PIRS: Python Interfaces for Reactor Simulations

Current capabilities and selected results

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15.09.14

Outline

1. What is PIRS and what it is for
2. PIRS current capabilities
3. Example
   - Geometry description
   - High-level interface to MCNP
   - High-level interface to SCF
4. Results for 3x3 minicore
5. Conclusions and outlook

What PIRS is

PIRS: Python Interfaces for Reactor Simulations

A set of packages for *Python* programming language, to facilitate *interaction* with reactor calculation codes.

Python

- www.python.org
- Free
- Interpreted
- Big community
- Lot of packages

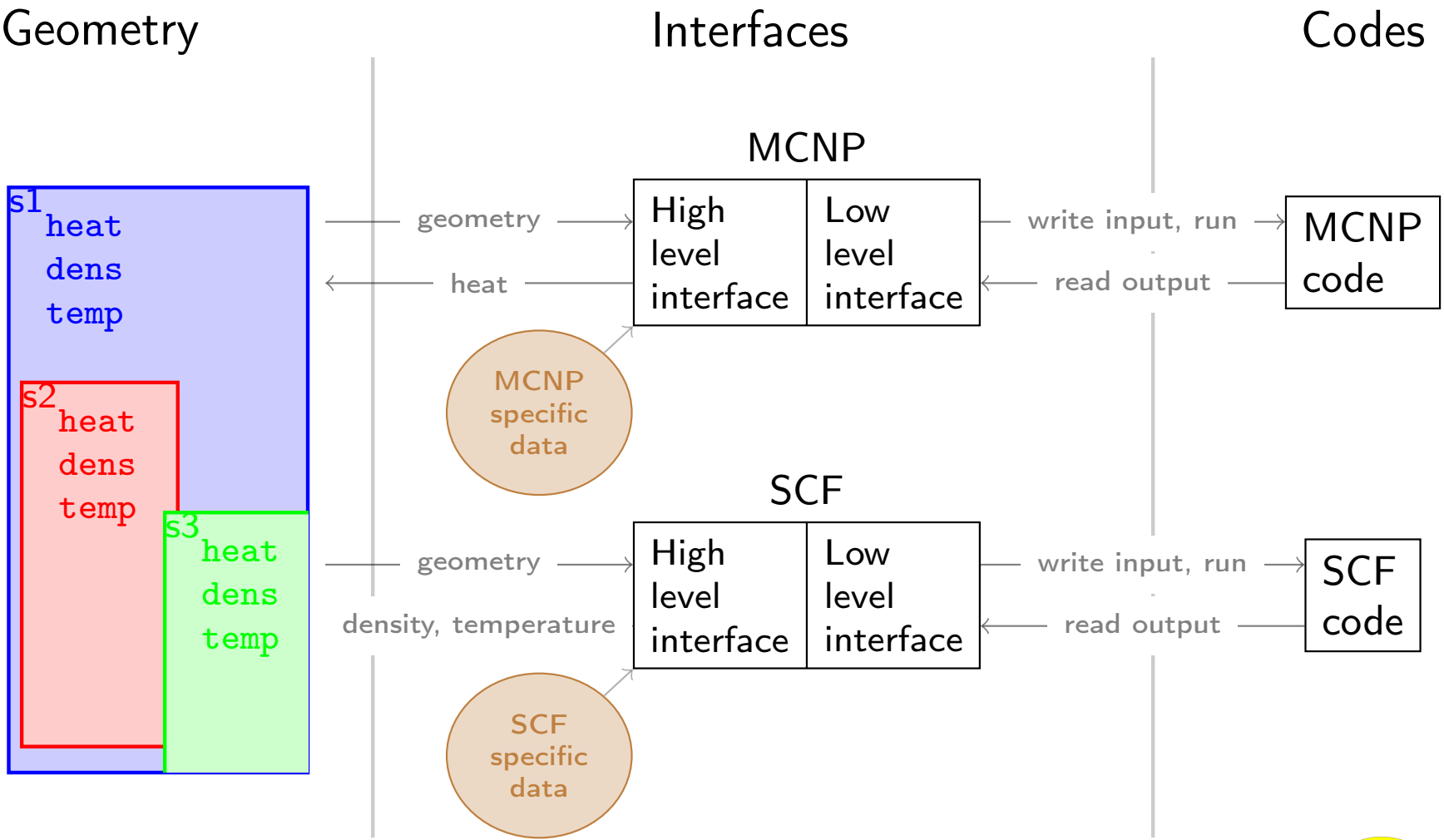
Interaction with code

- Model description
- Generation of Input file(s)
- Job submission
- Reading of calculation results

What PIRS is for

- Routine preparation of input files, reading output files
- Framework for coupled calculations

PIRS concept



PIRS current capabilites

Geometry definition

- Geometry described by
  - boxes with facets perpendicular to coordinate axes
  - cylinders with axes parallel to z (vertical) axis
- Dependent variables vertical distribution are presented by piece-wise constant functions
  - heat deposition
  - temperature
  - material density

Low-level interfaces

Classes to represent code input data, to start code, read code output

- MCNP 5
- SCF 2.5

PIRS current capabilites (contd.)

High-level interfaces

Classes to convert geometry to code-specific representation, start calculations and put results back to geometry.

- MCNP 5: any geometry can be converted into MCNP input file.
- SCF 2.5: for square bundle of vertical rods only.

Utils

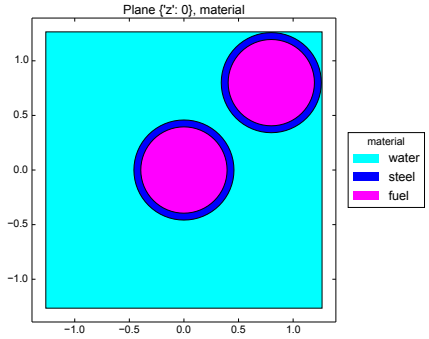
- geometry plotter
- plotter of vertical distributions
- dump and load models to and from hard drive

Geometry I

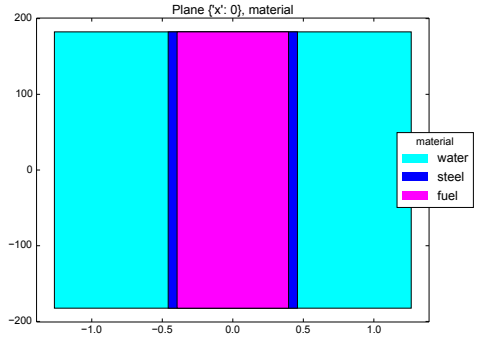
```
from pirs.solids import Box, Cylinder

cnt = Box(X=2.53, Y=2.53, Z=365, material = 'water')
r = Cylinder(R=0.4583, Z=365, material = 'steel')
f = Cylinder(R=0.3951, Z=365, material = 'fuel')

r.insert(f)
cnt.insert(r)

r2 = cnt.insert(r.copy_tree())
r2.pos.x = 0.8
r2.pos.y = 0.8

if __name__ == '__main__':
    from pirs.tools.plots import colormap
    pz = colormap(cnt, plane={'z':0})
    px = colormap(cnt, plane={'x':0}, aspect='auto')
    py = colormap(cnt, plane={'y':0}, aspect='auto')
    pz.get_figure().savefig('geom1_pz.pdf')
    px.get_figure().savefig('geom1_px.pdf')
```

Geometry I: plots

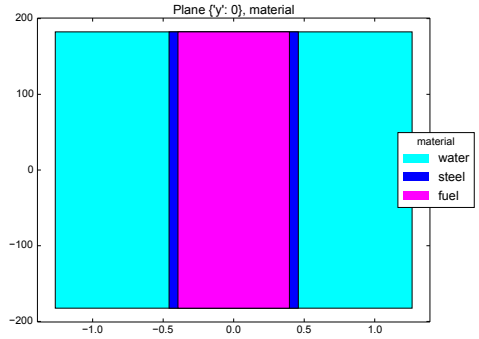
z plane



x plane



y plane

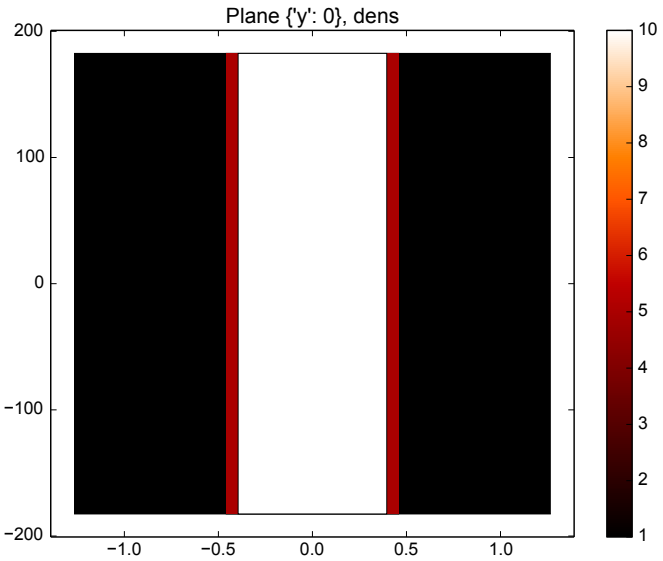


System variables

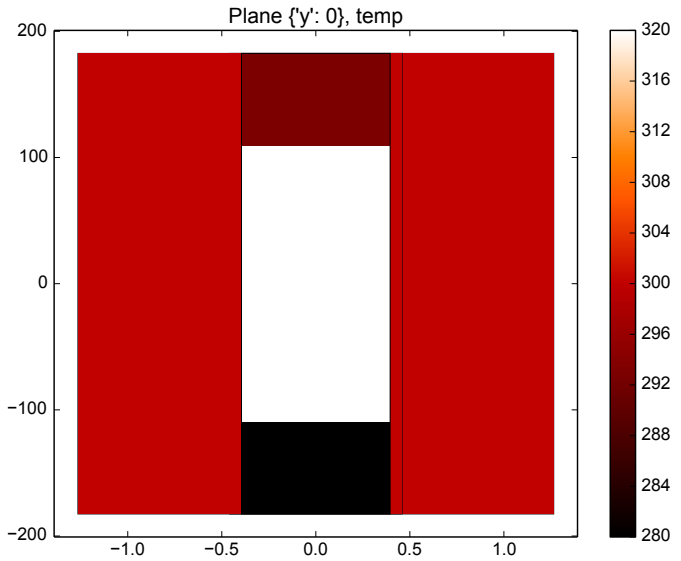
```
from geom1 import cnt

for v in cnt.values(True):
    v.temp.set_values(300.)

cnt.dens.set_values(1.0)
cnt.children[0].dens.set_values(5.0)
cnt.children[1].dens.set_values(5.0)

f1 = cnt.get_child((0,0))
f2 = cnt.get_child((1,0))

f1.temp.set_grid([1, 3, 1])
f1.temp.set_values([280, 320, 293])

f2.temp.set_grid([1, 2, 1])
f2.temp.set_values([275, 314, 293])

f1.dens.set_values(10.)
f2.dens.set_values(10.)

if __name__ == '__main__':
    from pirs.tools.plots import colormap
```

System variables: plot

density at plane y=0



temperature at plate y=0

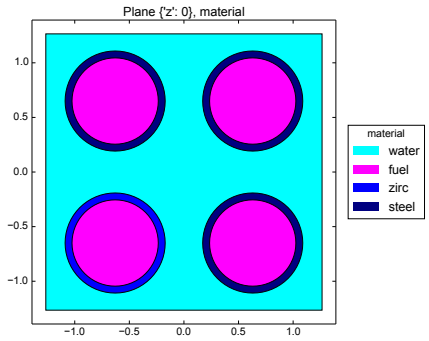


Geometry II

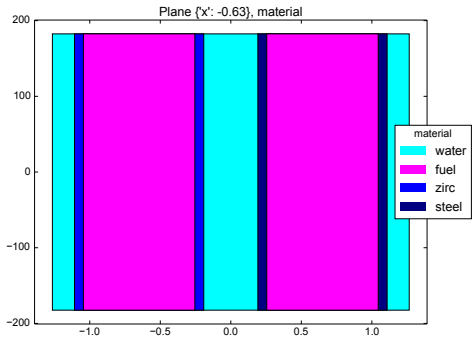
```
from geom2 import cnt

r1 = cnt.children[0]
r2 = cnt.children[1]

r1.material = 'zirc'
r1.ijk = (0, 0, 0)
r2.ijk = (1, 0, 0)
r2.pos *= 0.

cnt.grid.x = 1.26
cnt.grid.y = 1.30
cnt.grid.z = cnt.Z
r3 = cnt.grid.insert((1, 1, 0), r2.copy_tree())
r4 = cnt.grid.insert((0, 1, 0), r2.copy_tree())
# r4.R = 0.56

# cnt.grid.set_origin((0, -1, 0), (0.,-0.5,0.))
cnt.grid.center()
```

Geometry II: plots

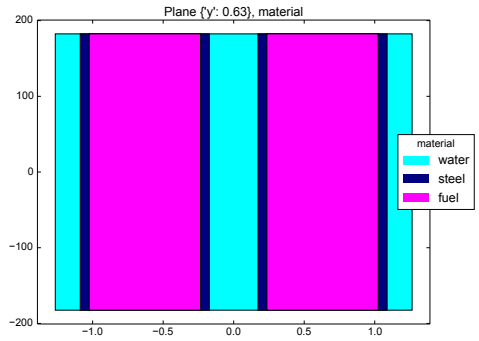
z plane



x plane at -1



y plane at 1



High-level interface to MCNP

```
from pirs import McnpInterface
from geom3 import cnt

mi = McnpInterface(cnt)

if __name__ == '__main__':
    mi.wp.prefix = 'm1_'
    mi.run('P')
```

High-level interface to MCNP: input file

```
MESSAGE:  datapath=/home/local/KIT/rx8040/data/mcnp/all_jeff

c title
1 0  -1 fill=1 imp:n=1
2 1 -1.0 -2 3 -4 5  fill=-1:2 0:1 0:0
c  k=0
     1 2 5 1
     1 5 5 1 imp:n=1 lat=1 u=1
3 0  -6 fill=3 imp:n=1 u=2
4 0  -7 fill=4 imp:n=1 u=3
5 2 -10.0 -8 imp:n=1 tmp=2.412856e-08 u=4
6 3 -10.0 8 -9 imp:n=1 tmp=2.757550e-08 u=4
7 4 -10.0 9 imp:n=1 tmp=2.524881e-08 u=4
8 1 -5.0 7 imp:n=1 tmp=2.585203e-08 u=3
9 1 -1.0 6 imp:n=1 tmp=2.585203e-08 u=2
10 0  -6 fill=6 imp:n=1 u=5
11 0  -7 fill=7 imp:n=1 u=6
12 5 -10.0 -10 imp:n=1 tmp=2.369769e-08 u=7
```

High-level interface to MCNP: input file continued

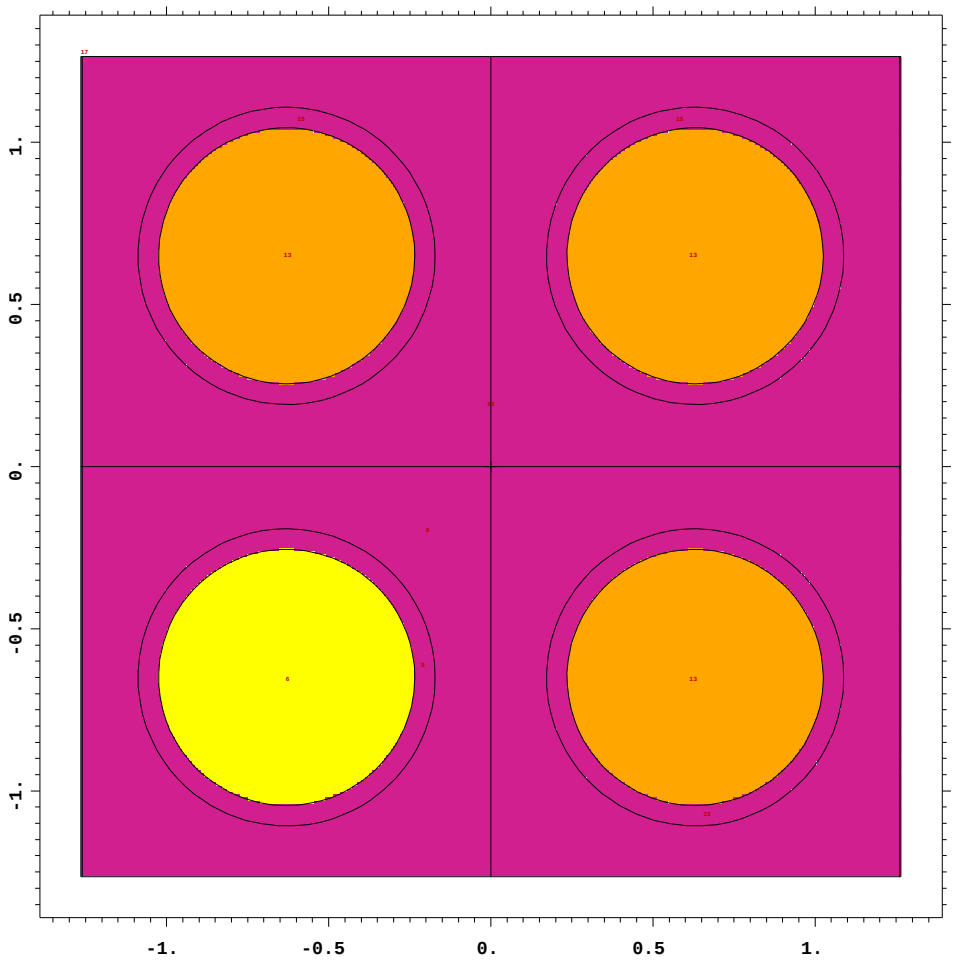
```
12 5 -10.0 -10 imp:n=1 tmp=2.369769e-08 u=7
13 6 -10.0 10 -11 imp:n=1 tmp=2.705846e-08 u=7
14 4 -10.0 11 imp:n=1 tmp=2.524881e-08 u=7
15 1 -5.0 7 imp:n=1 tmp=2.585203e-08 u=6
16 1 -1.0 6 imp:n=1 tmp=2.585203e-08 u=5
17 0  1 imp:n=0 tmp=2.526174e-08

c surfaces
1 rpp  -1.265  1.265  -1.265  1.265  -182.5  182.5
2 px  0.0
3 px  -1.26
4 py  0.0
5 py  -1.3
6 c/z  -0.63  -0.65  0.4583
7 c/z  -0.63  -0.65  0.3951
8 pz  -109.5
9 pz  109.5
10 pz  -91.25
11 pz  91.25
```

