OpenMC Workshop

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Outline

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Goals of the OpenMC Project

- Develop a Monte Carlo framework for reactor analysis that scales on leadership-class supercomputers (100,000+ cores)
- Provide a simple tool to analyze performance and limitations on proposed architectures
- Objectives:
  - Realistic physics
  - Modern programming style and data structures
  - Extensible for research purposes
  - Open source and freely available

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Characteristics of OpenMC

Current features

- Fixed source and k-eigenvalue calculations
- **Geometry**: CSG with second-order surfaces, universes, rotations/translations, rectangular/hexagonal lattices
- **Cross sections**: ACE format or multi-group
- **Physics**: neutron transport, $S(\alpha, \beta)$ thermal scattering, probability tables, target thermal motion
- Flexible general tally system
- **Parallelism**: Distributed/shared-memory via MPI/OpenMP
- Rich, extensible Python API
- **Input**: XML or Python API-driven
- **Output**: HDF5
- Multi-group cross section generation

Short-term

- HDF5 format cross sections
- Photon transport
- Depletion
- Transient-capability
- Temperature dependence
- Domain decomposition

Medium-term

- In-house nuclear data processing
- Thermal-hydraulics coupling
- Non-CSG deformable geometry
- Coupling with MOOSE

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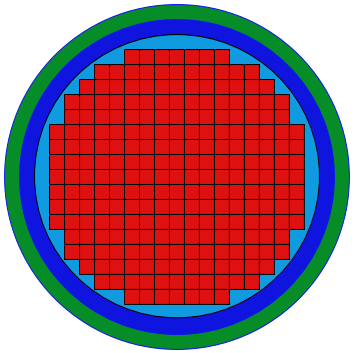
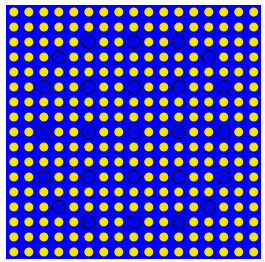
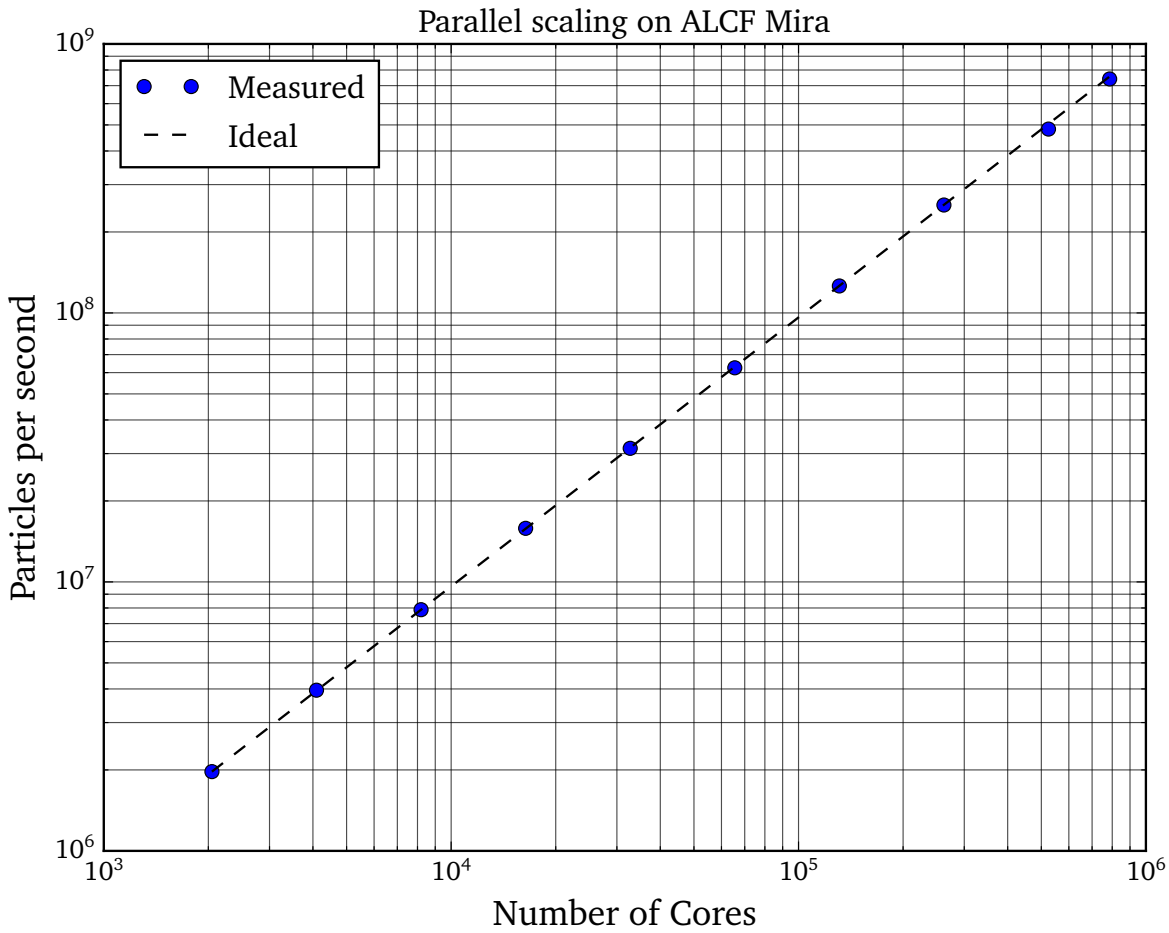
Parallel Performance


Core


Assembly

- Mira – #5 on TOP 500
- 49,152 nodes, 786,432 cores
- 4 hw threads/core = 3,145,728 threads



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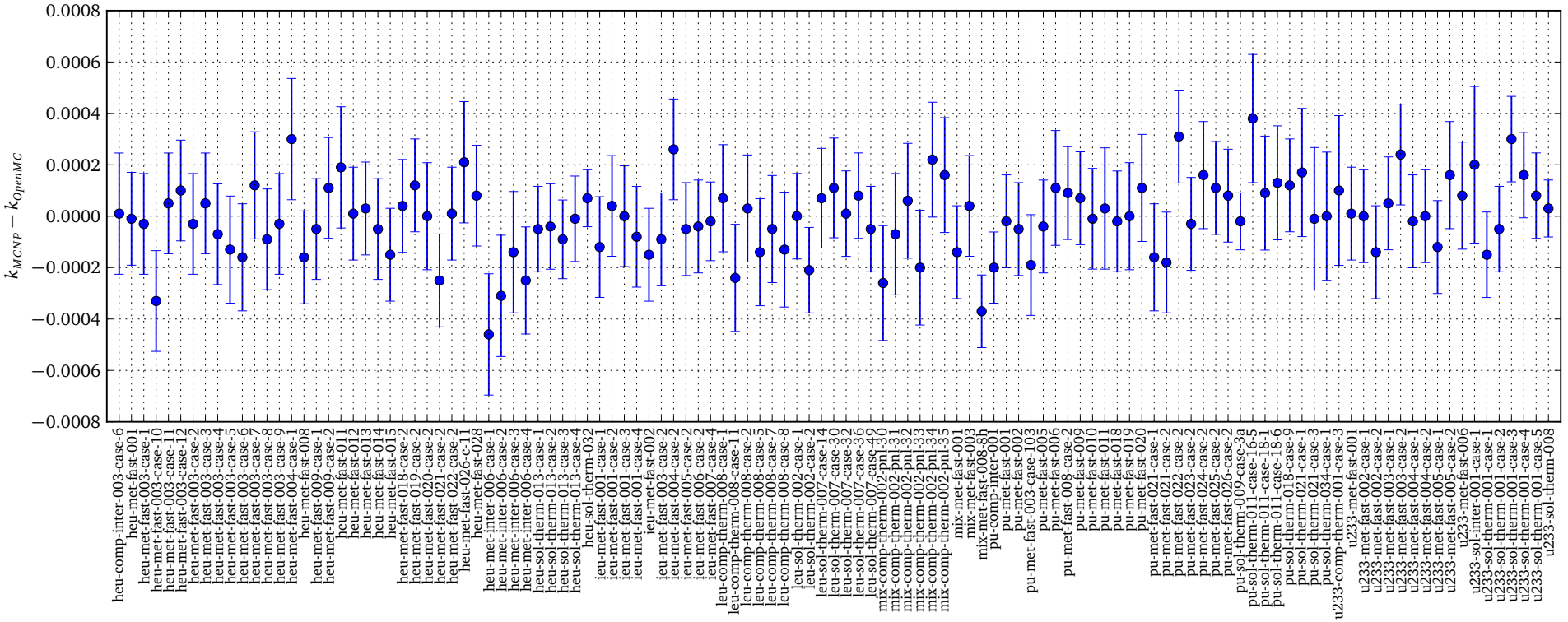
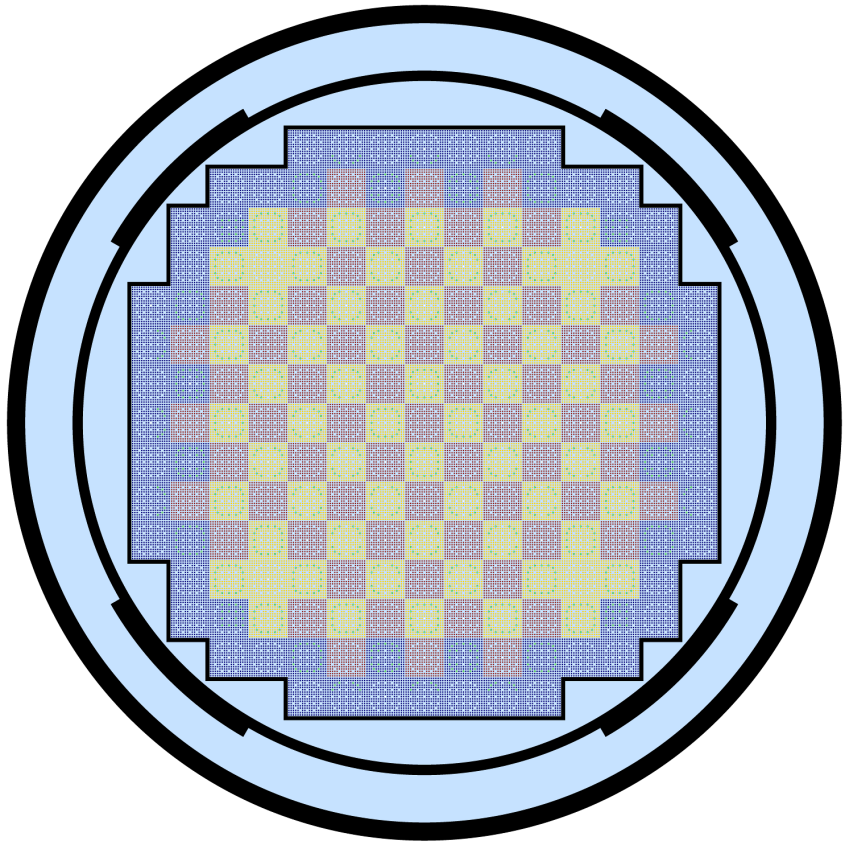
Validation and Verification

