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PIRS: Python Interfaces for Reactor Simulations

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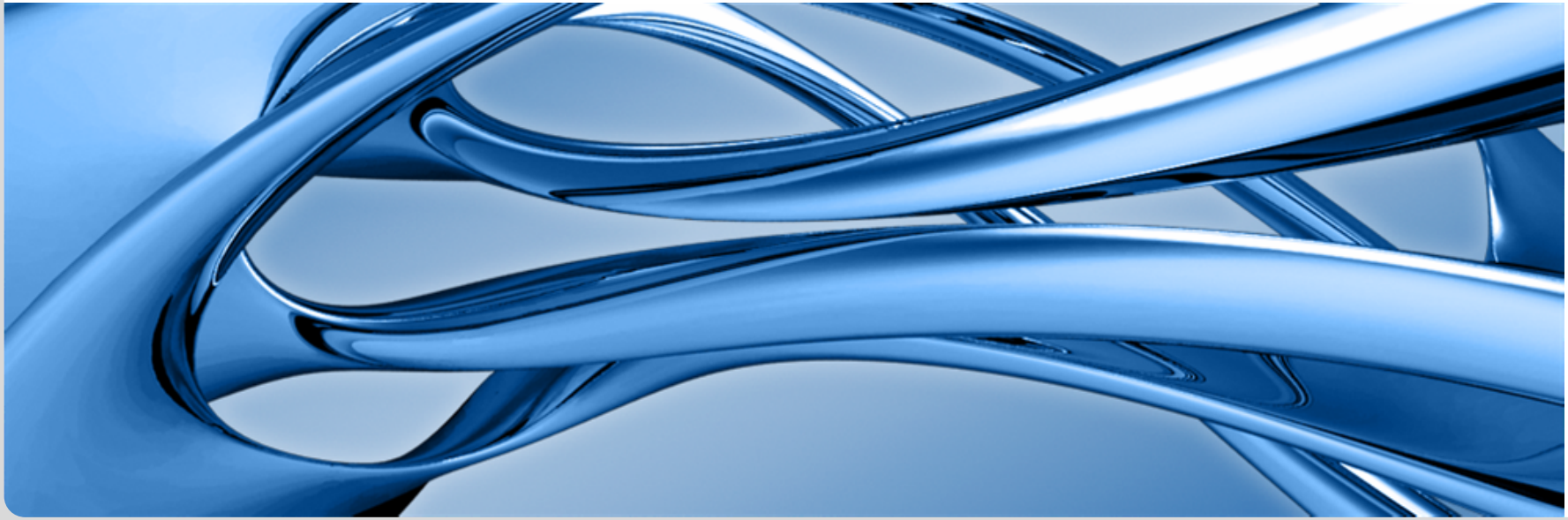


Content

- Introduction: what PIRS is, and what it is for
- PIRS concept
- Examples:
  - Python code to define fuel pin
  - Results of MCNP-SCF coupled calculations for assembly
- Current development status
- Ongoing work

