A new V&V philosophy for fusion nuclear data libraries

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JADE
• Nuclear data libraries and their V&V
• What is JADE?
• The Sphere Leakage benchmark
• JADE architecture and development

Looking ahead
• Our wish list
• Machine Learning
• Summary
JADE
Nuclear data libraries and their V&V

The nuclear data libraries production chain

Experimental points → Theoretical support → Evaluated continuous cross sections → [ENDF 6 format] → Point-wise/multi-group cross sections → [ACE format] → MC Transport codes

It is a complex procedure that require extensive Verification and Validation (V&V)
Nuclear data libraries and their V&V

The need for automation and standardization

- $10^3$ isotopes in a single library
- 1 .ACE file per isotope
- $10^2$ reactions per .ACE file (MT numbers)

$\sim 10^5$ different cross sections to be verified!

Heavy automation is a necessity, which, at the same time, is an opportunity for standardization
Nuclear data libraries and their V&V

The fission bias

Energy range

Different materials and cross sections

Fission rate

Fission products

EUROFER 97

Fusion rate

Tritium production

Activation issues

Heating on superconductive magnets
Nuclear data libraries and their V&V

The fission bias

Integral parameters representative of the entire system that simplifies the V&V process

- complex geometries that need to be fully modelled
- different regions with different needs
- a detailed spatial distribution of tallies is needed

Vast amount of tallies and energy/spatial discretization
What is JADE?

JADE is a python based software that aims to establish itself as a corner stone for a complete and extensive **automated and standardized V&V procedure** for nuclear data libraries, with a special focus towards fusion applications.

**ISSUES**

- Lack of Automation
- Effort Fragmentation
- Lack of Standardization
- Fission Bias
What is JADE?

The organization of the project

Implemented by means of a stage approach and > 1.5 ppy of total effort
What is JADE?

**JADE needs**

- Vast amount of benchmark to be automatically generated and run
- MCNP as transport code
- Vast amount of outputs
- Meaningful automatic post-processing
What is JADE?

Benchmarks suite

**TRANSPORT**

- Sphere Leakage
- C-model
- HCPB TBM
- WCLL TBM

**ACTIVATION**

- SPHERE SDDR
- ITER CYL SDDR
- OKTAVIAN
- FNG SDDR
What is JADE

Benchmarks suite

- Computational benchmarks
  - "Brute force"
    - Sphere Leakage
    - Sphere SDDR
    - ITER 1D
    - TBM
    - ITER Cylinder
  - 1D/2D benchmarks
    - C-model
  - 3D benchmarks
    - Oktavian TOF
    - FNG
- Experimental benchmarks
  - Single material
  - SDDR
  - ...

Verification

More XS tested

Higher physical relevance

Validation
The Sphere Leakage benchmark

Benchmark description

A uniform 0-14 MeV neutron point source is inserted at the center of a sphere composed entirely by a single isotope or a typical ITER material.

All isotopes provided by the nuclear data library under assessment are singularly tested.

Tallied quantities:
- Neutron and photon leakage flux (energy binned);
- Neutron and photon heating inside the sphere;
- Tritium and Helium production inside the sphere;
- DPA.
The Sphere Leakage benchmark

Excel formatted tables
The Sphere Leakage benchmark

Plot atlas
JADE architecture and development

General scheme
JADE Architecture and development

Open source

GitHub: https://github.com/dodu94/JADE

CoNDERC: https://nds.iaea.org/conderc/

JADE architecture and development

Automatic testing with pytest and coverage

- Help the stability of the code
- Increase trust on JADE results
- Sets a minimum quality standard for future contributors to the code
- Speed up introduction of new features (faster verification)
At each push on the main JADE branch:

• JADE is installed in a cloud Windows environment and the automatic testing is run (handled by GitHub)
• The documentation is rebuilt by ReadTheDocs and adjourned
JADE in numbers

12k Lines of code

9 Implemented benchmarks

2 Published papers


>10^6 CPU simulation hours worth of data that has been post-processed
Looking ahead
Next foreseeable steps

Expansion of the benchmarks suite

CoNDERC & SINBAD

MCNP6 → OpenMC → Linux
Monte Carlo codes like OpenMC are currently porting their code to GPU solvers. Simulation time could decrease by a few order of magnitudes! Leveraging the open source automation of benchmarks running and definition of acceptance test, ML algorithm could be introduced to support the libraries evaluation process.

An example of application is NucML\(^1\): [https://pedrojrv.github.io/nucml/index.html](https://pedrojrv.github.io/nucml/index.html)

\(^1\)Pedro Jr. Vicente-Valdez, Massimiliano Fratoni (UC Berkely, USA)
What it will be great to have

• A comprehensive, unified, user-friendly, open-source, ready to be used database of experiment (e.g., Conderc+SINBAD GitHub).
• A platform to provide feedback and record exchanges (e.g., GitHub).
• A collection of computational benchmark to use (e.g., 1D ITER).
• A standardized way to share and collect the different executed benchmarks in a common database (e.g., CONDERC) trying to avoid duplication.
• A closer collaboration with the different parties with periodic exchange (i.e., CCFE).
• Guidelines for the V&V of (fusion) libraries with clear acceptance criteria (e.g., C/E TBR : [0.95, 1.05]).
Summary

• JADE improves the standardization and the automation level in the field of nuclear data V&V (especially regarding fusion application).

