OpenMC demonstration

This notebook was created for the "Hands-on school on nuclear data from Research Reactors" course (organized by the Centre for Energy Research & Institute of Nuclear Techniques, and Budapest University of Technology and Economics, in Budapest, Hungary, September 25-29, 2023) of the "Accelerator and Research reactor Infrastructures for Education and Learning" (ARIEL) project.

The purpose of this notebook is to give a brief introduction to some of the functionality of OpenMC and its python API in JupyterLab environment through a very simple test case. This excercise is not at all intended as a comprehensive guide or tutorial, however it can provide some basic experience regarding the structure of an OpenMC input script.

Written by: Gergely KLUJBER, Budapest University of Technology and Economics - Institute of Nuclear Techniques

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OpenMC is an open source Monte Carlo neutron and photon transport simulation code.

It is capable of performing fixed source, k-eigenvalue, and subcritical multiplication calculations on models built using either a constructive solid geometry or CAD representation. OpenMC supports both continuous-energy and multigroup transport.

With OpenMC, you can calculate reaction rates, flux distribution in 3D, etc. in a detailed geometry.

Reference:

Paul K. Romano, Nicholas E. Horelik, Bryan R. Herman, Adam G. Nelson, Benoit Forget, and Kord Smith, "**OpenMC: A State-of-the-Art Monte Carlo Code for Research and Development,**" Ann. Nucl. Energy, 82, 90–97 (2015).

Useful links:

OpenMC online documentation
OpenMC source code on GitHub
Example Jupyter Notebooks
Zsolt Elter; Markus Preston; Erik Branger: Reactor Physics with Python (2021 edition)

Part I - Uranium sphere

STEP 0 - Initialize necessary python modules

In [1]:
```
# 'numpy' for arrays and some other stuff
import numpy as np

# 'matplotlib.pyplot' for plotting
from matplotlib import pyplot as plt

# 'os' for issuing system commands
import os

# OpenMC python API
import openmc
```

STEP 1 - Defining materials for the geometry

Different types of materials can be created with the `openmc.Material()` class.

The material objects contain information about e.g.:

- composition: `.add_nuclide()` and `.add_element()` ,
- density: `set_density()` ,
- S(a,b) treatment: `add_s_alpha_beta()` ,
- ...

The materials use in the model are bundled together in the `openmc.Materials()` object

This will be converted into an .xml file for the openmc application.

In [2]:
```
materials = openmc.Materials([])

# water
MAT_water=openmc.Material()
MAT_water.add_nuclide('H1', 0.6672, 'ao') # adding isotope
MAT_water.add_nuclide('O16', 0.3328, 'ao')
MAT_water.set_density('g/cm3', 9.978e-01)
MAT_water.add_s_alpha_beta('c_H_in_H2O')
materials.append(MAT_water)

# U fuel
MAT_fuel=openmc.Material()
MAT_fuel.add_nuclide('U235',0.27, 'wo')
MAT_fuel.add_nuclide('U238',0.73, 'wo')
MAT_fuel.set_density('g/cm3', 19.1)
materials.append(MAT_fuel)

# graphite
MAT_graphite=openmc.Material()
MAT_graphite.add_element('C', 1, 'ao') # adding element
MAT_graphite.set_density('g/cm3', 1.7)
MAT_graphite.add_s_alpha_beta('c_Graphite')
materials.append(MAT_graphite)

# Export materials to xml format file which will be used by openmc
materials.export_to_xml()
```

Tip: Examine 'materials.xml' in the file browser.

STEP 2 - Defining the geometry

In OpenMC, complex arbitrary 3D geometrical regions are defined using `Constructive Solid Geometry (CSG)`.
The geometry of a region is defined along the following steps:

- simple surfaces (planes, spheres, etc.) are defined,
- then half-spaces are defined using these surfaces,
- then complex regions are defined by doing boolean operations with the half-spaces

The different regions are described by `Cell` objects. Besides the region, these objects may store information about more complex sub-geometry (eg. in the form of a Universe, see below) and/or material properties.
Cells are bundled together into `Universe` objects. As mentioned previously, universes can be filled into cells.

In [3]:
```
# The final structure of the geometry needs to be a single universe.
root=openmc.Universe()

# Outer boundary of the problem
s_boundary_x1=openmc.XPlane(x0=-40,boundary_type='vacuum')
s_boundary_x2=openmc.XPlane(x0= 40,boundary_type='vacuum')
s_boundary_y1=openmc.YPlane(y0=-40,boundary_type='vacuum')
s_boundary_y2=openmc.YPlane(y0= 40,boundary_type='vacuum')
s_boundary_z1=openmc.ZPlane(z0=-40,boundary_type='vacuum')
s_boundary_z2=openmc.ZPlane(z0= 40,boundary_type='vacuum')

region_boundary = +s_boundary_x1 & -s_boundary_x2 & +s_boundary_y1 & -s_boundary_y2 & +s_boundary_z1 & -s_boundary_z2

# U sphere
sphere_1_radius=12
s_sphere_1=openmc.Sphere(r=sphere_1_radius)
cell_fuel=openmc.Cell(region=(-s_sphere_1))
cell_fuel.fill=MAT_fuel
root.add_cell(cell_fuel)

# reflector shell
sphere_2_radius=22
s_sphere_2=openmc.Sphere(r=sphere_2_radius)
cell_reflector=openmc.Cell(region=(-s_sphere_2 & +s_sphere_1))
cell_reflector.fill=MAT_graphite
root.add_cell(cell_reflector)

# some water
cell_workspace=openmc.Cell(region=(+s_sphere_2 & region_boundary ))
cell_workspace.fill=MAT_water
root.add_cell(cell_workspace)

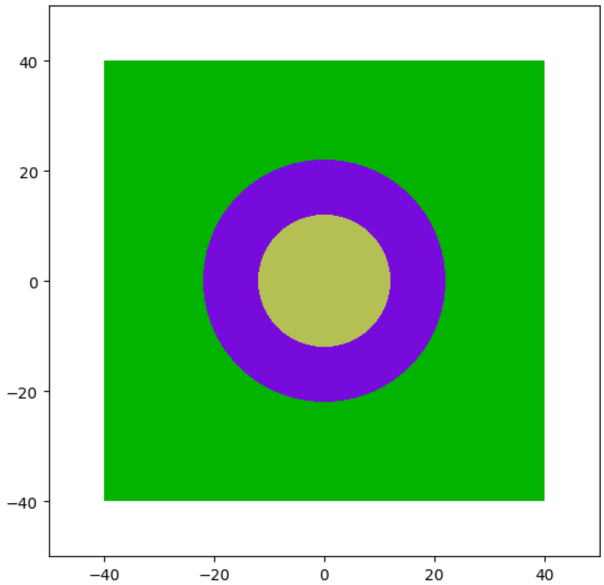
# The geometry needs to be exported into a xml file.
geometry = openmc.Geometry(root)
geometry.export_to_xml()
```

Tip: Examine 'geometry.xml' in the file browser.