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

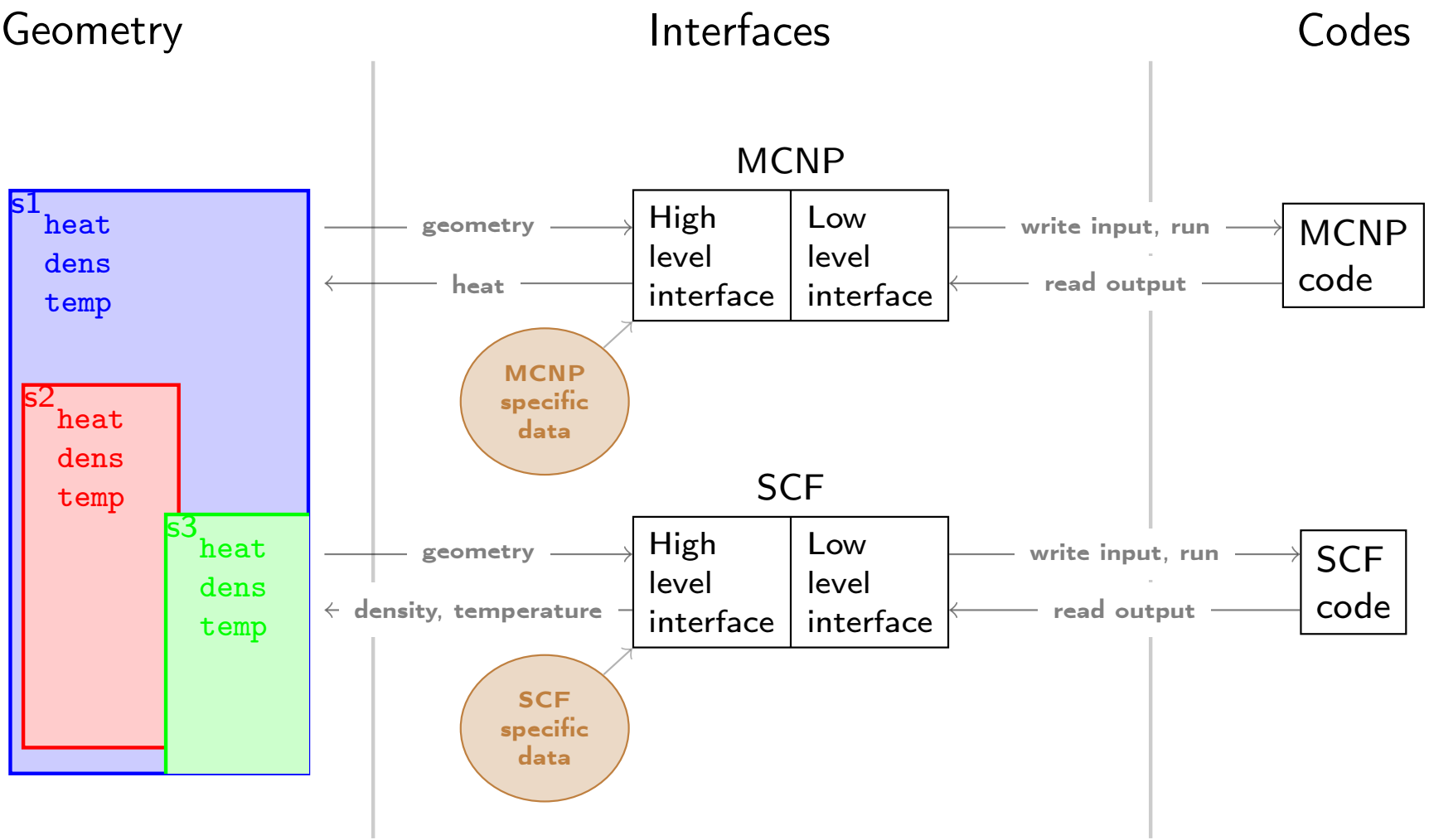
Interaction with code

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

What PIRS is for

- Routine preparation of input files
- Framework for coupled calculations

Concept


Geometry
Interfaces
Codes
s1
heat
dens
temp
s2
heat
dens
temp
s3
heat
dens
temp
MCNP
geometry
heat
High level interface
Low level interface
write input, run
read output
MCNP code
MCNP specific data
SCF
geometry
density, temperature
High level interface
Low level interface
write input, run
read output
SCF code
SCF specific data

Concept

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Classes provided by PIRS fall into three catogories

- To describe calculation geometry: Solids (Cylinder, Box) can be inserted into each other and positioned with respect to container.
- Low-level interfaces:
  - Assure correct syntax of input file,
  - "Know" command line parameters of the code,
  - provide functions to read output.
- High-level interfaces:
  - Conversion: geometry $\Longleftrightarrow$ low-level interfaces,
  - Interface to specify code-specific parameters

Example: simplified neutronics model of fuel pin

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Geometry definition:

```
from hpmc import Box, Cylinder

b = Box(X=1.2, Y=1.2, Z=110)
c = Cylinder(R=0.5, Z=100)
b.insert(0, c)

b.material = 'water'
c.material = 'fuel'

b.dens.set_grid([1, 1])
b.dens.set_values(1.)

c.temp.set_grid([1]*3)
c.temp.set_values([300, 500, 350])

c.heat.set_grid([1]*10)
```

