OpenMC Module: Description of OpenMC

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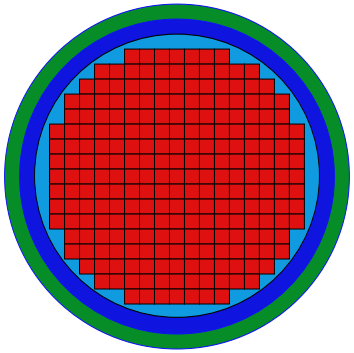
Goals of the OpenMC Project

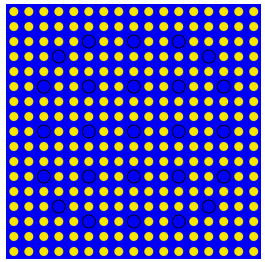
- Develop a Monte Carlo framework for reactor analysis that scales on leadership-class supercomputers (100,000+ cores)
- Provide a simple tool to analyze performance and limitations on proposed architectures
- Objectives:
  - Realistic physics
  - Modern programming style and data structures
  - Extensible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

Characteristics of OpenMC

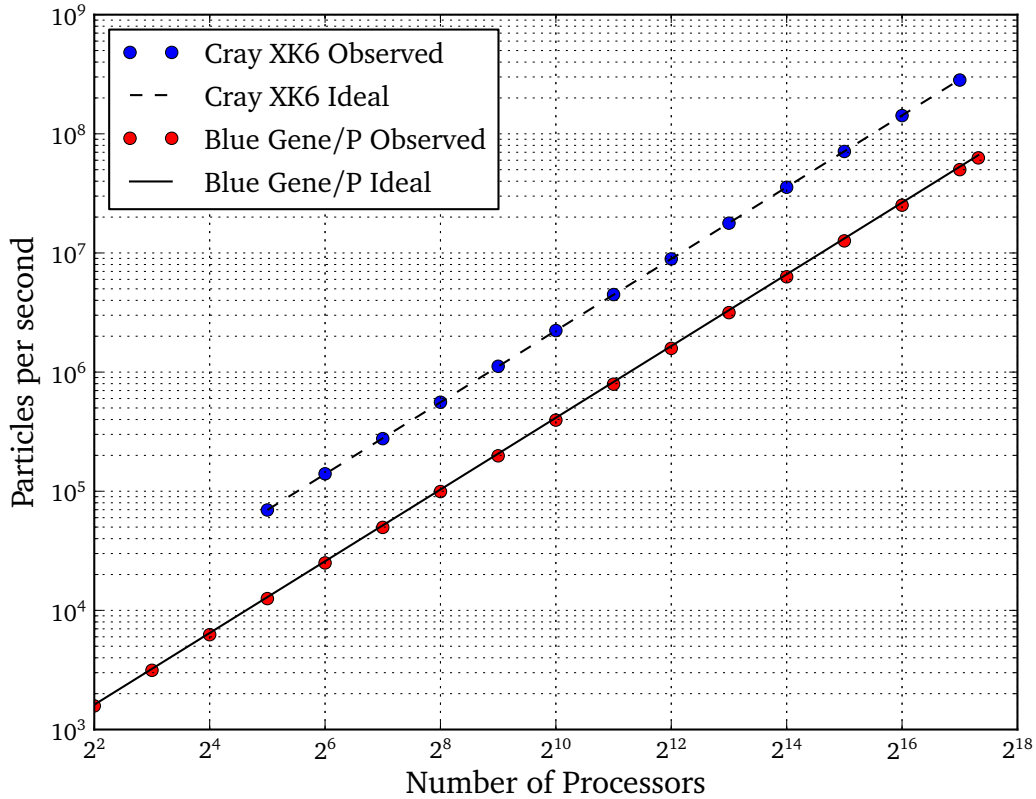
- Fixed source and k-eigenvalue calculations
- Geometry: constructive solid geometry, second-order surfaces
  - Universes and lattices
  - Rotations and translations
- Cross sections: ACE format (MCNP, Serpent)
- Physics: Only neutrons for now
  - $S(\alpha, \beta)$ thermal scattering
  - Unresolved resonance probability tables
  - Free gas thermal scattering
- Plotting: rasterization using find_cell
- Tallies:
  - Collision and path-length estimators
  - Surface and volume mesh tallies
- Distributed memory parallelism via MPI
- XML input format, HDF5 output format