Tip: The geometry can be visualized for example using the `openmc.Universe.plot()` member, as seen below:

In [4]:
```
root.plot(
    basis = 'xz',
    width =  (100, 100),
    pixels = (500, 500)
)
```

Out[4]: `<matplotlib.image.AxesImage at 0x7fe83277d2e0>`



STEP 3 - Defining the source

In [5]:
```
# Isotropic point source
source_n=openmc.Source(space=openmc.stats.Point((0,0,0)))
source_n.particle='neutron' # optional, as 'neutron' is the default
```

STEP 4 - Setting parameters of the simulation

In [6]:
```
settings = openmc.Settings()

# Criticality calculation
settings.batches = 600
settings.inactive = 100
settings.particles = 5000

# Source
settings.source = source_n

# Exporting the settings into a xml file.
settings.export_to_xml()
```

Tip: Examine 'settings.xml' in the file browser.

STEP 5 - Defining tallies ("*optional*")

Generally speaking, a Monte Carlo code is more than happy to run a simulation without calculating and outputting any quantities.
In case of OpenMC, a series if filters can be defined (energy, space, angle, isotope, etc.), through which it will collect contributions to the desired quantity.

In [7]:
```
# Without getting into the detailes of each object, let's define a tally to calculate the spatial distribution of the thermal neutron flux along y=0 plane

# Defining a spatial filter
x_min=-40
x_max=40
y_min=x_min
y_max=x_max
resolution=160
myMesh_xz=openmc.RegularMesh()
myMesh_xz.dimension=[resolution,1,resolution]
myMesh_xz.lower_left=[x_min,-2,y_min]
myMesh_xz.upper_right=[x_max,2,y_max]
meshfilter_xz=openmc.MeshFilter(myMesh_xz)

# ...and an energy filter for thermal energies
energybins_th=np.array([0., 0.625])
energy_filter_th = openmc.EnergyFilter(values=energybins_th)

# Defining the tally
tally_xz=openmc.Tally(name='thermal_flux')
tally_xz.filters = [meshfilter_xz,energy_filter_th]
tally_xz.scores = ['flux']

# Exporting the tally information into a xml file.
tallies=openmc.Tallies()
tallies.append(tally_xz)
tallies.export_to_xml()
```

Tip: Examine 'tallies.xml' in the file browser.

STEP 6 - Run the simulation

An OpenMC simulation can be initiated in a number of ways, for example by entering the `openmc` command in a system terminal, or by using the `openmc.run()` member inside the API. `Note` that the program will use the data defined in the '.xml' files, and it is independent from the Jupyter Lab or python environment. It is therefore important to make sure that any desired changes are registered in the '.xml' files.

