Scattering, Transport and Shielding

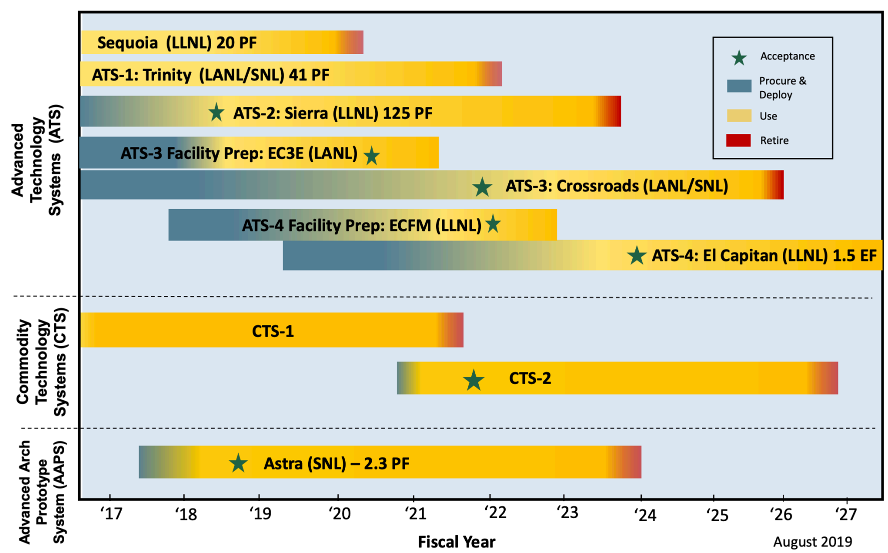
ASC Codes at LLNL and LANL
Jon Dahl (LANL)
•**Reactor Physics Codes**
Will Wieselquist (ORNL)
•**Naval Codes, KAPL and Bettis**
Michael Zerkle (NNL)

•**Thermal Scattering**
Ayman Hawari (NCSU)
•**Fast Elastic**
Yaron Danon (RPI)
•**Fe Scattering with Pulsed Spheres**
Carl Brune (Ohio U)

ASC Program Status and Needs - Jon Dahl

- Codes are being ported to massively parallel, HPC architectures.
  - V&V required at all stages: evaluations, processed libraries, transport methods.
    - SN and Monte Carlo codes are complimentary in crushing the bugs.
  - Tensions between speed and fidelity:
    - ML techniques leading to physics-on-the-fly may improve this situation.
- Transport code developers recognize the need for:
  - High-quality, well-tested nuclear data -- including new physics!
  - New algorithms, shared between transport codes and other parts of the pipeline.
  - Stronger partnerships within the nuclear data community.

Code	Description	Lab	POC
PARTISN	Particle Transport, Multigroup, Deterministic SN	LANL	Jon Dahl
Ardra	Particle Transport, Multigroup, Deterministic SN	LLNL	Teresa Bailey
MCATK	Monte Carlo, Combinatorial Geometry, Continuous Energy	LANL	Travis Trahan
Mercury	Monte Carlo, Combinatorial Geometry, Multigroup (hybrid) and Continuous Energy	LLNL	Patrick Brantley
MCNP	Monte Carlo, Combinatorial Geometry, Continuous Energy and Multigroup	LANL	Michael Rising



Nuclear Data used by SCALE Reactor Physics Codes - Will Wieselquist

ENDF/B
Physics data
Thermal scattering law, resonance data, energy distributions, fission yields, decay constants, decay energy

