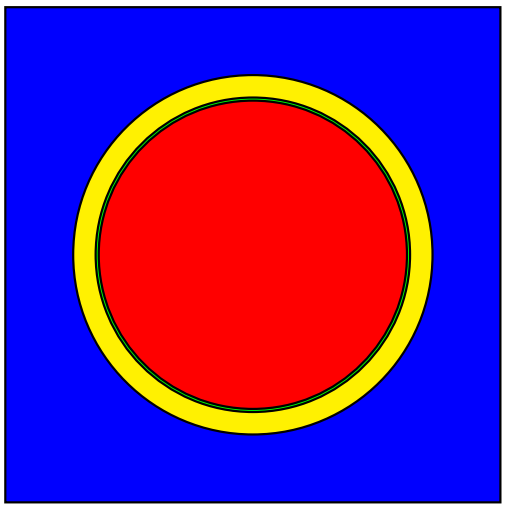
OpenMC Module: Basic Model Building

Computational Reactor Physics Group

Department of Nuclear Science and Engineering
Massachusetts Institute of Technology

Problem to Solve

- Simple pin-cell comprised of UO_2, clad and water
- **Objective**: Deterimine k_{eff} of pin-cell



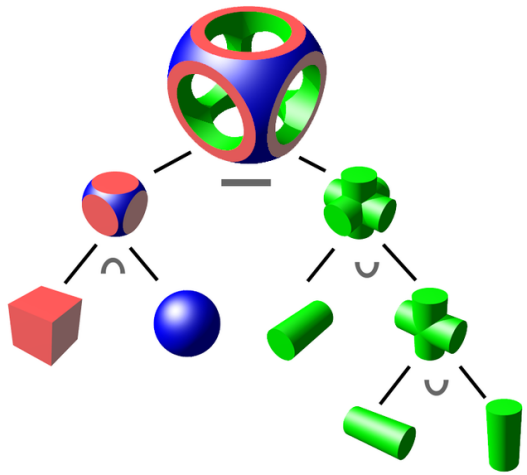
Material	Isotope	Composition Fraction (a or w)
Fuel	U-235	0.02115 (w)
Fuel	U-238	0.86032 (w)
Fuel	O-16	0.11852 (w)
Clad	Zr	elemental
Water	H-1	2.0 (a)
Water	O-16	1.0 (a)

w = weight fraction, a = atom fraction

Creating Geometry in OpenMC

- OpenMC uses constructive solid geometry
- Intersections of surfaces are used to create cells

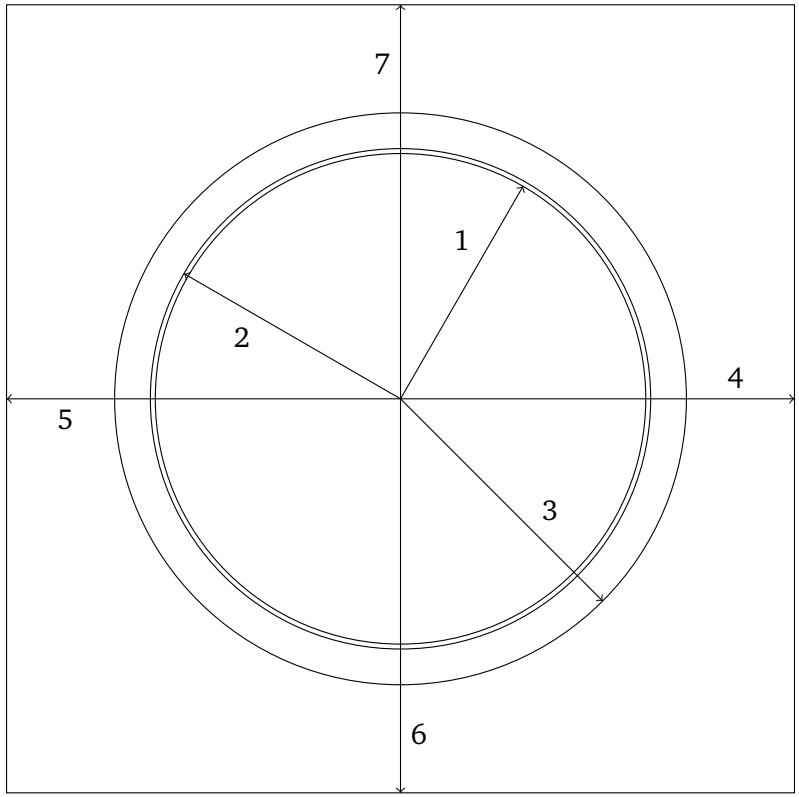
- List of surface types:
  - x-, y-, z-plane
  - general plane
  - x-, y-, z-cylinder
  - sphere
  - x-, y-, z-cone
- Each surface type takes difference arguments



