COMPUTING AND OPTIMIZATION IN NUCLEAR APPLICATIONS
Cross-Cutting Area

Vladimir Sobes
Department of Nuclear Engineering
University of Tennessee

NSSC3 Kickoff Meeting and Advisory Board Review
April 19-20, 2022

CONA Overview

Computing and Optimization in Nuclear Applications is truly a crosscutting theme in all aspects of nuclear security.

CONA methodologies efficiently utilize increased complexity in supercomputer architectures to advance monitoring, characterization, safeguards, controls, and design of nuclear systems.

Dramatic increases in simulation capabilities and computational methods (e.g. AI/ML) will accelerate the pace of scientific discovery in fundamental sciences and assist engineers in designing and optimizing nuclear security and non-proliferation systems with drastically improved performance, safety, and efficiency.

Through engagement in cross-cutting CONA research, students will develop the ability to work in multi-disciplinary teams and develop an understanding of fundamental nuclear phenomena that underpin the ability to develop cutting-edge computational models and development of optimized nuclear systems.

CONA Overview

AI/ML optimization in nuclear applications

Subtask 1
AI optimization of Networked Detection for Safeguards Applications
Supports RD and NMS

Subtask 2
Artificial Intelligence-based Identification of Nuclear Resonances
Supports NP-ND

Subtask 3
Neutron Spectra Tailoring Optimization for Exascale Computing
Supports NCH-NE

Computational methods for nuclear applications

Subtask 4
Stochastic Media Radiation Transport and Nuclear Signature Analysis
Supports NP-ND&RD

Subtask 5
Characterizing Reactor Fuel Isotopics and Corresponding Effluent Releases
Supports NCE-NE

Key Personnel

Berkeley
UNIVERSITY OF CALIFORNIA

THE UNIVERSITY OF TENNESSEE KNOXVILLE

THE UNIVERSITY OF NEW MEXICO

UNIVERSITY OF ILLINOIS URBANA-CHAMPAIGN

AF INSTITUTE OF TECHNOLOGY

Laboratory Partners*

Los Alamos NATIONAL LABORATORY EST. 1943

J. Conlin, E. Davis, N. Gibson, M. Grosskopf, W. Haeck, J. Hutchinson, B. Little, D. Neudecker, M. Paris, S. Ramsey, P. Talou, T. Urbatsch, J. Favorite, J. Bevins

Lawrence Livermore National Laboratory

D. Bleuel, P. Brantley, L. Dauffy, S. Dazeley, S. Labov, V. Mozin, M. Prasad, D. Shaughnessy, D. Siefman

OAK RIDGE National Laboratory

B. Betzler, D. Bowen, P. Hausladen, S. McConchie, R. Venkataraman, C. Weber, A. Worrall, K. Ziock, J. Brown, R. Bostelman, L. Evans, J. Nattress, M. Dion, K. Schmitt

Sandia National Laboratories

Z. Gastelum, A. Olson, J. Whetzel

BERKELEY LAB Lawrence Berkeley National Laboratory

R. Cooper, R. Hartman-Baker, K. Yellick, T. Joshi

*Identified during proposal process

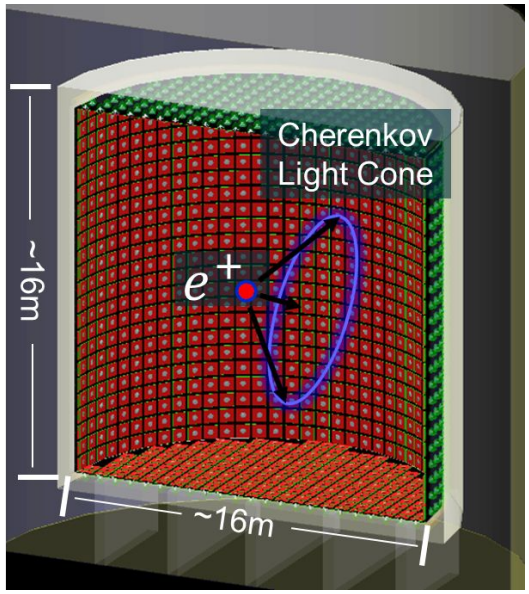
M&S of Wavelength Shifting Plates in a Water Cherenkov Detector

Supports NP-ND and RD
Ph.D. Students: Austin Mullen
Faculty Advisor: Dr. Jasmina Vujic