High-level interface to MCNP: input file continued

```
11 pz  91.25

c data cards
c materials
m1
c density 1.00000000000000e-05 g/cc, 5.97538539870074e-06 1/cm-barn
     1001.31c  1.00000e+00
m2
c density 1.00000000000000e-05 g/cc, 5.97538539870074e-06 1/cm-barn
     1001.31c  1.00000e+00
m3
c density 1.00000000000000e-05 g/cc, 5.97538539870074e-06 1/cm-barn
     1001.31c  7.88018e-01   1001.32c  2.11982e-01
m4
c density 1.00000000000000e-05 g/cc, 5.97538539870074e-06 1/cm-barn
     1001.31c  1.00000e+00
m5
c density 1.00000000000000e-05 g/cc, 5.97538539870074e-06 1/cm-barn
     1001.31c  1.00000e+00
m6
```

High-level interface to MCNP: plot 1

```
 09/15/14 04:46:05
c title

probid =  09/15/14 04:46:05
basis:   XY
( 1.000000, 0.000000, 0.000000)
( 0.000000, 1.000000, 0.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (     1.39,     1.39)
cell labels are
 cell names
```



MCNP-specific data

Data in general model

- geometry
- axial behaviour of system variables (temperature, density – to define MCNP geometry, heat – to define tallies)

What else MCNP needs

- Material specifications
- Boundary conditions
- Description of (criticality) source

Material specifications: water

```
from pirs.mcnp import Material

m1 = Material(('H', 2, 1),
              ('O', 1, 1))
m1.sdict[8018] = 8016
m1.thermal = 'lwtr'

m1.T = 300
print m1.card()

m1.T = 450
print m1.card()
```

Material specifications: water continued

```
m{0:<}
     1001.31c  1.99977e+00
     1002.31c  2.30000e-04
     8016.31c  9.97570e-01
     8017.31c  3.80000e-04
     8016.31c  2.05000e-03
mt{0:<} lwtr01.31t
m{0:<}
     1001.32c  9.72153e-01   1001.33c  1.02762e+00
     1002.32c  1.11810e-04   1002.33c  1.18190e-04
     8016.32c  4.84951e-01   8016.33c  5.12619e-01
     8017.32c  1.84730e-04   8017.33c  1.95270e-04
     8016.32c  9.96571e-04   8016.33c  1.05343e-03
mt{0:<} lwtr05.31t
```

Material specifications: steel

```
from pirs.mcnp import Material
# zircaloy-2, Table 5, p.7
zr = Material(('Zr', 98.23),
              ('Sn', 1.50),
              ('Fe', 0.12),
              ('Cr', 0.10),
              ('N',  0.05))

print zr.card()
```

Material specifications: steel continued

```
m{0:<}
      40090.31c  5.05393e+01
      40091.31c  1.10214e+01
      40092.31c  1.68464e+01
      40094.31c  1.70724e+01
      40096.31c  2.75044e+00
      50118.31c  3.63300e-01
      50122.31c  6.94500e-02
      50120.31c  4.88700e-01
      50112.31c  1.45500e-02
      50114.31c  9.90000e-03
      50115.31c  5.10000e-03
      50116.31c  2.18100e-01
      50117.31c  1.15200e-01
      50119.31c  1.28850e-01
      50124.31c  8.68500e-02
      26054.31c  7.01400e-03
      26056.31c  1.10105e-01
      26057.31c  2.54280e-03
      26058.31c  3.38400e-04
      24050.31c  4.34500e-03
      24052.31c  8.37890e-02
      24053.31c  9.50100e-03
```

Material specifications: mox

```
from pirs.mcnp import Material
# depleted u, mass fractions
ud = Material((92235,  0.2, 2),
              (92238, 99.8, 2))
# simplified o for oxide
o = Material(8016)
# pu
pu = Material((94239, 93.6, 2),
              (94240,  5.9, 2),
              (94241,  0.4, 2),
              (94242,  0.1, 2))
# oxides and mox
ux = Material((ud, 1), (o, 2))
px = Material((pu, 1), (o, 2))
mox = Material((ux, 0.5), (px, 0.5))
print mox.report()
# objective function
def obj(mix):
    a1 = mix.how_much(2, ZAID=[92235, 94239, 94241, 94243])
    a2 = mix.how_much(2, Z=[92, 94])
    return a1/a2 - 0.025
mox.tune(obj, [ux, px])
print mox.report()
```

Material specifications: mox continued

before tune() method

```
Mixture O-U-Pu
        <O-U       89.2383>: 0.5 mol
        <O-Pu      89.5943>: 0.5 mol
        total: 1.0 mol or 90.1910541098 g
Nuclide composition:
                    Nuclide       At.frac      Wgt.frac
        <    8016  15.8575>   6.66667e-01   1.18230e-01
        <   92235 233.0248>   3.37589e-04   8.79779e-04
        <   92238 236.0058>   1.66329e-01   4.39010e-01
        <   94239 236.9986>   1.56046e-01   4.13600e-01
        <   94240 237.9916>   9.79516e-03   2.60709e-02
        <   94241 238.9861>   6.61316e-04   1.76752e-03
        <   94242 239.9793>   1.64645e-04   4.41880e-04
```

after tune() method

```
Mixture O-U-Pu
        <O-U       89.2383>: 0.9755859375 mol
        <O-Pu      89.5943>: 0.0244140625 mol
        total: 1.0 mol or 90.0202779671 g
Nuclide composition:
                    Nuclide       At.frac      Wgt.frac
        <    8016  15.8575>   6.66667e-01   1.18454e-01
        <   92235 233.0248>   6.58694e-04   1.71986e-03
        <   92238 236.0058>   3.24537e-01   8.58209e-01
        <   94239 236.9986>   7.61941e-03   2.02336e-02
        <   94240 237.9916>   4.78279e-04   1.27541e-03
        <   94241 238.9861>   3.22908e-05   8.64685e-05
        <   94242 239.9793>   8.03929e-06   2.16171e-05
```

Set materials to high-level MCNP interface

```
from hmcnp1 import mi
from mcnp_water import m1 as w
from mcnp_zirc import zr
from mcnp_mox import mox

mi.materials['water'] = w
mi.materials['fuel'] = mox
mi.materials['steel'] = zr
mi.materials['zirc'] = zr

if __name__ == '__main__':
    mi.wp.prefix = 'm2_'
    mi.run('P')
```

MCNP input file

```
MESSAGE:  datapath=/home/local/KIT/rx8040/data/mcnp/all_jeff

c title
1 0  -1 fill=1 imp:n=1                                          $  container for None
2 1 -1.0 -2 3 -4 5  fill=-1:2 0:1 0:0
c  k=0
     1 2 5 1
     1 5 5 1 imp:n=1 lat=1 u=1                                  $  Lattice cell for Nor
3 0  -6 fill=3 imp:n=1 u=2                                      $  container for None
4 0  -7 fill=4 imp:n=1 u=3                                      $  container for None
5 2 -10.0 -8 imp:n=1 tmp=2.412856e-08 u=4                       $  layer of None
6 3 -10.0 8 -9 imp:n=1 tmp=2.757550e-08 u=4                     $  layer of None
7 4 -10.0 9 imp:n=1 tmp=2.524881e-08 u=4                        $  layer of None
8 5 -5.0 7 imp:n=1 tmp=2.585203e-08 u=3                         $  layer of None
9 1 -1.0 6 imp:n=1 tmp=2.585203e-08 u=2                         $  layer of lattice ele
10 0  -6 fill=6 imp:n=1 u=5                                     $  container for None
11 0  -7 fill=7 imp:n=1 u=6                                     $  container for None
12 6 -10.0 -10 imp:n=1 tmp=2.369769e-08 u=7                     $  layer of None
13 7 -10.0 10 -11 imp:n=1 tmp=2.705846e-08 u=7                  $  layer of None
14 4 -10.0 11 imp:n=1 tmp=2.524881e-08 u=7                      $  layer of None
15 5 -5.0 7 imp:n=1 tmp=2.585203e-08 u=6                        $  layer of None
16 1 -1.0 6 imp:n=1 tmp=2.585203e-08 u=5                        $  layer of lattice ele
17 0  1 imp:n=0 tmp=2.526174e-08                                $  layer of Container i

c surfaces
1 rpp  -1.265  1.265  -1.265  1.265  -182.5  182.5              $   None
2 px  0.0
3 px  -1.26
4 py  0.0
5 py  -1.3
```