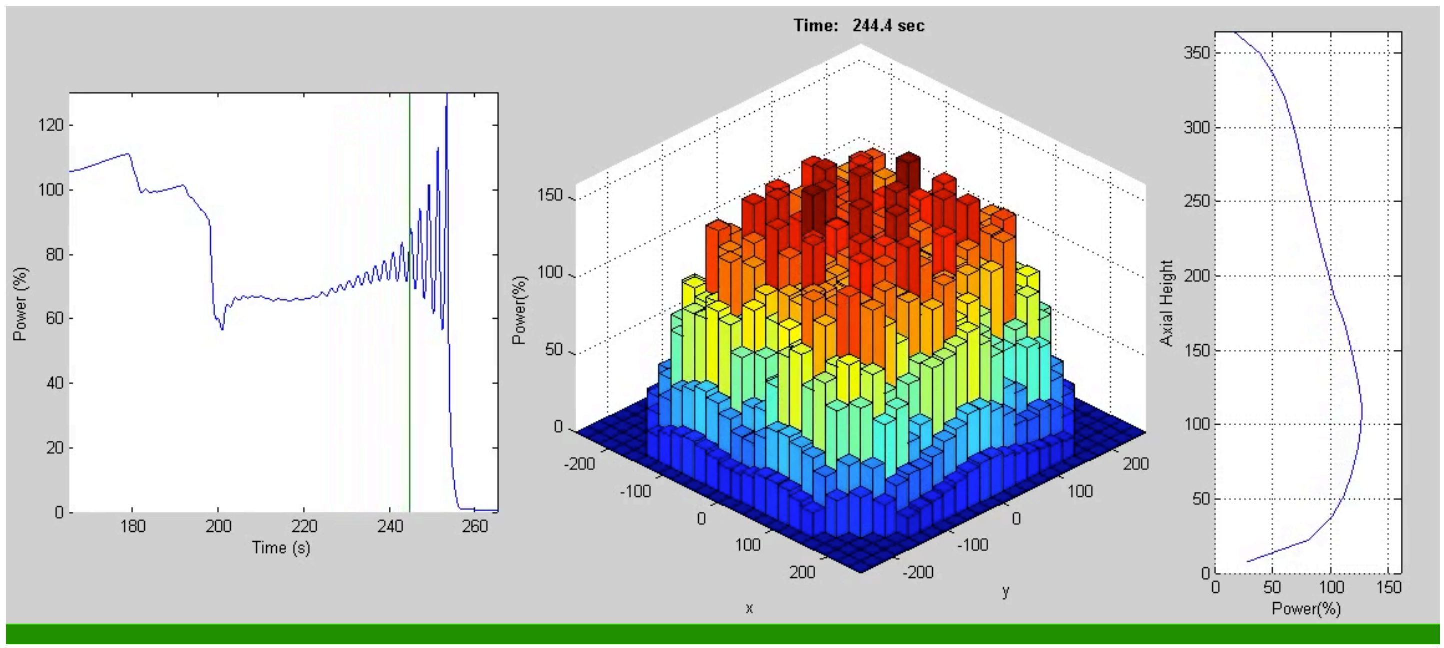
Activation (JEFF)
Isomeric cross sections, activation reactions

Kinetics
nuclide-specific beta, neutron precursor data

Energy Release
nuclide-specific energy per capture/fission

Mass (NIST)
natural abundance, atomic mass

- **Focus on ENDF/B completeness first**
  - SCALE would replace JEFF with ENDF/B activation
    FOA: *Model Oriented Nuclear Data Library (MONDL)*
  - Kinetics data is extremely relevant for advanced reactors: **High-priority?**
- **Improve decay, fission product yield, activation data.**
  - Improve fission gamma, capture gamma, Kerma
  - Is energy resolution for FPYs sufficient for advanced reactor applications?



NNL Transport Code - MC21

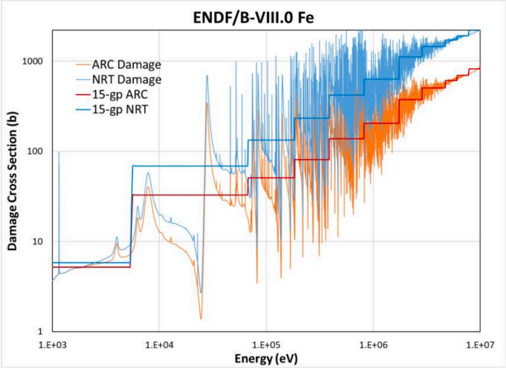
Michael L. Zerkle, Senior Advisor

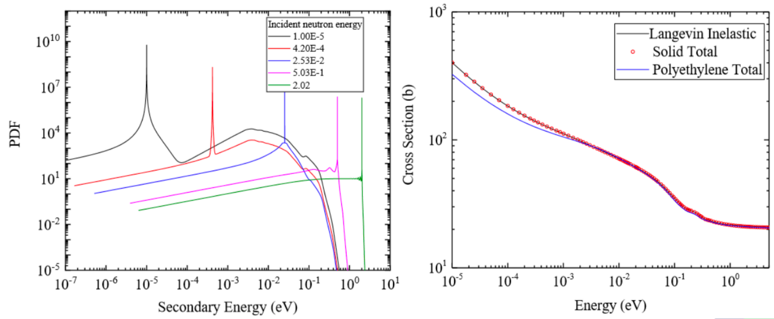
NNL Nuclear Data Needs

- Light water reactor materials
  - Zirconium, Hafnium
  - U-236 & Np-237 neutron capture
- Radiation shielding
  - Fe-56 cross sections
  - Scattering angular distributions
- Long-lived fission products (fission product credit)