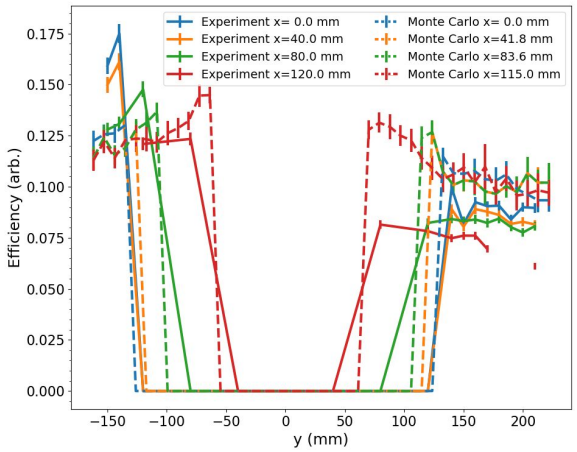
LLNL Mentor: Dr. Adam Bernstein

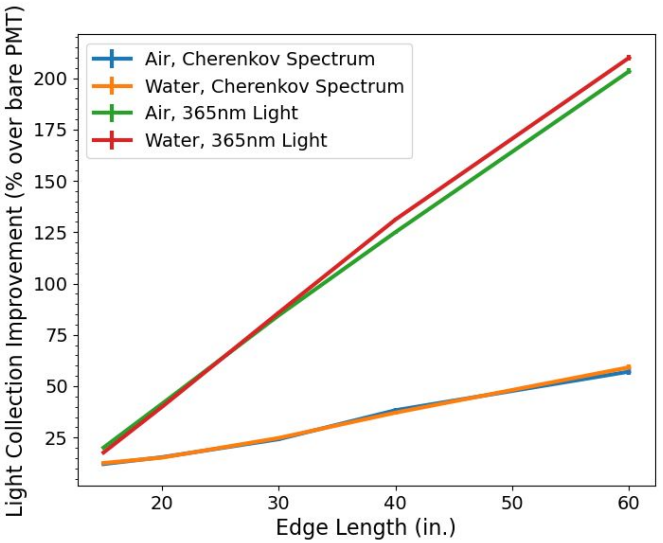
Goal: Simulating light collection efficiency of a wavelength shifting plate for inclusion in a large-scale water-Cherenkov detector.

- Monte Carlo model of photon behavior in the plate built in a Geant4 framework
- Model validated against experimental data
- Simulations used to predict behavior of wavelength shifting plates of various sizes, in various media, exposed to different light sources



Reflector	Light Increase	
	Experimental	Simulated
Yes	7.4 ± 0.7%	7.1 ± 0.2%
No	-0.08 ± 0.7%	-1.2 ± 0.2%
Yes & using Optical Grease	16.2 ± 0.7%	16.2 ± 0.2%





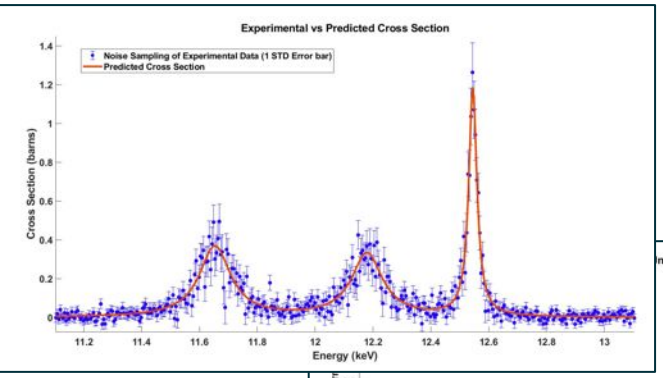
AI/ML-based Tool for Automated Resonance Identification (ATARI)

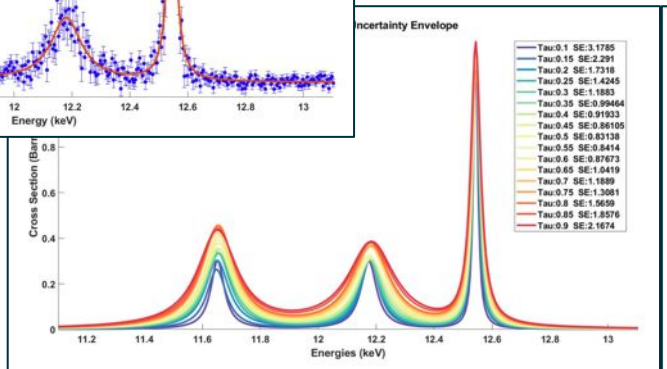
Supports NP-ND

UTK Student: Noah Walton
UTK Advisor: Dr. Vladimir Sobes
ORNL Mentor: Dr. Jesse Brown

NNSA-Relevant Outcomes

Produce quantitative and defendable uncertainty estimates which will be used to calculate confidence intervals for predictive radiation transport modeling for all NNSA applications.