- MCNP Criticality Benchmark Suite
  - 119 configurations — different spectra, materials, enrichment
  - Models built for all but two



Example: MIT BEAVRS Benchmark

- Radial enrichment zoning
- Guide tubes/instrument tubes
- Burnable absorbers/control rods
- Grid spacers, core support
- Core baffel, core barrel
- Thermal shield pads
- Reactor pressure vessel



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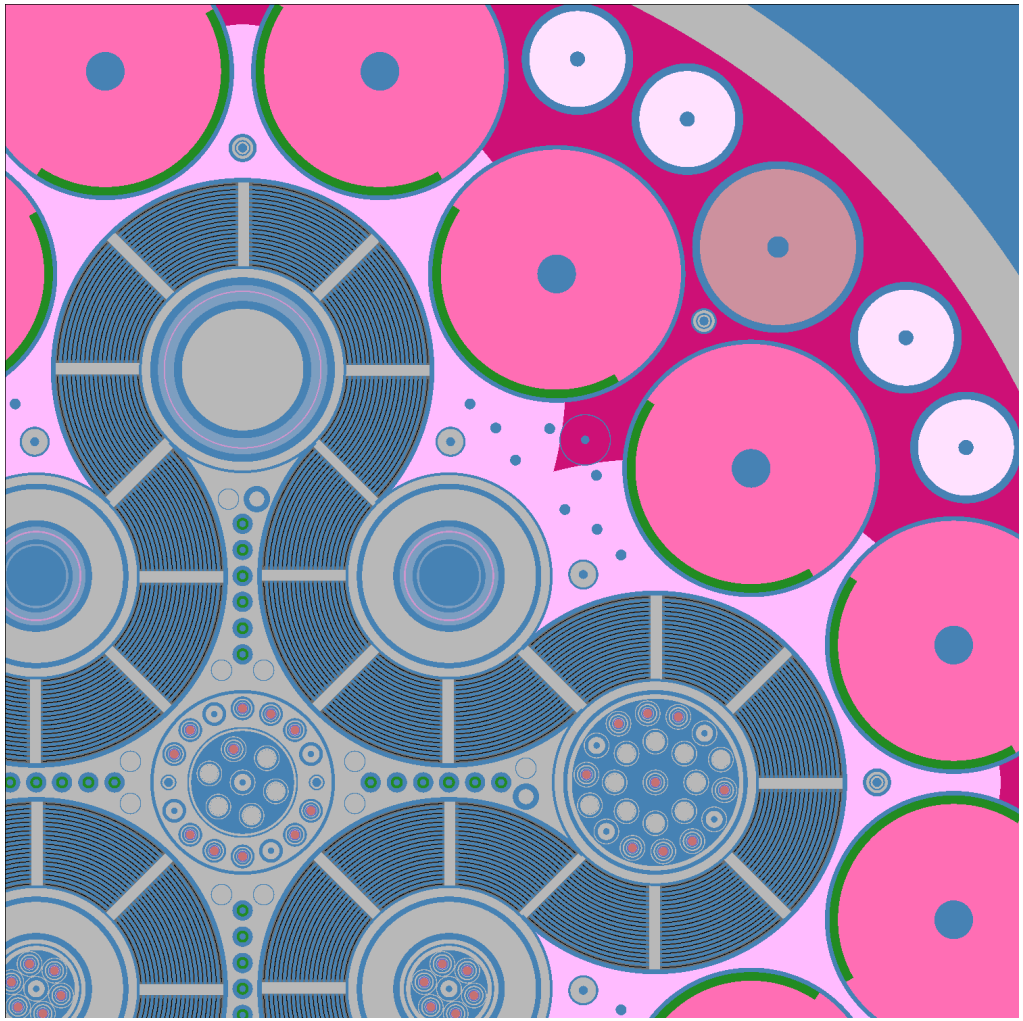
Example: Advanced Test Reactor



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Software Architecture

- ∼40,000 lines of **Fortran 2008** code
- Distributed-memory parallelism via **MPI**
- Shared-memory parallelism via **OpenMP**
- **CMake** build system for portability
- ∼20,000 lines of **Python** API
- Version control through **git**
- Code hosting, bug tracking through **GitHub**
  - `https://github.com/mit-crpg/openmc`
- Automatic documentation generation with **Sphinx**
  - `http://openmc.readthedocs.io`

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Resources

- User's Group: `openmc-users@googlegroups.com`
- Developer's Group: `openmc-dev@googlegroups.com`
- Documentation: `http://openmc.readthedocs.io`

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XML Input

- When you run **openmc** command, it looks for a set of XML files:
  - Paramters for the simulation — **settings.xml**
  - Material definitions — **materials.xml**
  - Geometric model, mapping of materials — **geometry.xml**
  - Determine which quantities to score — **tallies.xml**
  - Create geometry plots — **plots.xml**
- Writing XML files is now considered "old-school"

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Python API Input

- OpenMC includes a rich Python API that enables programmatic pre- and post-processing
- To construct input files (and analyze output) you, as the user, *must write a Python script* utilizing classes defined by the OpenMC API
- There are many benefits to using Python API over direct use of XML, e.g.,
  - All the usual benefits of Python – variables vs. hard-coded numbers, standard library, third-party packages
  - Run-time type checking
  - Perturbation or sensitivity studies
  - Extra features in our API – data analysis, multi-group cross section generation, nuclear data parsers, etc.
- **Caveat:** You need to know Python!

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Python 101

Python is often thought of as a "scripting" language

- Dynamically typed (type of variable interpreted at runtime)
- Implicitly typed (type of variable never declared)
- Case-sensitive (var and VAR are different)
- Object oriented (everything is an object)
- Containers are zero-indexed

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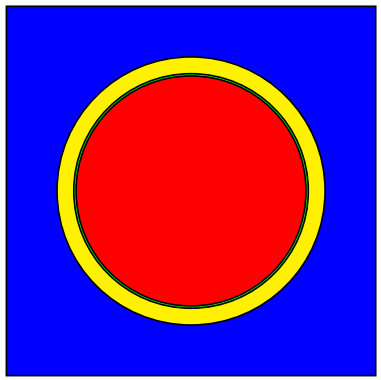
Problem to Solve

- Simple pin cell comprised:
  - UO_2 ($10.3\,g/cm^3$)
  - Clad ($6.55\,g/cm^3$)
  - Water ($0.701\,g/cm^3$)
- Dimensions:
  - Fuel OR $= 0.392\,18$ cm
  - Clad IR $= 0.400\,05$ cm
  - Clad OR $= 0.457\,20$ cm
  - Pitch $= 1.259\,84$ cm

Material	Isotope	Composition Fraction (a or w)
Fuel	U-235	0.02115 (w)
Fuel	U-238	0.86032 (w)
Fuel	O-16	0.11852 (w)
Clad	Zr	elemental
Water	H-1	2.0 (a)
Water	O-16	1.0 (a)

w = weight fraction, a = atom fraction



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Creating Materials

- Material defined as collection of nuclides (`openmc.Nuclide`) and/or elements (`openmc.Element`) with assigned atom/weight fractions
- Each nuclide/element has a `name` and `xs` which link it to an ACE file
  - `name` is a nuclide's or element's name (e.g., H-1 or Zr)
  - `xs` is the ACE file cross section extension (for temperature)
- Total density of material can be specified in units of `g/cc` or `atom/b-cm` (renormalization based on total density)
- Thermal scattering libraries should be assigned to moderator materials
- In many cases, specifying default cross section is useful

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Geometry and Material Assignments

- **Cell** defined by assigning a material/fill to a region
- **Region** defined as intersection, union, and/or complement surface half-spaces
- **Surface** is a locus of zeros of a function
  - Planes, e.g., $x - x_0 = 0$
  - Cylinders parallel to axis, e.g., $y^2 + z^2 - R^2 = 0$
  - Sphere, e.g., $x^2 + y^2 + z^2 - R^2 = 0$
  - Cones parallel to axis, e.g., $x^2 + z^2 - R^2 y^2 = 0$
  - General quadratic
- Surface **half-space** is the region whose points satisfy a positive/negative inequality of the surface equation
- Universes, rectangular/hexagonal lattices, rotation/translation

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Simulation Settings

- At a minimum, one should specify how many particles to run and initial starting source
- The `openmc.Settings` object contains these and other settings:
  - `Settings.source` – list of sources
  - `Settings.batches` – number of batches
  - `Settings.inactive` – number of inactive batches
  - `Settings.particles` – number of particles per batch

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Source Definitions

- The `openmc.Source` object allows one to specify separate spatial, angular, and energy distributions
  - Spatial distributions: independent (x, y, z), box, point
  - Angular distributions: independent (μ, ϕ), isotropic, monodirectional
  - Energy distributions: discrete, tabular, uniform, Maxwell, Watt

