CoNDERC
White paper & status

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The CoNDERC project  2018 - 2024

• The purpose of the project entitled Compilation of Nuclear Data Experiments for Radiation Characterisation is to provide and transfer into technology the experimental integral radiation information that can be used as part of the Validation and Verification processes of nuclear model and code systems, and to provide various schema to perform the V&V processes

• The aim is to provide all experimental methods, protocols, know how and calculational information in such computational ways that it can easily, seamlessly and rapidly be deployed in support of the many scientific systems that need them: model, inventory, transport, material sciences, Multiphysics code systems,…
Key elements

• Identify and compile a set of radiation characterization benchmarks (both computational and experimental) that includes spectral indices, reaction rates, decay heat, resonance integral, particle emissions, radiations source terms

• Assess and review the data, including quantification of uncertainties, then compile the data into computer format for dissemination

• Perform simulations of each benchmark cases with a suitable code system and nuclear libraries and produce a database/repository of the necessary input files to repeat those simulations for other settings
Lexical semantics: R&V&V

**Regression, Unit test:** with save outputs and results files, the current execution is compared to the above templates

**Verification:** analytical and semi-analytical solutions to an equation (Boltzmann, Bateman, Schrödinger, Dirac, etc.) may exist, to ensure that the simulation tool is solving the correct equation

**Validation:** combination of code, schema and processed nuclear data to produce results comparable to observables
Prompt, delayed, decay heat
   Integral power, power density, power deposition,..

Reaction rates, emitted particles rates and spectra
   Dose, particle fluence, dpa, activity, gas production, activation,
   depletion, breeding, radiation,..

Fission yields: cumulative and spontaneous, radionuclides yields
   Fission products, residual nuclei, transmutation,..
Benchmarks experiments

1. JAEA time dependent Fusion Neutron Source decay heat experiments (73 materials, 2/3 irradiation campaigns)
2. UCB DT-source NIF concrete (gamma dose rate)
3. Li(p,n) (up to 150 MeV) angular neutron yields
4. Fission pulse decay heat experiments ★
5. Fission delayed neutron experiments
6. Selected criticality experiment with reaction rates from ICSBEP, IRPhEP, REAL-IAEA, … ★
7. Experimental MACS from ASTRAL & KADoNiS ★

black to be done
blue done, work in progress
★ in this talk
Benchmarks experiments

8. Spectrum-averaged xs in reference spectra (e.g. Cf-252, ACCR, LR-0, etc.)
9. Resonance integrals (based on the Atlas, other experiments, compilation)
10. Resonance integrals and thermal xs based on kayzero database for NAA
11. Time dependent gamma measurements from PNNL (fission) and UK (fusion)
12. (γ,n) experimental data (Laser-Compton scattering from TUNL and New Subaru)
13. Integro-differential benchmark (from EXFOR or otherwise)
14. Shielding and leakage benchmarks from SINBAD (including models) ★
15. Reference spectra for computational analysis: 122 ★

black to be done
blue done, work in progress
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Compilation of Nuclear Data Experiments for Radiation Characterisation (CoNDERC)

The purpose of the CoNDERC project is to transfer into technology the experimental integral radiation information that can be used as part of the Validation and Verification processes of nuclear model and code systems, and to provide various schema to perform the V&V. Under the auspices of the IAEA Nuclear Data Section, individuals and institutions are assembling several of databases and code infrastructures based on their own V&V activities mainly associated with inventory, activation-transmutation, source term and radiation shielding R&D.
CoNDERC contributors

• A handful of experts and national laboratory generous contributions
Spectra

- The majority of neutron-application spectra stem from light-water assemblies, mock-ups, piles or reactors where the integral responses are strongly, if not solely, influenced by the energy ranges of the fission spectra, resonance range and thermal Maxwellian.

- Fusion spectra that have been obtained from magnetic confinement (MCF) or inertial confinement fusion (ICF) simulation and present typical D-D 2.5 MeV, or D-T 14 MeV peaks sometimes accompanied by a higher-energy tail, but also showing rather different slowing-down profiles.

- Accelerator-driven beam secondary spectra are important in their role in nuclear sciences, nuclear observables, materials research and medical applications.
Spectra

• 122 spectra from all over the World, all types, piles, NPPs, research reactor, spallation, FBRs, Maxwellian, Am-Be, at temperatures,

• one gamma from LMJ flash

• plots and numerical data
Spectra shape shifting
Spectra shape shifting

Reaction Rates below the Unresolved and Resolved Resonance Range are strongly impacted!!
Fission pulsed events

- 29 complete experimental datasets from the World over in one place
- Scobie 1971
- ...30 years
- Ohkawashi 2001
Experimental MACS from ASTRAL # KADONIS

- Second stage of KADONIS upgrade, 78 traditional + 58 activations (136)

- The $^{197}$Au($n,\gamma$) standard!! @$kT=30$ keV changed from 582±9 mb (Kadonis 0.3 and earlier) to 612±6 mb

https://exp-astro.de/astral/
Shielding

- Upon specific request of member states, beyond Keff and radiation shielding benchmark are now also considered in CoNDERC.
- Building from the existent: IAEA consultancy achievements, generous contributors and moving forward ensemble.
- MCNP6®, TRIPOLI-4® and OpenMC input decks have been developed for:
Shielding: e.g. Oktavian

• Computational
  - experimental data
  - expert crafted Monte Carlo input decks
  - validation Monte Carlo outputs
  - for different libraries

• Documentation
  - open litterature
  - open declassified report
  - figures
Shielding

- Oktavian
  Co X
  Zr ~

- Log-Log could be deceptive

- 10 to 50% !!
ICSBEP & reaction rates: beyond $K_{\text{eff}}$

• International Criticality Safety Benchmark Evaluation Project (ICSBEP)
• International Reactor Physics Experiment Evaluation Project (IRPhEP)
• Compile critical and subcritical benchmark experiment data into a standardized format to validate simulation tools and cross-section libraries
• In addition to criticality some benchmark evaluations also contain spectral indices and measured reaction rate data
• Another class of experimental data that can provide additional qualification of the underlying nuclear data and simulation tools
ICSBEP & reaction rates: beyond $K_{\text{eff}}$

- Good $K_{\text{eff}}$ C/E with small uncertainty
- More troubled spectral indices C/E
- Right for the wrong reasons?

![Graph showing C/E values for different benchmarks and spectral indexes](http://www.psi.ch/stars/2017.11.22/STARS/RD41-(15/16))

Example with different benchmarks

- Many benchmarks, all together: 17 quantities (12 $K_{\text{eff}}$, 5 spectral indexes)

Courtesy D. Rochman (PSI)
ICSBEP and IRPhEP Handbooks

- MCNP6®, TRIPOLI-4® and OpenMC input decks with reaction rate (spectral index) or pin power data

<table>
<thead>
<tr>
<th>Legacy Assembly Name</th>
<th>ICSBEP Benchmark Identifier</th>
</tr>
</thead>
<tbody>
<tr>
<td>Godiva</td>
<td>HEU-MET-FAST-001</td>
</tr>
<tr>
<td>Flattop-25</td>
<td>HEU-MET-FAST-028</td>
</tr>
<tr>
<td>Jezebel</td>
<td>Pu-MET-FAST-001</td>
</tr>
<tr>
<td>Flattop-Pu</td>
<td>Pu-MET-FAST-006</td>
</tr>
<tr>
<td>Thor</td>
<td>Pu-MET-FAST-008</td>
</tr>
<tr>
<td>‘dirty’ Jezebel</td>
<td>Pu-MET-FAST-002</td>
</tr>
<tr>
<td>Big-10</td>
<td>IEU-MET-FAST-007</td>
</tr>
<tr>
<td>Babcock &amp; Wilcox 15x15</td>
<td>LEU-COMP-THERM-008</td>
</tr>
<tr>
<td>Dimple-LWR</td>
<td>LEU-COMP-THERM-055</td>
</tr>
<tr>
<td>Jezebel-23</td>
<td>U233-MET-FAST-001</td>
</tr>
<tr>
<td>Flattop-23</td>
<td>U233-MET-FAST-006</td>
</tr>
<tr>
<td>Pu BR-1 core</td>
<td>FUND-IPPE-FR-MULT-RRR-001</td>
</tr>
</tbody>
</table>
Running strategy

• up to six MCNP6® “kcode”

• 50 million (50M) and 250 million (250M) active neutron histories
  - 5100 cycles (100 warmup cycles and 5000 active cycles) with either 10,000 or 50,000 neutrons per cycle
  - remaining jobs were run with 50 warmup cycles and 2,500,000 neutrons per cycle