Parallel Performance


Core

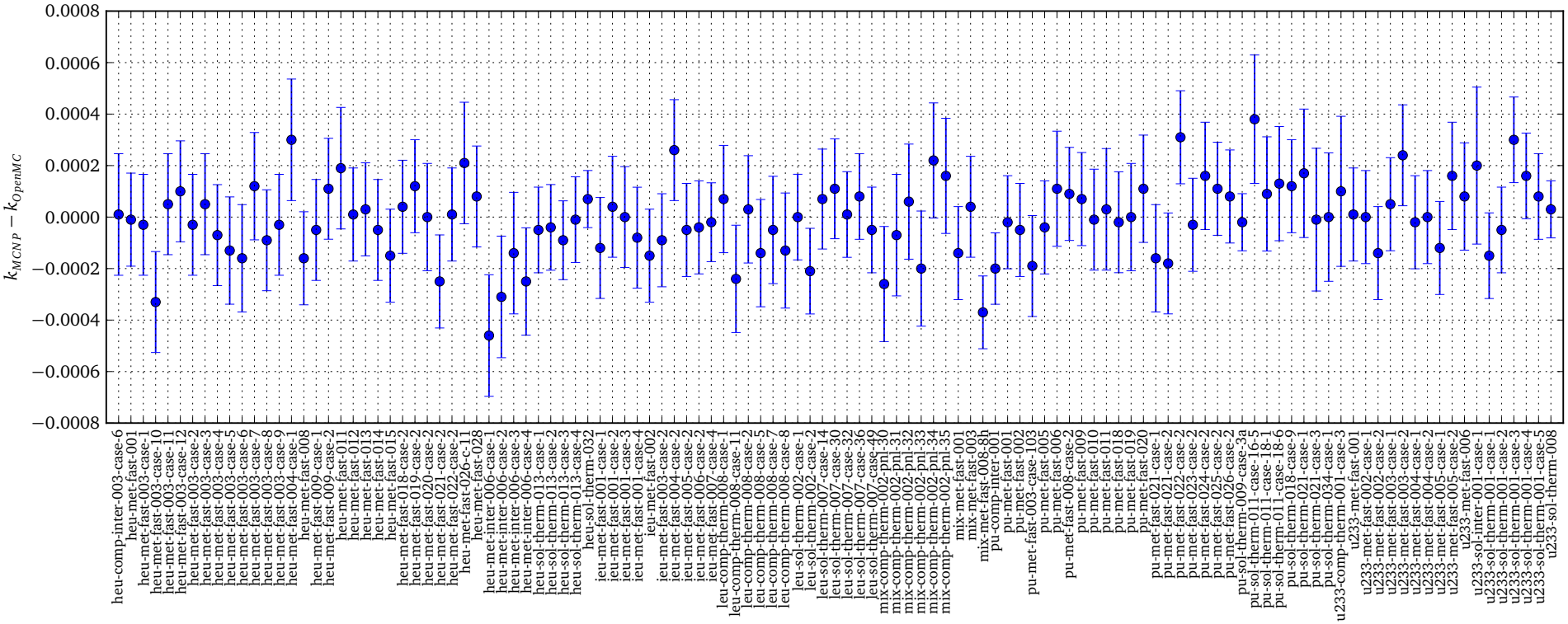

Assembly

- $2^{17} = 131,072$
- Cray XK6 = ORNL Jaguar
- Blue Gene/P = ANL Intrepid



Validation and Verification

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



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Obtaining OpenMC

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

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

- Ubuntu PPA:

```
sudo apt-add-repository ppa:paulromano/staging
sudo apt-get update
sudo apt-get install openmc
```

Compiling on Linux/Mac OS X

- ~30,000 lines of Fortran 2008 code
- All handled by a Makefile

```
cd openmc/src
make
```

- Optional dependencies
  - MPI for distributed-memory parallelism
  - HDF5 for portable standard binary output format
  - PETSc for CMFD acceleration
- Works with gfortran, Intel, IBM, Cray, PGI compilers
- On Mac OS X, can obtain compiler via Mac Ports

Compiling on Windows

- Uninstall Windows
- Install a better operating system, like Linux
- Follow previous directions

Compiling on Windows

- No native Windows binaries (yet)
- Options: Cygwin or MinGW (Minimalist GNU for Windows)
- Successful builds using both
- Visual Studio Port:
  `https://bitbucket.org/Lockee/openmc_vs2010`

Cross Sections

- You'll need:
  - A set of ACE format cross sections
  - A cross_sections.xml file
- Cross section data is not currently distributed with the code. Your options are:
  - Obtain JEFF data in ACE format from OECD/NEA
  - Use data from MCNP or Serpent
  - Process raw ENDF/B data into ACE format using NJOY

XML Input Format

- Unlike many nuclear codes, OpenMC uses a modular XML input format
  - Building a geometric model — **geometry.xml**
  - Define materials in problem — **materials.xml**
  - Settings paramters for the simulation — **settings.xml**
  - Determining which quantities to score — **tallies.xml**
  - Creating geometry plots — **plots.xml**

XML Basics

- XML = e**X**tensible **M**arkup **L**anguage
- Two kinds of information in a file:
  - *Markup*, like `<firstName>`, that describes the structure of the document, and
  - *Text*, like "Paul", that is the actual content of the document
- All text must be contained within *opening* and *closing* tags, e.g. `<firstName>Paul</firstName>`

XML Basics

- Nesting of elements usually represents logical relationships:

```
<?xml version="1.0"?>
<EmployeeDatabase>

  <!-- Information about our employees -->

  <employee>
    <firstName>Paul</firstName>
    <lastName>Romano</lastName>
    <age>26</age>
  </employee>

  <employee firstName="Li" lastName="Zhu" age="34" />

</EmployeeDatabase>
```

Configure Cross Section Data

- Download cross section data from website
- In this directory you will find a `cross_sections.xml`
- Open this file and change directory absolute path to your current directory path
  - You can type `echo $PWD` to determine this
- Set up cross section environmental variable
  - `export CROSS_SECTIONS=$PWD/cross_sections.xml`

Running your first simulation

- Executable compiled
  - Download source code from website
  - Navigate to `src` directory
  - Type `make`
- Navigate to directory with XML input files
  - Navigate to `examples` directory: `cd ../examples`
  - Go into `basic`: `cd basic`
- Run OpenMC to make sure code compiled correctly
  - `cd ../../src/openmc`

Online documentation

- When in doubt, check the user's guide!
- `http://mit-crpg.github.com/openmc`