Verification and Validation Activities with OpenMC

Paul K. Romano

Computational Scientist, Argonne National Laboratory

Technical Meeting on CoNDERC October 12, 2022



What is OpenMC?

A community developed, open source Monte Carlo particle transport code, primarily targeted at applications in nuclear science and engineering

OpenMC: Overview of features

- **Modes**: Fixed source, *k*-eigenvalue calculations, volume calculations, geometry plotting
- Geometry: Constructive solid geometry, CAD-based, unstructured meshes
- · Solvers: Neutron and photon transport, depletion
- Data: Continuous energy or multigroup cross sections, multipole for Doppler broadening
- Parallelism: Distributed/shared-memory via MPI/OpenMP

OpenMC: Unique attributes

What sets OpenMC apart from other codes?

- Programming interfaces (C/C++ and Python)
- Nuclear data interfaces and representation
- Tally abstractions
- Parallel performance
- Development workflow and governance

OpenMC: Community Resources

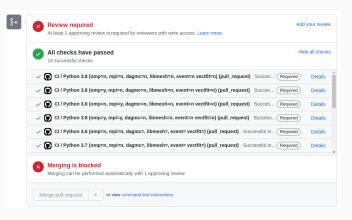
- Code: https://github.com/openmc-dev/openmc
- Documentation: https://docs.openmc.org
- Nuclear Data: https://openmc.org
- Forum: https://openmc.discourse.group
- · Slack: https://join.slack.com/t/openmc/signup

V&V and **QA** Activities

- 1. Continuous integration testing
- 2. Criticality benchmarks
- 3. Depletion comparisons
- 4. Shielding benchmarks
- 5. Automated model conversion

Continuous integration testing

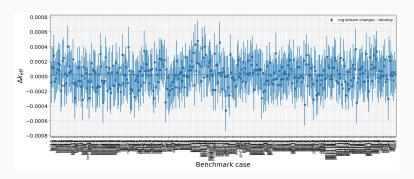
Every time a pull (change) request is made, a comprehensive set of regression and unit tests are run for a matrix of build/run configurations



Works well when no changes are expected in reference results

Changes in reference results

When a change in our reference results *are* expected (new physics, random number stream, etc.), we kick off a set of benchmark simulations to ensure everything agrees within uncertainty:



ICSBEP Benchmarks

 MIT hosts a collection of reactor physics benchmark models for OpenMC, including ~400 ICSBEP models:

Fuel	COMP	MET	SOL	MISC
HEU	7	72	48	0
LEU	6	0	32	0
IEU	1	12	0	0
PU	1	39	121	0
U233	1	10	7	0
MIX	8	27	0	0

Fuel	THERM	INTER	FAST	MIXED
HEU	48	11	68	0
LEU	38	0	0	0
IEU	0	0	13	0
PU	121	2	38	0
U233	7	1	10	0
MIX	6	1	28	0

CoNDERC Contributions

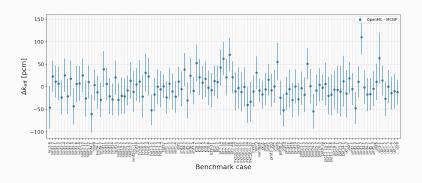
- A collection of ICSBEP/IRPhEP benchmark models were contributed to CoNDERC under the "beyond k_{eff}" section
- Emphasis placed on utilizing additional functionality:
 - · Plotting flux spectra in various materials
 - Built-in energy group structures
 - · Radial flux profile in a spherical mesh
 - Automated volume/mass checks compared to benchmark specifications
 - · Complex modeling functionality in OpenMC
 - · Use of third-party Python packages
 - Automated generation of parameterized models

Benchmark Automation

- · We also maintain a repository of validation scripts
 - openmc-run-benchmarks Run a collection of ICSBEP benchmarks using either OpenMC or MCNP and collect results
 - openmc-plot-benchmarks Plot results from openmc-run-benchmarks
- Running hundreds of benchmarks is as simple as executing a single command (and having a big computer!)

Automation: Code-to-code Comparison

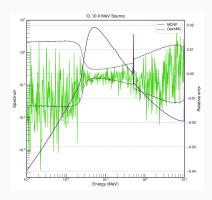
• OpenMC 0.13.1 vs MCNP 6.2 on ICSBEP benchmarks:

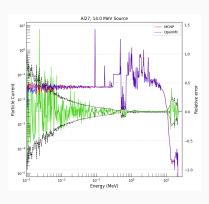


Simple Physics Comparisons

Validation scripts also include simple physics comparisons:

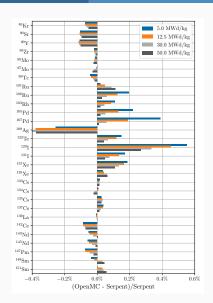
- Neutron/photon spectrum from a monoenergetic point source in a sphere
- · Secondary photon spectrum in broomstick model (coupled $n-\gamma$)





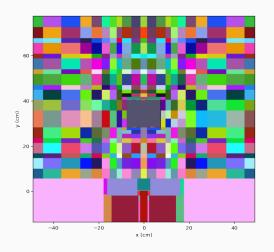
Depletion Code-to-code Comparison

Extensive code-to-code comparisons for depletion have been carried out with OpenMC and Serpent

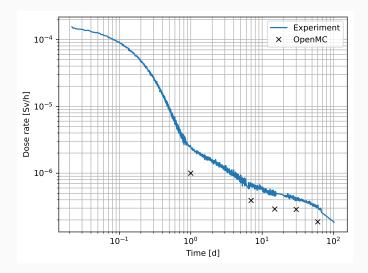


SINBAD Benchmarks

- As part of a new project funded by DOE/Fusion Energy Sciences, OpenMC models for SINBAD benchmarks are being developed
- · First one is "FNG dose":



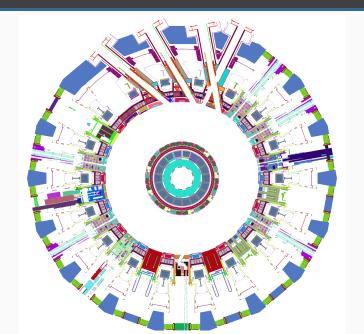
FNG Dose: Early Results



Automated Model Conversion

- Recently, we released a utility for converting MCNP models to OpenMC
- · Unlike csg2csg, directly utilizes OpenMC's Python API
- · Some MCNP features are not supported:
 - · Periodic boundary conditions
 - Hexagonal lattices
 - · Some macrobodies
 - · Source definitions, tallies, and most cards in the "data" section

Model Conversion: ITER E-lite



Model Conversion Opportunities

- General capability for model conversion opens up new opportunities:
 - · Maintaining a single "canonical" set of inputs
 - · Minimizing/eliminating model differences
 - Volume comparisons
 - · Mass comparisons
- Many code-to-code differences (esp. outliers) I've seen tend to be a result of modeling errors or inconsistencies
- Study different approaches in csg2csg, t4_geom_convert, and openmc_mcnp_adapter to learn from one another

Thank you!

Acknowledgments

- This research was supported by the Exascale Computing Project (17-SC-20-SC), a
 collaborative effort of two U.S. Department of Energy organizations (Office of Science and
 the National Nuclear Security Administration) responsible for the planning and preparation
 of a capable exascale ecosystem, including software, applications, hardware, advanced
 system engineering, and early testbed platforms, in support of the nation's exascale
 computing imperative.
- This material is based upon work supported by the US Department of Energy, Office of Science, Office of Fusion Energy Sciences under Award DE-AC02-06CH11357.
- We gratefully acknowledge the computing resources provided on Bebop, a highperformance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory.