15 cases with thermal scattering turned on and off, the effect on k_{eff} was generally less than 1% in k_{eff}, with the hightest case being 5.3% in k_{eff} for PE



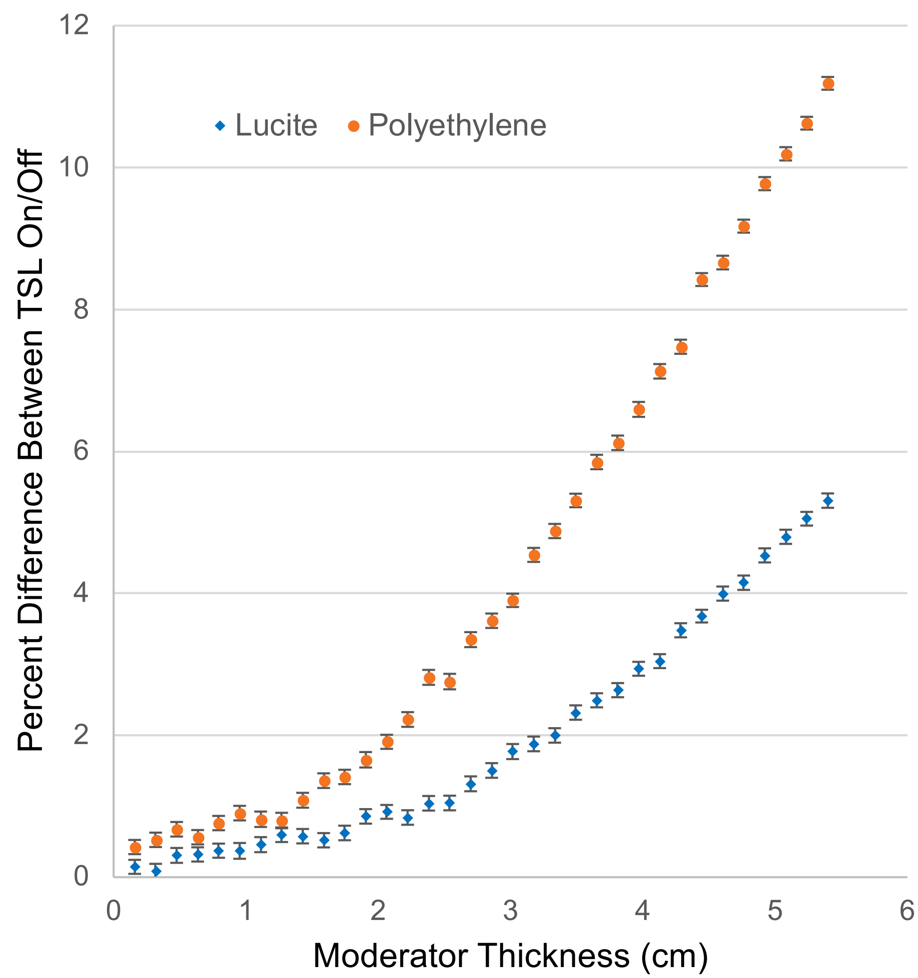
Optimizing TEX for TSL Validation

- Method:
  - Vary the thickness (x) of PE/Lucite moderator between Pu ZPPR plate layers in TEX design using MCNP6
  - Compare MCNP6 k_{eff} with and without NCState-generated TSLs (MT card) to find the largest effect



Results of TSL TEX Calculations

- TSL “off” gave higher k_{eff}
- Sensitivity to TSL increased with increasing moderator thickness, with large percentage gains seen after 2 cm thickness
- The most thermal TEX baseline case (2.54 cm PE) has a 2.76% k_{eff} sensitivity to PE TSL
- The TEX set-up is much more sensitive to PE thermal scattering than a similar amount of Lucite
  - Up to 11% difference with PE
  - Up to 5% difference with Lucite



Downselect to Four Configurations

- Criteria for choosing experimental configurations
  - TSL sensitivity
  - k_{eff} close to 1
  - Minimize partial Pu layers required for criticality
  - Height to Diameter (H/D) ratio of overall stack less than 2