source: Wikipedia

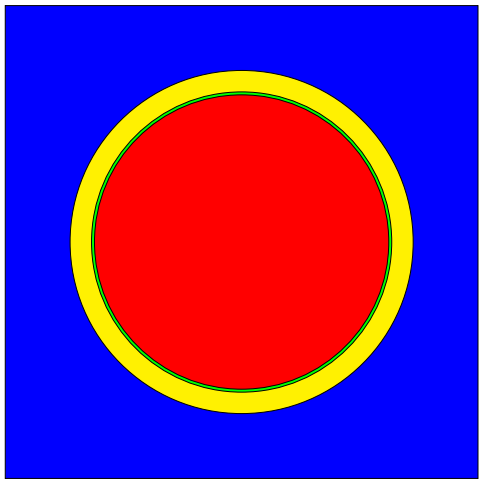
Pin-cell Surface Definitions

```
<surface id="1" type="z-cylinder" coeffs="0.0 0.0 0.39218" />
<surface id="2" type="z-cylinder" coeffs="0.0 0.0 0.40005" />
<surface id="3" type="z-cylinder" coeffs="0.0 0.0 0.45720" />
<surface id="4" type="x-plane" coeffs="-0.62992" boundary="reflective" />
<surface id="5" type="x-plane" coeffs=" 0.62992" boundary="reflective" />
<surface id="6" type="y-plane" coeffs="-0.62992" boundary="reflective" />
<surface id="7" type="y-plane" coeffs=" 0.62992" boundary="reflective" />
<surface id="8" type="z-plane" coeffs="-5.0" boundary="reflective" />
<surface id="9" type="z-plane" coeffs=" 5.0" boundary="reflective" />
```



Pin-cell Cell Definitions

```
<cell id="1" material="1" surfaces="-1 8 -9" />
<cell id="2" material="void" surfaces="1 -2 8 -9" />
<cell id="3" material="2" surfaces="2 -3 8 -9" />
<cell id="4" material="3" surfaces="3 4 -5 6 -7 8 -9" />
```



- Fuel — Material 1
  - Inside Surface 1 (-1)
  - Above -z plane (8)
  - Below +z plane (-9)
- Gap — No Material (*void*)
  - Outside Surface 1 (1)
  - Inside Surface 2 (-2)
  - Above -z plane (8)
  - Below +z plane (-9)
- Clad — Material 2
  - Outside Surface 2 (2)
  - Inside Surface 3 (-3)
  - Above -z plane (8)
  - Below +z plane (-9)
- Coolant — Material 3
  - Outside Surface 3 (3)
  - Right -x plane (4)
  - Left +x plane (-5)
  - Above -y plane (6)
  - Below +y plane (-7)
  - Above Bottom (8)
  - Below Top (-9)

Pin-cell geometry.xml File

```
<?xml version="1.0" encoding="UTF-8"?>
<geometry>

  <!-- Surfaces -->
  <surface id="1" type="z-cylinder" coeffs="0.0 0.0 0.39218" /> <!-- fuel radius -->
  <surface id="2" type="z-cylinder" coeffs="0.0 0.0 0.40005" /> <!-- clad iradius -->
  <surface id="3" type="z-cylinder" coeffs="0.0 0.0 0.45720" /> <!-- clad oradius -->
  <surface id="4" type="x-plane" coeffs="-0.62992" boundary="reflective" />
  <surface id="5" type="x-plane" coeffs=" 0.62992" boundary="reflective" />
  <surface id="6" type="y-plane" coeffs="-0.62992" boundary="reflective" />
  <surface id="7" type="y-plane" coeffs=" 0.62992" boundary="reflective" />
  <surface id="8" type="z-plane" coeffs="-5.0" boundary="reflective" />
  <surface id="9" type="z-plane" coeffs=" 5.0" boundary="reflective" />

  <!-- Cells -->
  <cell id="1" material="1" surfaces="-1 8 -9" /> <!-- fuel -->
  <cell id="2" material="void" surfaces="1 -2 8 -9" /> <!-- gas gap -->
  <cell id="3" material="2" surfaces="2 -3 8 -9" /> <!-- clad -->
  <cell id="4" material="3" surfaces="3 4 -5 6 -7 8 -9" /> <!-- coolant -->

</geometry>
```