Example: simplified neutronics model of fuel pin

MCNP interface:

```
from hpmc import McnpInterface
from mcnp import Material

m = McnpInterface(b)

u = Material((92235,  0.5, 2),
             (92238, 95.5, 2))

o = Material('O')
h = Material('H')

f = u + 2*o
w = h*2 + o
w.thermal = 'lwtr'
```

```
f.sdict[8018] = 8016
w.sdict[8018] = 8016

m.materials['fuel'] = f
m.materials['water'] = w

m.bc['radial'] = '*'

m.adc.append('ksrc 0 0 0')
m.adc.append('kcode 500 1. 20 100')

m.run('P')

r = m.run('R')
```

Example: simplified neutronics model of fuel pin

Generated MCNP input file

```
c title
1 0  -3 4 -5 6 -2 1 fill=1 imp:n=1
2 0  -7 fill=2 imp:n=1 u=1
3 1 -1.0 -8 imp:n=1 tmp=2.585203e-08 u=2
4 2 -1.0 8 -9 imp:n=1 tmp=4.308671e-08 u=2
5 3 -1.0 9 imp:n=1 tmp=3.016070e-08 u=2
6 4 -1.0 -10 7 imp:n=1 tmp=2.585203e-08 u=1
7 4 -1.0 10 7 imp:n=1 tmp=2.585203e-08 u=1
8 0  11 (3:-4:5:-6:2:-1) imp:n=0 tmp=2.585203e-08

c surfaces
1 pz  -55.0
2 pz  55.0
*3 px  0.6
*4 px  -0.6
*5 py  0.6
*6 py  -0.6
7 rcc  0.0  0.0  -50.0  0.0  0.0  100.0  0.5
8 pz  -16.666666667
9 pz  16.666666667
10 pz  0.0
11 pz  -1055.01817881

c data cards
c materials
m1                      $ mixture U-O at 300 K
      92235.31c 5.0000000e-01
      92238.31c 9.5500000e+01
       8016.31c 1.9951400e+00
       8017.31c 7.6000000e-04
       8016.31c 4.1000000e-03
```

```
m2                      $ mixture U-O at 500 K
      92235.31c 3.9962042e-01  92235.40c 1.0037958e-01
      92238.31c 7.6327500e+01  92238.40c 1.9172500e+01
       8016.31c 1.5945974e+00   8016.40c 4.0054263e-01
       8017.31c 6.0742304e-04   8017.40c 1.5257696e-04
       8016.31c 3.2768874e-03   8016.40c 8.2311256e-04
m3                      $ mixture U-O at 350 K
      92235.31c 5.0000000e-01
      92238.31c 9.5500000e+01
       8016.31c 1.9951400e+00
       8017.31c 7.6000000e-04
       8016.31c 4.1000000e-03
m4                      $ mixture H-O at 300.0 K
       1001.31c 1.9997700e+00
       1002.31c 2.3000000e-04
       8016.31c 9.9757000e-01
       8017.31c 3.8000000e-04
       8016.31c 2.0500000e-03
mt4 lwtr01.31t          $ thermal data at 293.606K
c tallies
fmesh14:n               $ heat in ('/', 0)
     geom=cyl
     origin=0.0 0.0 -50.0
     axs=0.0 0.0 1.0
     vec=1.0 0.0 0.0
     imesh= 0.5
     jmesh= 10.0 20.0 30.0 40.0 50.0 60.0
            70.0 80.0 90.0 100.0
     kmesh= 1.0
fm14 -1 0 -6 -8
prdmp j j 1             $ write mctal file
ksrc 0 0 0
kcode 500 1. 20 100
```