Moderator Material	Thickness (cm)	Pu Layers	Height/ Diameter (H/D) of Stack	TSL Sensitivity (% k_{eff})
PE	4.28625	6	0.77	7.48
PE	5.08	10	1.60	10.19
Lucite	4.1275	7	0.89	3.04
Lucite	5.715	9	1.59	6.15

TEX TSL Conclusions and Current Work

- TEX baseline thermal case (Experiment #5, completed June 2017) will be the most sensitive Pu benchmark to PE TSL at 2.76% in ICSBEP
- Additional TEX configurations with thicker PE can get sensitivities up to 11%, as predicted by MCNP6
- TEX Configurations with Lucite could get up to 6% k_{eff} TSL sensitivity

- LLNL is currently working on a preliminary design report (CED-1) documenting the proposed experiments, due in Q4

Optimizing TEX for Intermediate Fission Fraction

- The maximum intermediate fission fraction for the TEX baseline experiments with PE was 43%

Thickness of PE Plates (in)	Thermal Fission Fraction (<0.625 eV)	Intermediate Fission Fraction (0.625 eV-100 KeV)	Fast Fission Fraction (>100 KeV)
0 (no PE)	0.09	0.17	0.74
1/16	0.14	0.38	0.49
3/16	0.27	0.43	0.30
7/16	0.48	0.33	0.19
1	0.67	0.21	0.12

- LLNL/IRSN TEX collaboration
  - IRSN is designing a variation of a TEX experiment to approximate MOX elemental and isotopic compositions
  - IRSN had success using alumina (Al_2O_3) as a moderator and reflector to maximize intermediate fission fraction
  - IRSN developed and used a machine-learning based parameterization tool, called PROMETHEE, to design the experiments

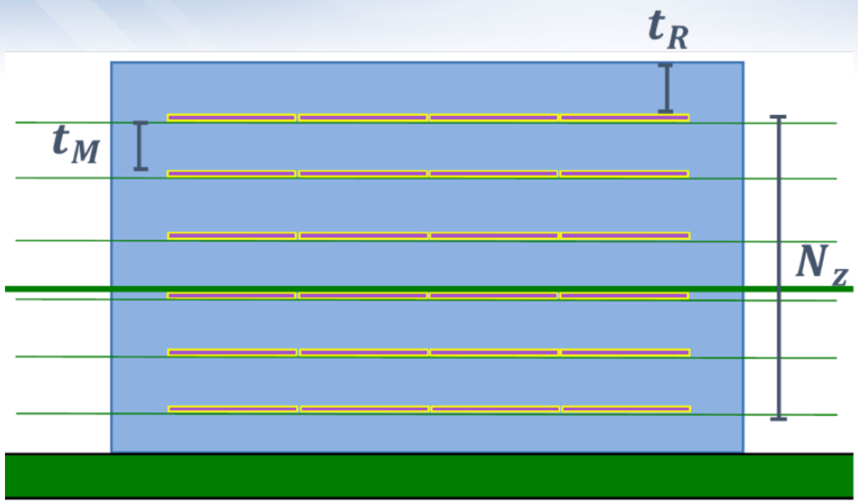
Optimizing TEX for Intermediate Fission Fraction