In [8]:
```
option=2
if option==1 :
    !openmc
else:
    openmc.run()
```

```
                                %%%%%%%%%%%%%%%
                           %%%%%%%%%%%%%%%%%%%%%%%%
                        %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                      %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                    %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                   %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
                                    %%%%%%%%%%%%%%%%%%%%%%%%
                                     %%%%%%%%%%%%%%%%%%%%%%%%
                 ###############      %%%%%%%%%%%%%%%%%%%%%%%%
                ##################     %%%%%%%%%%%%%%%%%%%%%%%
                ###################     %%%%%%%%%%%%%%%%%%%%%%%
                ####################     %%%%%%%%%%%%%%%%%%%%%%
                #####################     %%%%%%%%%%%%%%%%%%%%%
                ######################     %%%%%%%%%%%%%%%%%%%%
                #######################     %%%%%%%%%%%%%%%%%%
                 #######################     %%%%%%%%%%%%%%%%%
                 ######################     %%%%%%%%%%%%%%%%%
                  ####################     %%%%%%%%%%%%%%%%%
                    #################     %%%%%%%%%%%%%%%%%
                     ###############     %%%%%%%%%%%%%%%%
                       ############     %%%%%%%%%%%%%%%
                          ########     %%%%%%%%%%%%%%
                                      %%%%%%%%%%%

                 | The OpenMC Monte Carlo Code
       Copyright | 2011-2022 MIT, UChicago Argonne LLC, and contributors
         License | https://docs.openmc.org/en/latest/license.html
         Version | 0.13.2
        Git SHA1 | 030f73a8690ed19e91806e46c8caf338d252e74a
       Date/Time | 2023-09-26 14:05:45
   MPI Processes | 1
  OpenMP Threads | 12

Reading settings XML file...
Reading cross sections XML file...
Reading materials XML file...
Reading geometry XML file...
Reading H1 from /root/nndc_hdf5/H1.h5
Reading O16 from /root/nndc_hdf5/O16.h5
Reading U235 from /root/nndc_hdf5/U235.h5
Reading U238 from /root/nndc_hdf5/U238.h5
Reading C0 from /root/nndc_hdf5/C0.h5
Reading c_H_in_H2O from /root/nndc_hdf5/c_H_in_H2O.h5
Reading c_Graphite from /root/nndc_hdf5/c_Graphite.h5
Minimum neutron data temperature: 294 K
Maximum neutron data temperature: 294 K
Reading tallies XML file...
Preparing distributed cell instances...
Reading plot XML file...
Writing summary.h5 file...
Maximum neutron transport energy: 20000000 eV for H1
Initializing source particles...

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

  Bat./Gen.      k            Average k
  =========   ========   ====================
        1/1    1.28163
        2/1    1.10348
        3/1    1.03581
        4/1    1.03798
        5/1    0.97284
        6/1    1.02702
        7/1    0.98032
        8/1    1.00016
        9/1    1.01197
       10/1    0.98504
       11/1    0.94865
       12/1    1.03436
       13/1    0.98976
       14/1    1.02623
       15/1    0.97389
       16/1    0.98534
       17/1    1.00742
       18/1    0.97816
       19/1    1.02089
       20/1    1.00529
       21/1    1.03735
       22/1    1.01508
       23/1    0.99139
       24/1    1.02007
       25/1    1.00952
       26/1    0.99204
       27/1    0.99516
       28/1    1.03267
       29/1    0.98586
       30/1    1.01499
       31/1    1.01107
       32/1    0.98814
       33/1    1.00495
       34/1    0.97347
       35/1    0.99745
       36/1    0.99658
       37/1    1.00593
       38/1    0.98486
       39/1    0.97613
       40/1    1.02846
       41/1    1.00867
       42/1    1.00996
       43/1    1.01530
       44/1    1.01995
       45/1    1.00991
       46/1    0.97765
       47/1    0.97820
       48/1    0.99616
       49/1    1.00545
       50/1    1.01856
       51/1    0.97477
       52/1    0.99719
```

```
     53/1    0.99489
     54/1    0.99484
     55/1    0.98983
     56/1    1.00777
     57/1    0.98348
     58/1    1.01840
     59/1    1.01630
     60/1    0.99120
     61/1    1.01262
     62/1    1.00231
     63/1    0.99081
     64/1    1.03419
     65/1    1.00590
     66/1    1.03320
     67/1    0.99098
     68/1    0.97685
     69/1    1.00113
     70/1    1.00632
     71/1    1.03678
     72/1    1.00678
     73/1    1.01079
     74/1    1.00745
     75/1    0.98521
     76/1    1.00943
     77/1    0.98305
     78/1    0.97221
     79/1    1.00362
     80/1    0.97617
     81/1    1.03377
     82/1    0.98608
     83/1    1.01172
     84/1    0.99627
     85/1    0.99552
     86/1    0.99624
     87/1    0.99505
     88/1    1.02616
     89/1    1.01494
     90/1    1.00570
     91/1    1.02766
     92/1    0.98041
     93/1    0.99590
     94/1    1.00834
     95/1    1.00192
     96/1    0.98382
     97/1    0.97761
     98/1    0.99698
     99/1    1.02858
    100/1    0.97563
    101/1    0.99641
    102/1    1.00898    1.00269 +/- 0.00629
    103/1    1.02244    1.00928 +/- 0.00752
    104/1    0.98590    1.00343 +/- 0.00790
    105/1    1.00932    1.00461 +/- 0.00623
    106/1    0.99302    1.00268 +/- 0.00544
    107/1    1.01274    1.00411 +/- 0.00482
    108/1    0.97590    1.00059 +/- 0.00546
    109/1    0.97519    0.99777 +/- 0.00558
    110/1    1.02875    1.00086 +/- 0.00588
    111/1    1.00646    1.00137 +/- 0.00534
    112/1    1.01179    1.00224 +/- 0.00495
    113/1    0.97657    1.00027 +/- 0.00496
    114/1    1.02113    1.00176 +/- 0.00483
    115/1    1.01710    1.00278 +/- 0.00461
    116/1    1.00301    1.00279 +/- 0.00432
    117/1    0.98252    1.00160 +/- 0.00423
    118/1    0.99459    1.00121 +/- 0.00400
    119/1    0.96576    0.99935 +/- 0.00422
    120/1    0.99784    0.99927 +/- 0.00401
    121/1    1.00328    0.99946 +/- 0.00381
    122/1    0.99401    0.99921 +/- 0.00365
    123/1    1.01073    0.99971 +/- 0.00352
    124/1    0.97943    0.99887 +/- 0.00347
    125/1    0.99902    0.99888 +/- 0.00333
    126/1    0.97543    0.99797 +/- 0.00333
    127/1    1.02173    0.99885 +/- 0.00332
    128/1    0.98434    0.99834 +/- 0.00324
    129/1    1.00077    0.99842 +/- 0.00313
    130/1    1.01737    0.99905 +/- 0.00309
    131/1    0.99728    0.99899 +/- 0.00299
    132/1    0.98648    0.99860 +/- 0.00292
    133/1    1.02982    0.99955 +/- 0.00298
    134/1    1.00303    0.99965 +/- 0.00289
    135/1    0.98273    0.99917 +/- 0.00285
    136/1    1.01050    0.99948 +/- 0.00279
    137/1    1.01351    0.99986 +/- 0.00274
    138/1    1.02055    1.00041 +/- 0.00272
    139/1    1.03465    1.00128 +/- 0.00279