• JADE is a consolidated open-source tool built for the community by the community. If you are interested in collaborating do not hesitate to contact us. Let’s join forces.

• V&V on many libraries has been already performed by JADE (i.e., FENDL3.1d, FENDL3.2, JEFF-3.3., JEFF-4.0T1). Few inconsistencies and discrepancies were spotted and reported. More work is planned.

• We sincerely appreciate the effort put in place by NEA, IAEA, SINBAD to modernize the experimental database and the collaboration with the different parties to continue the development of JADE.
GitHub: https://github.com/dodu94/JADE
READ THE DOCS: https://readthedocs.org/

Any Questions?
Thank you for your kind attention!
Backup slides
JADE application to production cases

Proof of concept

Tested libraries:
- FENDL v2.1
- FENDL v3.0
- FENDL v3.1d
- ENDF VII.1

Known errors in the FENDL v3.1d were re-spotted by JADE consistency checks

Paper:
JADE application to production cases

Proof of concept

Some examples where the leakage neutron flux results differed significantly among the tested libraries.
JADE application to production cases

FENDL v3.2 release (BETA)

**SPHERE LEAKAGE COMPARISON RECAP**

<table>
<thead>
<tr>
<th>ZAID</th>
<th>TALLIES</th>
<th>T production</th>
<th>He ppm production</th>
<th>DPA production</th>
<th>Neutron heating F6</th>
<th>Gamma heating F6</th>
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<tbody>
<tr>
<td>M901</td>
<td>Polyethylene, Non-borated</td>
<td>-0.01%</td>
<td>0.01%</td>
<td>0.02%</td>
<td>0.02%</td>
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</tr>
<tr>
<td>M900</td>
<td>Natural silicon</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td>0.00%</td>
<td></td>
</tr>
<tr>
<td>M101</td>
<td>SS316L(N)-IG</td>
<td>0.57%</td>
<td>4.18%</td>
<td>79.12%</td>
<td>98.41%</td>
<td>2.38%</td>
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<tr>
<td>M203</td>
<td>Boron carbide (Bc)</td>
<td>9.68%</td>
<td>0.79%</td>
<td>100.00%</td>
<td>100.00%</td>
<td>-0.01%</td>
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<tr>
<td>M200</td>
<td>Ordinary concrete</td>
<td>1.52%</td>
<td>10.47%</td>
<td>87.15%</td>
<td>87.53%</td>
<td>-8.15%</td>
</tr>
<tr>
<td>M400</td>
<td>Water</td>
<td>0.57%</td>
<td>16.37%</td>
<td>-2.82%</td>
<td>6.00%</td>
<td>-3.24%</td>
</tr>
</tbody>
</table>

Important differences in key neutron related quantities were spotted for typical ITER materials when comparing the old and new release of FENDL libraries

**Paper:**

Effect of the higher neutron heating in the steel layers of the ITER 1D model.

B-10 accounts only for 0.00036 % (in mass) of SS316L(N)-IG and at the same time SS316L(N)-IG is composed by 45 different isotopes. Without systematic and automated testing it would have been more difficult to track the origin of the issue.
### JADE application to production cases

#### FENDL v3.2 official release

<table>
<thead>
<tr>
<th>ZAID</th>
<th>Symbol</th>
<th>TALLIES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>T production</td>
</tr>
<tr>
<td>M101</td>
<td>SS316(N)/IG</td>
<td>8.59%</td>
</tr>
<tr>
<td>M200</td>
<td>Ordinary Concrete</td>
<td>-0.27%</td>
</tr>
<tr>
<td>M203</td>
<td>Boron Carbide</td>
<td>13.13%</td>
</tr>
<tr>
<td>M400</td>
<td>Water</td>
<td>1.10%</td>
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<tr>
<td>M900</td>
<td>Natural Silicon</td>
<td>0.00%</td>
</tr>
<tr>
<td>M901</td>
<td>Polyethylene, non-borated</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

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<table>
<thead>
<tr>
<th>ZAID</th>
<th>Symbol</th>
<th>TALLIES</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>T production</td>
</tr>
<tr>
<td>3007</td>
<td>Li-7</td>
<td>-0.01%</td>
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<tr>
<td>4009</td>
<td>Be-9</td>
<td>0.04%</td>
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<tr>
<td>5010</td>
<td>B-10</td>
<td>5.12%</td>
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<tr>
<td>5011</td>
<td>B-11</td>
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<tr>
<td>6012</td>
<td>C-12</td>
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<td>6013</td>
<td>C-13</td>
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<td>7014</td>
<td>N-14</td>
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<tr>
<td>7015</td>
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<tr>
<td>8016</td>
<td>O-16</td>
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<tr>
<td>8017</td>
<td>O-17</td>
<td>0.00%</td>
</tr>
<tr>
<td>8018</td>
<td>O-18</td>
<td>-91.74%</td>
</tr>
</tbody>
</table>
Difference in neutron heating are clearly visible in water both in ITER1D and HCPB TBM benchmarks.

IAEA nuclear data section is considering for the O-16 cross section to either to:

• Switch to ENDFVIII.0 evaluation;
• Correct NJOY processing routine for KERMA data