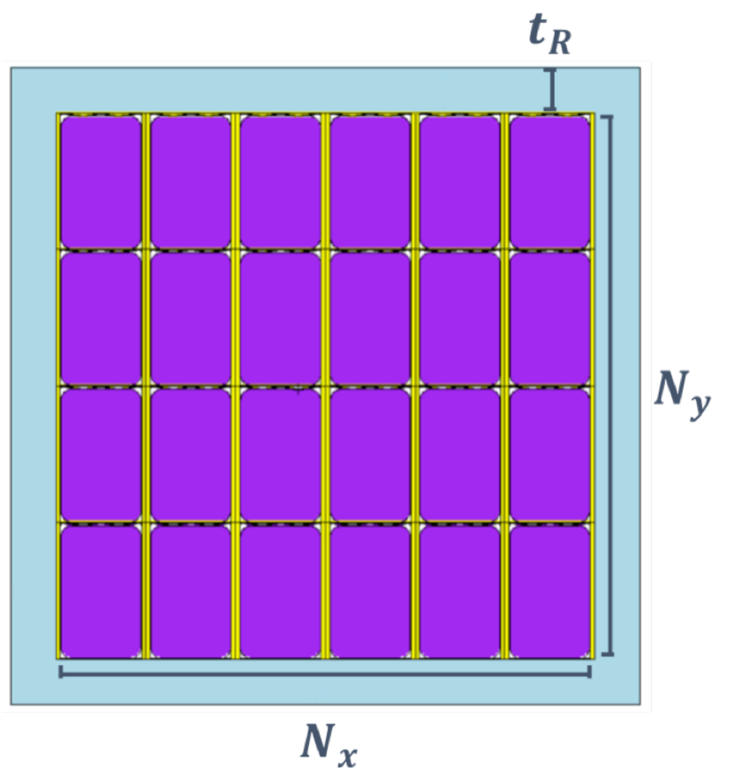
- Originally the plan was to use PROMETHEE to design TEX configurations using alumina as a moderator and reflector that optimized intermediate fission fraction
  - Unfortunately, the LLNL computer security firewalls prevented us from using PROMETHEE (no fault of the code!)

- Therefore, we developed a novel Python-based machine-learning code, Optimus, that creates and reads MCNP6 files
  - Goal of intelligently varying a given set of parameters to create a critical experiment

Inputs to Optimus

- Goals for the configurations:
  - Multiplication factor, ($0.98 \le k_{eff} \le 1.02$)
  - > 50% of fission in the intermediate region (0.625 eV < E < 100 keV)
- Constraints:
  - Up to 1167 Pu-ZPPR plates
  - Assembly height to diameter ratio < 2
  - Layers fit within the 35” x 35” footprint of the vertical lift machine
- By changing the following parameters:
  - Number of plates in the x (N_x), y (N_y), and layers (N_z)
  - Moderator thickness (t_M)
  - Reflector thickness (t_R)