MCNP input file continued 1

```
5 py  -1.3
6 c/z  -0.63  -0.65  0.4583
7 c/z  -0.63  -0.65  0.3951
8 pz  -109.5
9 pz  109.5
10 pz  -91.25
11 pz  91.25

c data cards
c materials
m1                                                          $  H-O at 300.0 K
     1001.31c  1.99977e+00
     1002.31c  2.30000e-04
     8016.31c  9.97570e-01
     8017.31c  3.80000e-04
     8016.31c  2.05000e-03
mt1 lwtr01.31t                                              $  thermal data at 293
m2                                                          $  O-U-Pu at 280 K
     92235.31c  6.58694e-04
     92238.31c  3.24537e-01
     8016.31c  6.50391e-01
     94239.31c  7.61941e-03
     94240.31c  4.78279e-04
     94241.31c  3.22908e-05
     94242.31c  8.03929e-06
     8016.31c  1.62760e-02
m3                                                          $  O-U-Pu at 620 K as
     92235.31c  5.19063e-04   92235.32c  1.39631e-04
     92238.31c  2.55741e-01   92238.32c  6.87960e-02
     8016.31c  5.12519e-01   8016.32c  1.37871e-01
     94239.31c  6.00423e-03   94239.32c  1.61518e-03
```

MCNP input file continued 2

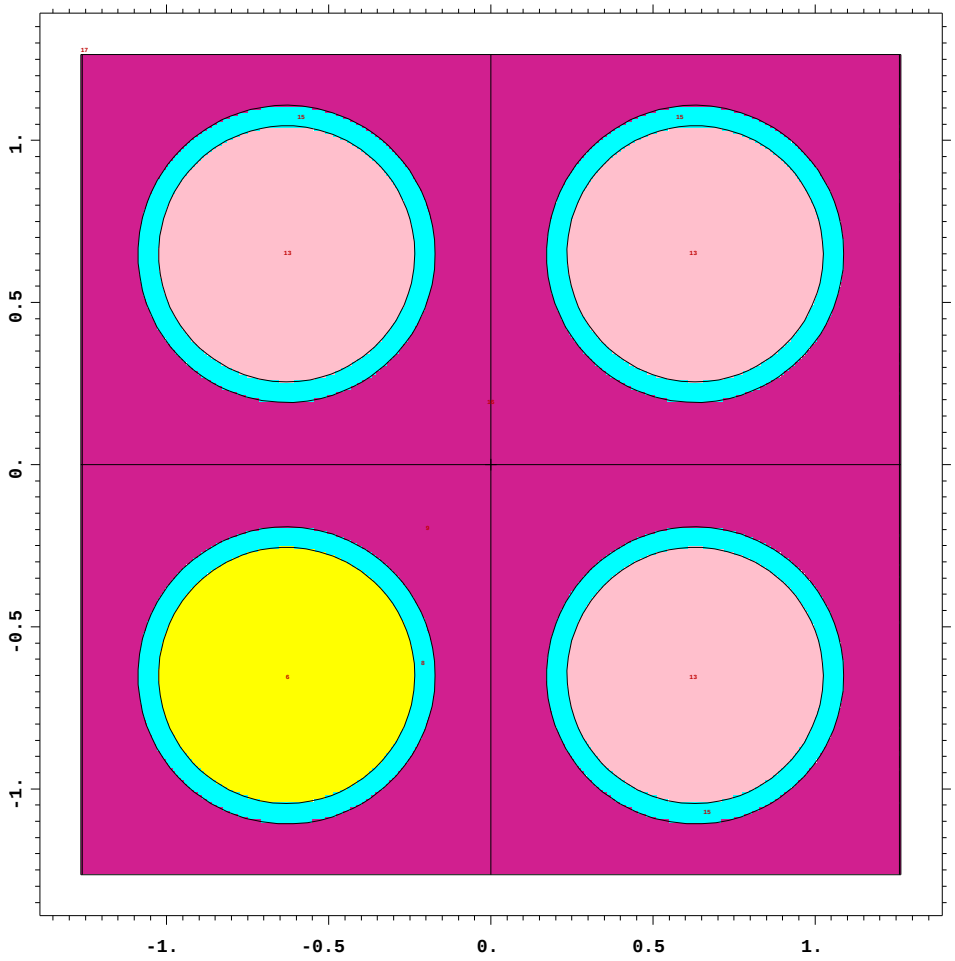
```
     94239.31c  6.00423e-03   94239.32c  1.61518e-03
     94240.31c  3.76893e-04   94240.32c  1.01387e-04
     94241.31c  2.54457e-05   94241.32c  6.84508e-06
     94242.31c  6.33510e-06   94242.32c  1.70419e-06
     8016.31c  1.28258e-02   8016.32c  3.45023e-03
m4                                                          $  O-U-Pu at 293 K
     92235.31c  6.58694e-04
     92238.31c  3.24537e-01
     8016.31c  6.50391e-01
     94239.31c  7.61941e-03
     94240.31c  4.78279e-04
     94241.31c  3.22908e-05
     94242.31c  8.03929e-06
     8016.31c  1.62760e-02
m5                                                          $  Zr-Sn-Fe- at 300.0 K
     40090.31c  5.05393e+01
     40091.31c  1.10214e+01
     40092.31c  1.68464e+01
     40094.31c  1.70724e+01
     40096.31c  2.75044e+00
     50118.31c  3.63300e-01
     50122.31c  6.94500e-02
     50120.31c  4.88700e-01
     50112.31c  1.45500e-02
     50114.31c  9.90000e-03
     50115.31c  5.10000e-03
     50116.31c  2.18100e-01
     50117.31c  1.15200e-01
     50119.31c  1.28850e-01
     50124.31c  8.68500e-02
     26054.31c  7.01400e-03
```

MCNP input file continued 3

```
     94241.31c  3.22908e-05
     94242.31c  8.03929e-06
     8016.31c  1.62760e-02
m7                                                                    $  O-U-Pu at 314 K  as
     92235.31c  5.60481e-04   92235.32c  9.82127e-05
     92238.31c  2.76147e-01   92238.32c  4.83891e-02
     8016.31c  5.53416e-01   8016.32c  9.69747e-02
     94239.31c  6.48334e-03   94239.32c  1.13607e-03
     94240.31c  4.06967e-04   94240.32c  7.13125e-05
     94241.31c  2.74762e-05   94241.32c  4.81463e-06
     94242.31c  6.84061e-06   94242.32c  1.19868e-06
     8016.31c  1.38492e-02   8016.32c  2.42679e-03
c tallies
c kcode 500  1.0  20  100  j  j  100000  j
prdmp j j 1                                                           $  write mctal file
```

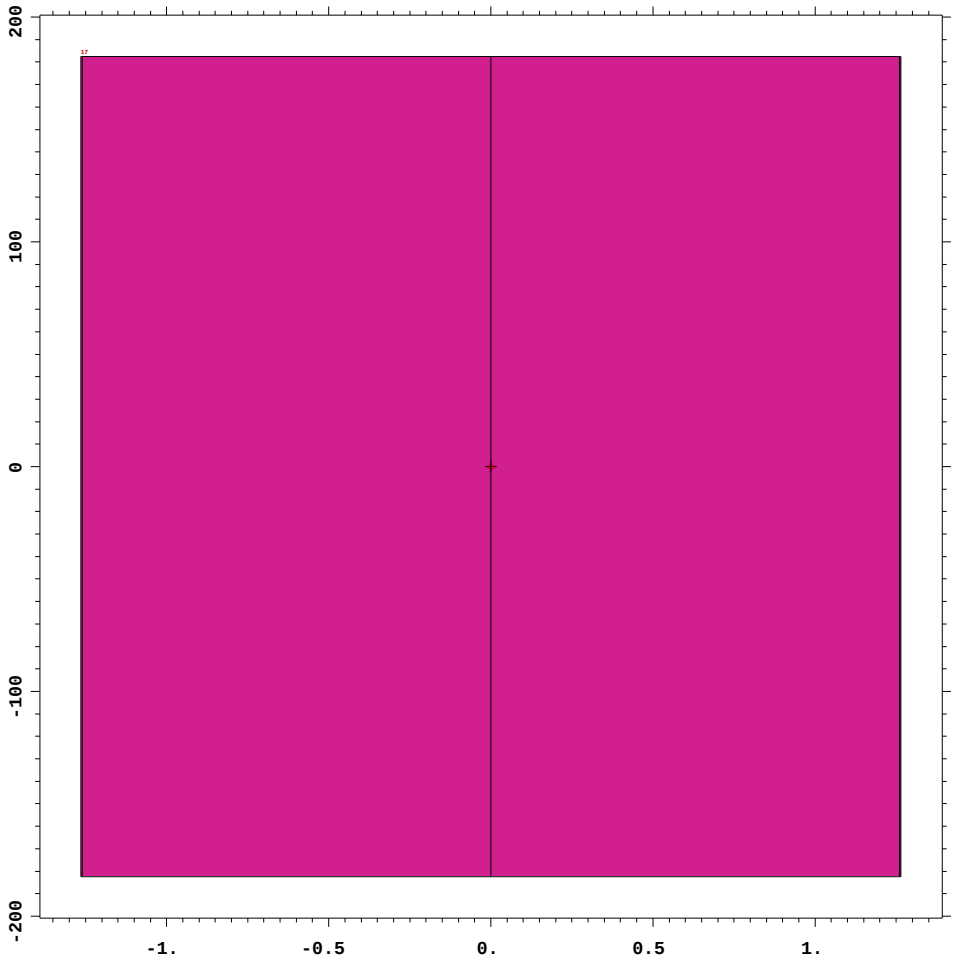
MCNP plot 1

```
 09/15/14 04:46:15
c title

probid =  09/15/14 04:46:15
basis:   XY
( 1.000000, 0.000000, 0.000000)
( 0.000000, 1.000000, 0.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (     1.39,     1.39)
cell labels are
 cell names
```



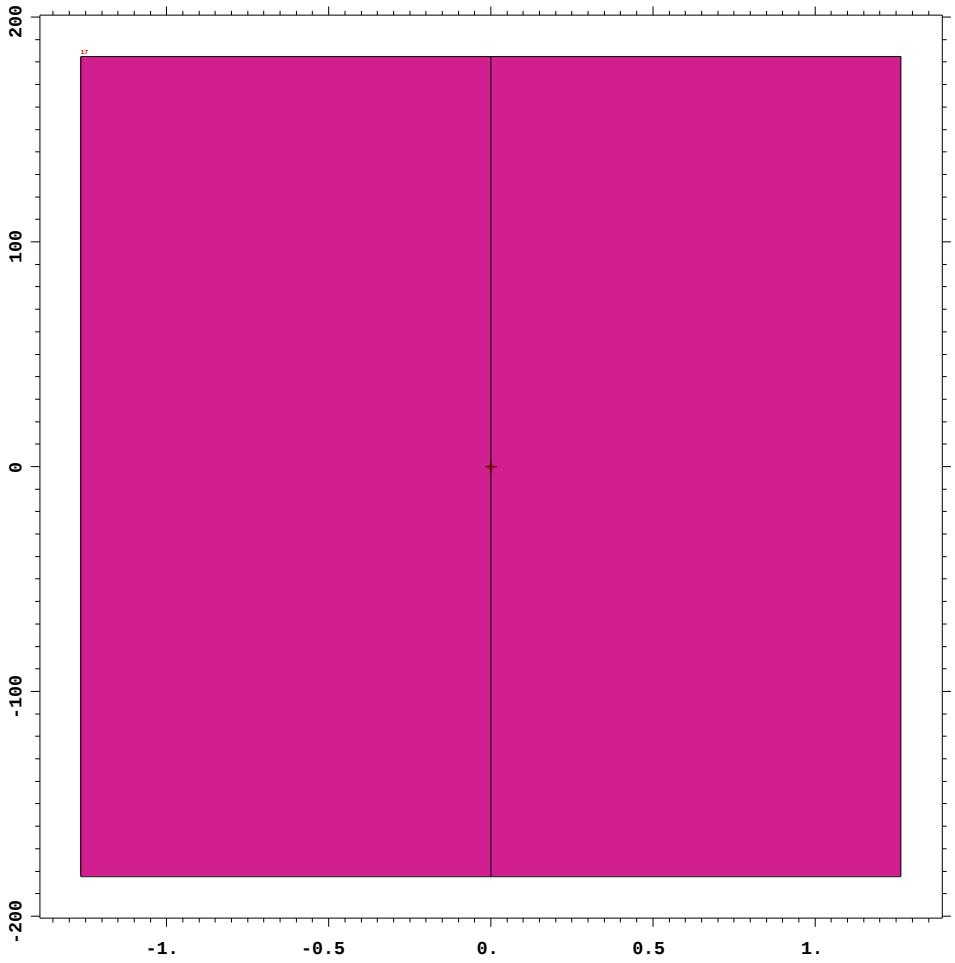
MCNP plot 2

```
 09/15/14 04:46:15
c title


probid =  09/15/14 04:46:15
basis:   XZ
( 1.000000, 0.000000, 0.000000)
( 0.000000, 0.000000, 1.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (     1.39,   200.75)
cell labels are
 cell names
```



MCNP plot 3

```
 09/15/14 04:46:15
c title


probid =  09/15/14 04:46:15
basis:   YZ
( 0.000000, 1.000000, 0.000000)
( 0.000000, 0.000000, 1.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (     1.39,   200.75)
cell labels are
 cell names
```



Set boundary conditions to high-level MCNP interface

```
from hmcnp2 import mi

mi.bc['radial'] = '*'
mi.bc['axial'] = ''

if __name__ == '__main__':
    mi.wp.prefix = 'm3_'
    mi.run('P')
```

MCNP input file

without boundary conditions

```
3 px  -1.26
4 py  0.0
5 py  -1.3
6 c/z  -0.63  -0.65  0.4583
7 c/z  -0.63  -0.65  0.3951
8 pz  -109.5
9 pz  109.5
10 pz  -91.25
11 pz  91.25

c data cards
c materials
m1
     1001.31c  1.99977e+00
     1002.31c  2.30000e-04
     8016.31c  9.97570e-01
```

with boundary conditions

```
*3 px  1.265
*4 px  -1.265
*5 py  1.265
*6 py  -1.265
7 px  0.0
8 px  -1.26
9 py  0.0
10 py  -1.3
11 c/z  -0.63  -0.65  0.4583
12 c/z  -0.63  -0.65  0.3951
13 pz  -109.5
14 pz  109.5
15 pz  -91.25                $  H-O at 300.0 K
16 pz  91.25

c data cards
c materials
m1
     1001.31c  1.99977e+00
     1002.31c  2.30000e-04
     8016.31c  9.97570e-01
```

Specify additional cards for MCNP input

```
from hmcnp3 import mi
# additional cell cards
mi.acc.append('c commented cell card')

# additional surface cards
mi.asc.append('c commented surface card')

# additional data cards
ksrc = 'ksrc '
for v in mi.gm.values(True):
    if v.material == 'fuel':
        x, y, z = v.abspos().car
        ksrc += '  {0} {1} {2}'.format(x, y, z-v.Z*0.49)
        ksrc += '  {0} {1} {2}'.format(x, y, z)
        ksrc += '  {0} {1} {2}'.format(x, y, z+v.Z*0.49)
mi.adc.append(ksrc)

# kcode card
mi.kcode.active = True # otherwise commented
mi.kcode.Nh = 1000 # histories per cycle
mi.kcode.Ncs = 20 # cycles to skip
mi.kcode.Nct = 100 # total num of cycles

if __name__ == '__main__':
    mi.wp.prefix = 'm4_'
    mi.run('P')
```

MCNP input file

Additional cell cards

```
*3 px  1.265                                                    $   None
*4 px  -1.265                                                   $   None
*5 py  1.265                                                    $   None
*6 py  -1.265                                                   $   None
```

Additional surface cards

```
     1002.31c  2.30000e-04
     8016.31c  9.97570e-01
     8017.31c  3.80000e-04
     8016.31c  2.05000e-03
mt1 lwtr01.31t                                                  $  thermal data at 293
m2                                                              $  O-U-Pu at 280 K
     92235.31c  6.58694e-04
```

Additional data cards

```
     -178.85  0.63 -0.65 0.0  0.63 -0.65 178.85  0.63 0.65 -178.85  0.63 0.65
     0.0  0.63 0.65 178.85  -0.63 0.65 -178.85  -0.63 0.65 0.0  -0.63 0.65
     178.85
```