Mo-95	Tc-99	Ru-101	Rh-103
Cs-133	Cs-135	Pr-141	Nd-143
Nd-145	Sm147	Sm-145	Sm-150
Sm-152	Eu-153		

- Irradiation damage (DPA)
- Thermal scattering law data

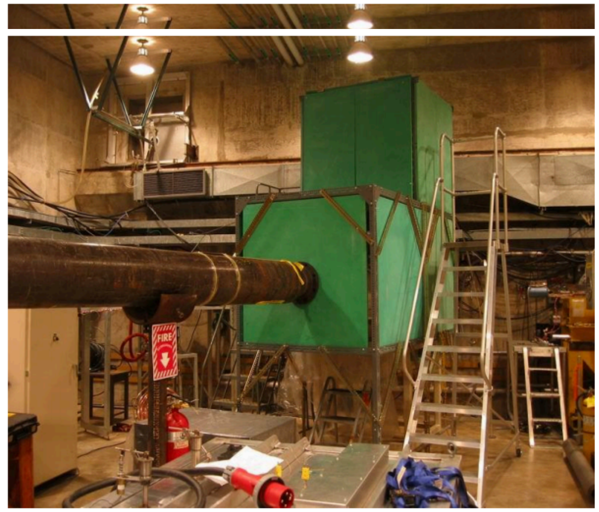


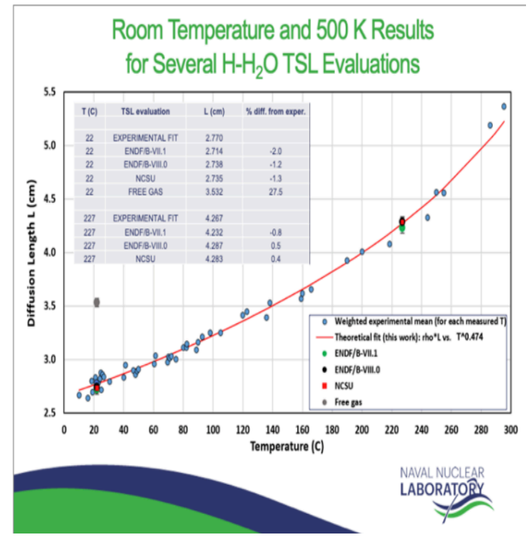


TSL for heavy paraffinic oil (C. A. Manring, PHYSOR-2018)

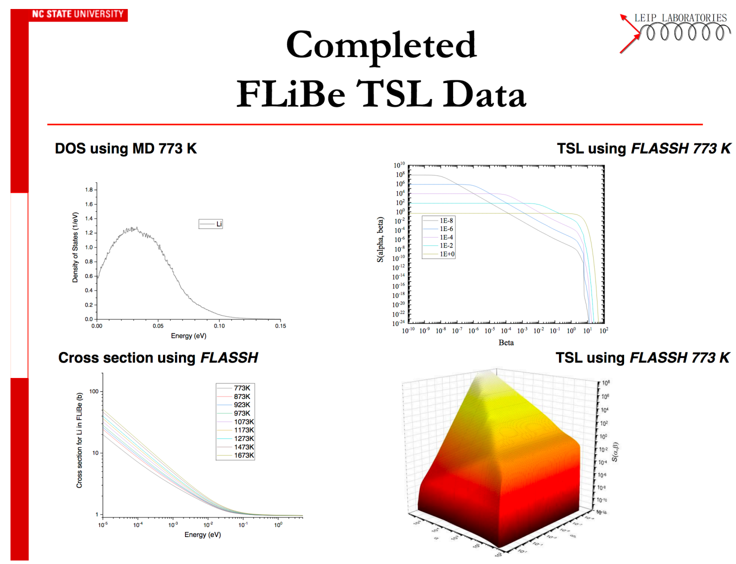
Thermal Neutron Scattering Law Methods and Evaluations

