

OpenMC Module: Basic Model Building

Computational Reactor Physics Group

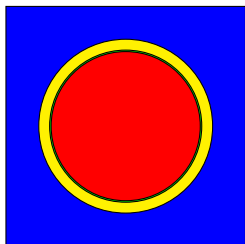
Department of Nuclear Science and Engineering
Massachusetts Institute of Technology

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Problem to Solve

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



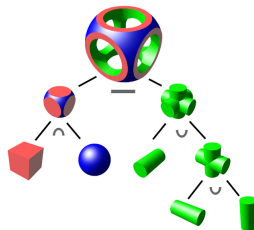
■ Fuel ■ Clad ■ Water

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

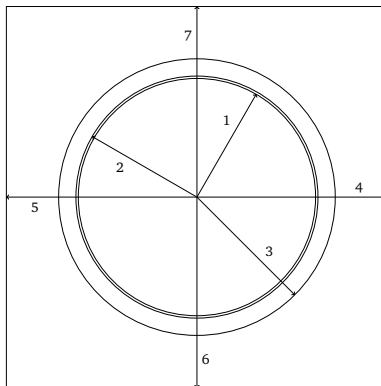
- OpenMC uses constructive solid geometry
- Intersections of surfaces are used to create cells
- List of surface types:
 - x-, y-, z-plane
 - general plane
 - x-, y-, z-cylinder
 - sphere
 - x-, y-, z-cone
- Each surface type takes difference arguments



source: Wikipedia

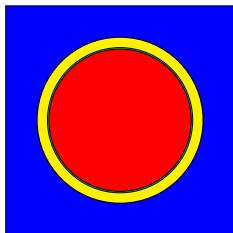
Pin-cell Surface Definitions

```
<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>

  <!-- Parameters for criticality calculation -->
  <eigenvalue batches="120" 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      888888b.      .d88b.      888888b.      888Y888888P888      888
888      888      888      "88b      d8P      Y8b      888      "88b      888      Y888P      888      888
888      888      888      888888888      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
```