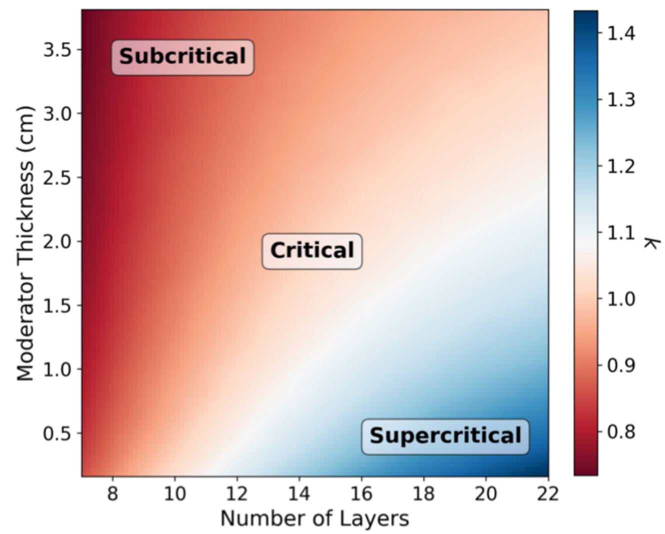
Optimization

- Optimization involves minimizing an objective function

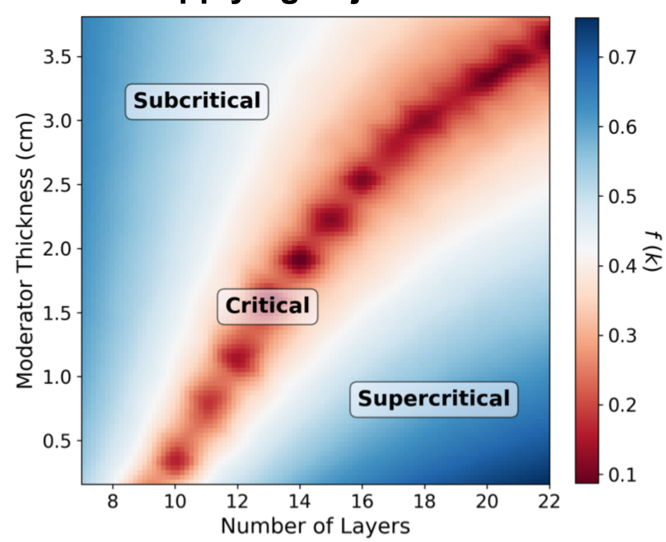
$$f(k) = |k - 1|^x$$

- Powell's Method used for minimization
  - – Linear search algorithm
  - – Does not use or compute the gradient
    - Unlike quasi-Newton minimization methods (such as Nelder-Mead or BFGS)
- Determines the local minima, corresponding to the configurations which are closest to critical (locally)