Ayman I. Hawari



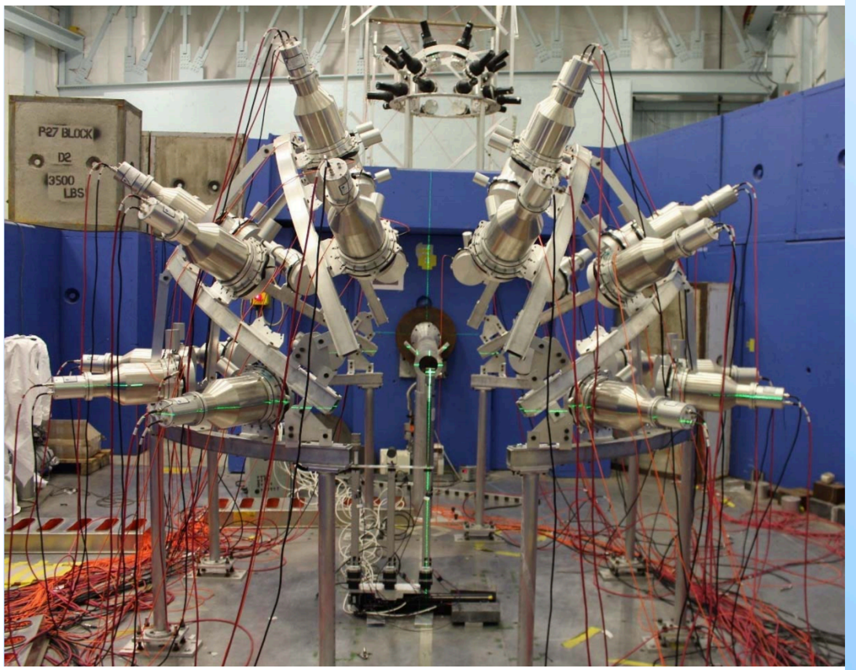


Material	ENDF Library Name	Evaluation Basis	Institution
Beryllium metal	tsl-Be-metal.endf	DFT/LD	NCSU
Beryllium oxide (beryllium)	tsl-BeinBeO.endf	DFT/LD	NCSU
Beryllium oxide (oxygen)	tsl-OinBeO.endf	DFT/LD	NCSU
Light water (hydrogen)	tsl-HinH2O.endf	MD	CAB
Light water ice (hydrogen)	tsl-HinIceIh.endf	DFT/LD	BAPL
Light water ice (oxygen)	tsl-OinIceIh.endf	DFT/LD	BAPL
Heavy water (deuterium)	tsl-DinD2O.endf	MD	CAB
Heavy water (oxygen)	tsl-OinD2O.endf	MD	CAB
Polymethyl Methacrylate (Lucite)	tsl-HinC5O2H8.endf	MD	NCSU
Polyethylene	tsl-HinCH2.endf	MD	NCSU
Crystalline graphite	tsl-graphite.endf	MD	NCSU
Reactor graphite (10% porosity)	tsl-reactor-graphite-10P.endf	MD	NCSU
Reactor graphite (30% porosity)	tsl-reactor-graphite-30P.endf	MD	NCSU
Silicon carbide (silicon)	tsl-CinSiC.endf	DFT/LD	NCSU
Silicon carbide (carbon)	tsl-SiinSiC.endf	DFT/LD	NCSU
Silicon dioxide (alpha phase)	tsl-SiO2-alpha.endf	DFT/LD	NCSU
Silicon dioxide (beta phase)	tsl-SiO2-beta.endf	DFT/LD	NCSU
Yttrium hydride (hydrogen)	tsl-HinYH2.endf	DFT/LD	BAPL
Yttrium hydride (yttrium)	tsl-YinYH2.endf	DFT/LD	BAPL
Uranium dioxide (oxygen)	tsl-OinUO2.endf	DFT/LD	NCSU
Uranium dioxide (uranium)	tsl-UinUO2.endf	DFT/LD	NCSU
Uranium nitride (nitrogen)	tsl-NinUN.endf	DFT/LD	NCSU
Uranium nitride (uranium)	tsl-UinUN.endf	DFT/LD	NCSU



