Attila neutronics simulations and validation, 3-D ITER machine and ports modeling with preliminary results

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Topics

• Deterministic versus Monte Carlo methods in nuclear analysis: *Pros and Cons*

• ATTLA code:
  • *Features and Capabilities*

• Results of Benchmarking ATTLA
  • 3 Fusion Integral Experiments *(comparison to experimental Data and MCNP Results)*
  • ITER CAD-Model *(Comparison to the UW DAG-MCNPX CAD-based Results as well as other CAD-Based MCNP codes)*

• Examples of ATTLA application for diagnostics ports

• Capability of ATTLA for activation and dose rate calculation

• Summary
Advantages and Disadvantages

**Deterministic codes**

**Advantages:**
- Fluxes and responses are calculated everywhere. No need to redo separate runs if additional responses are needed.
- Shorter time to run a case compared to Monte Carlo methods.

**Disadvantages:**
- Large disk space is required to store angular flux
- Ray effect due to angular discretization
- Cross section should be shielded particularly in resonance regions

**Monte Carlo codes**

**Advantages:**
- Complex geometry can be modeled accurately. However, extensive effort is needed to generate the appropriate “geometry cards”. This is why CAD-based versions are in progress.

**Disadvantages:**
- Fluxes and responses are calculated at pre-selected locations

Visualization of the responses requires generating many tallies at various planes. Progress to improve this limitation is currently implemented in MCNP-5
What is Attila?

- A finite element discrete ordinates (Sn/Pn) neutron, gamma and charged particle transport code using 3D unstructured grids (tetrahedral meshes)
- Geometry input from CAD (Solid Works, ProE)
- Complete visualization of the solution field (e.g. Flux, current response function, etc.)
- Supplied by Transpire Inc., (Gig Harbor, WA, USA)
Some New Features (under testing)

- **Integrated Activation Capability**
  - Extension of current Integrated depletion module (similar to ORIGEN) to include decay source terms

- **Group-wise Adaptive $S_N$ Order**
  - For ITER, can run 14 MeV source bin at a high $S_n$ order to transport the primary flux

- **Distributed Memory Parallel**
  - Linear scaling achieved on test version up to 256 processors
  - A primary motivation is to distribute memory resources
Benchmarks Experiments (FNG Facility)

Experiments performed at the FNG facility, ENEA, Frascati Italy
Measurements of many reactions rates
Measured Reactions

- Zr-90(n,2n)Zr-89, Eth~12 MeV
- Ni-58(n,2n)Ni-57, Eth~12 MeV
- Nb-93(n,2n)Nb-92, Eth~ 9 MeV
- Al-27(n,a)Na-24, Eth~ 5 MeV
- Fe-56(n,p)Mn-56, Eth~ 3 MeV
- Ni-58(n,p)Co-58, Eth~ 0.5 MeV
- In115(n,n’), Eth~ 0.2 MeV
- Au197(n,g), All energies

The accuracy in predicting these reactions is a good measure of how well the neutron spectrum and energy-dependent reactions rates are predicted.
Tungsten Experiment (Attila’s Model and Calculation)

Calculations:

Quadrature:
S12

XS Scattering:
P3

Number of Cells:
14681 cells for Nb, Ni, Au, Fe, In Foils
19398 cells For Zr, Al, Mn foils

Cells and three iso-surfaces are shown
Examples of Calculated/Experimental (C/E) values

Zr-90(n,2n) Zr-89 Reaction Rate

Al-27(n,a) Na-24 Reaction Rate

Al-27 (n,a) Na-24 Reaction Rate

Ni-58(n,p) Co-58 Reaction Rate

Foil Position from front Edge, (cm)

Penetration Depth Along Central Axis, (cm)

Nuclear Data: FENDL2.1
Response Function: IRDF-90

Tungsten Expt.