Defining Tallies

Tallies are defined as combinations of *filters* and *scores*

$$X = \underbrace{\int d\mathbf{r} \int d\mathbf{\Omega} \int dE}_{\text{filters}} \underbrace{f(\mathbf{r}, \mathbf{\Omega}, E)}_{\text{scores}} \psi(\mathbf{R}, \mathbf{\Omega}, E)$$

- Filters: cell, material, energy, outgoing energy, mesh, ...
- Scores: flux, total, fission, nu-fission, scatter, absorption, scattering moments, individual reactions, ...
- Can also specify nuclides

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Plotting Geometry

- OpenMC can be run in plotting mode to create either slice or voxel plots
- Slice plots are `.ppm` files – usually best to convert to `.png`

Running OpenMC

With a complete set of inputs, we can run OpenMC by either

1. Dropping into a terminal and running `openmc`
2. Calling `openmc.run()`

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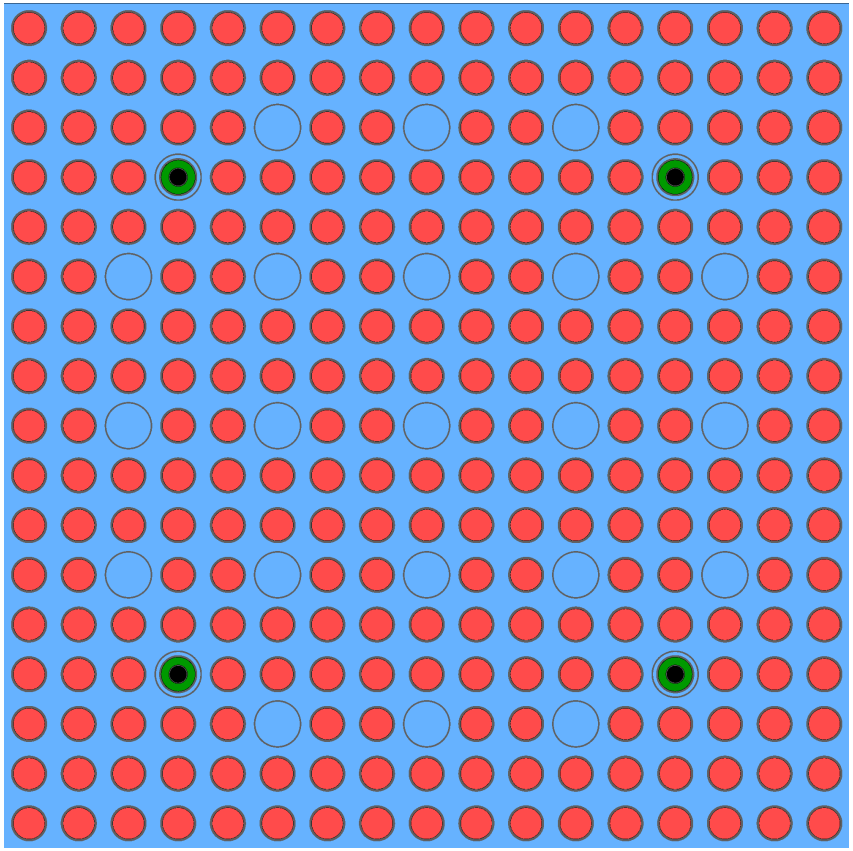
Lattices

Pin cells are cool, but some physics can only be captured in a lattice calculation. This section will show how to construct and tally lattices in OpenMC.



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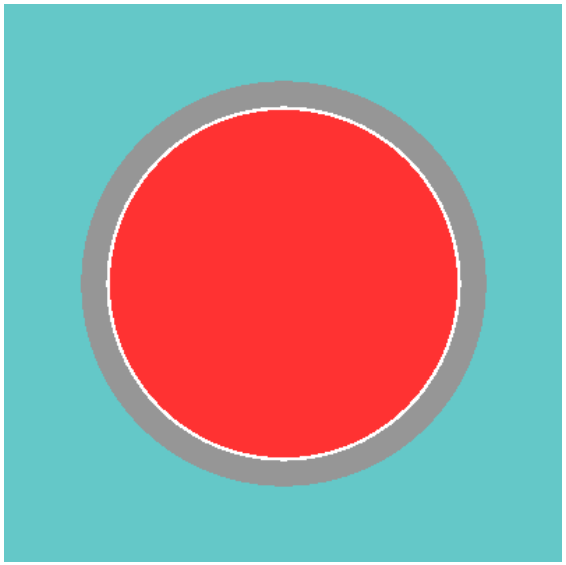
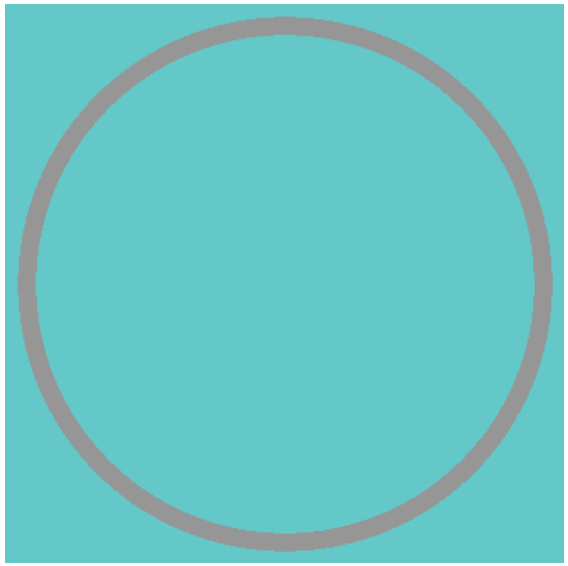
Piece-by-piece

Build each component of your lattice in its own universe, and test it as you go along

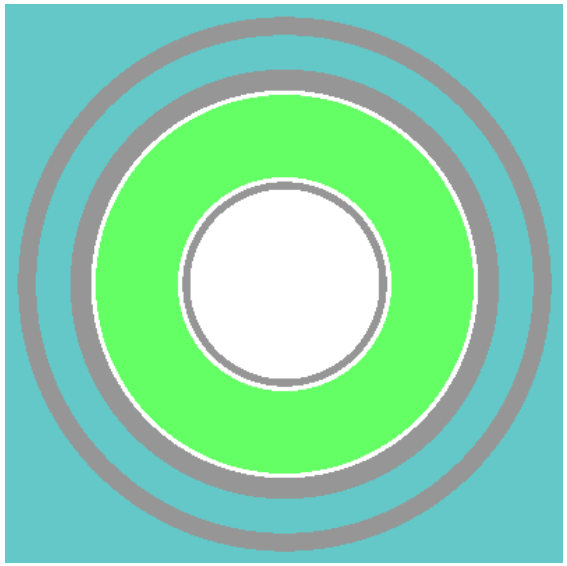
Fuel pin:



Guide tube:



Burnable absorber:



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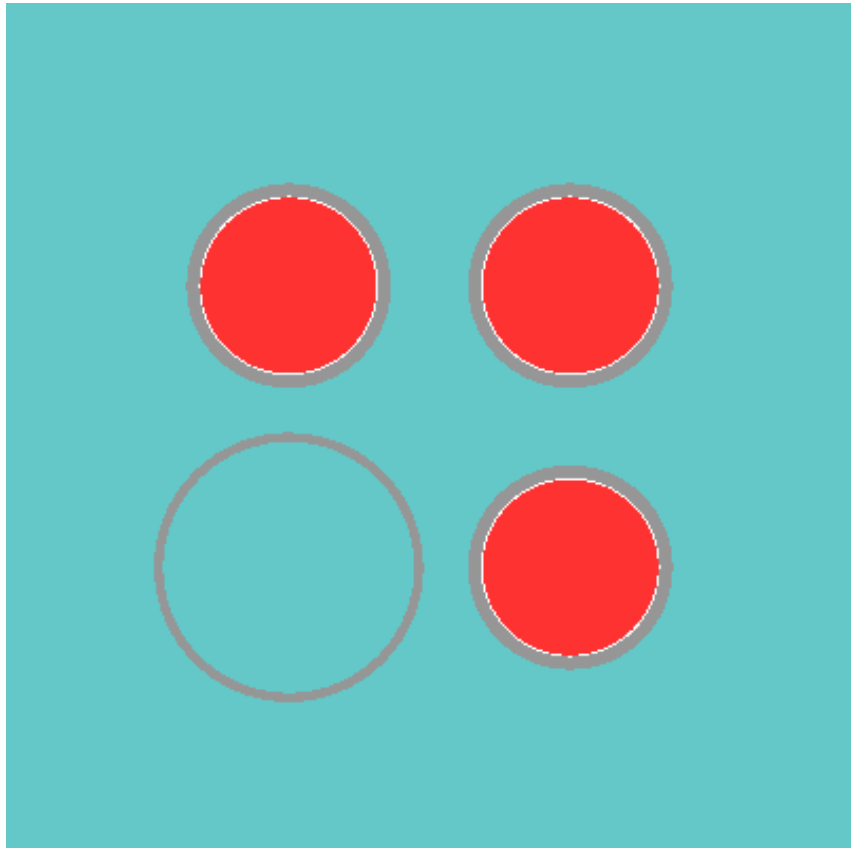
A simple lattice

```
lattice = openmc.RectLattice()
lattice.dimension = [2, 2]
lattice.lower_left = [0.0, 0.0]
lattice.pitch = [pitch]*2
lattice.universes = [
    [fuel_pin,   fuel_pin],
    [guide_tube, fuel_pin]
]
lattice.outer = all_water
```