Tallies for MCNP input

```
from hmcnp4 import mi

# set heat meshes
for v in mi.gm.values():
    if v.material == 'fuel':
        v.heat.set_grid([1]*20)

if __name__ == '__main__':
    mi.wp.prefix = 'm5_'
    mi.run('R', tasks=3)

    from pirs.tools import dump
    dump('m5_.dump', gm=mi.gm)


    from pirs.tools.plots import colormap
    hx1 = colormap(mi.gm, plane={'x':-0.63}, var='heat', aspect='auto')
    hx2 = colormap(mi.gm, plane={'x': 0.63}, var='heat', aspect='auto')
    hy1 = colormap(mi.gm, plane={'y':-0.63}, var='heat', aspect='auto')
    hy2 = colormap(mi.gm, plane={'y': 0.63}, var='heat', aspect='auto')
    hx1.get_figure().savefig('hmcnp5_hx1.pdf')
    hx2.get_figure().savefig('hmcnp5_hx2.pdf')
    hy1.get_figure().savefig('hmcnp5_hy1.pdf')
    hy2.get_figure().savefig('hmcnp5_hy2.pdf')
else:
    from pirs.tools import load
    mi.gm = load('m5_.dump')['gm']
```

MCNP input file with tallies

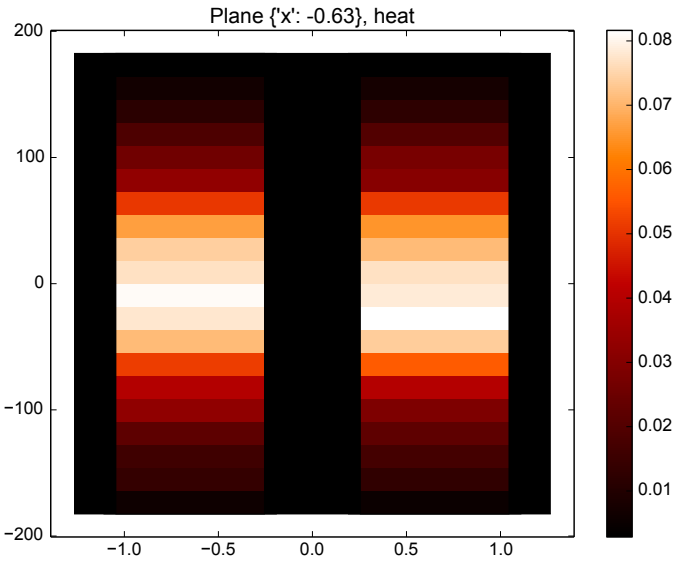
```
     jmesh= 0.0 1.265
     kmesh= -164.25 -146.0 -127.75 -109.5 -91.25 -73.0 -54.75 -36.5 -18.25 -0.0
     18.25 36.5 54.75 73.0 91.25 109.5 127.75 146.0 164.25 182.5
fm14 -1 0 -6 -8
kcode 1000  1.0  20  100  j  j  100000  j
prdmp j j 1                                                    $  write mctal file
ksrc   -0.63 -0.65 -178.85  -0.63 -0.65 0.0  -0.63 -0.65 178.85  0.63 -0.65
     -178.85  0.63 -0.65 0.0  0.63 -0.65 178.85  0.63 0.65 -178.85  0.63 0.65
     0.0  0.63 0.65 178.85  -0.63 0.65 -178.85  -0.63 0.65 0.0  -0.63 0.65
     178.85
```

MCNP meshtal file

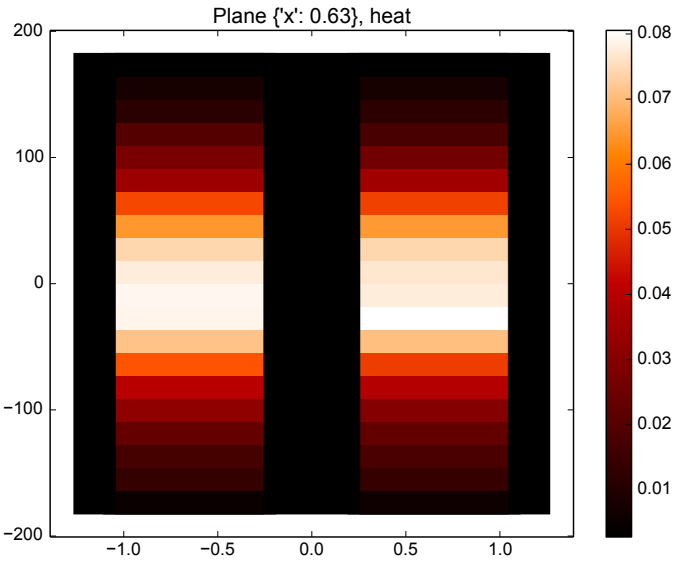
```
-1.262    -0.632   100.375 0.00000E+00 0.00000E+00
-1.262    -0.632   118.625 0.00000E+00 0.00000E+00
-1.262    -0.632   136.875 0.00000E+00 0.00000E+00
-1.262    -0.632   155.125 0.00000E+00 0.00000E+00
-1.262    -0.632   173.375 0.00000E+00 0.00000E+00
-1.262     0.632  -173.375 0.00000E+00 0.00000E+00
-1.262     0.632  -155.125 0.00000E+00 0.00000E+00
-1.262     0.632  -136.875 0.00000E+00 0.00000E+00
-1.262     0.632  -118.625 0.00000E+00 0.00000E+00
-1.262     0.632  -100.375 0.00000E+00 0.00000E+00
-1.262     0.632   -82.125 0.00000E+00 0.00000E+00
-1.262     0.632   -63.875 0.00000E+00 0.00000E+00
-1.262     0.632   -45.625 0.00000E+00 0.00000E+00
-1.262     0.632   -27.375 0.00000E+00 0.00000E+00
-1.262     0.632    -9.125 0.00000E+00 0.00000E+00
-1.262     0.632     9.125 0.00000E+00 0.00000E+00
-1.262     0.632    27.375 0.00000E+00 0.00000E+00
-1.262     0.632    45.625 0.00000E+00 0.00000E+00
-1.262     0.632    63.875 0.00000E+00 0.00000E+00
-1.262     0.632    82.125 0.00000E+00 0.00000E+00
-1.262     0.632   100.375 0.00000E+00 0.00000E+00
-1.262     0.632   118.625 0.00000E+00 0.00000E+00
-1.262     0.632   136.875 0.00000E+00 0.00000E+00
-1.262     0.632   155.125 0.00000E+00 0.00000E+00
-1.262     0.632   173.375 0.00000E+00 0.00000E+00
-0.630    -0.632  -173.375 5.74785E-03 8.46687E-02
-0.630    -0.632  -155.125 1.36505E-02 5.42823E-02
-0.630    -0.632  -136.875 1.60058E-02 5.19930E-02
-0.630    -0.632  -118.625 2.21769E-02 4.28544E-02
-0.630    -0.632  -100.375 3.25456E-02 3.63517E-02
-0.630    -0.632   -82.125 3.95603E-02 3.18629E-02
```

MCNP results

x plane at -1



x plane at 1



High-level interface to SCF

```
from pirs import ScfInterface
from hmcnp5 import mi

si = ScfInterface(mi.gm)

if __name__ == '__main__':
    si.wp.prefix = 's1_'
    si.run('r')
```

Limitations

- Rectangular container (i.e. an instance of the pirs.solids.Box() class)
- Rods inserted into grid element centers, no empty grid elements.
- Container and rods (and all internal structure) have the same height.

SCF input file: channels

```
&channel_layout
file = this_file
channel_number         channel_area    wetted_perimeter    heated_perimeter    x_position    y_position
             1    2.25560841552e-05     0.0071989595657     0.0071989595657           1.1           1.2
             2    4.44971683104e-05     0.0143979191314     0.0143979191314           1.1           1.2
             3    2.25560841552e-05     0.0071989595657     0.0071989595657           1.1           1.2
             4    4.95571683104e-05     0.0143979191314     0.0143979191314           1.1           1.2
             5    9.78143366208e-05     0.0287958382628     0.0287958382628           1.1           1.2
             6    4.95571683104e-05     0.0143979191314     0.0143979191314           1.1           1.2
             7    2.25560841552e-05     0.0071989595657     0.0071989595657           1.1           1.2
             8    4.44971683104e-05     0.0143979191314     0.0143979191314           1.1           1.2
             9    2.25560841552e-05     0.0071989595657     0.0071989595657           1.1           1.2
!
file = this_file
channel    max_40_x_(neighbour+gap+distance)
      1                                    2    0.001567    0.009475    4    0.001767    0.009575    /
      2                                    3    0.001567    0.009475    5    0.003434    0.009575    /
      3                                    6    0.001767    0.009575    /
      4                                    5    0.003834    0.009475    7    0.001767    0.009575    /
      5                                    6    0.003834    0.009475    8    0.003434    0.009575    /
      6                                    9    0.001767    0.009575    /
      7                                    8    0.001567    0.009475    /
      8                                    9    0.001567    0.009475    /
      9                                    /
!
!
```