Autonomous Design of Nuclear Measurement Systems

Supports RD and NMS

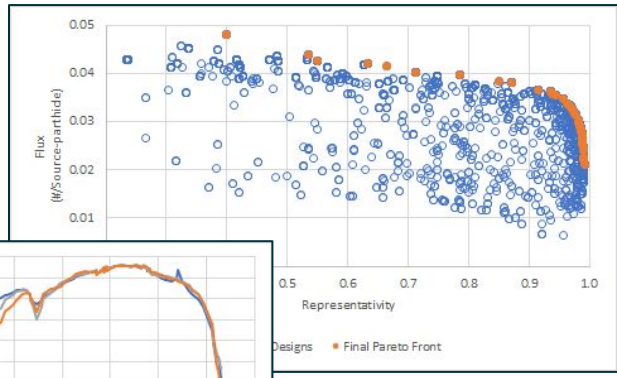
UTK Student: Alex Depillis
UTK Advisor: Dr. Vladimir Sobes
LANL Mentor: Dr. Jesson Hutchinson

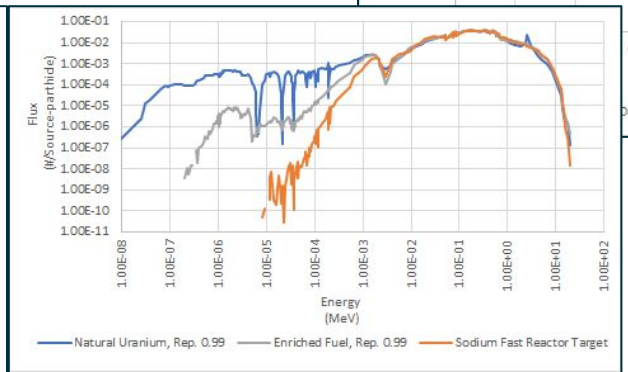
NNSA-Relevant Outcomes

An AI optimization algorithm is able to improve the performance of measurement systems by systematically changing their design.

Dr. Sobes

Dr. Bogetic





Neutron Spectra Tailoring Optimization for Exascale Computing

Supports NP-ND and NCE-NE

Ph.D. Student: Austin Williams
Faculty Advisor: Dr. Sandra Bogetic

LANL Mentor: Dr. Jeffrey Favorite
ORNL Mentor: Dr. Rike Bostelmann

Goal: Expanding Optimization Metaheuristic methodology for Energy Tuning Assemblies (ETA) design with AI/ML and GPU Monte Carlo capabilities, by developing:

- Optimization algorithm to take into account uncertainty in the nuclear data (neutrons and photons)
- New framework (alternative to COEUS) for GNOWEE to include alternative transport codes (MCNP, SCALE, etc.), and GPU based MC
- ETA optimization design capabilities for Criticality Experiments, source driven multiplication systems and designs for facilities as NIF and HFIR

Work performed in the Fall ‘21 and Spring ‘22 semester by the student:

- Creating a “toolkit” that has UQ capability using the sandwich rule for eigenvalue and fixed-source problems
- Started developing AI to use with GNOWEE for systems optimized to have low uncertainty

Quantitative Imaging

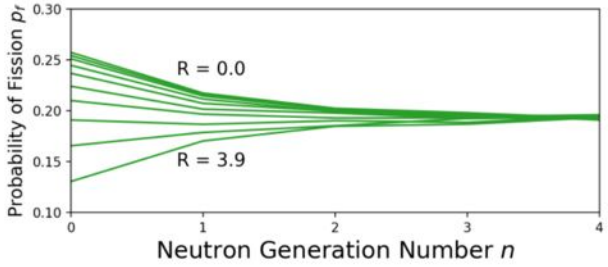
Quantitative, Real-time Associated Particle Imaging

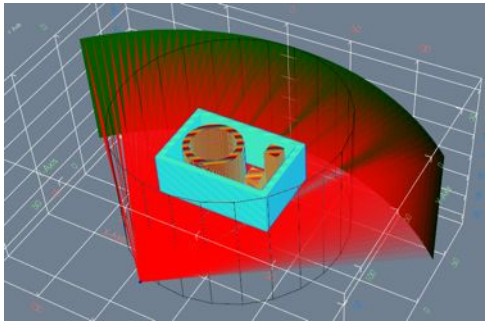
Supports RD

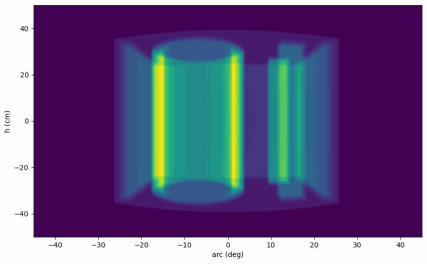
UTK Student: Aaron Nowack
UTK Advisor: Dr. Jason Hayward
ORNL Mentor: Dr. Paul Hausladen

NNSA-Relevant Outcomes

Extend point kinetics framework appropriate for associated particle imaging to produce real-time, quantitative estimates of nuclear material properties







Quantitative Gamma Imaging of Uranium

Supports RD

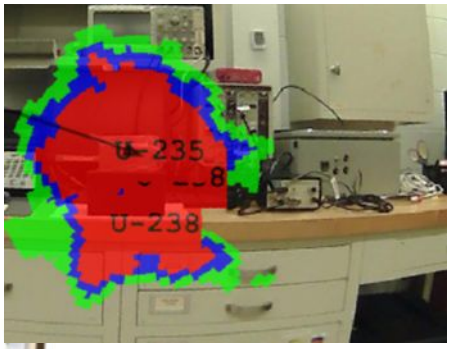
UTK Student: Jonathan Mitchell
UTK Advisor: Dr. Jason Hayward
ORNL Mentor: Dr. K. Schmidtt

NNSA-Relevant Outcomes

Produce quantitative estimates of nuclear material properties from combined Compton and coded-aperture imaging of kg quantities of uranium as data is collected

Dr. Hayward

THE UNIVERSITY OF TENNESSEE KNOXVILLE



OAK RIDGE National Laboratory

Reactor and Radiation Monitoring

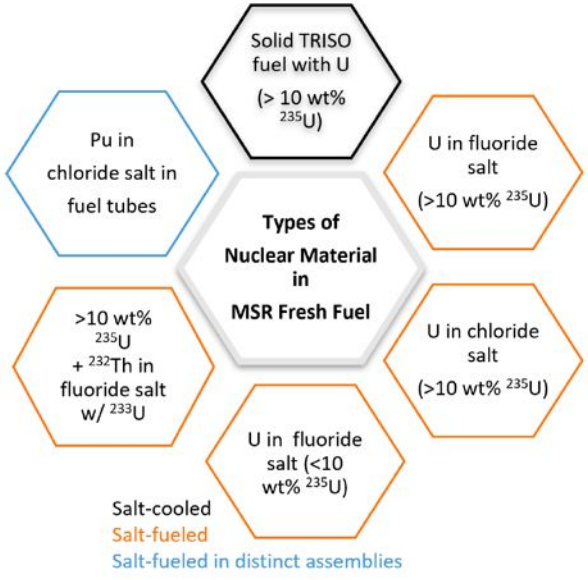
Liquid-Fueled Molten Salt Reactor Monitoring System

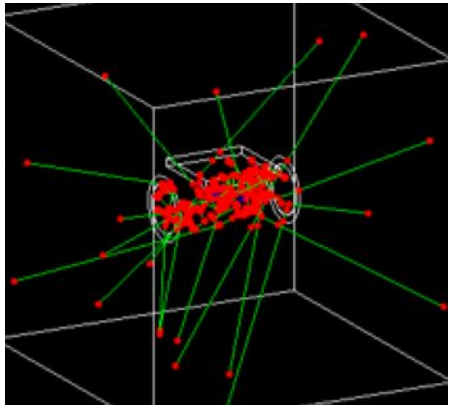
Supports NCH-NE and RD

UTK Student: Karen Hogue
UTK Advisor: Dr. Jason Hayward
ORNL Mentor: Dr. Louise Evans

NNSA-Relevant Outcomes

Design a proof-of-concept feed monitoring system to account for and quantify fertile and fissile material in salt additions to a liquid-fueled molten salt reactor