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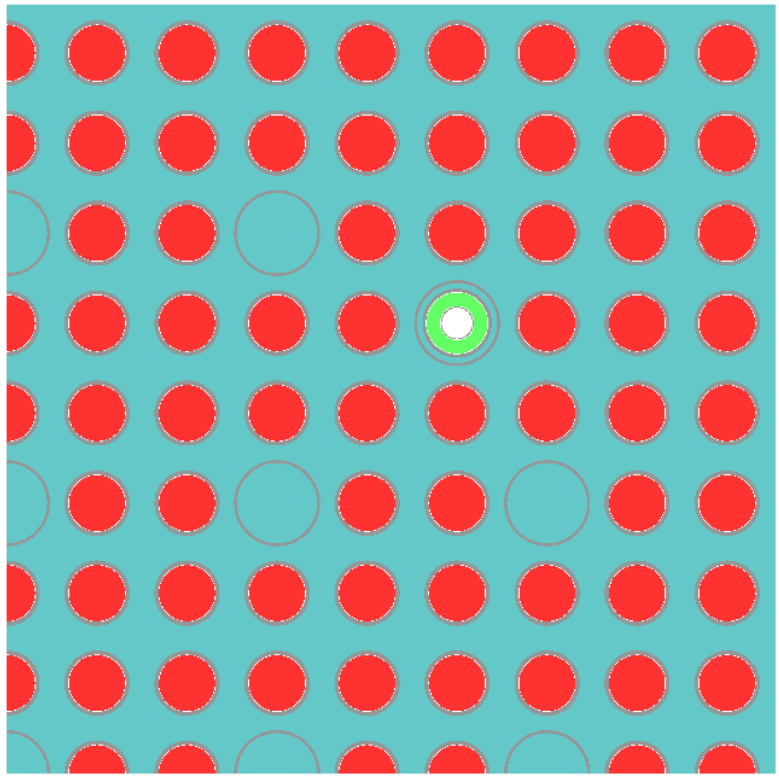
The quarter assembly

```
lattice = openmc.RectLattice()
lattice.dimension = [9, 9]
lattice.pitch = [pitch]*2
lattice.outer = all_water
lattice.lower_left = [-pitch/2.0]*2
lattice.universes = [
    [fuel_pin for i in range(9)] for j in range(9)]
lattice.universes[2][0] = guide_tube
lattice.universes[2][3] = guide_tube
lattice.universes[5][0] = guide_tube
lattice.universes[5][3] = guide_tube
lattice.universes[5][6] = guide_tube
lattice.universes[8][0] = guide_tube
lattice.universes[8][3] = guide_tube
lattice.universes[8][6] = guide_tube
lattice.universes[3][5] = burn
```



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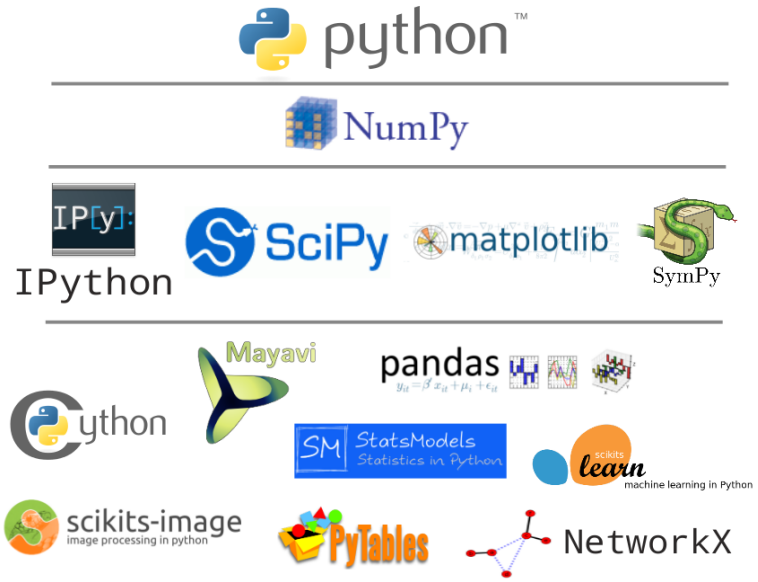
Leverage the Python Ecosystem

- Python API is built to serve your data processing needs
- Enables **tight coupling** with **Python's ecosystem** of scientific computing packages
- We will interactively explore OpenMC's features to **accelerate data workflows**



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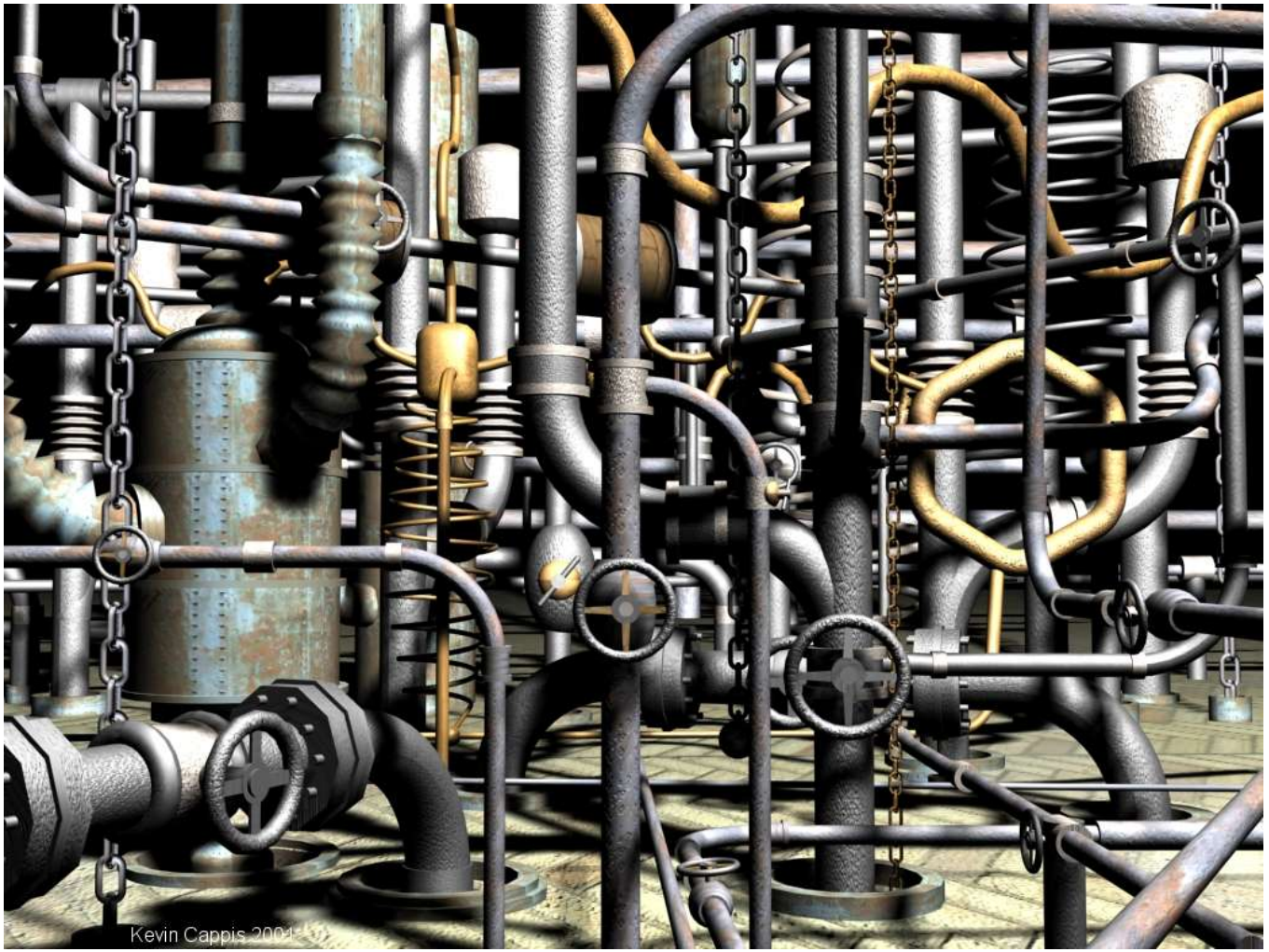
Everything You Need to Build a Data Pipeline!



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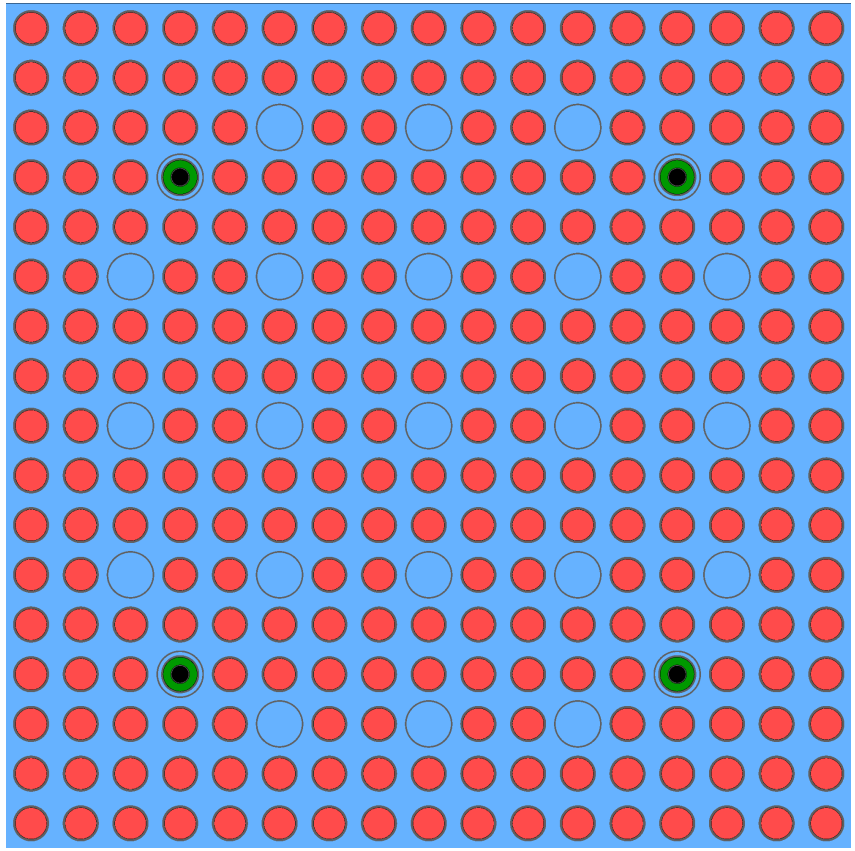
Data Processing Demo Case Study

- A 17 $\times$ 17 PWR fuel assembly
- Pin cells comprised of:
  - UO2 fuel
  - Helium gap
  - Zircaloy clad
  - Light water moderator
  - Pyrex burnable poisons
- A variety of tallies for us to interactively analyze



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StatePoint and Summary Files

StatePoint Files

- HDF5 output files with **source sites** and **tally data**
- Output **statepoint.*.h5** files for some or all batches
- Easily processed with `openmc.StatePoint`

Summary Files

- HDF5 output files with **geometric** and **materials**
- Output **summary.h5** file at beginning of simulation
- Easily processed with `openmc.Summary`

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Simulation Metadata

- Metadata in a `StatePoint`
  - Various estimators for k_{eff} (*i.e.*, `StatePoint.k_combined`)
  - Simulation parameters (*i.e.*, # batches, #particles / batch, etc.)
  - Simulation date, time, version, etc.