• These jobs were stopped/continued after 450, 2050, 4050 and 10050 cycles, for a total of 1 billion (1B), 5 billion (5B), 10 billion (10B) and 25 billion (25B) active histories, respectively

• For a given f4 tally we also specify an identical *f4 tally. Division of the *f4 tally result by the f4 tally result yields the average energy for that reaction <E>
PMF1 (Jezebel Rev 4) - MCNP6® & ENDF/B-VIII.0

- Spectral index variation with increasing neutron histories
- 50 million to 25 billion, 25x10^9
- \( \langle E \rangle \) 8.5 MeV – 2%
  deemed acceptable
PMF1 (Jezebel) - MCNP6® & ENDF/B-VIII.0

- Zoom out
- 50 million to 25 billion $25 \times 10^9$
  - $\langle E \rangle$ 8.5 MeV – 2%
  - $\langle E \rangle$ 10.7 MeV - 10%
  - $\langle E \rangle$ 14 MeV - 30%
Jezebel PMF1 central region flux

- Histories x 500
- High tail – sharp decrease
- Low tail – more scattered but has the potential to notably impact capture, fission
- Span 5 decades
## Spectral Indices: Jezebel PMF1

- Shaded area
- Good C/C +/-2%
- C/E divergence -5% to 25% increase with energy

<table>
<thead>
<tr>
<th>Central Region Spectral Index</th>
<th>Measured value</th>
<th>MCNP6® Calculated Average Energy, MeV</th>
<th>MCNP6®</th>
<th>TRIPOLI-4®</th>
<th>C/C</th>
<th>C/E</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMF1 (Jezebel)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$^{238}\text{U}(n,\gamma) / ^{235}\text{U}(n,f)$</td>
<td>0.0677</td>
<td>0.87</td>
<td>0.0644</td>
<td>0.0644</td>
<td>1.01</td>
<td><strong>0.95</strong></td>
</tr>
<tr>
<td>$^{238}\text{U}(n,f) / ^{235}\text{U}(n,f)$</td>
<td>0.2133(23)</td>
<td>3.3</td>
<td>0.2120</td>
<td>0.2122</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>$^{238}\text{U}(n,2n) / ^{235}\text{U}(n,f)$</td>
<td>0.0106</td>
<td>8.5</td>
<td>0.0132</td>
<td>0.0131</td>
<td>0.98</td>
<td><strong>1.25</strong></td>
</tr>
<tr>
<td>$^{237}\text{Np}(n,f) / ^{235}\text{U}(n,f)$</td>
<td>0.9835(140)</td>
<td>2.3</td>
<td>0.9769</td>
<td>0.9776</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>$^{239}\text{Pu}(n,f) / ^{235}\text{U}(n,f)$</td>
<td>1.4609(13)</td>
<td>1.9</td>
<td>1.4273</td>
<td>1.4275</td>
<td>1.00</td>
<td>0.98</td>
</tr>
<tr>
<td>$^{55}\text{Mn}(n,\gamma) / ^{235}\text{U}(n,f)$</td>
<td>0.00235(3)</td>
<td>0.83</td>
<td>0.00282</td>
<td>0.00283</td>
<td>1.02</td>
<td>1.20</td>
</tr>
<tr>
<td>$^{63}\text{Cu}(n,\gamma) / ^{235}\text{U}(n,f)$</td>
<td>0.00989(6)</td>
<td>0.91</td>
<td>0.0101</td>
<td>0.0101</td>
<td>1.01</td>
<td>1.02</td>
</tr>
<tr>
<td>$^{169}\text{Tm}(n,\gamma) / ^{235}\text{U}(n,f)$</td>
<td>0.0931</td>
<td>0.69</td>
<td>0.1061</td>
<td>0.1059</td>
<td>1.02</td>
<td>1.14</td>
</tr>
<tr>
<td>$^{169}\text{Tm}(n,2n) / ^{235}\text{U}(n,f)$</td>
<td>0.00313</td>
<td>10.7</td>
<td>0.00371</td>
<td>0.00375</td>
<td>0.98</td>
<td>1.19</td>
</tr>
</tbody>
</table>
Conclusions

- Live web portal, explicit with graphics, tables, datasets
- Deployable data streams, full download
- V&V codes inputs & outputs
- Experimental information in computer forms
- Safe repository
- Partly accessible through GitHub

- Priority next?
Thank you for your attention!