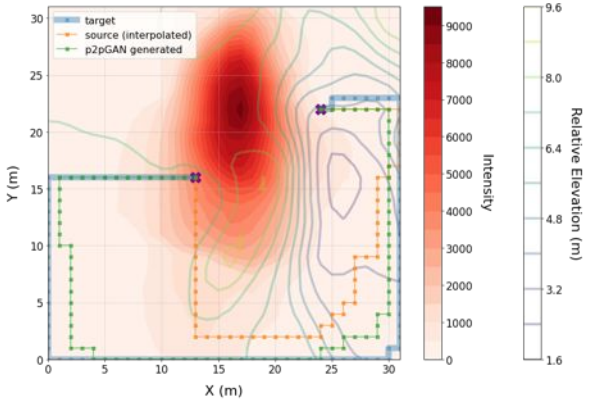
Wide-area Sensor Networks for Radiation Monitoring

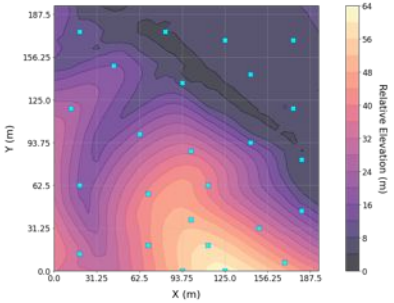
Supports RD

UTK Student: David Raji
UTK Advisor: Dr. Jason Hayward
BNL Mentor: Dr. Ren Cooper

NNSA-Relevant Outcomes

Design wide-area sensor networks and multi-objective optimization for environmentally-distributed radiation source terms; path planning, positioning sensors



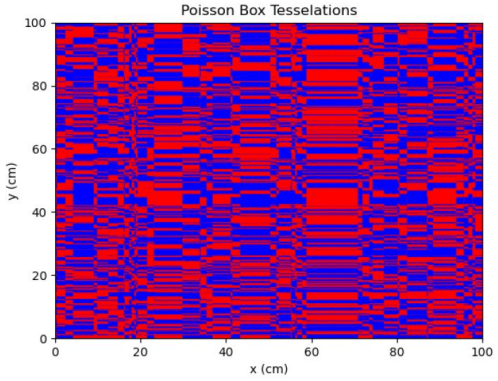


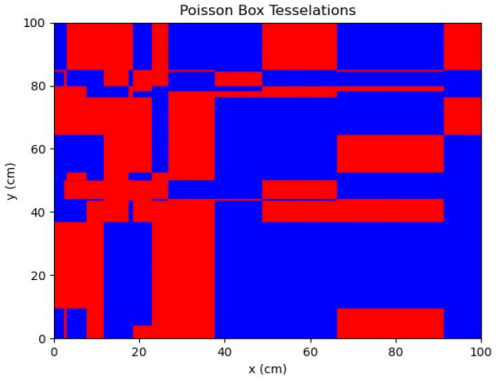
Radiation Transport in Stochastic Media and Nuclear Signatures in Nonproliferation

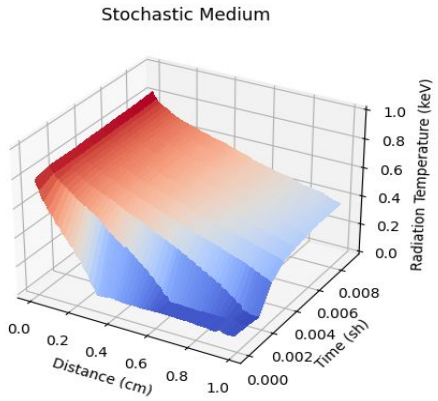
Supports NP-ND and RD

Student: Dominic Lioce - Undergraduate Fellow UNM (2021-22)
Graduate Fellow UCB (Fall 2022)
Faculty Advisor: Anil K. Prinja (UNM)
Laboratory Mentor: Patrick Brantley (LLNL)

- Thermal radiation transport in turbulent material mixtures presents a forefront challenge to the national lab mission: ICF capsule experiments, weapons performance, explosive fireball modeling.
- Current radiation transport capabilities cannot adequately resolve subgrid processes associated with turbulent fluid-solid material mixtures.
- Robust stochastic material treatments and accurate radiation transport solutions will advance radiation-hydrodynamics models in national lab codes.