    140/1    0.99833    1.00121 +/- 0.00272
    141/1    1.01919    1.00165 +/- 0.00269
    142/1    0.99061    1.00139 +/- 0.00264
    143/1    1.01537    1.00171 +/- 0.00260
    144/1    1.02426    1.00222 +/- 0.00259
    145/1    0.98826    1.00191 +/- 0.00255
    146/1    1.00030    1.00188 +/- 0.00249
    147/1    0.98645    1.00155 +/- 0.00246
    148/1    0.98601    1.00123 +/- 0.00243
    149/1    0.99559    1.00111 +/- 0.00239
    150/1    0.99473    1.00098 +/- 0.00234
    151/1    0.96151    1.00021 +/- 0.00242
    152/1    1.00403    1.00028 +/- 0.00238
    153/1    1.01463    1.00055 +/- 0.00235
    154/1    1.03404    1.00117 +/- 0.00238
    155/1    0.99910    1.00114 +/- 0.00234
    156/1    0.99929    1.00110 +/- 0.00230
    157/1    1.00101    1.00110 +/- 0.00226
    158/1    0.98799    1.00088 +/- 0.00223
    159/1    1.01545    1.00112 +/- 0.00221
    160/1    0.98570    1.00087 +/- 0.00218
    161/1    1.04999    1.00167 +/- 0.00229
```

```
162/1    1.01595    1.00190 +/- 0.00227
163/1    0.97880    1.00153 +/- 0.00226
164/1    1.01574    1.00176 +/- 0.00224
165/1    1.00563    1.00182 +/- 0.00220
166/1    0.99847    1.00176 +/- 0.00217
167/1    1.01520    1.00197 +/- 0.00215
168/1    0.99267    1.00183 +/- 0.00212
169/1    0.98788    1.00163 +/- 0.00210
170/1    0.99955    1.00160 +/- 0.00207
171/1    1.00143    1.00159 +/- 0.00204
172/1    0.99160    1.00146 +/- 0.00202
173/1    1.01200    1.00160 +/- 0.00199
174/1    1.02153    1.00187 +/- 0.00198
175/1    0.96960    1.00144 +/- 0.00200
176/1    0.99495    1.00135 +/- 0.00198
177/1    1.02009    1.00160 +/- 0.00197
178/1    0.98641    1.00140 +/- 0.00195
179/1    1.01115    1.00153 +/- 0.00193
180/1    1.03575    1.00195 +/- 0.00196
181/1    1.01875    1.00216 +/- 0.00194
182/1    0.99284    1.00205 +/- 0.00192
183/1    0.98816    1.00188 +/- 0.00191
184/1    1.02749    1.00218 +/- 0.00191
185/1    0.99998    1.00216 +/- 0.00188
186/1    0.98760    1.00199 +/- 0.00187
187/1    0.98272    1.00177 +/- 0.00186
188/1    1.00844    1.00184 +/- 0.00184
189/1    1.03202    1.00218 +/- 0.00185
190/1    1.00631    1.00223 +/- 0.00183
191/1    1.03094    1.00254 +/- 0.00184
192/1    0.99251    1.00243 +/- 0.00182
193/1    1.00888    1.00250 +/- 0.00180
194/1    1.02312    1.00272 +/- 0.00180
195/1    1.01013    1.00280 +/- 0.00178
196/1    1.01737    1.00295 +/- 0.00177
197/1    0.97927    1.00271 +/- 0.00177
198/1    0.99352    1.00262 +/- 0.00175
199/1    1.00448    1.00263 +/- 0.00173
200/1    1.02879    1.00290 +/- 0.00174
201/1    1.00781    1.00294 +/- 0.00172
202/1    0.99536    1.00287 +/- 0.00170
203/1    1.02848    1.00312 +/- 0.00171
204/1    0.99888    1.00308 +/- 0.00169
205/1    1.00329    1.00308 +/- 0.00167
206/1    0.99294    1.00298 +/- 0.00166
207/1    1.01333    1.00308 +/- 0.00165
208/1    0.97771    1.00285 +/- 0.00165
209/1    0.99570    1.00278 +/- 0.00164
210/1    1.01105    1.00286 +/- 0.00162
211/1    1.00622    1.00289 +/- 0.00161
212/1    1.00552    1.00291 +/- 0.00159
213/1    1.01528    1.00302 +/- 0.00158
214/1    0.98397    1.00285 +/- 0.00158
215/1    1.02926    1.00308 +/- 0.00158
216/1    1.00333    1.00308 +/- 0.00157
217/1    0.98309    1.00291 +/- 0.00156
218/1    0.98906    1.00280 +/- 0.00156
219/1    0.97212    1.00254 +/- 0.00156
220/1    0.99882    1.00251 +/- 0.00155
221/1    1.01736    1.00263 +/- 0.00154
222/1    0.98963    1.00252 +/- 0.00153
223/1    0.95881    1.00217 +/- 0.00156
224/1    1.00812    1.00222 +/- 0.00155
225/1    1.00638    1.00225 +/- 0.00154
226/1    0.99737    1.00221 +/- 0.00153
227/1    1.04108    1.00252 +/- 0.00154
228/1    1.00404    1.00253 +/- 0.00153
229/1    0.99509    1.00247 +/- 0.00152
230/1    0.99927    1.00245 +/- 0.00151
231/1    0.98471    1.00231 +/- 0.00150
232/1    1.00581    1.00234 +/- 0.00149
233/1    1.02255    1.00249 +/- 0.00149
234/1    0.99867    1.00246 +/- 0.00148
235/1    1.01491    1.00255 +/- 0.00147
236/1    0.99009    1.00246 +/- 0.00146
237/1    0.99032    1.00237 +/- 0.00146
238/1    0.99461    1.00232 +/- 0.00145
239/1    0.98988    1.00223 +/- 0.00144
240/1    1.01944    1.00235 +/- 0.00143
241/1    0.99662    1.00231 +/- 0.00142
242/1    0.99818    1.00228 +/- 0.00141
243/1    1.01566    1.00237 +/- 0.00141
244/1    0.96351    1.00210 +/- 0.00142
245/1    0.99154    1.00203 +/- 0.00141
246/1    0.99890    1.00201 +/- 0.00141
247/1    1.00044    1.00200 +/- 0.00140
248/1    0.98418    1.00188 +/- 0.00139
249/1    0.97294    1.00168 +/- 0.00140
250/1    0.99037    1.00161 +/- 0.00139
251/1    1.03967    1.00186 +/- 0.00140
252/1    0.97135    1.00166 +/- 0.00141
253/1    0.99331    1.00161 +/- 0.00140
254/1    0.98876    1.00152 +/- 0.00139
255/1    1.02387    1.00167 +/- 0.00139
256/1    1.01750    1.00177 +/- 0.00139
257/1    0.97105    1.00157 +/- 0.00139
258/1    0.99431    1.00153 +/- 0.00138
259/1    1.00044    1.00152 +/- 0.00137
260/1    0.98739    1.00143 +/- 0.00137
261/1    1.00330    1.00144 +/- 0.00136
262/1    1.00018    1.00143 +/- 0.00135
263/1    1.03289    1.00163 +/- 0.00136
264/1    1.02468    1.00177 +/- 0.00136
265/1    0.99105    1.00170 +/- 0.00135
266/1    0.99217    1.00165 +/- 0.00134
267/1    0.97713    1.00150 +/- 0.00134
268/1    0.98419    1.00140 +/- 0.00134
269/1    1.00744    1.00143 +/- 0.00133
270/1    0.98151    1.00131 +/- 0.00133
```

```
271/1    1.00695    1.00135 +/- 0.00132
272/1    0.99254    1.00130 +/- 0.00131
273/1    1.01201    1.00136 +/- 0.00131
274/1    1.02114    1.00147 +/- 0.00131
275/1    1.01504    1.00155 +/- 0.00130
276/1    1.03647    1.00175 +/- 0.00131
277/1    0.97834    1.00162 +/- 0.00131
278/1    0.97504    1.00147 +/- 0.00131
279/1    1.00344    1.00148 +/- 0.00130
280/1    0.99879    1.00146 +/- 0.00129
281/1    1.02359    1.00158 +/- 0.00129
282/1    0.97611    1.00144 +/- 0.00129
283/1    1.01673    1.00153 +/- 0.00129
284/1    1.01613    1.00161 +/- 0.00128
285/1    1.00412    1.00162 +/- 0.00128
286/1    1.01589    1.00170 +/- 0.00127
287/1    1.01519    1.00177 +/- 0.00127
288/1    0.99634    1.00174 +/- 0.00126
289/1    0.97738    1.00161 +/- 0.00126
290/1    1.00535    1.00163 +/- 0.00125
291/1    0.99359    1.00159 +/- 0.00125
292/1    0.99589    1.00156 +/- 0.00124
293/1    1.00308    1.00157 +/- 0.00124
294/1    0.97705    1.00144 +/- 0.00124
295/1    0.98437    1.00135 +/- 0.00123
296/1    1.01095    1.00140 +/- 0.00123
297/1    0.99426    1.00137 +/- 0.00122
298/1    0.98250    1.00127 +/- 0.00122
299/1    0.98314    1.00118 +/- 0.00122
300/1    0.99129    1.00113 +/- 0.00121
301/1    1.00063    1.00113 +/- 0.00121
302/1    1.01379    1.00119 +/- 0.00120