SCF input file: rods

```
file = this_file
rod_number   material_type   outer_diameter   power_fraction   x_position   y_position
         1                1         0.009166              0.1        -0.63        -0.65
         2                1         0.009166              0.1         0.63        -0.65
         3                1         0.009166              0.1         0.63         0.65
         4                1         0.009166              0.1        -0.63         0.65
!
file = this_file
rod   max_6_x_(channel+fraction)
  1                           1   0.25   2   0.25   4   0.25   5   0.25   /
  2                           2   0.25   3   0.25   5   0.25   6   0.25   /
  3                           5   0.25   6   0.25   8   0.25   9   0.25   /
  4                           4   0.25   5   0.25   7   0.25   8   0.25   /
!
file = this_file
```

SCF input file: power axial profile

```
file = this_file
time   inlet_flow
!
file = this_file
channel_number   time   inlet_flow
!
file = this_file
time   heat_flux_factor
!
file = this_file
power_map_time
!
file = this_file
axial_cell_number   rod_number    power_map
                1             1   0.00574785
                2             1    0.0136505
                3             1    0.0160058
                4             1    0.0221769
                5             1    0.0325456
                6             1    0.0395603
```

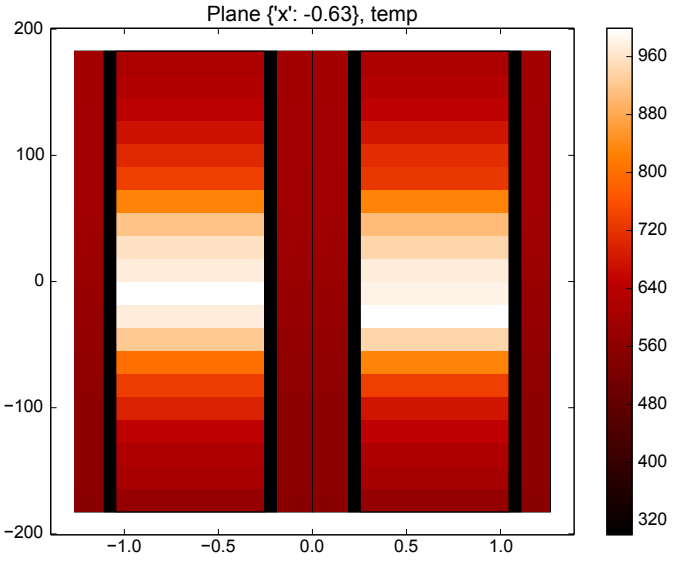
SCF-specific parameters

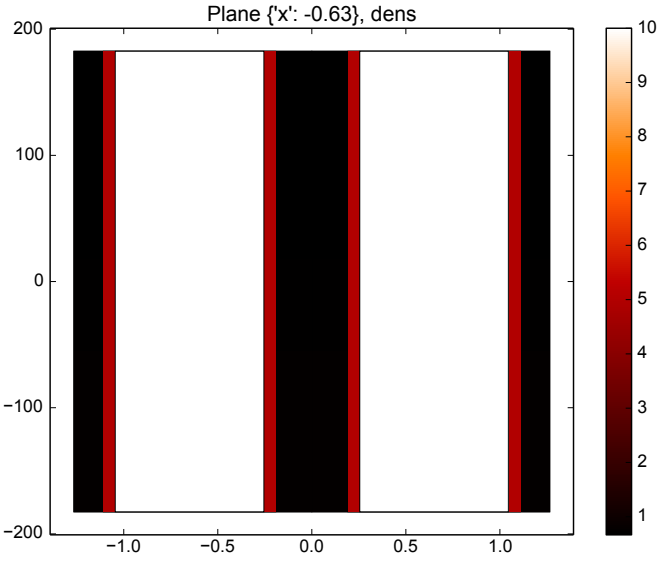
```
from hscf1 import si

# set boundary conditions
si.find('total_power')[0].value = 7e4*4 # W
si.find('average_heat_flux')[0].value = 0.0
si.find('inlet_temperature')[0].value = 280 # C
si.find('inlet_flow_rate')[0].value = 0.28*4 # g/sec
si.find('inlet_mass_flux')[0].value = 0.
si.find('set_driving_pressure_condition')[0].state = 'set_pure_flow_condition'
si.find('exit_pressure')[0].value = 15.45e6 # Pa
si.find('v', 'pressure_drop')[0].value = 0.
si.find('inlet_boron_concentration')[0].value = 0.
si.find('heat_fraction_moderator')[0].value = 0.

si.find('number_of_fuel_nodes')[0].value = 10

# variables:
si.find('blasius_laminar_prefactor')[0].value = 64.0
si.find('blasius_laminar_reynolds_exponent')[0].value = -1.0
si.find('blasius_laminar_constant')[0].value = 0

si.find('blasius_turbulent_prefactor')[0].value = 0.316
si.find('blasius_turbulent_reynolds_exponent')[0].value = -0.25
si.find('blasius_turbulent_constant')[0].value = 0

si.find('dittus_boelter_prefactor')[0].value = 0.023
si.find('dittus_boelter_reynolds_exponent')[0].value = 0.8
si.find('dittus_boelter_prandtl_exponent')[0].value = 0.4
si.find('dittus_boelter_constant')[0].value = 0.

si.find('set_buoyancy')[0].state = 0
```

SCF-specific parameters: rod material specifications

```
from pirs.scf2 import RodMaterial
from hscf2 import si

cld = RodMaterial()
cld.fp = 'benpwr'
cld.fd = -1
cld.ct = -1
cld.cp = 'zircaloy'

si.materials['steel'] = cld
si.materials['zirc'] = cld

if __name__ == '__main__':
    si.wp.prefix = 's3_'
    si.run('R')

    from pirs.tools import dump
    dump('s3_.dump', gm=si.gm)

    from pirs.tools.plots import colormap
    fltr = lambda e: e.material not in ['zirc', 'steel']
    tz  = colormap(si.gm, plane={'z':1},     var='temp', aspect='auto')#  , filter_=fltr
    tx1 = colormap(si.gm, plane={'x':-0.63}, var='temp', aspect='auto')#  , filter_=fltr
    tx2 = colormap(si.gm, plane={'x': 0.63}, var='temp', aspect='auto')#  , filter_=fltr
    ty1 = colormap(si.gm, plane={'y':-0.63}, var='temp', aspect='auto')#  , filter_=fltr
    ty2 = colormap(si.gm, plane={'y': 0.63}, var='temp', aspect='auto')#  , filter_=fltr
    tz.get_figure().savefig('hscf3_tz.pdf')                             #
    tx1.get_figure().savefig('hscf3_tx1.pdf')                           #
    tx2.get_figure().savefig('hscf3_tx2.pdf')                           #
    ty1.get_figure().savefig('hscf3_ty1.pdf')                           #
    ty2.get_figure().savefig('hscf3_ty2.pdf')                           #
```