Real-time Feature Selection and Classification

Supports RD

Ph.D. Student: John Leland

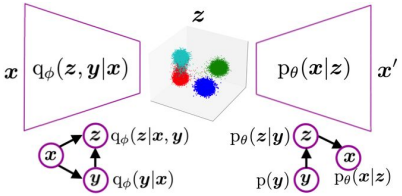
Starting in Fall 2022

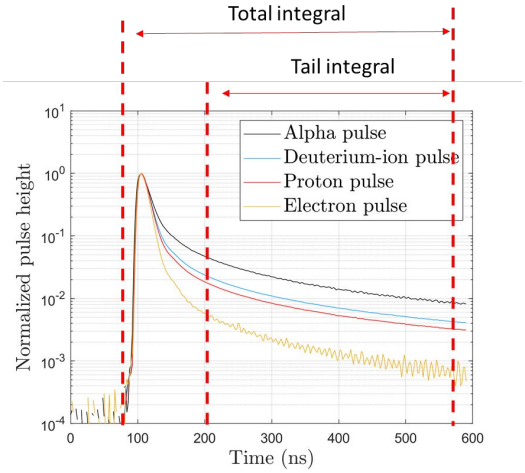
Faculty Advisor: Dr. Angela Di Fulvio

SNL Mentor: Dr. Zoe Gastelum

Goal: We propose to develop adaptive feature-selection algorithms capable of selecting domain-relevant features while not limiting the number of data labels.

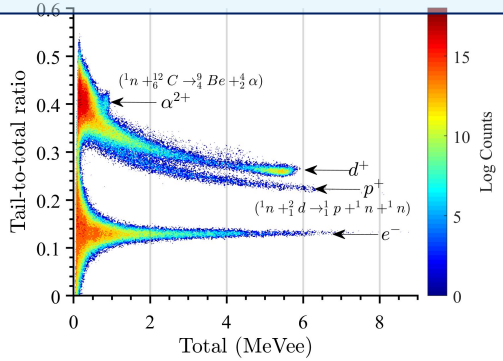
- Applicable to 1-D and 2-D data and hybrid streaming data sets from multiple domains
- Example application to pulse shape discrimination (PSD) in radiation detection:
  - No need to optimize the discrimination of the PSD for each data set
  - To be implemented on open-FPGA digitizers for online application



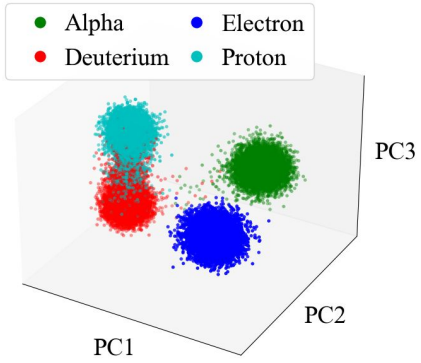


Template pulses with different delayed fluorescence

14.1 MeV neutrons detected by a deuterated stilbene crystal



Charge-integration PSD



Machine-learning PSD

Training Neural Networks for Neutron Spectrum Unfolding

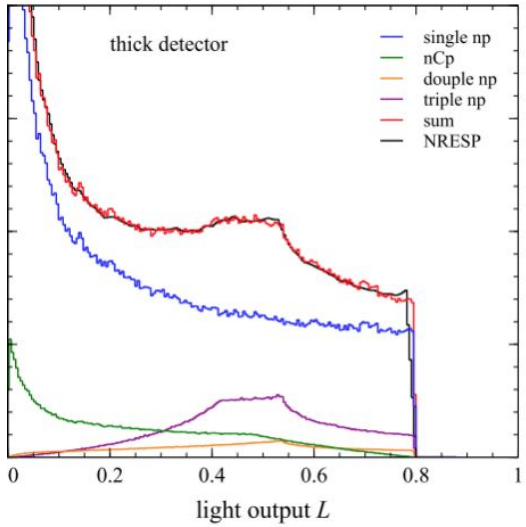
Supports NP-ND and RD

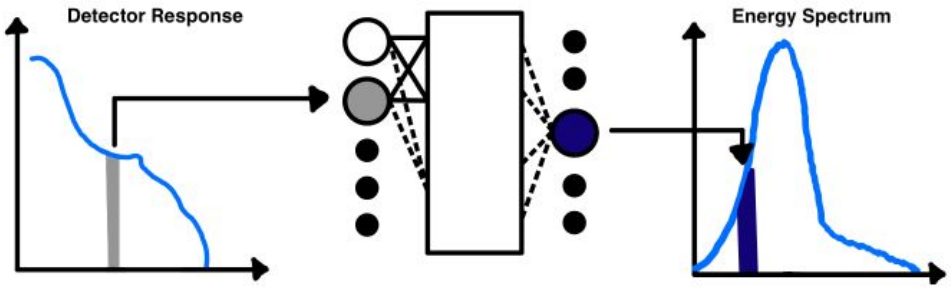
Undergradate Student: James McGreivy (UCB)
Faculty Advisor: Dr. Juan Manfredi (AFIT)
LLNL Mentor: Dr. Daniel Siefman