- Metadata in a `Summary`
  - Complete description of model geometry and materials
  - Methods to retrieve `Material`, `Surface`, `Cell`, etc. objects
  - **Link metadata** with `Tally` objects using `StatePoint.link_with_summary(...)`

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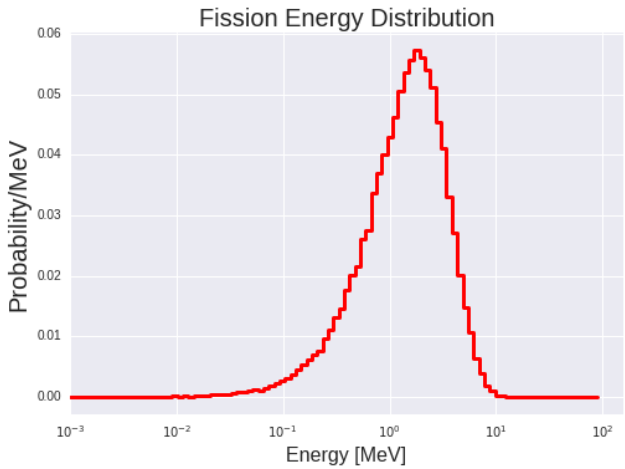
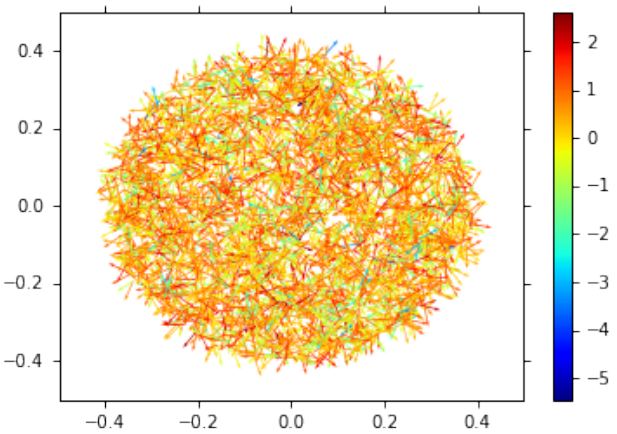
Neutron Source Sites

- A `StatePoint` contains complete **source bank** for current batch
- Access source sites with `StatePoint.source` property
- Each **source site** includes the following data:
  - Spatial location `xyz`
  - Angular trajectory `uvw`
  - Energy [MeV] `E`
- Source sites can be left out of statepoint files to save space





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Extracting Tallies from a StatePoint

- A `StatePoint` encapsulates metadata and `Tally` objects
- The `StatePoint.tallies` property is a Python dictionary of `Tally` objects indexed by integer ID
- The `StatePoint.get_tally(...)` method is highly recommended over direct access to `tallies` property
- Retrieves the first `Tally` found in the `StatePoint` matching one or more of the following descriptors:
  - Integer ID
  - String name
  - One or more `Filters`
  - One or more nuclides
  - One or more scores

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Inspecting Tallies

- View description of `Tally` with Python's `print(...)` method
- A few key `Tally` properties:
  - `Tally.id` - integer ID
  - `Tally.name` - string name
  - `Tally.scores` - list of scores
  - `Tally.nuclides` - list of nuclides
  - `Tally.filters` - list of `Filters`
  - `Tally.mean` - **3D array of sample means**
  - `Tally.std_dev` - **3D array of standard deviations**
- The sample means and uncertainties are stored in NumPy arrays indexed by filter bin, nuclide and score

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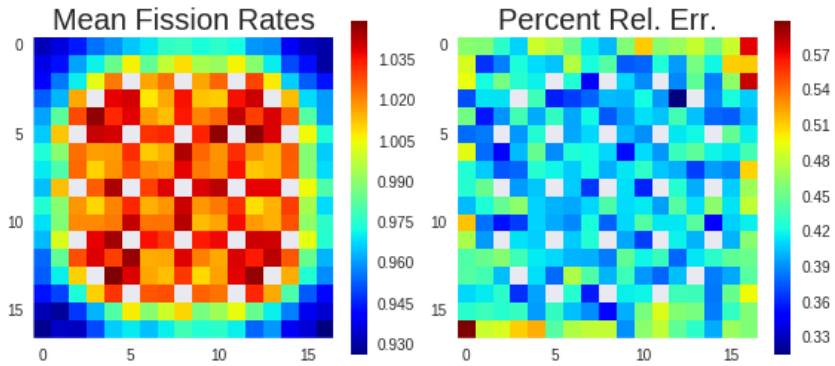
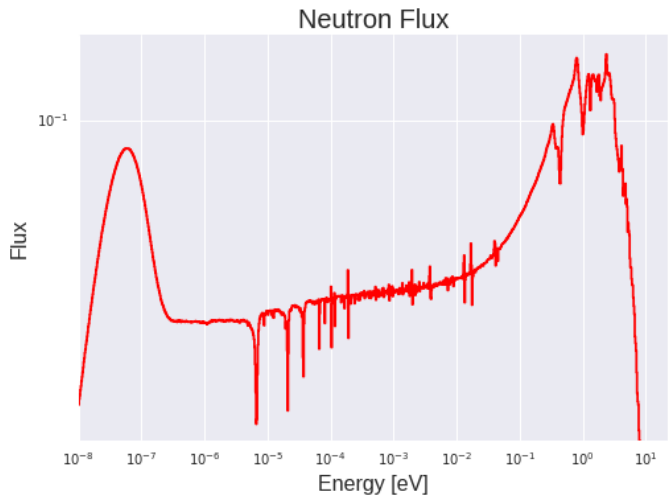
Plotting Tally Data

- Python API closes the gap between your tally data and a rich variety of plotting tools:
  - **matplotlib** - Python's *de facto* general purpose plotting package
  - **seaborn** - High-level statistical graphics interface
  - **bokeh** - Interactive visualization in the browser
  - **statsmodels** - Statistical plotting inspired by R
- Share your coolest visualizations with the OpenMC community!





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Pandas DataFrames for Tally Data

Problem: Tallies are Opaque

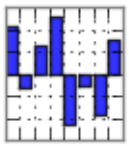
- OpenMC tally data is stored by filter, nuclide and score
- Difficult to rapidly index contiguous tally data arrays
- Need to quickly inspect data to debug simulation data workflows

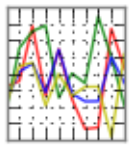
Solution: Pandas DataFrames

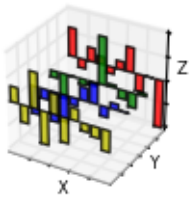
- Pandas `DataFrame` containers inspired by R
- A 2D data structure of columns and rows
- Includes an amazing assortment of features:
  - Mixed type data (*i.e.*, strings, integers)
  - Fancy indexing, slicing and subsetting
  - And a LOT more!

pandas

$$y_{it} = \beta' x_{it} + \mu_i + \epsilon_{it}$$







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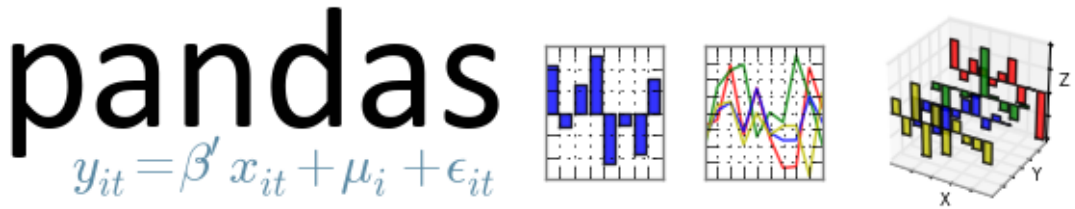
OpenMC + Pandas

- OpenMC `Tally` objects can construct a `DataFrame` with columns for filters, nuclides, and scores
- Each row corresponds to a sample mean and uncertainty for one combination of filter, nuclide and score bins
- Retrieve a Pandas `DataFrame` from tally data with `Tally.get_pandas_dataframe()`