Streaming Expt.
Examples of Calculated/Experimental (C/E) values

**Bulk Shield Experiment**

- **Nb-93(n,2n) Nb-92 Reaction Rate**
- **Fe-56(n,p)Mn-56 Reaction Rate**
- **Al-27(n,α)Na-24 Reaction Rate**
- **Ni-58(n,p)Co-58 Reaction Rate**
### Average Estimates for the C/E Values and Deviation from Experiment

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Calculation Method</th>
<th>Tungsten</th>
<th>Experiment</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Streaming</td>
<td>Channel</td>
<td>Cavity</td>
<td>Bulk Shield</td>
</tr>
<tr>
<td>Zr-90(n,2n)Zr-89</td>
<td><strong>MCNP</strong></td>
<td>2%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-6%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ni-58(n,2n)Ni-57</td>
<td><strong>MCNP</strong></td>
<td>-1%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-6%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nb-93(n,2n)Nb-92</td>
<td><strong>MCNP</strong></td>
<td>1%</td>
<td>-4%</td>
<td>-6%</td>
<td>-10%</td>
<td>-13%</td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-9%</td>
<td>-13%</td>
<td>-10%</td>
<td>-13%</td>
<td></td>
</tr>
<tr>
<td>Al-27(n,a)Na-24</td>
<td><strong>MCNP</strong></td>
<td>3%</td>
<td>-10%</td>
<td>-7%</td>
<td>-11%</td>
<td>-13%</td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-7%</td>
<td>-20%</td>
<td>-11%</td>
<td>-13%</td>
<td></td>
</tr>
<tr>
<td>Fe-56(n,p)Mn-56</td>
<td><strong>MCNP</strong></td>
<td>-4%</td>
<td></td>
<td></td>
<td></td>
<td>-11%</td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-14%</td>
<td></td>
<td></td>
<td></td>
<td>-14%</td>
</tr>
<tr>
<td>Ni-58(n,p)Co-58</td>
<td><strong>MCNP</strong></td>
<td>6%</td>
<td>4%</td>
<td>3%</td>
<td>-7%</td>
<td>-8%</td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-4%</td>
<td>-6%</td>
<td>-3%</td>
<td>-8%</td>
<td></td>
</tr>
<tr>
<td>In-115(n,n')In-115m</td>
<td><strong>MCNP</strong></td>
<td>-6%</td>
<td></td>
<td></td>
<td></td>
<td>-23%</td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-18%</td>
<td></td>
<td></td>
<td></td>
<td>-25%</td>
</tr>
<tr>
<td>Au-197(n,g)Au-198</td>
<td><strong>MCNP</strong></td>
<td>-1%</td>
<td>3%</td>
<td>7%</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td><strong>Attila</strong></td>
<td>-10%</td>
<td>9%</td>
<td>10%</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Largest Deviation From Expt. Data
ATTLILA: ~-25%,  MCNP: ~-23%

Largest Between ATTLILA and MCNP  ~ -12%
Benchmarking ATTLA with the ITER CAD-Model and Comparison to MCNP Results

The 40-degree Solid Works CAD model of ITER

The Blanket Shield Modules (BSM) and divertor CAD model integrated in the 40-degree CAD model
Mesh Scheme used in the calculation:

\sim 500,000 mesh

Layering techniques is used to reduce mesh counts

D-T plasma Source and its Strength
Scalar Flux: Multiply by 1.7753E20

• Neutron Flux (solution) can be visualized at any location or at any plane

• Hot spots can be identified—Modification in the design can be altered to minimize these spots
Comparison to MCNPX-CGM CAD-Based Results (UW)

Neutron Wall Loading (NWL) at First Wall

Average (MW/m²)
- ATTILA: 0.57 (NAR: 0.55)
- MCNP (UW): 0.51 ~11% Dif.

Peak Values (MW/m²)
- I/B: ATTILA 0.64 (NAR: 0.60)
  MCNP (UW) 0.57 ~13% Dif.
- O/B: ATTILA 0.84 (NAR: 0.78)
  MCNP (UW) 0.74 ~14% Dif.
Comparison to DAG-MCNPX CAD-Based Results (UW)

Neutron Flux and Total Heating in the Inboard Target Part of the Divertor Segment

<table>
<thead>
<tr>
<th></th>
<th>Flux ([10^{13} \text{n/cm}^2\text{s}])</th>
<th>Heating (n+g) ([\text{kW}])</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ATTILA (Sn40Sn16)</td>
<td>MCNP(UW)</td>
</tr>
<tr>
<td>1</td>
<td>12.1</td>
<td>10.4 ± 0.56%</td>
</tr>
<tr>
<td>2</td>
<td>6.06</td>
<td>5.88 ± 1.1%</td>
</tr>
<tr>
<td>3</td>
<td>7.56</td>
<td>6.83 ± 0.58%</td>
</tr>
<tr>
<td>4</td>
<td>3.61</td>
<td>3.17 ± 0.70%</td>
</tr>
<tr>
<td></td>
<td>TOT.</td>
<td>239.34</td>
</tr>
</tbody>
</table>