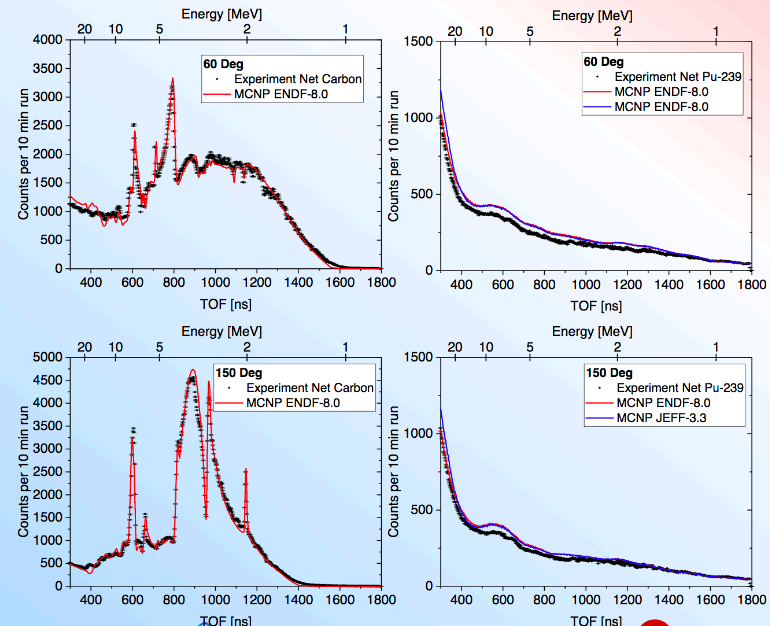
Experiments with Neutron Induced Neutron Emission

Y. DANON



^{239}Pu results

- **The ^{239}Pu neutron emission yield is similar in shape to the ^{235}U yield**
- **The simulations are higher than the experimental data.**
- **Careful attention to the encapsulation of this sample**



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Copper KeV scattering measurement

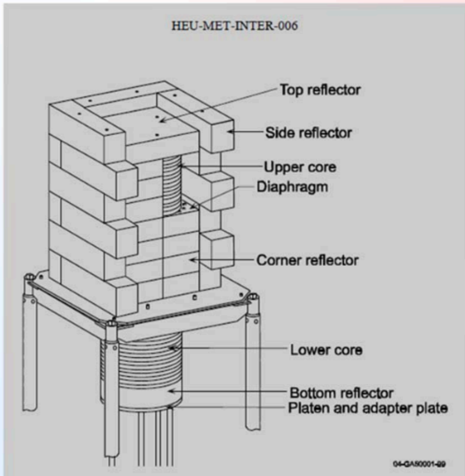


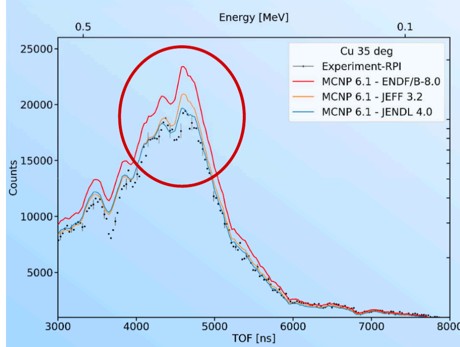
Figure 6. Schematic Cutaway of Zeus before Assembly.

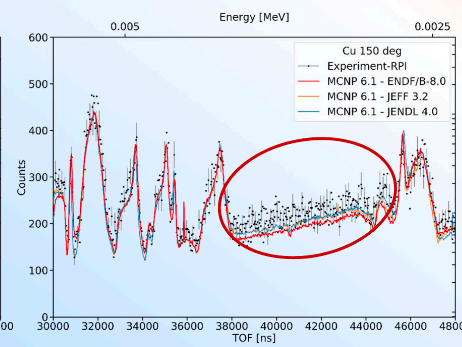
Motivation – Zeus benchmark

- Intermediate energy benchmark with HEU and graphite plates and a copper reflector
- Discrepancies in the critical benchmark
- Possible issues in the angular distribution

Copper scattering closer look

- Closer look shows some discrepancies between experiment and evaluations at the low and high keV energy range
  - Near 250 keV differences between evaluations at some angles
  - Near 3 keV the evaluations seem low at all angles





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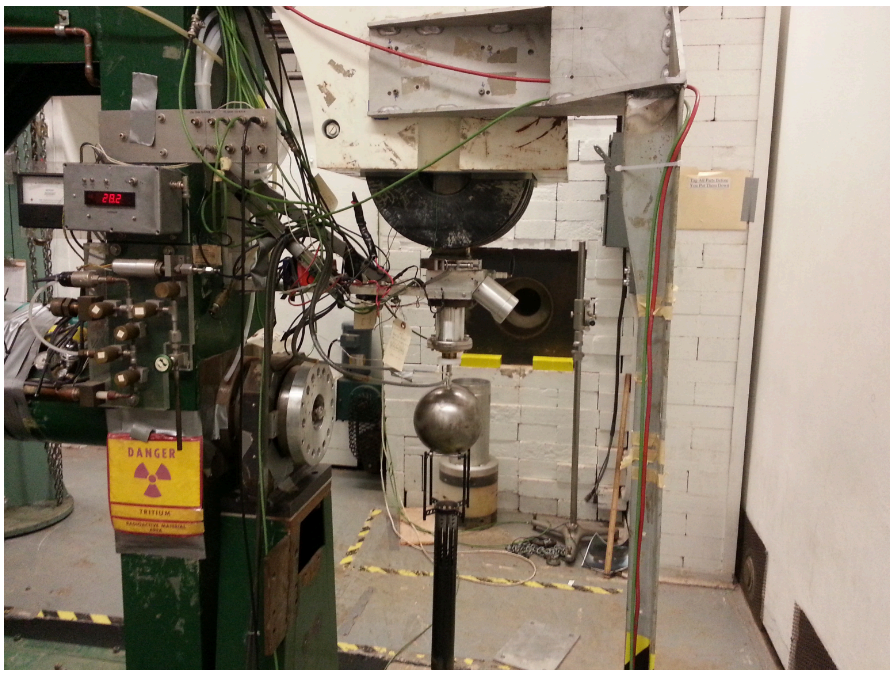
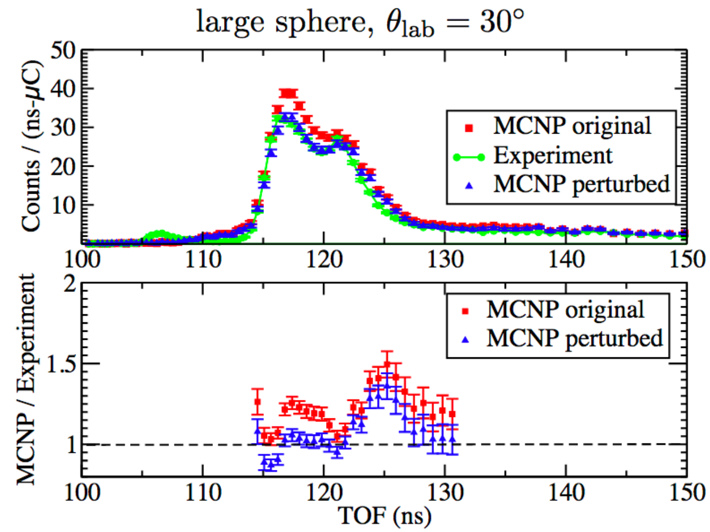
Neutron Transport Studies in Fe using Pulsed Spheres

Carl R. Brune



Adjusting the Simulation



- Adjusting the ENDF/BVII.1 ^{56}Fe elastic cross section down by 10%, and the inelastic up by 15% (keeping the total cross section constant), leads to a much better description of the experimental data.
- Note that systematic errors in the data are estimated to be 3-5%.

Scattering, Transport and Shielding

- Code improvements: speed, data size, what data is needed (tension between fidelity and code performance).
- Machine learning opportunity? Compression of thermal scattering data, scattering angular distributions, etc.
- Improve capture γ data, full cascades needed (instead of averages)? Better γ energy/multiplicity data. More input from applications needed (detectors, DP, reactors…)
- Getting Kerma right
- Is the energy resolution for fission product yields sufficient for advanced reactors?

Scattering, Transport and Shielding

- Shielding has been neglected, important for costs (time and money) for applications
- Lack of good shielding benchmarks (impacting nuclear data, ^{56}Fe)
- Quasi-differential, quasi-integral (pulsed spheres) measurements are important, pulsed neutron die-away
- Not every benchmark/validation effort needs to be gold standard to inform nuclear data
- University involvement, lab/university collaborations

  Feeds talent pipeline