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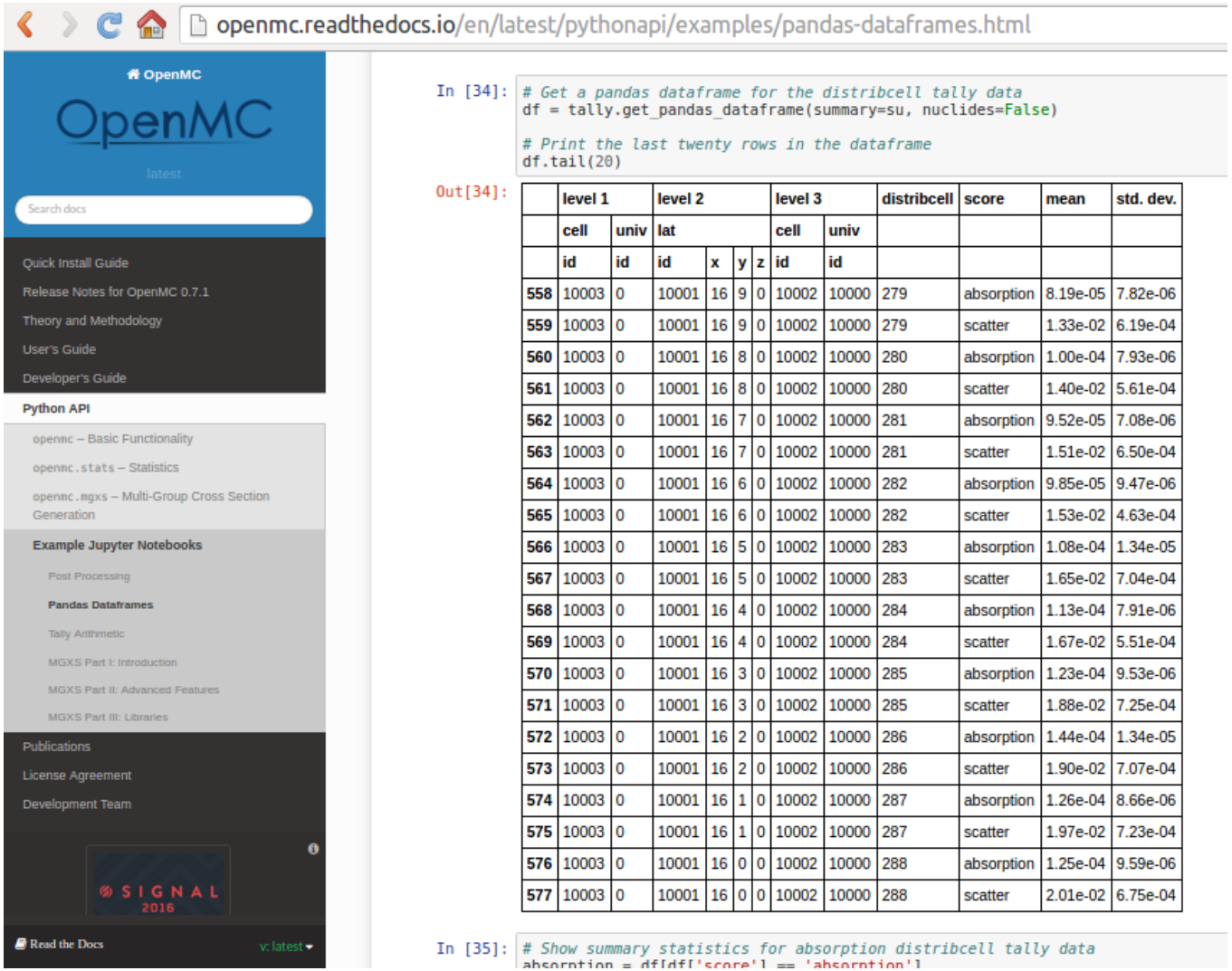
OpenMC + Pandas (Cont.)



In [34]:
```
# Get a pandas dataframe for the distribcell tally data
df = tally.get_pandas_dataframe(summary=su, nuclides=False)

# Print the last twenty rows in the dataframe
df.tail(20)
```

Out[34]:

	level 1		level 2				level 3		distribcell	score	mean	std. dev.
	cell	univ	lat				cell	univ				
	id	id	id	x	y	z	id	id				
558	10003	0	10001	16	9	0	10002	10000	279	absorption	8.19e-05	7.82e-06
559	10003	0	10001	16	9	0	10002	10000	279	scatter	1.33e-02	6.19e-04
560	10003	0	10001	16	8	0	10002	10000	280	absorption	1.00e-04	7.93e-06
561	10003	0	10001	16	8	0	10002	10000	280	scatter	1.40e-02	5.61e-04
562	10003	0	10001	16	7	0	10002	10000	281	absorption	9.52e-05	7.08e-06
563	10003	0	10001	16	7	0	10002	10000	281	scatter	1.51e-02	6.50e-04
564	10003	0	10001	16	6	0	10002	10000	282	absorption	9.85e-05	9.47e-06
565	10003	0	10001	16	6	0	10002	10000	282	scatter	1.53e-02	4.63e-04
566	10003	0	10001	16	5	0	10002	10000	283	absorption	1.08e-04	1.34e-05
567	10003	0	10001	16	5	0	10002	10000	283	scatter	1.65e-02	7.04e-04
568	10003	0	10001	16	4	0	10002	10000	284	absorption	1.13e-04	7.91e-06
569	10003	0	10001	16	4	0	10002	10000	284	scatter	1.67e-02	5.51e-04
570	10003	0	10001	16	3	0	10002	10000	285	absorption	1.23e-04	9.53e-06
571	10003	0	10001	16	3	0	10002	10000	285	scatter	1.88e-02	7.25e-04
572	10003	0	10001	16	2	0	10002	10000	286	absorption	1.44e-04	1.34e-05
573	10003	0	10001	16	2	0	10002	10000	286	scatter	1.90e-02	7.07e-04
574	10003	0	10001	16	1	0	10002	10000	287	absorption	1.26e-04	8.66e-06
575	10003	0	10001	16	1	0	10002	10000	287	scatter	1.97e-02	7.23e-04
576	10003	0	10001	16	0	0	10002	10000	288	absorption	1.25e-04	9.59e-06
577	10003	0	10001	16	0	0	10002	10000	288	scatter	2.01e-02	6.75e-04

In [35]:
```
# Show summary statistics for absorption distribcell tally data
absorption = df[df['score'] == 'absorption']
```

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Manipulating Tallies - Tally Slicing

- A `Tally` may contain more data than is needed for some downstream calculations
- **Tally "slicing"** extracts a subset of data from a `Tally` object
- The `Tally.get_slice(...)` method is designed to arbitrarily slice `Tally` objects by `Filter` bin(s), nuclide(s) or score(s)
- Slice out data for U-235 from a `Tally` with multiple nuclides:
  - `slice = tally.get_slice(nuclides=['U-235'])`
- The "sliced" tally data is encapsulated within a fully expressive `Tally`, while the original `Tally` remains intact

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Manipulating Tallies - Tally Summation

- It may be useful to sum across a `Tally` for some downstream calculations (*i.e.*, nuclides, scores, etc.)
- **Tally "summation"** sums a subset of data in a `Tally` object
- The `Tally.summation(...)` method is designed to arbitrarily sum `Tally` objects across `Filter` bin(s), nuclide(s) or score(s)
- Sum data for U-235 and U-238 from a `Tally`:
  - `sum = tally.summation(nuclides=['U-235', 'U-238'])`
- The "summed" tally data is encapsulated within a fully expressive `Tally`, while the original `Tally` remains intact

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Manipulating Tallies - Tally Arithmetic

- Many data workflows require the arithmetic combination of multiple tallies
- **Tally "arithmetic"** applies binary operations to `Tally` objects
- Tally arithmetic automatically performs **uncertainty propagation** through each operation
- Add two `Tally` objects and divide by a third:
  - `tallyD = (tallyA + tallyB) / tallyC`
- The resultant tally data is encapsulated within a fully expressive `Tally`, while the original `Tally` operands remains intact
- **Fast** and **efficient** with **NumPy vectorization**

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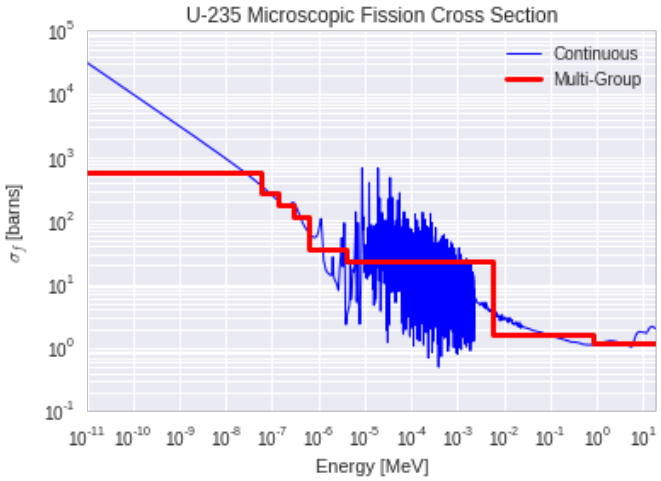
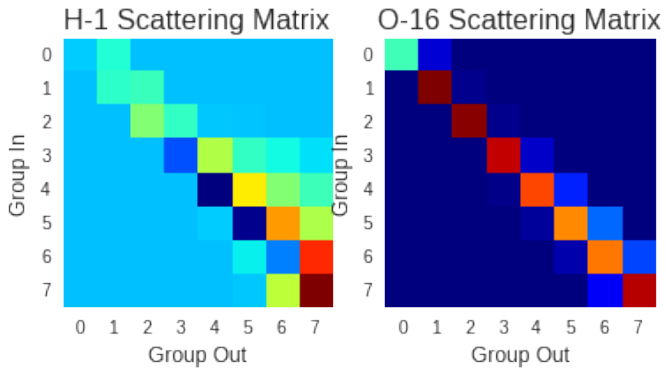
Multi-Group Cross Section Generation





- New `openmc.mgxs` package to calculate **multi-group cross sections** (MGXS)
- Built atop of Python API using tally arithmetic, slicing, etc.
- Tight integration with custom Pandas `DataFrames`
- **Fast** and **efficient** with **NumPy vectorization**
- Designed for next-gen **high-fidelity neutron transport codes**