From M Youssef, R. Feder and T. Wareing, *Benchmarking the CAD-based ATTILA Discrete Ordinates Code with Experimental Data of Fusion Experiments and to MCNP Results in Simulated ICENES-2007, Istanbul, Turkey*
Comparison to DAG-MCNPX CAD-Based Results (UW)

Neutron Flux and Total Heating in the Central Dome Part of the Divertor Segment

<table>
<thead>
<tr>
<th></th>
<th>Flux [10^{13} n/cm^2.s]</th>
<th>Heating (n+g) [kW]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ATTILA (Sn40Sn16)</td>
<td>MCNP(UW)</td>
</tr>
<tr>
<td>1</td>
<td>8.60</td>
<td>8.80 ± 0.47%</td>
</tr>
<tr>
<td>2</td>
<td>6.79</td>
<td>6.83 ± 0.52%</td>
</tr>
<tr>
<td>3</td>
<td>3.75</td>
<td>3.92 ± 0.56%</td>
</tr>
<tr>
<td>4</td>
<td>268</td>
<td>268 ± 1.1</td>
</tr>
</tbody>
</table>

From M. Youssef, R. Feder and T. Wareing, *Benchmarking the CAD-based ATILIA Discrete Ordinates Code with Experimental Data of Fusion Experiments and to MCNP Results in Simulated ICENES-2007, Istanbul, Turkey*
### Present CAD-based Neutronics Tools

<table>
<thead>
<tr>
<th>Institution</th>
<th>Country</th>
<th>Code Name</th>
<th>Type</th>
<th>CAD-based Method</th>
</tr>
</thead>
<tbody>
<tr>
<td>FZK</td>
<td>Germany</td>
<td>McCad</td>
<td>Monte Carlo-MCNP</td>
<td>Automated Translation Method</td>
</tr>
<tr>
<td>ASIPP</td>
<td>China</td>
<td>MCAM</td>
<td>Monte Carlo-MCNP</td>
<td>Automated Translation Method</td>
</tr>
<tr>
<td>UW</td>
<td>USA</td>
<td>DAG-MCNPX</td>
<td>Monte Carlo-MCNP</td>
<td>Direct geometry utilization</td>
</tr>
<tr>
<td>JAEA</td>
<td>Japan</td>
<td>GEOMIT</td>
<td>Monte Carlo-MCNP</td>
<td>Automated Translation Method</td>
</tr>
<tr>
<td>UCLA/PPPL-Transpire</td>
<td>USA</td>
<td>ATTLA</td>
<td>Deterministic</td>
<td>unstructured tetrahedral meshes generated by CAD software and used as input</td>
</tr>
</tbody>
</table>

* Direct translation of CAD model to input cards describing geometry for MCNP

** Direct geometry utilization: approach changes the MCNP software, replacing its core geometry routines
Comparison of CAD-Based Codes in the Divertor. (Results are Normalized to UW Results)

- Differences are generally within ~10%
- ASIPP gives on the average larger values than UW
- ATIILA gives consistent results (no Biasing)

From P.P.H. Wilson, R. Feder, U. Fischer, M. Loughlin, L. Petrizzi, Y. Wu, M. Youssef
STATE-OF-THE-ART 3-D NEUTRONICS ANALYSIS METHODS FOR FUSION ENERGY SYSTEMS, to presented at ISFNT-8
Comparison of CAD-Based Codes in calculating the total flux in the equatorial port.

Three regions are represented: two shielding regions (<50cm, 50-100cm) and a streaming region (>100cm).

