OpenMC Workshop

ANS Student Conference

April 13, 2023

Workshop overview

- Intro (slides)
- Intro to geometry in OpenMC (slides)
- Reactor pin cell (interactive)
- Tallies (interactive)

Time-permitting:

- Briefer on depletion (slides)
- Depletion (interactive)
- Fixed source mode (interactive)
- Nuclear data (interactive)
- Volume calculations (interactive)

Logistics

Instructors:

- **MIT**: Gavin Ridley (ridley@mit.edu)
- **ANL**: April Novak (anovak@anl.gov)

Asking Questions:

- onlinequestions.org (room number TBD)

Interactive Sessions

- You will be using **JupyterHub** for demonstrations and (optionally) take-home exercises
- Instructor will give live demo for each session, and you can follow along in your own Jupyter Lab instance (dual monitor / side-by-side)
- The URL provided to you will be available all week but will be shutdown at the end of the week — "notebooks" can be downloaded at anytime

Login: **https://nsecluster.mit.edu/jhub/**

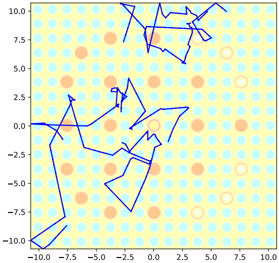
Monte Carlo Particle Transport

- Analysis of nuclear reactors, fusion devices, radiation shielding, and other problems relies on ability to solve particle transport equations
    - *Deterministic methods:* discrete ordinates, method of characteristics, collision probability method, diffusion theory
    - *Monte Carlo (MC) method:* directly simulate life of individual particles using known probability distributions
- MC method confers a number of benefits:
    - Use of continuous-energy interaction data (no grouping necessary)
    - No spatial approximations necessary
    - Parallelization is "simple" since particles do not interact with one another
    - Some classes of problems are very difficult to solve at all with deterministic methods (e.g., high-energy physics)
- Biggest impediment to wider use is *time to solution*

Adoption of MC

- As computers continually improve in performance over time, the scope of problems amenable to solution by MC has increased as well
- Lots of activity in the research community on MC methods, and plenty of new codes:
  - **U.S.**: OpenMC (*), MC21 (NNL), Shift (ORNL), Mercury (LLNL)
  - **China**: RMC (Tsinghua), SuperMC (FDS)
  - **Europe**: Serpent (VTT), Tripoli (IRSN/CEA)
  - **South Korea**: PRAGMA (SNU)

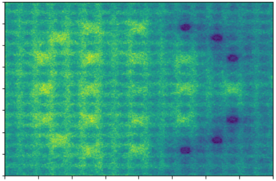
Neutral Particle Transport



What we simulate, e.g. a PWR fuel assembly

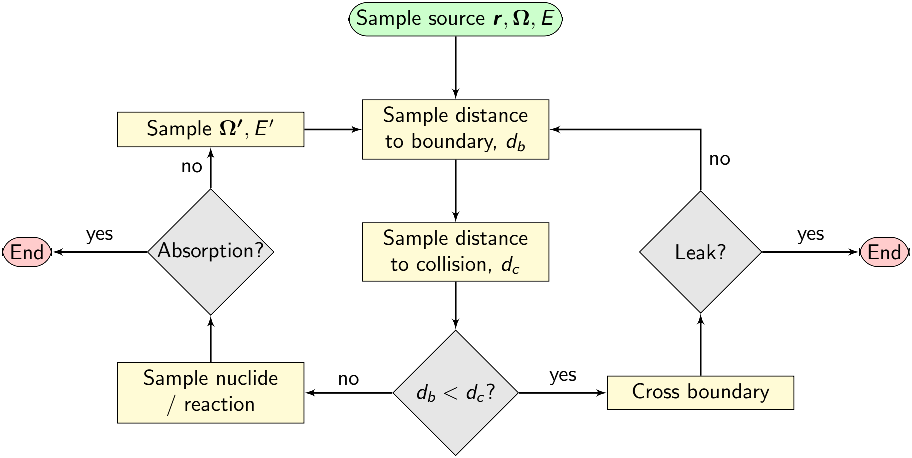
$\longrightarrow$

average many tracks



Example output: thermal flux distribution

Neutral particle transport



Tallies

Monte Carlo is well-suited to calculating volume integral quantities of the form:

$$X = \int d\boldsymbol{r} \int d\boldsymbol{\Omega} \int dE \ f(\boldsymbol{r}, \boldsymbol{\Omega}, E)\psi(\boldsymbol{r}, \boldsymbol{\Omega}, E)$$

During a simulation, physical quantities of interest (called *tallies* or *detectors*) are accumulated as:

$$\hat{X} = \frac{1}{N} \sum_{i \in T} w_i \ell_i f_i$$

Monte Carlo Statistics

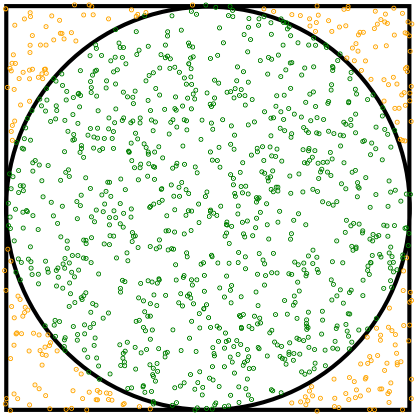
At the end of a simulation, we have a set of realizations for each tally, $\hat{X}_1, \hat{X}_2, \ldots, \hat{X}_N$. We can calculate mean and variance as

$$\bar{X} = \frac{1}{N} \sum_{i=1}^{N} \hat{X}_i$$

$$s_X^2 = \frac{1}{N-1} \left(\frac{1}{N} \sum_{i=1}^{N} \hat{X}_i^2 - \bar{X}^2 \right)$$

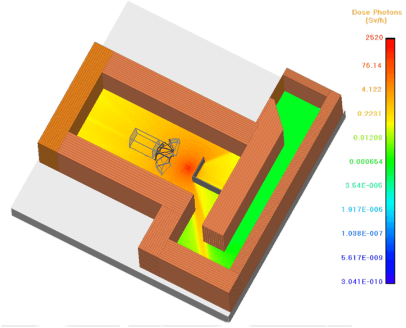
Monte Carlo Statistics

- Calculate π by sampling!
- $A = \pi r^2$
- Probability of being in circle proportional to its area
- Is inside? $\hat{x}^2 + \hat{y}^2 < 1$
- I sample 500 points, 393 land inside
- $\hat{\pi} \approx 4 \cdot 393/500 = 3.144$
- $s_{\hat{\pi}} = \sqrt{\frac{1}{499}(.804 - .646)} \approx .02$



Problem Types

- For **fixed source** problems, the source of particles is known *a priori*, e.g., 100 neutrons/sec from an isotropic point source
- When fission chain reaction neutrons are the primary source, like in a reactor, an iterative approach is required



For example, medical radiation sources are fixed source problems.

[0] Image: https://www.physicsforums.com/threads/mcnp-diagnostic-x-ray-tube-simulation.948590/

Eigenvalue Problem

What they teach in nuclear engineering 101

$$k = \eta f p \epsilon P_{FNL} P_{TNL}$$

What OpenMC simulates (pretty much real life!)

$$\begin{aligned}\frac{1}{v}\frac{\partial\psi}{\partial t} + \hat{\Omega}\cdot\nabla\psi + \Sigma_t(\mathbf{r},E)\psi(\mathbf{r},\boldsymbol{\Omega},E,t) = \\ + \int_0^\infty dE' \int_{4\pi} d\Omega' \nu_s \Sigma_s(\mathbf{r},\boldsymbol{\Omega}\cdot\boldsymbol{\Omega}',E'\to E)\psi(\mathbf{r},\boldsymbol{\Omega}',E',t) \\ + \frac{\chi(E)}{4\pi \color{red}{k}}\int_0^\infty dE'\nu\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',t) \\ + s(\mathbf{r},\boldsymbol{\Omega},E,t)\,.\end{aligned}$$

k Eigenvalue Algorithm

Guess initial source distribution and k
for $i = 1 \to n_{generations}$ **do**
  for $j = 1 \to n_{particles}$ **do**
    Sample neutron from source bank
    Track neutron until death, at each **collision** storing

$$n = \left\lfloor \frac{\nu\Sigma_f}{\Sigma_t} + \xi \right\rfloor \quad \text{fission sites}$$

  Sample $N = n_{particles}$ neutrons from N' fission sites collected
  Calculate $k^{(i)} = N'/N$

Inactive generations

- Our goal is to estimate physical quantities (e.g., ^{235}U fission rate) resulting from a source
- In the generation algorithm, we have to wait until the spatial distribution of source sites converges (otherwise, our results would be biased by the arbitrary source guess)
- Simulation is broken up into *inactive* and *active* generations
- For problems with large dominance ratio, hundreds of generations may need to be discarded [1]

[1] rule of thumb: many scattering events to cross problem means larger dominance ratio

Objectives

The overarching objectives of the OpenMC project:

- Open source contribution model, freely available
- Extensible for research purposes
- Adopt best practices for software development
- Ease of installation, minimize third-party dependencies
- High performance, scalable on HPC resources
- Use best physics models when possible
- Fun to use, and thriving user and developer community!

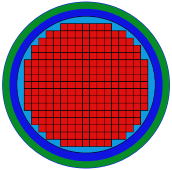
OpenMC: Overview of features

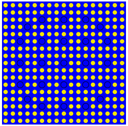
- **Modes**: Fixed source, k-eigenvalue calculations, volume calculations, geometry plotting
- **Geometry**: Constructive solid geometry, CAD-based, unstructured mesh (tallies only)
- **Solvers**: Neutron and photon transport, depletion, stochastic volume calculation
- **Data**: Continuous energy or multigroup cross sections, multipole for Doppler broadening

What makes OpenMC unique?

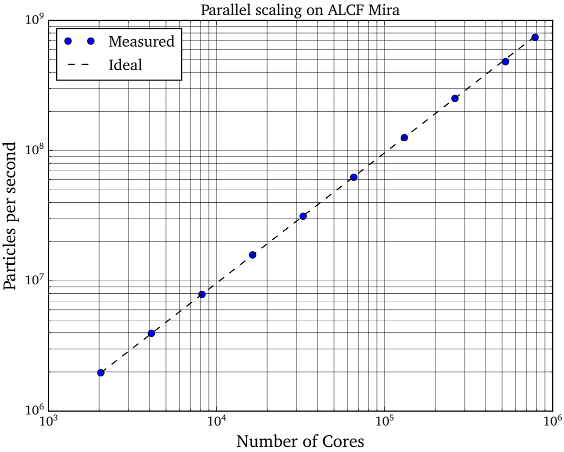
- Programming interfaces (C/C++ and Python)
- Nuclear data interfaces and representation
- Tally abstractions
- Parallel performance
- Development workflow and governance

Parallel Performance

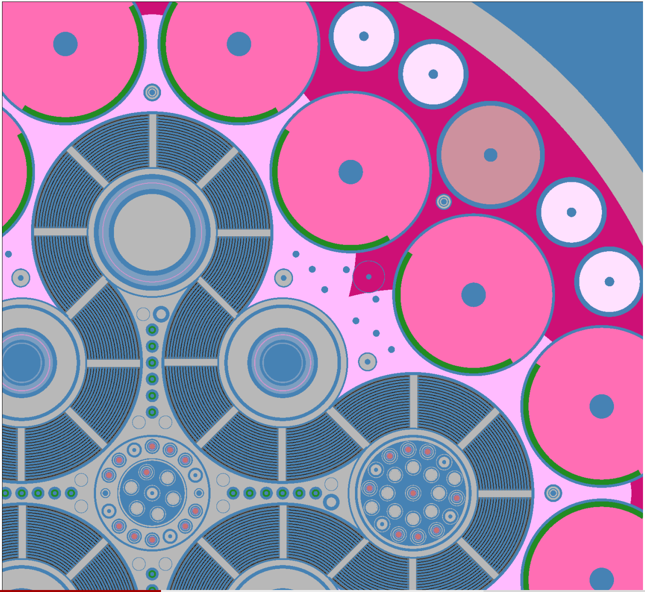

Core


Assembly

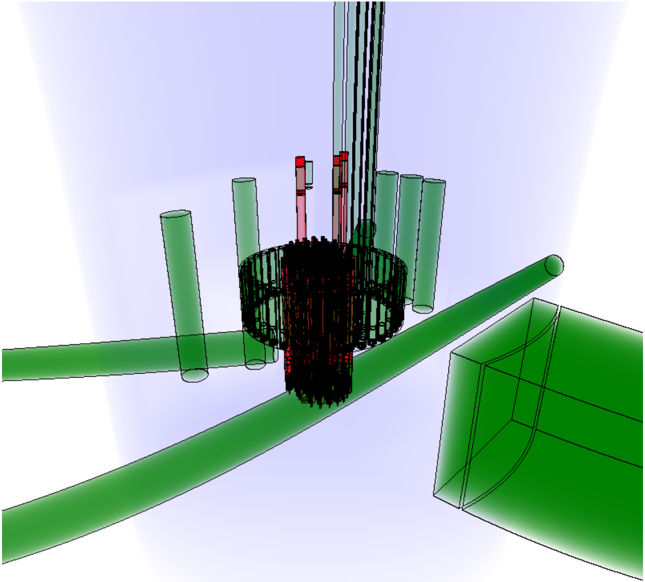
- ALCF Mira supercomputer
- 49,152 nodes, 786,432 cores
- 4 hw threads/core = 3,145,728 threads



Example: Advanced Test Reactor



Example: JSI TRIGA



Software Architecture

- Mixed **C++** and **Python** codebase
- **CMake** build system for portability
- Distributed-memory parallelism via **MPI**
- Shared-memory parallelism via **OpenMP**
- Version control through **git**
- Code hosting, bug tracking through **GitHub**
- Regression/unit tests run on **GitHub Actions** CI platform

Upcoming developments

- GPU porting (Exascale Computing Project)
- Multiphysics coupling
- Fusion shutdown dose rate (SDR) calculations
- Unstructured mesh support
- Methods to support molten salt reactor design

Resources

- **Code:** https://github.com/openmc-dev/openmc
- **Docs:** https://docs.openmc.org
- **Nuclear Data:** https://openmc.org
- **Forum:** https://openmc.discourse.group