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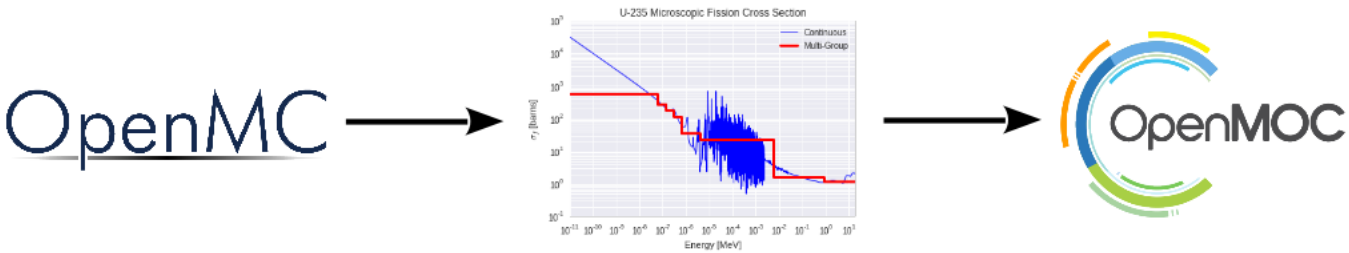
Pipelining OpenMC MGXS to OpenMOC

- MIT CRPG's OpenMOC deterministic neutron transport code is fully equipped to easily make use of `openmc.mgxs`
- Compute OpenMC MGXS `Library` with 5-10 lines of Python
- Inject MGXS `Library` into OpenMOC with 1 line of Python
- **Use a single constructive solid geometry for both OpenMC and OpenMOC calculations**



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Outline

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Installation on Ubuntu

For users with Ubuntu 15.04 or later, a binary package for OpenMC is available through a Personal Package Archive (PPA) and can be installed through the APT package manager.

```
sudo apt-add-repository ppa:paulromano/staging
```

```
sudo apt-get update
```

```
sudo apt-get install openmc
```

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Building from Source

To compile from source you will need a Fortran compiler (e.g gfortran v4.6 or greater), CMake and an HDF5 library compiled with your Fortran compiler (and optionally MPI).

```
git clone https://github.com/mit-crpg/openmc.git
```

```
cd openmc && git checkout master
```

```
mkdir build && cd build && cmake .. && make
```

For more details, see `http://openmc.readthedocs.io/en/latest/`

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Question and Bugs

Questions can be submitted to the OpenMC User group on Google Groups

- Search for OpenMC on https://groups.google.com/
- or https://groups.google.com/forum/#!forum/openmc-users

Bugs or interest in new features can be reported on the github page by creating a New Issue

- https://github.com/mit-crpg/openmc/issues
- For bugs, please include input file reproducing the error
- For new features, new developers are always welcome!

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OpenMC Papers at PHYSOR 2016

- **Monday Afternoon, 4:25pm (Columbine)** J.Walsh, B.Forget, K.Smith, F.Brown: *On-The-Fly Doppler Broadening of Unresolved Resonance Region Cross Sections Via Probability Band Interpolation*
- **Monday Evening 6:00pm** P.Romano: *Efficacy of Hardware Threading for Monte Carlo Particle Transport Calculations on Multi- And Many-Core Systems*
- **Wednesday Morning, 11:50am (Columbine)** Z.Liu, K.Smith, B.Forget: *A Cumulative Migration Method for Computing Rigorous Transport Cross Sections and Diffusion Coefficients for LWR Lattices with Monte Carlo*
- **Wednesday Afternoon, 2:20pm (Sawtooth)** W.Boyd, P.Romano, S.Harper: *Equipping OpenMC for the Big Data Era*
- **Thursday Morning, 8:00am (Columbine)** M.Ellis, D.Gaston, B.Forget, K.Smith: *Continuous Temperature Representation in Coupled OpenMC/MOOSE Simulations*

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Other CRPG Papers at PHYSOR 2016

- **Monday Afternoon, 4:25pm (Camas)** S.Shaner, G.Gunow, K.Smith, B.Forget: *Verification of the 3D Method of Characteristics Solver in OpenMOC*
- **Tuesday Morning, 9:15am (Columbine)** K.Smith: *Nodal Diffusion Methods: Understanding Numerous Unpublished Details*
- **Tuesday Afternoon, 1:30pm (Columbine)** P.Ducru, V.Sobes, B.Forget, K.Smith: *On Methods for Conversion to Multipole Formalism*
- **Thursday Morning, 8:25am (Boiler)** G.Gunow, S.Shaner, B.Forget, K.Smith: *Reducing 3D MOC Storage Requirements with Axial On-the-Fly Ray Tracing*

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Upcoming Features

- On-the-fly Doppler Broadening
- Domain Decomposition
- Multiphysics
- Differential Tallies
- Depletion
- Transient Analysis

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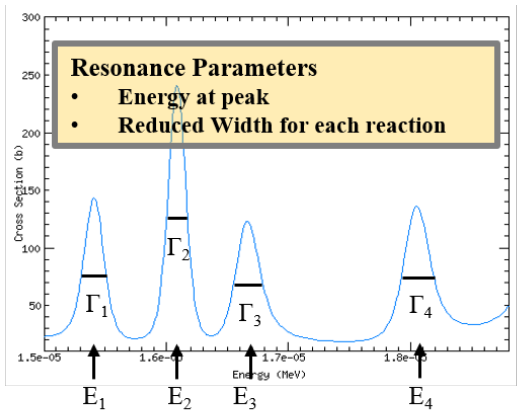
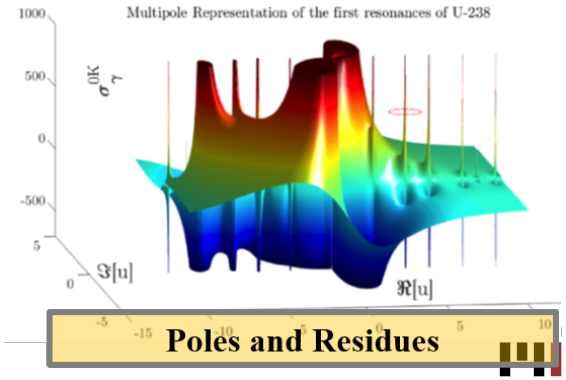
Doppler Broadening

- On-the-fly Doppler broadening based on the windowed multipole method (300 of the 423 nuclides in ENDF/BVII.1)
- On-the-fly URR sampling or equiprobable E-T surfaces
- Kernel Reconstruction for remaining 100 nuclides
- Currently developing an HDF5 library format to replace ACE files





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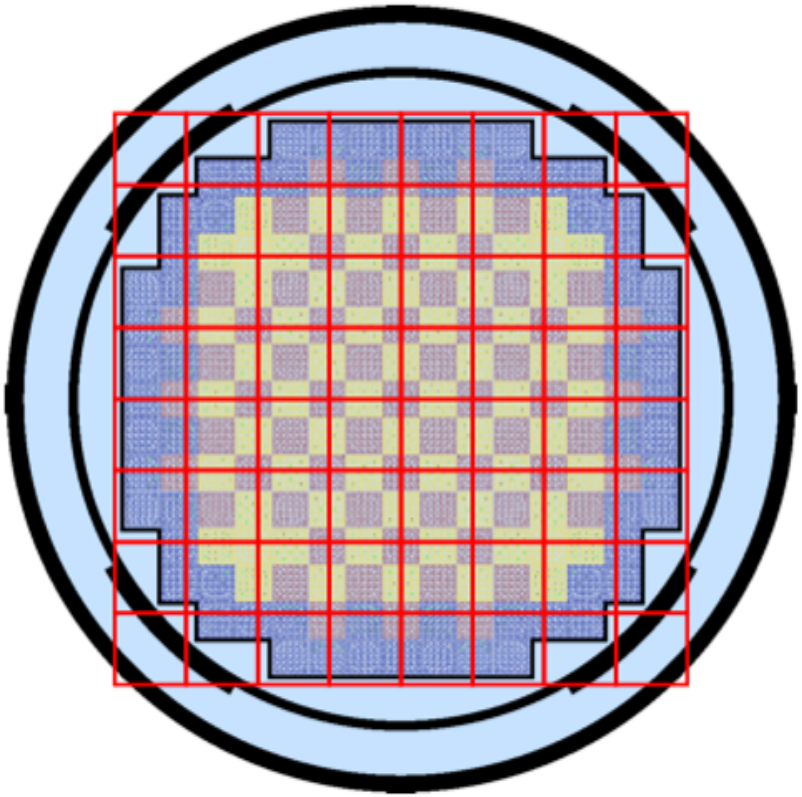
Domain Decomposition

- Arbitrary mesh domain decomposition for distributing memory from tallies and material compositions
- Load balancing achieved by domain replication
- Currently under review



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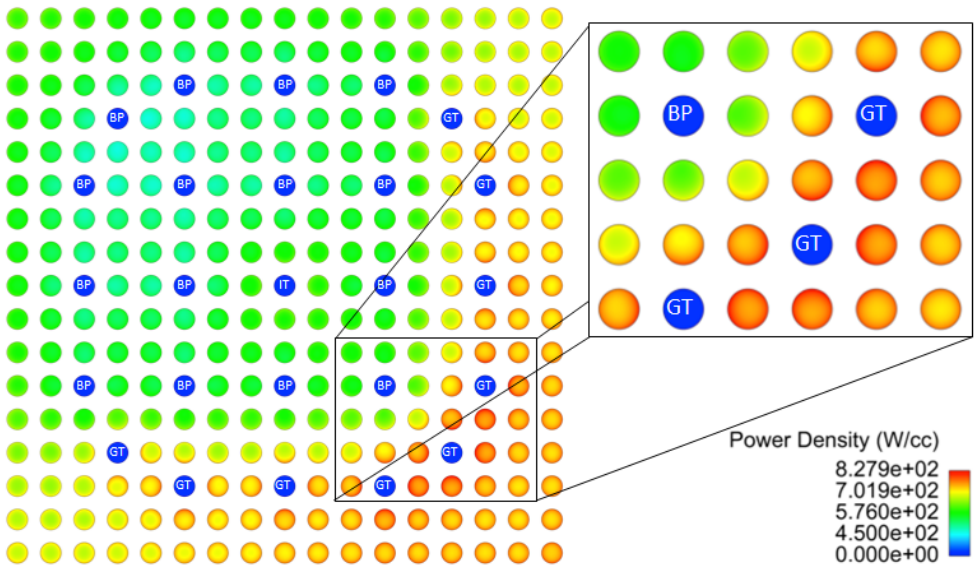
Multiphysics