Example: simplified neutronics model of fuel pin

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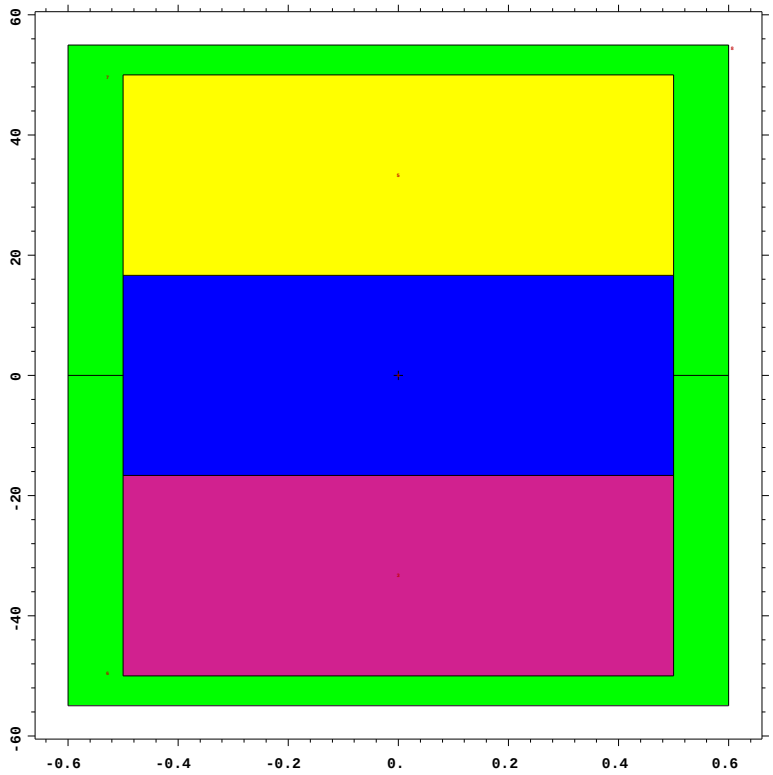
Geometry plot generated with MCNP

```
 09/10/13 13:02:39
c title

probid =  09/10/13 13:02:39
basis:   XZ
( 1.000000, 0.000000, 0.000000)
( 0.000000, 0.000000, 1.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (     0.66,    60.50)
cell labels are
 cell names
```



Example: results for coupled MCNP-SCF calculations

Coupled MCNP – SCF calculations, organized with PIRS

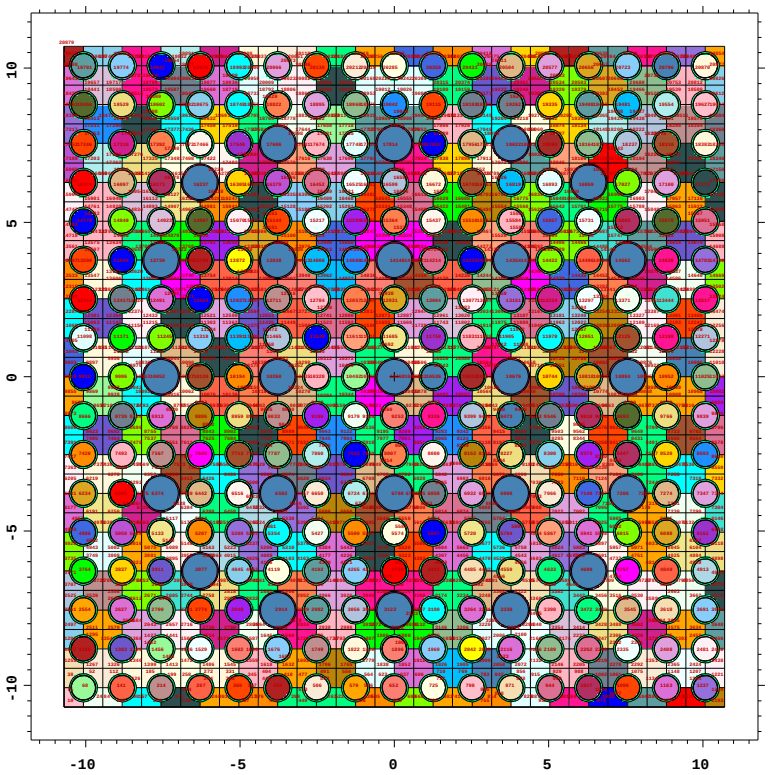
- Model: PWR assembly 17x17,
- moderator channels,
- two different types of fuel pins,
- boron in coolant,
- Coolant-centered subchannels,
- non-uniform axial mesh,
- Calculations conducted on a linux desktop
- relaxation scheme for power axial distribution with varying relaxation parameter and increasing statistical precision