Creating Materials in OpenMC

- Total density of material can be specified in units of `g/cc` or `atom/b-cm`
- Either isotopes or natural elements (OpenMC automatically expands them) are specified
- Each isotope/element has a `name` and `xs` attribute which links it to an ACE file via the `cross_sections.xml` file
  - `name` is an isotope's or element's name (e.g.,H-1 or Zr)
  - `xs` is the ACE file cross section extension (for temperature)
- Each isotope/element is given a weight fraction or atom fraction (OpenMC automatically renormalizes to a sum of one)
- Finally thermal scattering libraries are available with `sab` attribute

Pin-cell `materials.xml` File

```
<?xml version="1.0" encoding="UTF-8"?>
<materials>

  <!-- UO2 -->
  <material id="1">
    <density value="10.3" units="g/cc" />
    <nuclide name="U-235" xs="70c" wo="0.02115" />
    <nuclide name="U-238" xs="70c" wo="0.86032" />
    <nuclide name="O-16" xs="70c" wo="0.11852" />
  </material>

  <!-- Zirconium -->
    <material id="2">
    <density value="6.55" units="g/cc" />
    <element name="Zr" xs="70c" ao="1" />
  </material>

  <!-- Water -->
  <material id="3">
    <density value="0.701" units="g/cc" />
    <nuclide name="H-1" xs="70c" ao="2.0" />
    <nuclide name="O-16" xs="70c" ao="1.0" />
    <sab name="lwtr" xs="70t" />
  </material>

</materials>
```

Basic OpenMC Settings for Eigenvalue Calculation

- `cross sections` path to `cross_sections.xml` file relative to execution directory
- `batches`: total number of batches to run
- `inactive`: number of batches to discard
- `particles`: number of neutron histories per batch to simulate
- Initial source must be specified (e.g., from file, box/point, angle, energy)

More options discussed in later modules and in User's Guide

Pin-cell `settings.xml` File

- 120 total batches, discard 20 with 1000 neutron histories per batch
- Starting source guess is a uniform across geometry

```
<?xml version="1.0" encoding="UTF-8"?>
<settings>

  <!-- Path for cross section library -->
  <cross_sections> ../../data/cross_sections.xml </cross_sections>

  <!-- Parameters for criticality calculation -->
  <eigenvalue batches="120" generations_per_batch="1" inactive="20" particles="1000" />

  <!-- Starting source (default energy is Watt, default angle is isotropic) -->
  <source>
    <space type="box">
      <parameters> -0.62992 -0.62992 -5.0 0.62992 0.62992 5.0 </parameters>
    </space>
  </source>

</settings>
```

Nuclide data `cross_sections.xml` File

- directory: root director of ace files
- alias: `materials.xml` file links here
- awr: atomic weight ratio
- location: line number where isotope begins
- name: isotope zaid and extension
- path: relative path of ACE file from root
- temperature: isotope temp. in MeV
- zaid: isotope ZAID ID

```
<?xml version="1.0" ?>
<cross_sections>
  <directory>/opt/mcnp/data</directory>
  <filetype>ascii</filetype>
  <ace_table alias="H-1.70c" awr="0.999167" location="1" name="1001.70c" path="endf70a"
       temperature="2.5301e-08" zaid="1001"/>
  <ace_table alias="H-1.72c" awr="0.999167" location="4115" name="1001.72c" path="endf70a
       " temperature="7.7556e-08" zaid="1001"/>
  <ace_table alias="H-2.70c" awr="1.9968" location="10286" name="1002.70c" path="endf70a"
        temperature="2.5301e-08" zaid="1002"/>
  <ace_table alias="H-3.70c" awr="2.989596" location="23704" name="1003.70c" path="
       endf70a" temperature="2.5301e-08" zaid="1003"/>
  <ace_table awr="0.999167" location="2637033" name="lwtr.10t" path="endf70sab" zaid="0"/>

</cross_sections>
```

Let's Run OpenMC!

1. Make sure OpenMC is compiled
2. Make sure you have the XML input files created
3. Navigate to the directory containing input files
4. Execute OpenMC!