303/1    0.99778    1.00117 +/- 0.00120
304/1    1.00076    1.00117 +/- 0.00119
305/1    1.02455    1.00129 +/- 0.00119
306/1    1.04035    1.00148 +/- 0.00120
307/1    1.02738    1.00160 +/- 0.00120
308/1    1.00122    1.00160 +/- 0.00119
309/1    0.96001    1.00140 +/- 0.00120
310/1    1.01295    1.00146 +/- 0.00120
311/1    1.03012    1.00159 +/- 0.00120
312/1    1.00063    1.00159 +/- 0.00120
313/1    0.97961    1.00148 +/- 0.00120
314/1    1.03769    1.00165 +/- 0.00120
315/1    1.01003    1.00169 +/- 0.00120
316/1    1.00553    1.00171 +/- 0.00119
317/1    0.98013    1.00161 +/- 0.00119
318/1    0.99595    1.00158 +/- 0.00118
319/1    0.98750    1.00152 +/- 0.00118
320/1    0.98580    1.00145 +/- 0.00118
321/1    0.99347    1.00141 +/- 0.00117
322/1    0.99640    1.00139 +/- 0.00117
323/1    0.97529    1.00127 +/- 0.00117
324/1    0.99652    1.00125 +/- 0.00116
325/1    1.01588    1.00132 +/- 0.00116
326/1    1.02026    1.00140 +/- 0.00116
327/1    0.99504    1.00137 +/- 0.00115
328/1    1.01901    1.00145 +/- 0.00115
329/1    0.97282    1.00132 +/- 0.00115
330/1    0.99849    1.00131 +/- 0.00115
331/1    1.01412    1.00137 +/- 0.00114
332/1    1.02403    1.00147 +/- 0.00114
333/1    0.99978    1.00146 +/- 0.00114
334/1    1.01396    1.00151 +/- 0.00113
335/1    0.98075    1.00142 +/- 0.00113
336/1    1.01123    1.00146 +/- 0.00113
337/1    0.98677    1.00140 +/- 0.00113
338/1    0.97300    1.00128 +/- 0.00113
339/1    0.98064    1.00120 +/- 0.00113
340/1    0.99956    1.00119 +/- 0.00112
341/1    0.98311    1.00111 +/- 0.00112
342/1    1.01318    1.00116 +/- 0.00112
343/1    0.97700    1.00107 +/- 0.00112
344/1    1.02742    1.00117 +/- 0.00112
345/1    0.97027    1.00105 +/- 0.00112
346/1    1.02228    1.00113 +/- 0.00112
347/1    0.99117    1.00109 +/- 0.00111
348/1    0.99270    1.00106 +/- 0.00111
349/1    0.99553    1.00104 +/- 0.00111
350/1    1.02895    1.00115 +/- 0.00111
351/1    0.97731    1.00105 +/- 0.00111
352/1    1.00393    1.00107 +/- 0.00110
353/1    0.99496    1.00104 +/- 0.00110
354/1    0.99001    1.00100 +/- 0.00109
355/1    1.01863    1.00107 +/- 0.00109
356/1    1.00974    1.00110 +/- 0.00109
357/1    1.00958    1.00113 +/- 0.00109
358/1    1.01103    1.00117 +/- 0.00108
359/1    1.00217    1.00118 +/- 0.00108
360/1    1.01133    1.00121 +/- 0.00107
361/1    0.99298    1.00118 +/- 0.00107
362/1    0.99107    1.00114 +/- 0.00107
363/1    0.99509    1.00112 +/- 0.00106
364/1    1.00038    1.00112 +/- 0.00106
365/1    1.00622    1.00114 +/- 0.00106
366/1    1.02488    1.00123 +/- 0.00106
367/1    0.99840    1.00122 +/- 0.00105
368/1    0.98619    1.00116 +/- 0.00105
369/1    0.99556    1.00114 +/- 0.00105
370/1    0.98119    1.00107 +/- 0.00104
371/1    1.01586    1.00112 +/- 0.00104
372/1    0.99806    1.00111 +/- 0.00104
373/1    1.01742    1.00117 +/- 0.00104
374/1    1.04181    1.00132 +/- 0.00104
375/1    1.00605    1.00133 +/- 0.00104
376/1    1.01406    1.00138 +/- 0.00104
377/1    0.98897    1.00134 +/- 0.00103
378/1    0.98527    1.00128 +/- 0.00103
379/1    1.00669    1.00130 +/- 0.00103
```

```
380/1    0.98801    1.00125 +/- 0.00102
381/1    1.00453    1.00126 +/- 0.00102
382/1    0.99602    1.00124 +/- 0.00102
383/1    0.97995    1.00117 +/- 0.00102
384/1    1.00579    1.00118 +/- 0.00101
385/1    1.00656    1.00120 +/- 0.00101
386/1    1.00808    1.00123 +/- 0.00101
387/1    0.97941    1.00115 +/- 0.00101
388/1    1.03895    1.00128 +/- 0.00101
389/1    1.01188    1.00132 +/- 0.00101
390/1    1.00443    1.00133 +/- 0.00101
391/1    1.00330    1.00134 +/- 0.00100
392/1    1.00902    1.00136 +/- 0.00100
393/1    1.00709    1.00138 +/- 0.00100
394/1    0.98161    1.00132 +/- 0.00099
395/1    0.99490    1.00129 +/- 0.00099
396/1    1.00119    1.00129 +/- 0.00099
397/1    1.01434    1.00134 +/- 0.00099
398/1    1.00915    1.00136 +/- 0.00098
399/1    0.98320    1.00130 +/- 0.00098
400/1    1.01004    1.00133 +/- 0.00098
401/1    0.96535    1.00121 +/- 0.00098
402/1    0.98264    1.00115 +/- 0.00098
403/1    0.98089    1.00108 +/- 0.00098
404/1    1.01615    1.00113 +/- 0.00098
405/1    0.99322    1.00111 +/- 0.00098
406/1    1.00660    1.00113 +/- 0.00097
407/1    1.00117    1.00113 +/- 0.00097
408/1    0.98161    1.00106 +/- 0.00097
409/1    1.00224    1.00107 +/- 0.00096
410/1    1.00346    1.00107 +/- 0.00096
411/1    1.01356    1.00111 +/- 0.00096
412/1    1.03753    1.00123 +/- 0.00096
413/1    1.01916    1.00129 +/- 0.00096
414/1    1.01738    1.00134 +/- 0.00096
415/1    1.00271    1.00134 +/- 0.00096
416/1    0.99649    1.00133 +/- 0.00095
417/1    0.97317    1.00124 +/- 0.00096
418/1    0.96881    1.00114 +/- 0.00096
419/1    1.01869    1.00119 +/- 0.00096
420/1    0.99844    1.00118 +/- 0.00095
421/1    1.00047    1.00118 +/- 0.00095
422/1    0.98672    1.00114 +/- 0.00095
423/1    1.01711    1.00119 +/- 0.00095
424/1    0.98991    1.00115 +/- 0.00094
425/1    1.00402    1.00116 +/- 0.00094
426/1    0.98846    1.00112 +/- 0.00094
427/1    1.00130    1.00112 +/- 0.00094
428/1    1.00123    1.00112 +/- 0.00093
429/1    0.97163    1.00103 +/- 0.00094
430/1    1.01643    1.00108 +/- 0.00093
431/1    1.01057    1.00111 +/- 0.00093
432/1    0.99238    1.00108 +/- 0.00093
433/1    0.98968    1.00105 +/- 0.00093
434/1    1.00664    1.00106 +/- 0.00092
435/1    0.98930    1.00103 +/- 0.00092
436/1    1.00519    1.00104 +/- 0.00092
437/1    1.00865    1.00106 +/- 0.00092
438/1    1.02612    1.00114 +/- 0.00092
439/1    1.02828    1.00122 +/- 0.00092
440/1    1.00711    1.00124 +/- 0.00092
441/1    0.99197    1.00121 +/- 0.00091
442/1    1.01917    1.00126 +/- 0.00091
443/1    0.99247    1.00123 +/- 0.00091
444/1    0.98377    1.00118 +/- 0.00091
445/1    0.97692    1.00111 +/- 0.00091
446/1    1.02093    1.00117 +/- 0.00091
447/1    0.99319    1.00115 +/- 0.00091
448/1    0.98156    1.00109 +/- 0.00090
449/1    1.01317    1.00113 +/- 0.00090
450/1    1.02736    1.00120 +/- 0.00090
451/1    0.97185    1.00112 +/- 0.00090
452/1    0.99295    1.00109 +/- 0.00090
453/1    1.00827    1.00111 +/- 0.00090
454/1    0.99043    1.00108 +/- 0.00090
455/1    0.99955    1.00108 +/- 0.00090
456/1    1.01297    1.00111 +/- 0.00089
457/1    1.00095    1.00111 +/- 0.00089
458/1    0.98665    1.00107 +/- 0.00089
459/1    0.96317    1.00097 +/- 0.00089
460/1    0.99292    1.00094 +/- 0.00089
461/1    1.02262    1.00100 +/- 0.00089
462/1    0.99369    1.00098 +/- 0.00089
463/1    0.99005    1.00095 +/- 0.00089
464/1    1.00909    1.00098 +/- 0.00088
465/1    0.97296    1.00090 +/- 0.00089
466/1    0.98949    1.00087 +/- 0.00088
467/1    1.00930    1.00089 +/- 0.00088