Example: results for coupled MCNP-SCF calculations

Horizontal cross-section of MCNP model:

```
 09/10/13 17:32:56
c title


probid =  09/10/13 17:32:29
basis:   XY
( 1.000000, 0.000000, 0.000000)
( 0.000000, 1.000000, 0.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (    11.78,    11.78)
cell labels are
 cell names
```

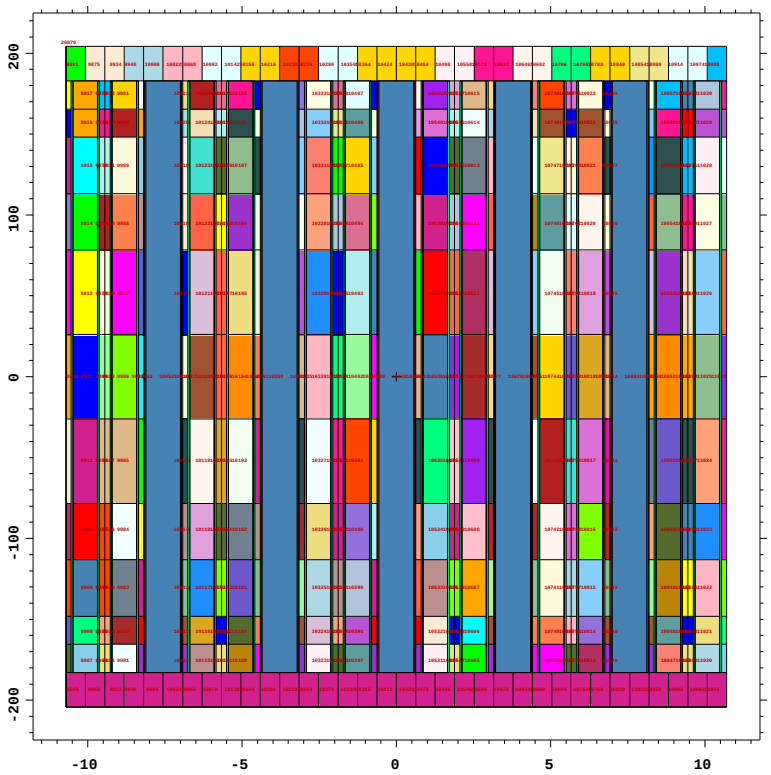


Example: results for coupled MCNP-SCF calculations

Vertical cross-section of MCNP model:

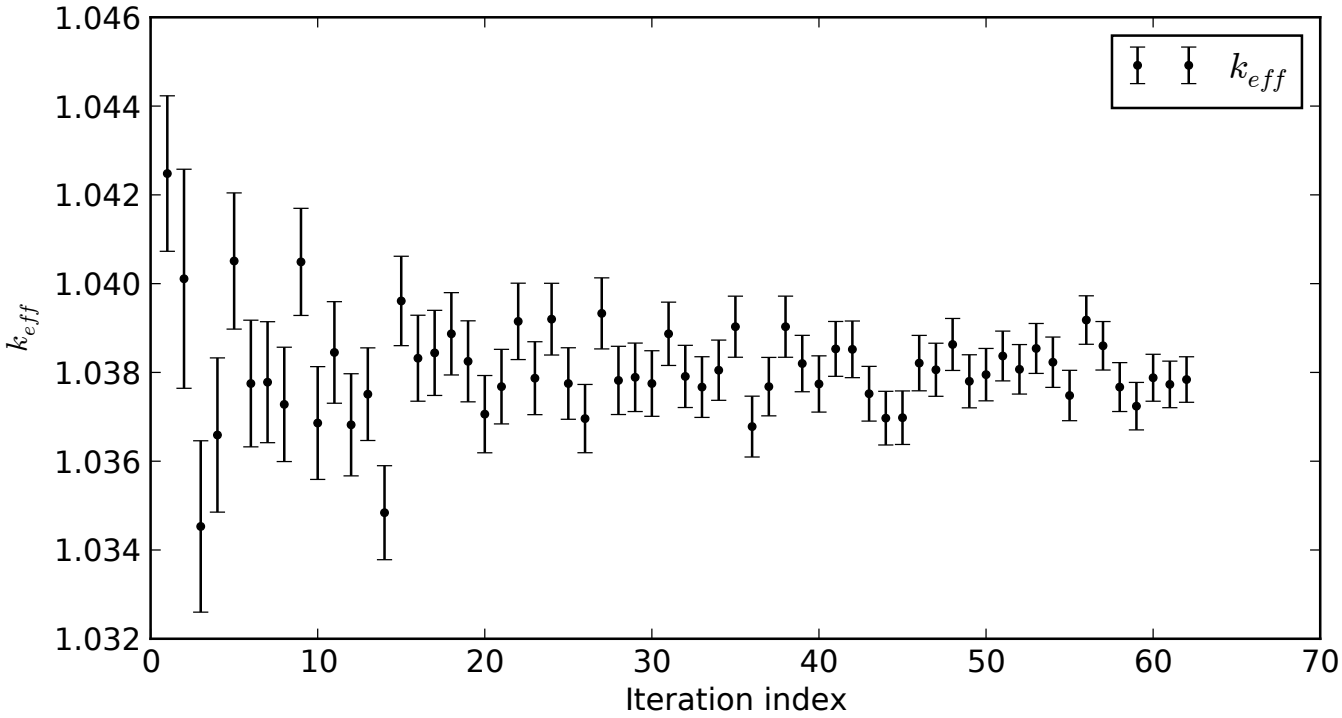
```
 09/10/13 17:32:58
c title


probid =  09/10/13 17:32:29
basis:   XZ
( 1.000000, 0.000000, 0.000000)
( 0.000000, 0.000000, 1.000000)
origin:
(     0.00,     0.00,     0.00)
extent = (    11.78,   224.73)
cell labels are
 cell names
```



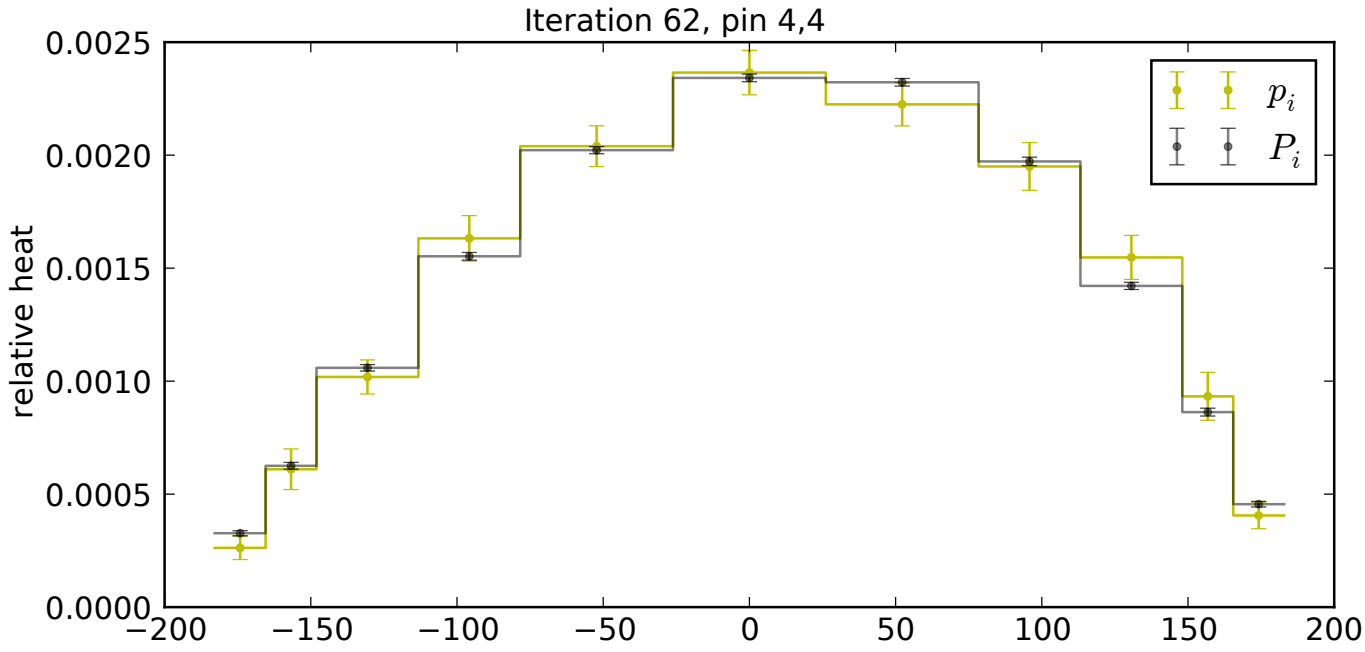
Example: results for coupled MCNP-SCF calculations