Before applying objective function

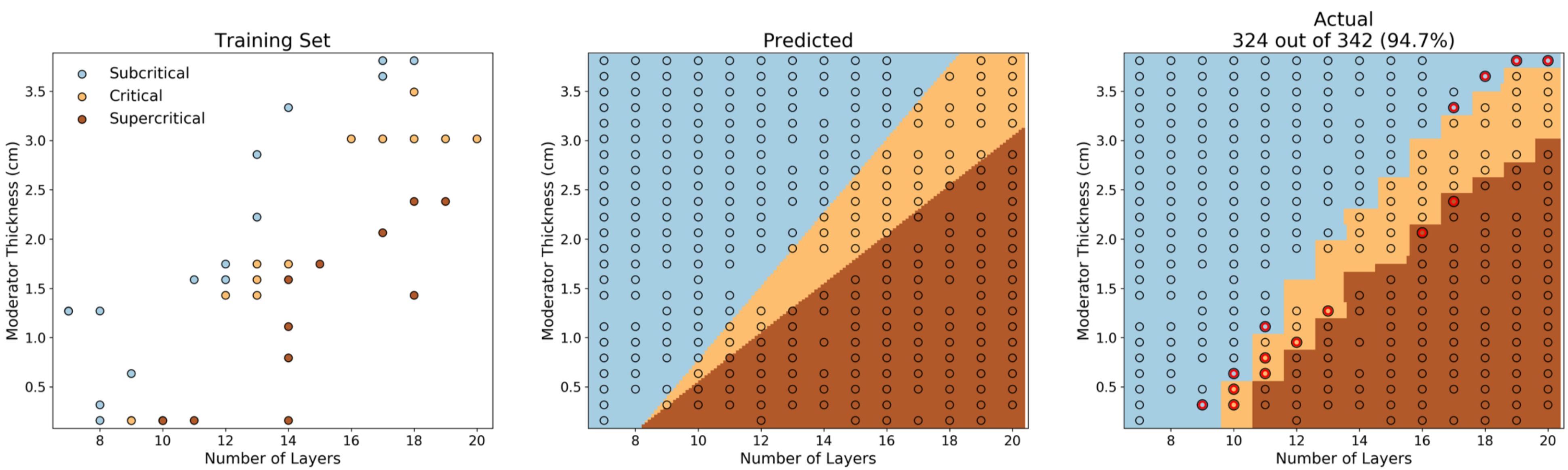


After applying objective function



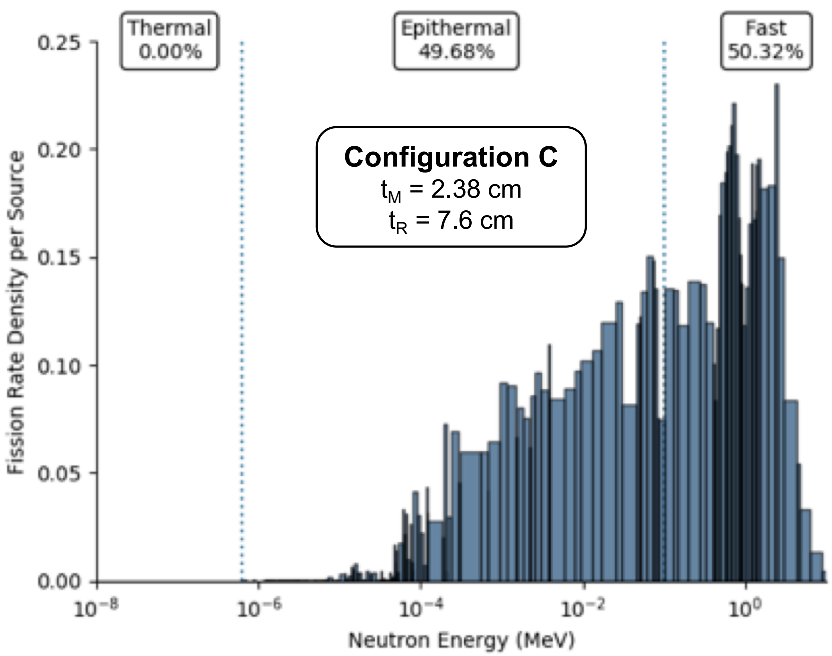
Machine Learning

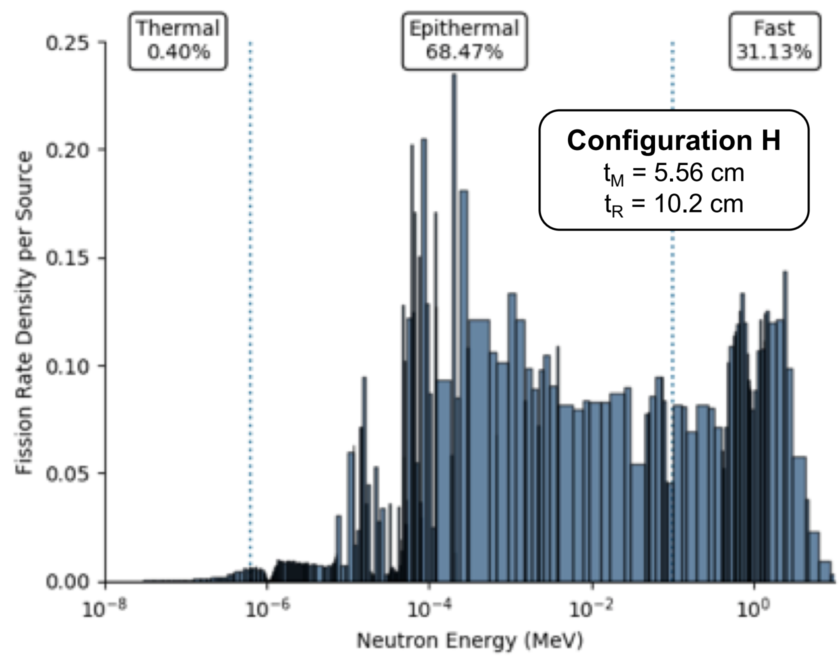
- Machine learning involves prediction through fitting training data
- Logistic regression was used to classify configurations as subcritical ($k < 0.98$), critical ($0.98 \leq k \leq 1.02$), and supercritical ($k > 1.02$)
- The process is demonstrated below for $k(N_z, t_M)$ where 324 out of 342 configurations were predicted accurately (94.7%)



Many Critical Configurations Identified

ID	N_x	N_y	Layers	Moderator Thickness t_M (cm)	Reflector Thickness t_R (cm)	Inter Fraction	Fast Fraction
A	9	6	19	2.54	7.6	0.51	0.49
B	9	6	20	4.45	12.7	0.66	0.34
C	10	6	17	2.38	7.6	0.50	0.50
D	10	6	17	4.60	12.7	0.66	0.33
E	11	7	12	2.22	10.2	0.50	0.50
F	11	7	15	4.76	10.2	0.67	0.33
G	12	8	11	2.86	10.2	0.56	0.44
H	12	8	12	5.56	10.2	0.68	0.31





Conclusions

- Using the Pu ZPPR plates and alumina moderator and reflector, intermediate fission fractions up to 70% are possible
- Depending on the thickness of alumina moderator, the intermediate fission spectrum can be shifted into the resolved or unresolved region
- Optimus was used to quickly parameterize the inputs, read the outputs, and converge on solutions without human intervention
- Optimus is a significant cost and time saver for critical experiment design