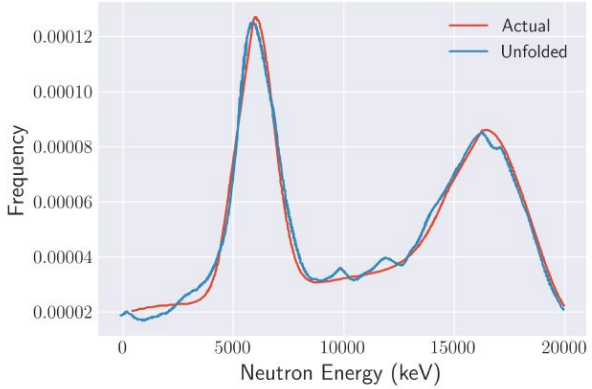
Goal: Unfolding neutron energy spectra with machine learning and minimal *a priori* information

- Geant4 model of organic scintillator with updated proton/carbon light yields from recent measurements
- Simulation-generated detector responses as training data for neural network
- Recent presentation at ANS 2022 Student Conference

For more details see Poster #14







Future projects: *Natural language processing for nuclear science literature (LBNL), Energy spectrum tuning with ATHENA for radiation effects testing (LLNL), characterizing effluents from CANDU reactors (ORNL)*

NSSC Success Story
Dr. Sandra Bogetic

Ph.D.
UCB, 2020

Postdoc
LLNL, 20/21

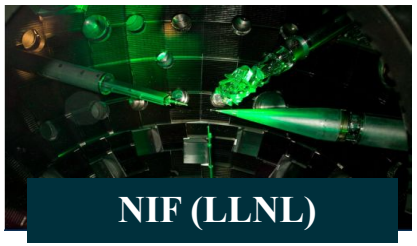
Asst. Prof.
UTK, 2021

Development of neutron spectra tailoring software package and its experimental validation and verification for neutron tailoring experiments at the NIF. Spectral shaping methods can expand the capabilities of existing facilities to cover new mission spaces - neutron cross section measurements, detector characterization, radiation damage studies, BNCT, etc.

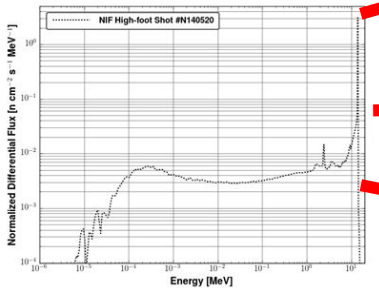
Faculty Advisor:
Dr. Jasmina Vujic

Lab Mentors LLNL:
Dr. L. Dauffy
Dr. D. Shaughnessy
Dr. C. Yaemans

Collaborators:
Dr. L. Bernstein
Dr. J. Bevins



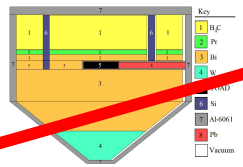
Neutron Sources Available, NIF

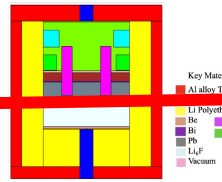


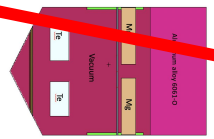
Experimental validation of ETAs using 14 MeV NIF beams and sets of activation foils

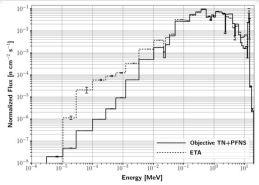
Energy Tuning Assembly (ETA)

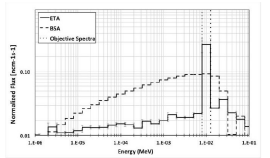
Tailored Spectra to match Objective Spectrum

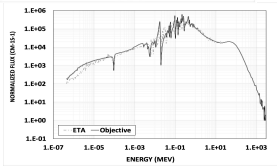












Acknowledgements

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