Results in the port plug and shield are nearly identical for all the methods. There is a substantial discrepancy across all the results in the streaming region. It could be due to various variance reduction schemes in the Monte Carlo methods. Attila results are systematically lower than the others.
Conclusions of Benchmarking

**Integral Experiments:**

Maximum Deviation from Experimental Values: ATTIILA: ~-25%, MCNP: ~-23%. Max. Difference between ATTIILA and MCNP ~ -12%

**ITER CAD Model (Difference between ATTIILA and MCNP):**

- Neuron Wall Load: Max. ~15%
- Divertor neutron flux: Max. ~14%, Total Nuclear Heating: ~ 15%
- BSM and Shield at Equatorial port: ~ 5%
- Large difference at deep locations behind shield(~30%)
Applications

Attila's Solid Works neutronics CAD model of the Upper Port Central Tube Visible-IR Endoscope.

On the right a section through the model is taken that shows the installation gaps and shield module water supply lines.
Results are shown on a log10 scale and need to be scaled by $1.78 \times 10^{20}$. Higher flux at the rear flange is from steaming down 20mm installation gaps between the port plug and the ITER Upper Port extension.
Attila’s CAD Model and Attila results for ITER RF Antenna

Straps around the RF Antenna represents steaming paths. It is tapered to reduce this effect.

To reduce the neutron flux to level at which the dose due to activation was less than 100\(\mu\)Sv/hr requires an attenuation of at least 10 orders of magnitude.

The lighter shades are indicative of higher intensity neutron flux.

M. Loughlin
New Version of ATTILA can perform Activation and Dose Rate calculations (procedures)

**Step 1**
- Neutron transport calculation

**Step 2**
- Terminal Restart File
- Gamma Source Calculation
- Input File

**Step 3**
- Dose Rate Calculation

**Neutron only calculation** (gammas could optionally be run)
- Performed using fendl_29n cross section set (current limitation)
- Generate terminal restart file

**Unique activation source** computed in each tetrahedral element
- Activation source may be visualized by energy group
- User may specify which mesh regions to activate
- Multiple time steps can be specifies (irradiation history): burn-decay-burn-decay, etc

**Transport the gamma source at a given decay time step and calculate dose rate**
- Computational mesh must be the same as in Steps 1 and 2
- Material properties can be different
- Gamma only calculation using the 217 group FENDL 2.1 library
- Energy group collapse permitted
Example: 14 MeV Neutron source, 1 m-thick SS316 (1)

Activation Gamma Ray Source (Step 2)
Example: 14 MeV Neutron source, 1 m-thick SS316 (2)
Benchmarking the FNG Shutdown Experiment with ATTILA (in progress)

Instrumentation for dose rate and decay gamma flux measurements

- 14 MeV Point Source
- Mock up Block
- Perspex
- Stainless steel AISI-316
- Cavity
- Streaming channel
- Neutron source
- G-M dose rate meter (1st campaign)
- TLD / activation foils (1st campaign)
- Dose rate meter (2nd campaign)
- Gamma spectrometer (2nd campaign)
**Irradiation History of First Campaign**

During May 8-10, 2000, the mock-up was irradiated by 14 MeV neutrons for a total of 18 hours in three days. The total neutron production was $1.815 \times 10^{15}$. The

Comparison of measured and calculated dose rate up to ~ 2 month following irradiation in first campaign

**Measurements:** G-M, TLD

**Calculation:** (MCNP-with different cross section library)
Summary

ATTILA is the only available 3-D deterministic code based on FEM with unstructured tetrahedral meshes generated from CAD-based input file. It compares favorably with other CAD-based Stochastic codes and can be used as high quality-assured code in modern nuclear analysis for complex geometry such as ITER. From benchmarking, Integral Experiments:

Maximum Deviation from Experimental Values: ATTILA: ~-25%, MCNP: ~-23%. Max. Difference between ATTILA and MCNP ~ -12%

**ITER CAD Model (Difference between ATTILA and other CAD-Based MCNP):** For Neuron Wall Load, Divertor neutron flux and nuclear heating: Max. ~14-15%, For flux in BSM and Shield at Equatorial port: ~ 5%, but large difference up to ~60% in the streaming zone behind shield

**Limitations:** Reflective boundaries and source specifications at any arbitrary boundary surfaces need to be implemented. Large disk space requirements. Shared-memory-parallel version is under testing

**In Progress:** Using ATTILA for Designing the Diagnostics Ports in ITER. Benchmarking ATTILA for Activation and Dose Calculations using FNG shutdown experiment. Using ATTILA for dose rate calculation of diagnostics ports. ATTILA can as well be used for TBM design