- OpenMC was built as a library and incorporated as a MultiApp in MOOSE
- Functional expansion tallies were implemented to transfer data between CSG and FEM
- Continuous material tracking was implemented to allow for continuously varying temperature and nuclide densities within a CSG cell



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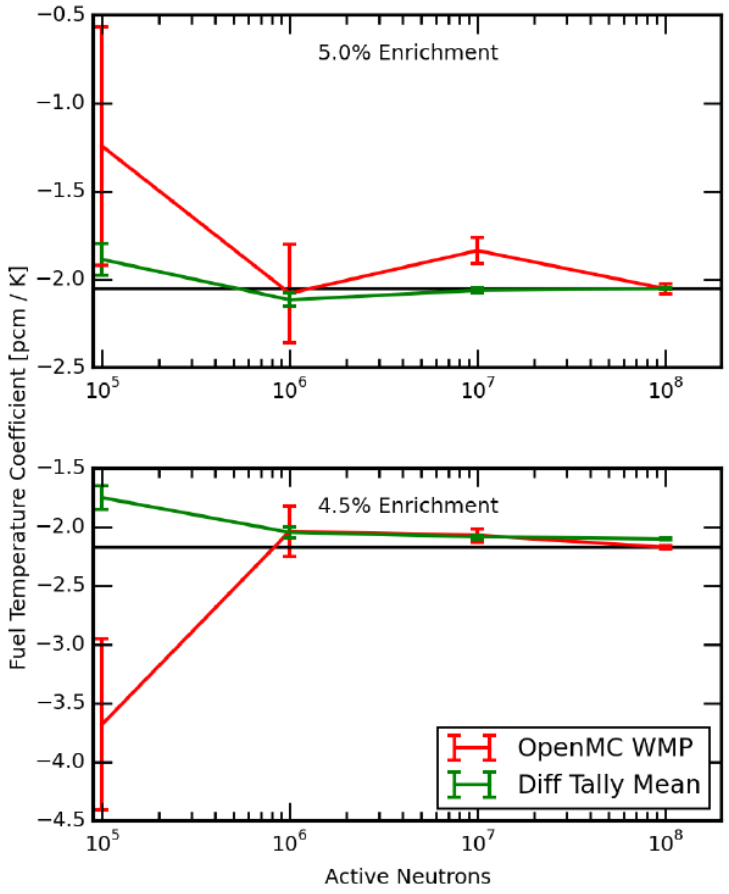
Differential Tallies

- Implemented differential tallies to tally first order derivatives with density changes
- Extended to include temperature using first order derivatives of the multipole equations
- OpenMC will thus be able to provide accurate temperature and density reactivity coefficients in a single run
- Can also provide cross section temperature derivatives

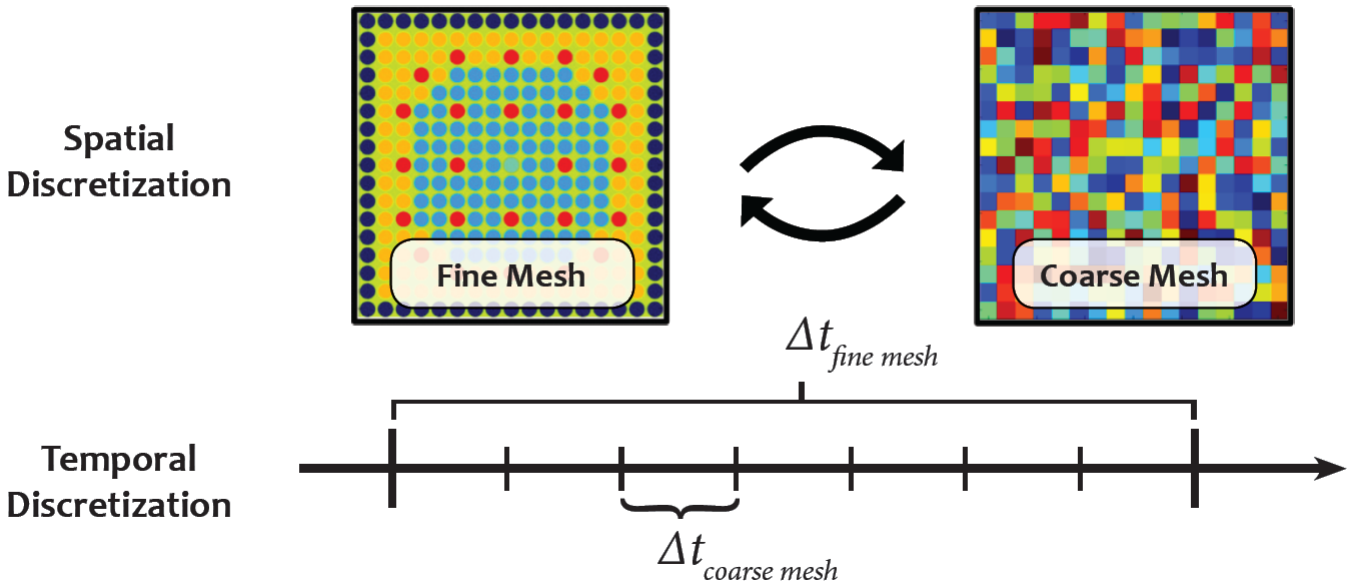


Depletion

When will OpenMC add depletion?

Transient Analysis

- Implementing multigrid amplitude function approach where the CMFD operator will be advanced on fine time steps with parameters updated from OpenMC on coarse time steps



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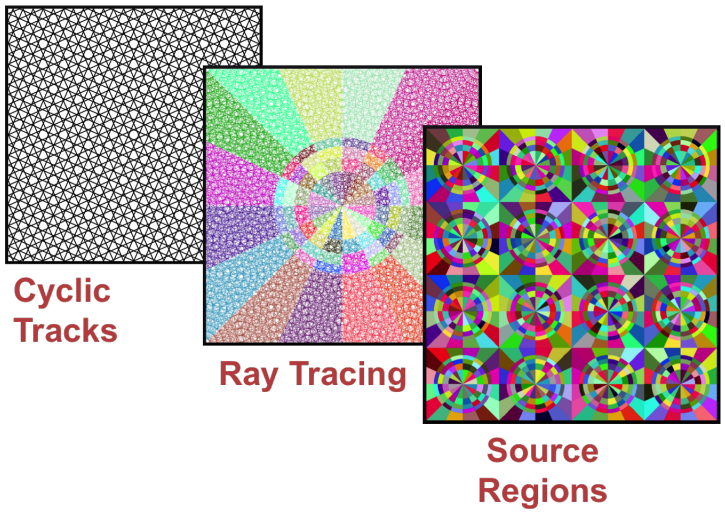
Other MIT-CRPG code - OpenMOC

- A Method of Characteristics code platform for solving the multigroup 2D and 3D form of the neutron transport equation.
- MOC: "Monte Carlo on Rails"
- Fast and accurate deterministic transport simulations.
- Ongoing development of data pipeline between OpenMC and OpenMOC to utilize multigroup XS generated from OpenMC.



OpenMOC

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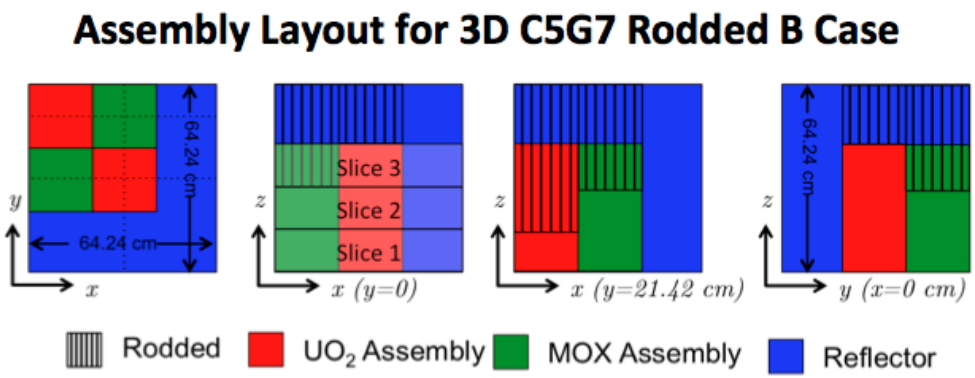
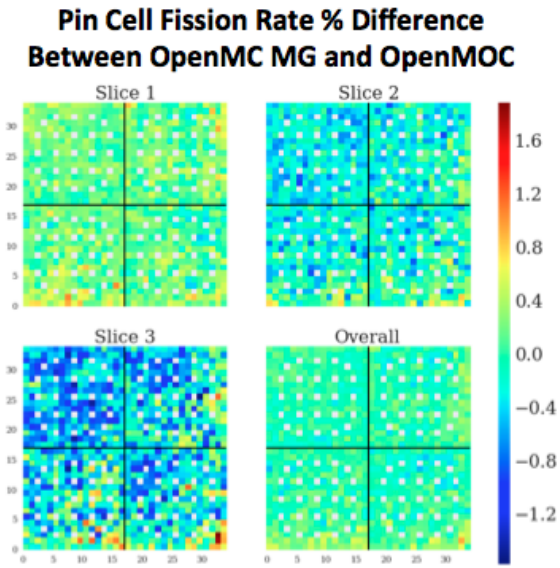
Cross-code verification - OpenMC MG and OpenMOC

- Multigroup Monte Carlo solver recently added to OpenMC by Adam Nelson.
- Allows for cross-code comparison with deterministic transport codes, such as OpenMOC.





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