Behaviour of k_{eff} with N–TH iterations



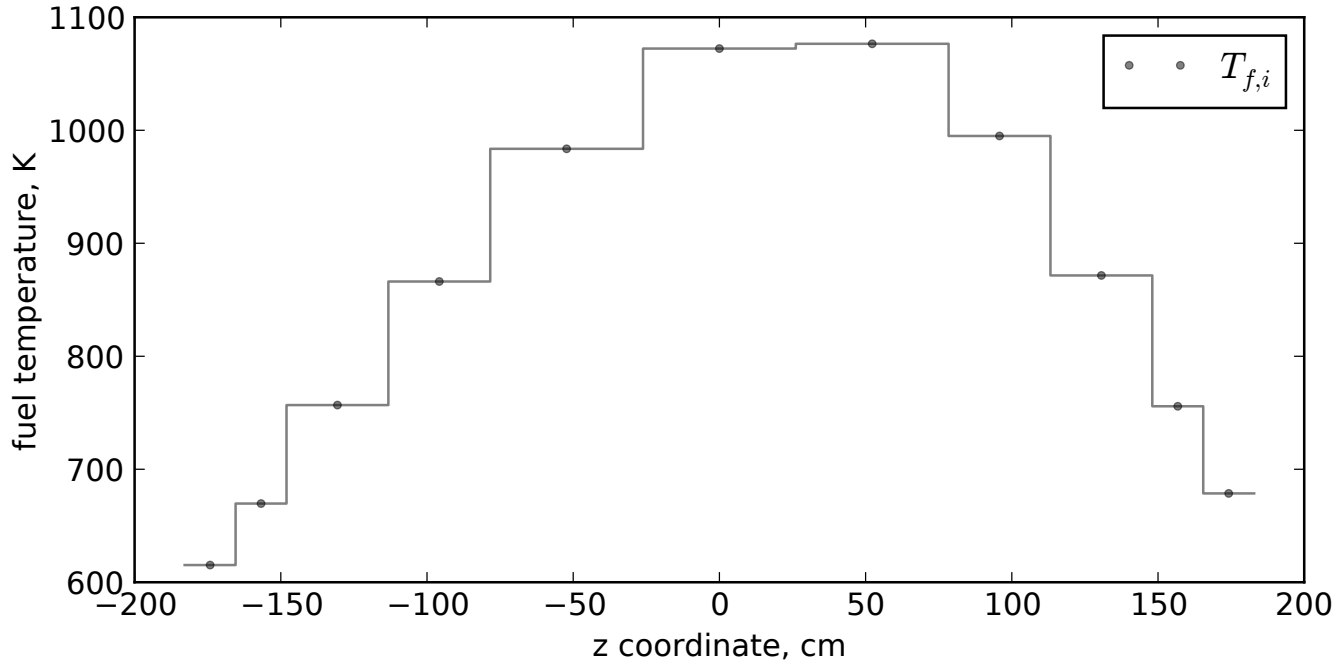
Example: results for coupled MCNP-SCF calculations