SCF-specific parameters: SCF results

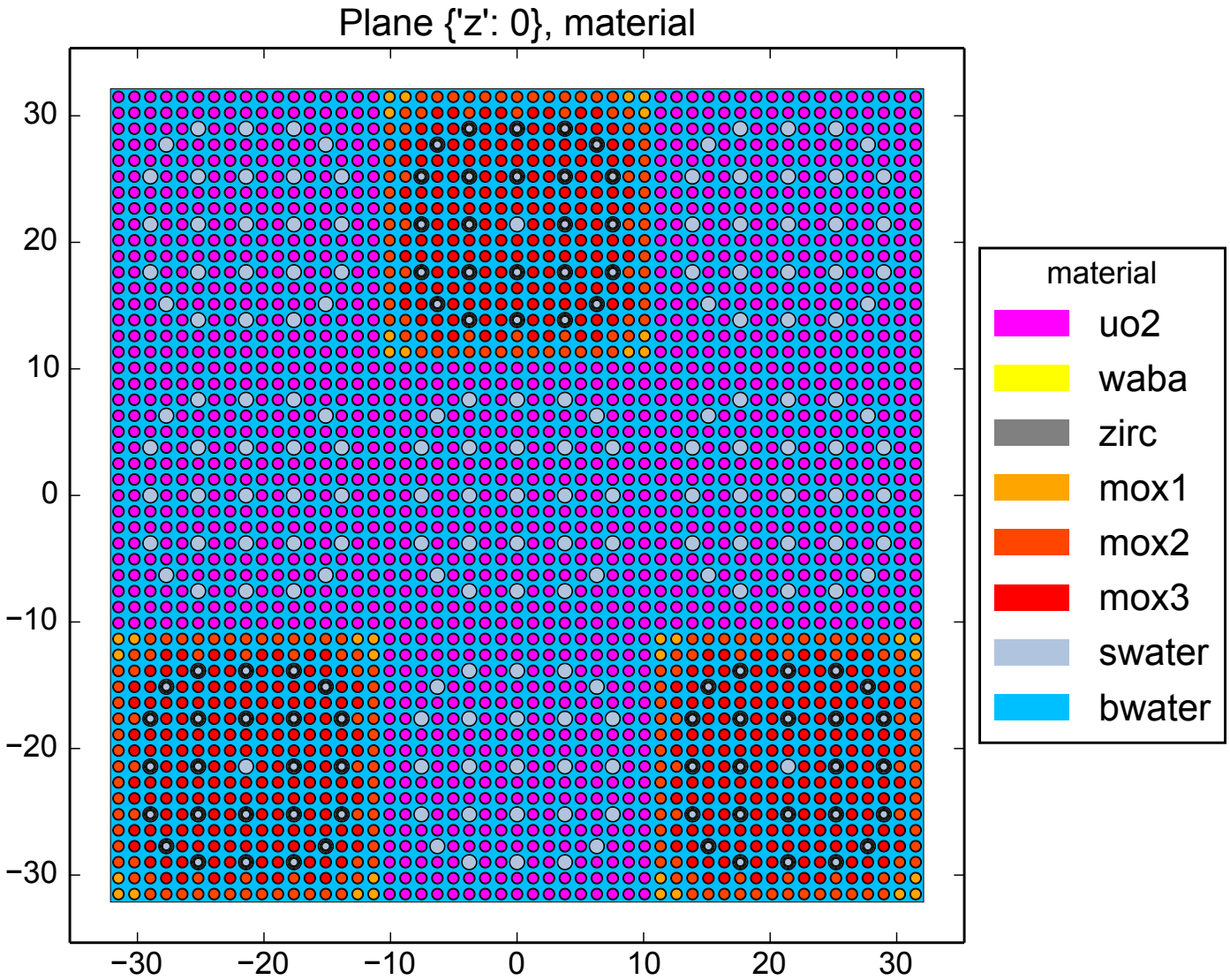




Data exchange between interfaces

```
from pirs.tools import dump
from hscf3 import si
from hmcnp5 import mi

mi.wp.prefix = 'cm_'
si.wp.prefix = 'cs_'

I = 0
while I < 5:
    # mcnp run
    mi.gm = si.gm.copy_tree()
    mr = mi.run('R', tasks=3)
    # relaxed power
    for (em, es) in zip(mr.heats(), si.gm.heats()):
        h = 0.5 *em.heat + 0.5 * es.heat
        es.heat.update(h)
    # scf run
    si.run('R')
    # store results
    dump('{}_coupling.dump'.format(I),
         Keff = mi.keff(),
         mr = mr,
         sr = si.gm,
         I = I)

    I += 1
```

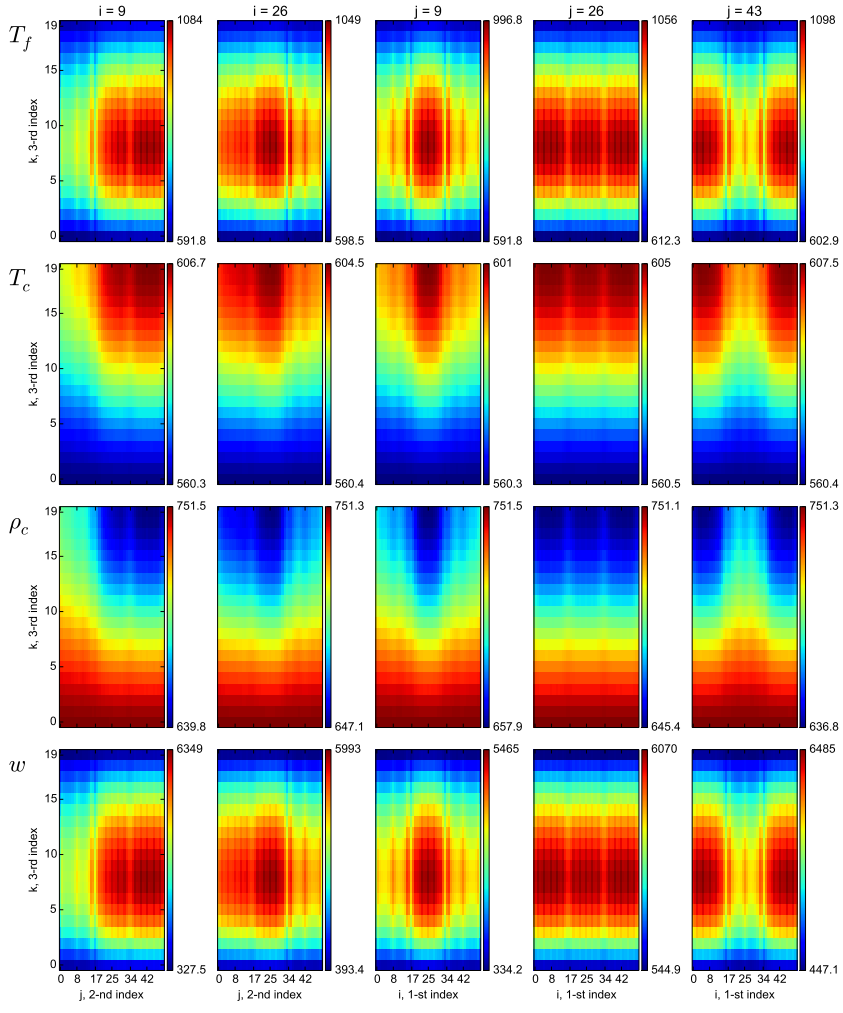
3x3 minicore model



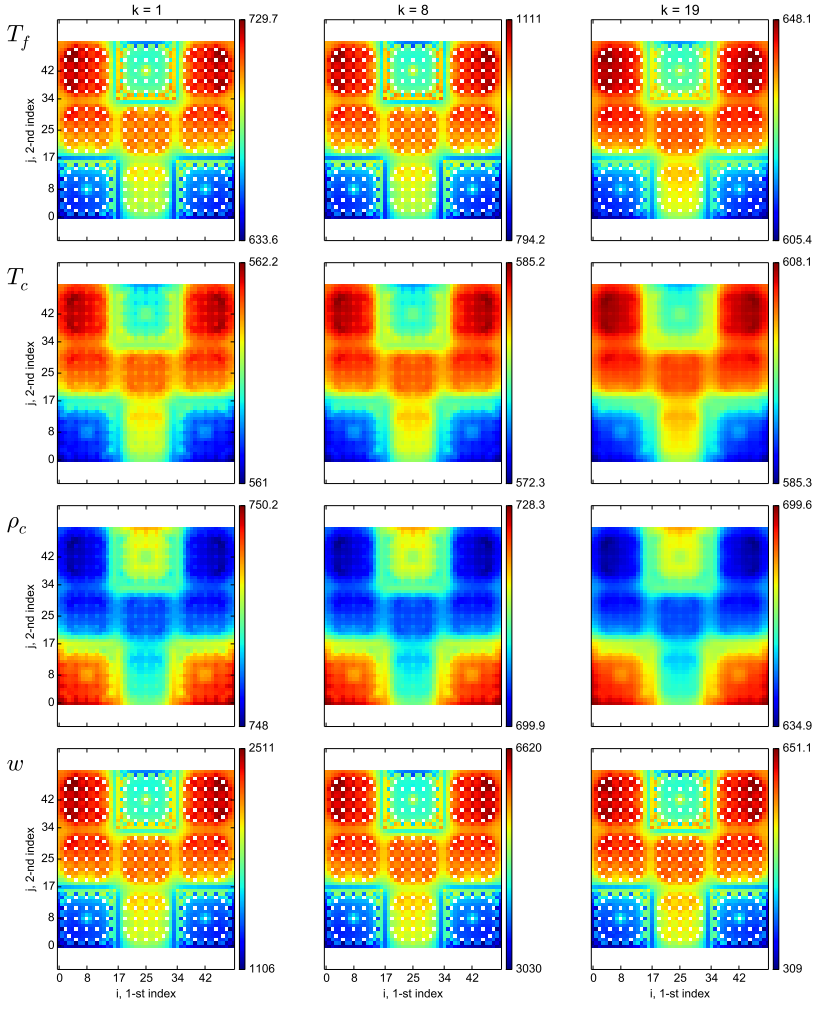
PWR assembly model

- PIRS deployed on a cluster, MCNP jobs queued to a job submission system
- Long MCNP initialization time due to huge amount of cells
- Good agreement with other results (see D1.9)

Results, vertical profile



Results, horizontal profile



Conclusion and outlook

- MCNP interface (low- and high-level) can be used as stand-alone tool to facilitate preparation of complex input files (e.g. 1/4 of the core).
- SCF interface mature enough to treat square bundles. Ideas to generalization tested but not implemented.
- Limitations due to MCNP number of cells
  - MCNP 6?
  - SERPENT-2
- PIRS is a tool for fast implementation of coupled MCNP-SCF calculations for geometries from one-pin to minicore.
- Documentation is (partly) written.