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.

<table>
<thead>
<tr>
<th>Code</th>
<th>Description</th>
<th>Lab</th>
<th>POC</th>
</tr>
</thead>
<tbody>
<tr>
<td>PARTISN</td>
<td>Particle Transport, Multigroup, Deterministic SN</td>
<td>LANL</td>
<td>Jon Dahl</td>
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<td>Ardra</td>
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<td>LLNL</td>
<td>Teresa Bailey</td>
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<td>MCATK</td>
<td>Monte Carlo, Combinatorial Geometry, Continuous Energy</td>
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<td>Travis Trahan</td>
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<td>Mercury</td>
<td>Monte Carlo, Combinatorial Geometry, Multigroup (hybrid) and Continuous Energy</td>
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<td>Patrick Brantley</td>
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<td>MCNP</td>
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<td>LANL</td>
<td>Michael Rising</td>
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</tbody>
</table>
• 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 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

<table>
<thead>
<tr>
<th>Material</th>
<th>ENDF Library Name</th>
<th>Evaluation Basis</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Beryllium metal</td>
<td>tsi-Be-metal.endf</td>
<td>DFT/LD</td>
<td>NCSU</td>
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<td>Beryllium oxide (beryllium)</td>
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<td>Beryllium oxide (oxygen)</td>
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<td>MD</td>
<td>CAB</td>
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<td>Heavy water (hydrogen)</td>
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<td>Reactor graphite (30% porosity)</td>
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<td>Silicon carbide (carbon)</td>
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<td>NCSU</td>
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<td>Silicon dioxide (alpha phase)</td>
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<td>Silicon dioxide (beta phase)</td>
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Completed FliBe TSL Data
Experiments with Neutron Induced Neutron Emission

Y. Danon

- The $^{239}$Pu neutron emission yield is similar in shape to the $^{238}$U yield.
- The simulations are higher than the experimental data.
- Careful attention to the encapsulation of this sample.
Copper KeV scattering measurement

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
Neutron Transport Studies in Fe using Pulsed Spheres

Carl R. Brune

Adjusting the Simulation

large sphere, $\theta_{\text{lab}} = 30^\circ$

- 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 $\gamma$ data, full cascades needed (instead of averages)? Better $\gamma$ 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