468/1    1.03335    1.00098 +/- 0.00088
469/1    1.01633    1.00102 +/- 0.00088
470/1    0.98051    1.00097 +/- 0.00088
471/1    0.99292    1.00094 +/- 0.00088
472/1    1.02199    1.00100 +/- 0.00088
473/1    0.98989    1.00097 +/- 0.00088
474/1    1.01055    1.00100 +/- 0.00087
475/1    0.98361    1.00095 +/- 0.00087
476/1    0.99534    1.00094 +/- 0.00087
477/1    0.97888    1.00088 +/- 0.00087
478/1    1.00146    1.00088 +/- 0.00087
479/1    0.99846    1.00087 +/- 0.00087
480/1    1.00464    1.00088 +/- 0.00086
481/1    0.99893    1.00088 +/- 0.00086
482/1    1.02105    1.00093 +/- 0.00086
483/1    1.00293    1.00094 +/- 0.00086
484/1    1.02137    1.00099 +/- 0.00086
485/1    0.96059    1.00088 +/- 0.00086
486/1    1.05369    1.00102 +/- 0.00087
487/1    1.00650    1.00103 +/- 0.00087
488/1    1.00606    1.00105 +/- 0.00087
```

```
489/1    0.98259    1.00100 +/- 0.00087
490/1    0.98532    1.00096 +/- 0.00086
491/1    0.98926    1.00093 +/- 0.00086
492/1    1.00757    1.00095 +/- 0.00086
493/1    1.02562    1.00101 +/- 0.00086
494/1    0.99250    1.00099 +/- 0.00086
495/1    1.00422    1.00100 +/- 0.00086
496/1    0.98869    1.00097 +/- 0.00086
497/1    1.03204    1.00104 +/- 0.00086
498/1    0.99564    1.00103 +/- 0.00085
499/1    1.00964    1.00105 +/- 0.00085
500/1    1.02252    1.00111 +/- 0.00085
501/1    0.99941    1.00110 +/- 0.00085
502/1    0.98342    1.00106 +/- 0.00085
503/1    1.00118    1.00106 +/- 0.00085
504/1    1.00742    1.00107 +/- 0.00085
505/1    0.97859    1.00102 +/- 0.00085
506/1    1.00928    1.00104 +/- 0.00084
507/1    1.01288    1.00107 +/- 0.00084
508/1    0.97980    1.00101 +/- 0.00084
509/1    1.00373    1.00102 +/- 0.00084
510/1    1.01327    1.00105 +/- 0.00084
511/1    0.99456    1.00104 +/- 0.00084
512/1    1.02239    1.00109 +/- 0.00084
513/1    1.00671    1.00110 +/- 0.00083
514/1    0.97995    1.00105 +/- 0.00083
515/1    1.00630    1.00106 +/- 0.00083
516/1    0.97881    1.00101 +/- 0.00083
517/1    0.99628    1.00100 +/- 0.00083
518/1    1.02458    1.00105 +/- 0.00083
519/1    1.01596    1.00109 +/- 0.00083
520/1    1.02459    1.00115 +/- 0.00083
521/1    1.00459    1.00115 +/- 0.00083
522/1    1.01617    1.00119 +/- 0.00082
523/1    1.01702    1.00123 +/- 0.00082
524/1    1.00246    1.00123 +/- 0.00082
525/1    1.00520    1.00124 +/- 0.00082
526/1    0.99963    1.00124 +/- 0.00082
527/1    0.99937    1.00123 +/- 0.00082
528/1    1.01369    1.00126 +/- 0.00081
529/1    0.98110    1.00121 +/- 0.00081
530/1    1.03672    1.00130 +/- 0.00082
531/1    0.98124    1.00125 +/- 0.00082
532/1    1.01083    1.00127 +/- 0.00081
533/1    0.99178    1.00125 +/- 0.00081
534/1    1.02303    1.00130 +/- 0.00081
535/1    1.00211    1.00130 +/- 0.00081
536/1    0.96683    1.00122 +/- 0.00081
537/1    0.99358    1.00120 +/- 0.00081
538/1    1.04142    1.00130 +/- 0.00081
539/1    0.97575    1.00124 +/- 0.00081
540/1    0.99910    1.00123 +/- 0.00081
541/1    0.98544    1.00120 +/- 0.00081
542/1    0.99406    1.00118 +/- 0.00081
543/1    0.95960    1.00109 +/- 0.00081
544/1    1.02417    1.00114 +/- 0.00081
545/1    0.98467    1.00110 +/- 0.00081
546/1    0.98710    1.00107 +/- 0.00081
547/1    1.01120    1.00109 +/- 0.00081
548/1    0.98328    1.00105 +/- 0.00081
549/1    1.01183    1.00108 +/- 0.00081
550/1    0.99746    1.00107 +/- 0.00081
551/1    1.00360    1.00108 +/- 0.00080
552/1    0.99827    1.00107 +/- 0.00080
553/1    0.99851    1.00106 +/- 0.00080
554/1    1.02910    1.00113 +/- 0.00080
555/1    0.99420    1.00111 +/- 0.00080
556/1    0.98783    1.00108 +/- 0.00080
557/1    1.00948    1.00110 +/- 0.00080
558/1    0.99377    1.00108 +/- 0.00079
559/1    1.00335    1.00109 +/- 0.00079
560/1    0.98863    1.00106 +/- 0.00079
561/1    0.95030    1.00095 +/- 0.00080
562/1    0.96729    1.00088 +/- 0.00080
563/1    0.99682    1.00087 +/- 0.00080
564/1    0.99004    1.00085 +/- 0.00080
565/1    0.99932    1.00084 +/- 0.00079
566/1    1.02662    1.00090 +/- 0.00079
567/1    0.99460    1.00089 +/- 0.00079
568/1    1.02770    1.00094 +/- 0.00079
569/1    0.99399    1.00093 +/- 0.00079
570/1    1.03103    1.00099 +/- 0.00079
571/1    1.01878    1.00103 +/- 0.00079
572/1    0.98353    1.00099 +/- 0.00079
573/1    1.00997    1.00101 +/- 0.00079
574/1    0.99053    1.00099 +/- 0.00079
575/1    0.98598    1.00096 +/- 0.00079
576/1    1.01111    1.00098 +/- 0.00079
577/1    1.00094    1.00098 +/- 0.00078
578/1    0.98186    1.00094 +/- 0.00078
579/1    0.98371    1.00090 +/- 0.00078
580/1    0.98553    1.00087 +/- 0.00078
581/1    0.97883    1.00082 +/- 0.00078
582/1    0.98449    1.00079 +/- 0.00078
583/1    1.01779    1.00083 +/- 0.00078
584/1    0.99532    1.00081 +/- 0.00078
585/1    1.01923    1.00085 +/- 0.00078
586/1    1.02183    1.00090 +/- 0.00078
587/1    1.02864    1.00095 +/- 0.00078
588/1    1.03545    1.00102 +/- 0.00078
589/1    1.00669    1.00104 +/- 0.00078
590/1    1.02018    1.00107 +/- 0.00078
591/1    1.01906    1.00111 +/- 0.00078
592/1    1.00958    1.00113 +/- 0.00078
593/1    0.99834    1.00112 +/- 0.00077
594/1    0.97846    1.00108 +/- 0.00077
595/1    1.00409    1.00108 +/- 0.00077
596/1    0.99519    1.00107 +/- 0.00077
597/1    0.99994    1.00107 +/- 0.00077
```

```
      598/1    1.02981    1.00113 +/- 0.00077
      599/1    1.01100    1.00115 +/- 0.00077
      600/1    0.99017    1.00112 +/- 0.00077
 Creating state point statepoint.600.h5...

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

 Total time for initialization     = 2.7232e-01 seconds
   Reading cross sections          = 2.4004e-01 seconds
 Total time in simulation          = 3.5674e+01 seconds
   Time in transport only          = 3.5333e+01 seconds
   Time in inactive batches        = 4.7086e+00 seconds
   Time in active batches          = 3.0966e+01 seconds
   Time synchronizing fission bank = 1.9422e-01 seconds
     Sampling source sites         = 1.6838e-01 seconds
     SEND/RECV source sites        = 2.4077e-02 seconds
   Time accumulating tallies       = 2.6337e-02 seconds
   Time writing statepoints        = 8.4221e-03 seconds
 Total time for finalization       = 5.3142e-02 seconds
 Total time elapsed                = 3.6005e+01 seconds
 Calculation Rate (inactive)       = 106189 particles/second
 Calculation Rate (active)         = 80734.6 particles/second

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

 k-effective (Collision)     = 1.00096 +/- 0.00067
 k-effective (Track-length)  = 1.00112 +/- 0.00077
 k-effective (Absorption)    = 1.00176 +/- 0.00069
 Combined k-effective        = 1.00137 +/- 0.00054
 Leakage Fraction            = 0.01085 +/- 0.00007
```