{path_to_openmc_root}/src/openmc

Standard Output — Header Information

```
      .d88888b.                             888b     d888  .d8888b.
     d88P" "Y88b                            8888b   d8888 d88P  Y88b
     888     888                            88888b.d88888 888    888
     888     888 88888b.   .d88b.  88888b.  888Y88888P888 888
     888     888 888 "88b d8P  Y8b 888 "88b 888 Y888P 888 888
     888     888 888  888 88888888 888  888 888  Y8P  888 888    888
     Y88b. .d88P 888 d88P Y8b.     888  888 888   "   888 Y88b  d88P
      "Y88888P"  88888P"   "Y8888  888  888 888       888  "Y8888P"
-----------------888-------------------------------------------------------
                 888
                 888

     Developed At:  Massachusetts Institute of Technology
     Version:       0.5.1
     Git SHA1:      4a5ad36f74fd2c50a7ab49a43107b610e7e6ec2c
     Date/Time:     2013-03-23 19:55:48

 ===============================================================================
 ======================>     INITIALIZATION     <=======================
 ===============================================================================

 Reading settings XML file...
 Reading cross sections XML file...
 Reading geometry XML file...
 Reading materials XML file...
 Building neighboring cells lists for each surface...
 Loading ACE cross section table: 92235.70c
 Loading ACE cross section table: 92238.70c
 Loading ACE cross section table: 8016.70c
 Loading ACE cross section table: 40090.70c
 Loading ACE cross section table: 40091.70c
 Loading ACE cross section table: 40092.70c
 Loading ACE cross section table: 40094.70c
 Loading ACE cross section table: 40096.70c
 Loading ACE cross section table: 1001.70c
 Loading ACE cross section table: lwtr.70t
 Creating unionized energy grid...
 Initializing source particles...
```

- Version and execution information
- Input files are read and processed
- Cross sections are loaded into memory

Standard Output — Header Information

```
================================================================================
====================>     K EIGENVALUE SIMULATION     <====================
================================================================================

 Bat./Gen.      k(batch)            Average k
 =========   ========   ====================
       1/1    1.37743
       2/1    1.23928
         ....
      18/1    1.30948
      19/1    1.37513
      20/1    1.35739
      21/1    1.25861
      22/1    1.23967    1.24914 +/- 0.00947
      23/1    1.34688    1.28172 +/- 0.03303
      24/1    1.28363    1.28220 +/- 0.02336
         ....               ...
     110/1    1.31772    1.31056 +/- 0.00453
     111/1    1.33785    1.31086 +/- 0.00449
     112/1    1.33253    1.31110 +/- 0.00444
     113/1    1.31805    1.31117 +/- 0.00439
     114/1    1.38429    1.31195 +/- 0.00442
     115/1    1.32248    1.31206 +/- 0.00437
     116/1    1.32758    1.31222 +/- 0.00433
     117/1    1.26614    1.31175 +/- 0.00431
     118/1    1.36733    1.31232 +/- 0.00430
     119/1    1.31629    1.31236 +/- 0.00426
     120/1    1.30628    1.31230 +/- 0.00422
Creating state point statepoint.120.binary...
```

- Inactive Batches (tracklength k-eff reported)
- Active Batches begin
- K-eff is accumulated
- Binary output file written

Standard Output — Results Information

```
=======================================================================
====================>     SIMULATION FINISHED     <====================
=======================================================================


====================>     TIMING STATISTICS     <====================

Total time for initialization     =  3.2280E+00 seconds
  Reading cross sections          =  3.0860E+00 seconds
  Unionizing energy grid          =  7.9000E-02 seconds
Total time in simulation          =  2.5496E+01 seconds
  Time in transport only          =  2.5478E+01 seconds
  Time in inactive batches        =  4.2360E+00 seconds
  Time in active batches          =  2.1260E+01 seconds
  Time synchronizing fission bank =  6.0000E-03 seconds
    Sampling source sites         =  5.0000E-03 seconds
    SEND/RECV source sites        =  1.0000E-03 seconds
  Time accumulating tallies       =  0.0000E+00 seconds
Total time for finalization       =  0.0000E+00 seconds
Total time elapsed                =  2.8724E+01 seconds
Calculation Rate                  =  4706.62 neutrons/second

============================>     RESULTS     <============================

k-effective (Collision)     =  1.31513 +/-  0.00378
k-effective (Track-length)  =  1.31230 +/-  0.00422
k-effective (Absorption)    =  1.31639 +/-  0.00239
Combined k-effective        =  1.31563 +/-  0.00229
Leakage Fraction            =  0.00000 +/-  0.00000
```