STEP 7 - Post processing

Some information is displayed during simulation as well as at the end of the calculation regarding the criticality calculation, but everything else needs to be extracted from the output files.

We are going to use the `statepoint.*.h5` binary file, which contains all results, but the tally outputs can be found also in the 'tallies.out' file.

Tip: Examine the contents 'tallies.out' file in the file browser.

In [9]:
```
160*160
```

Out[9]: 25600

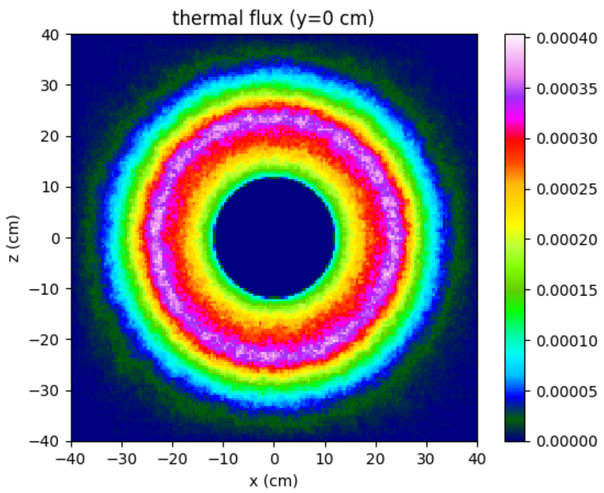
In [10]:
```
# Extracting data...
with openmc.StatePoint('statepoint.'+str(settings.batches)+'.h5') as sp:
    tally_flux_xz = sp.get_tally(name='thermal_flux')
    keff=sp.keff
    print("total run time :",int(np.round(sp.runtime['total'])),'s')
sp.close()
print('k_eff =',np.round(keff.n,5),' +/- ',np.round(keff.s,5))

# Processing data...
dataframe_xz=tally_flux_xz.get_pandas_dataframe()
tally_mean_values_xz=dataframe_xz['mean'].values.reshape((resolution,resolution))

# Displaying data...
plt.imshow(tally_mean_values_xz, interpolation='nearest', extent=[x_min,x_max,y_max,y_min]) # NOTE: 'extent' parameter is "visual", it doesn't affect the data r
plt.gca().invert_yaxis() # tally data order is different than drawing direction
plt.title('thermal flux (y=0 cm)')
plt.set_cmap('gist_ncar') # prism, gist_ncar
plt.xlabel('x (cm)')
plt.ylabel('z (cm)')
plt.colorbar()
```

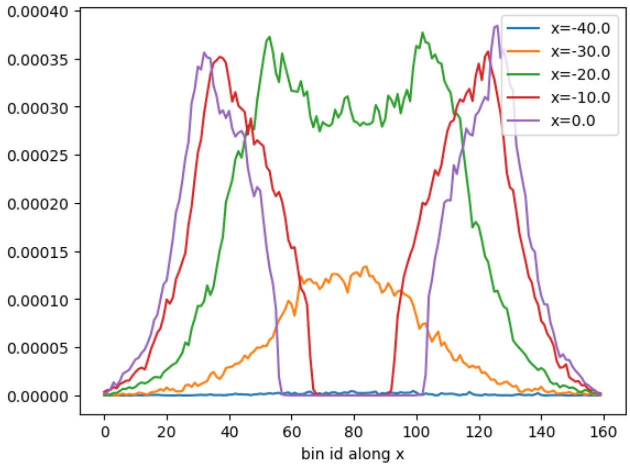
```
total run time : 36 s
k_eff = 1.00137  +/-  0.00054
```

Out[10]: <matplotlib.colorbar.Colorbar at 0x7fe8754aebe0>



In [37]:
```
for i in range(1,101,20):
    df=dataframe_xz[dataframe_xz['mesh 1','z']==i]
    datax=df['mean'].values.reshape((resolution))
    plt.plot(datax,label='x='+str(i/2-40.5))

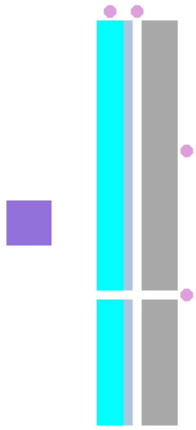
plt.xlabel('bin id along x')
plt.legend()
plt.show()
```

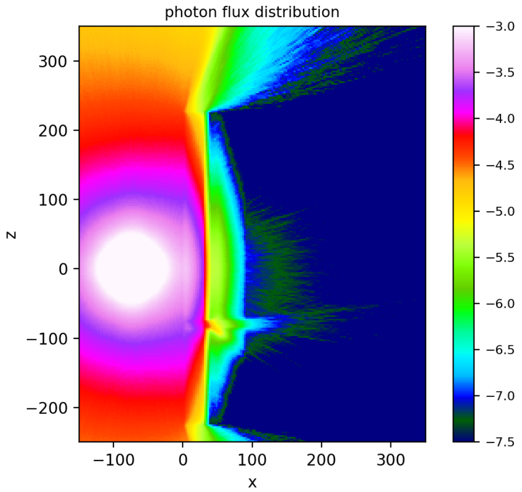


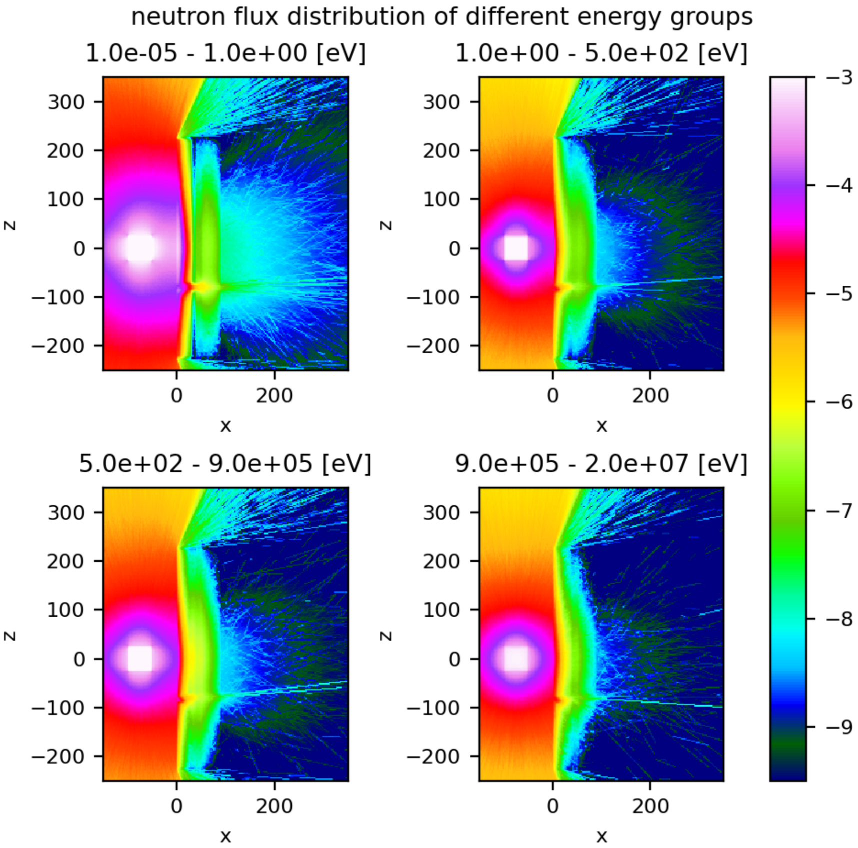
Part II - shielding example

One of the advantages of the Monte Carlo method is that small details can be included in the model. The effect of eg. a small gap/tunnel (like a tube for wires) would be extremely difficult to estimate with deterministic methods.

In this example, instead of k-eigenvalue calculation, a fixed source calculation was performed in a geometry with shielding materials, and photon- and neutron flux distributions were calculated, as seen below:

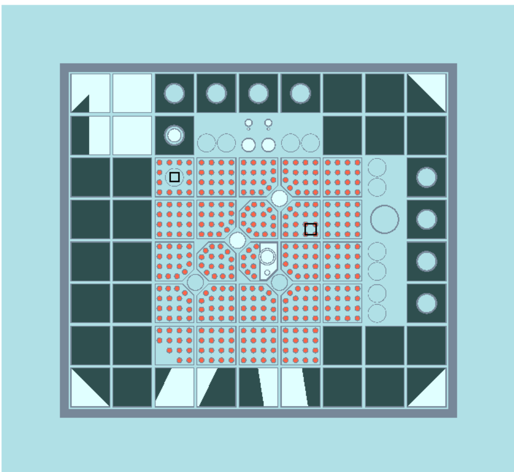


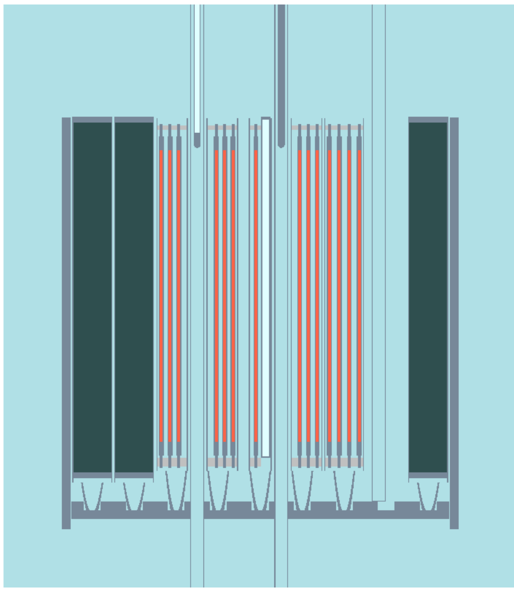




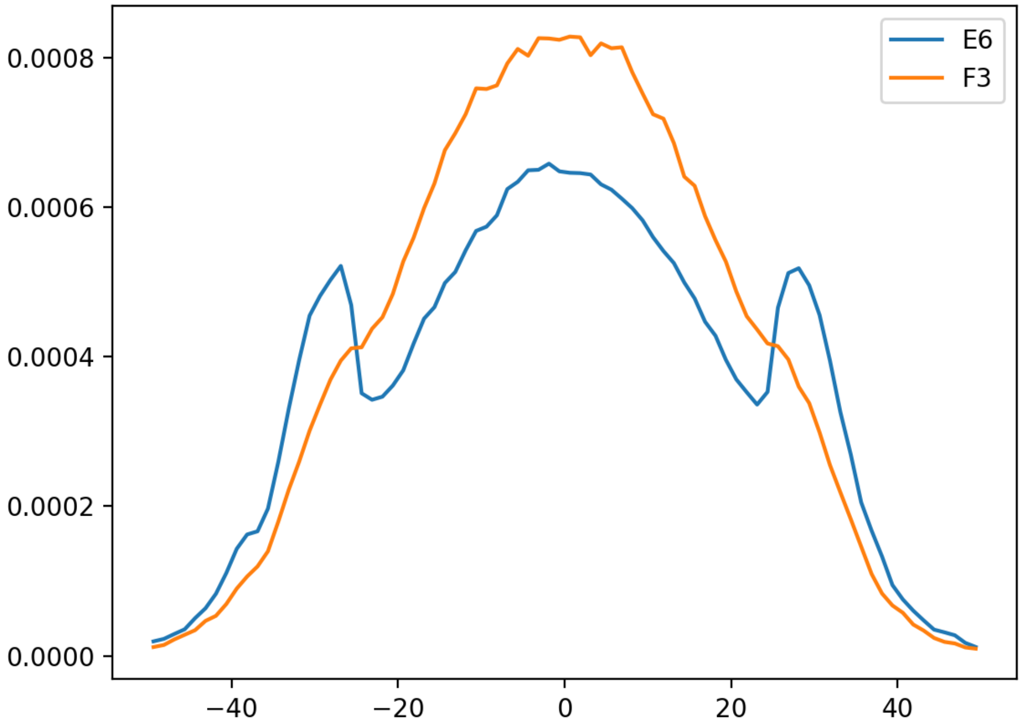
Part II - BME Training Reactor

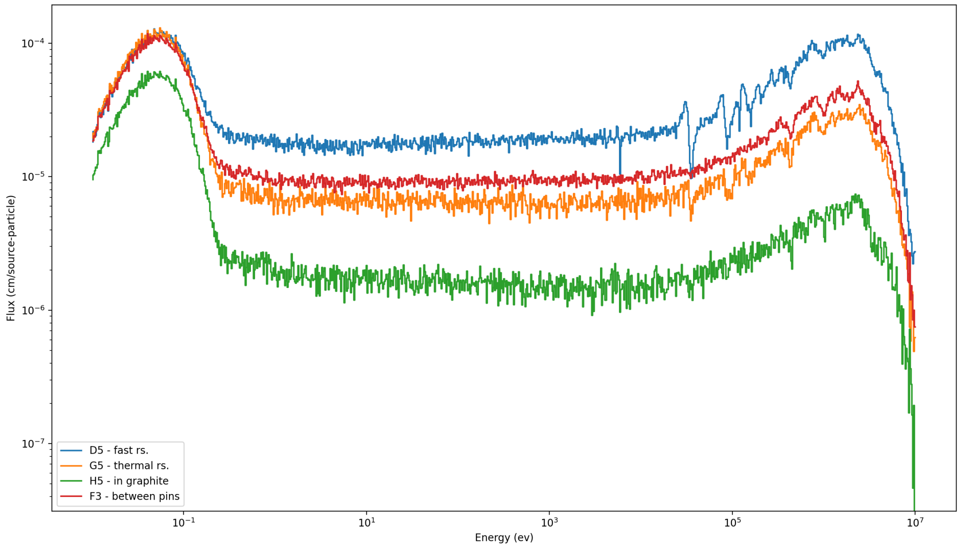
In this example, the active core of the BME Training Reactor was modelled with all rods withdrawn, and flux distributions were estimated in different measurement positions inside the fuel assemblies:





And the results:


E6
F3
0.0008
0.0006
0.0004
0.0002
0.0000
−40
−20
0
20
40


D5 - fast rs.
G5 - thermal rs.
H5 - in graphite
F3 - between pins
Flux (cm/source-particle)
Energy (ev)
10⁻⁴
10⁻⁵
10⁻⁶
10⁻⁷
10⁻¹
10¹
10³
10⁵
10⁷

```
In [ ]:
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