Axial distribution of heat deposition in one fuel pin



Example: results for coupled MCNP-SCF calculations

Axial distribution of fuel temperature in the same pin



Example: results for coupled MCNP-SCF calculations

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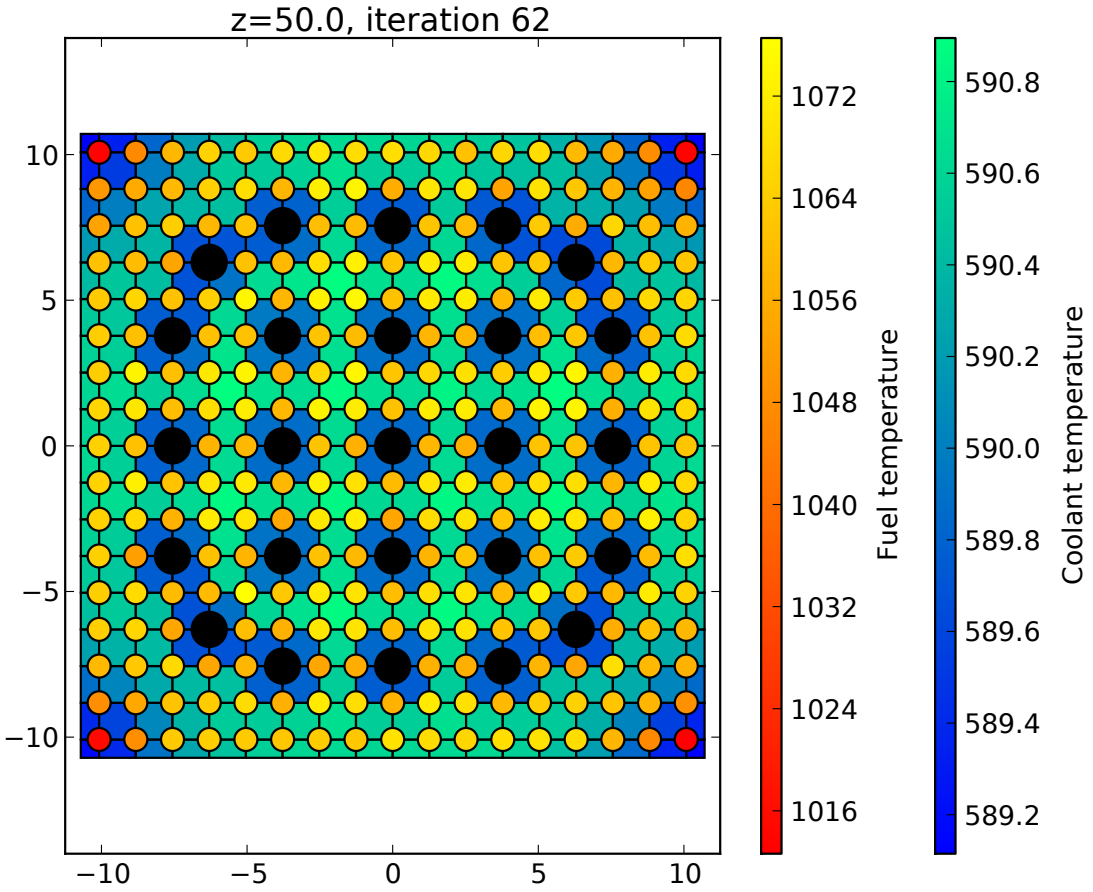
Temperature map



Current development status

Governed by HPMC project: Monte-Carlo neutronics and sub-channel TH modelling of PWR assembly and core.

Interface to MCNP

- handles any geometry represented by boxes and cylinders
- Repeated structure can be modelled as lattice
- Description of materials
  - Convenient definition of composition
  - Automatic choice of suffixes and interpolation of XS
- Reads meshtal

Means to set up geometry

- Cylinder: vertical cylinder of finite height
- Box: rectangular parallelepiped with facets perpendicular to axes
- meshes to represent temperature, density and heat axial profiles

Interface to SCF

- Only for PWR-like geometries
- Reads output.txt

Ongoing work

Current

- calculation of a minicore $\rightarrow$ optimization of MCNP and SCF interfaces

Plans

- Interface to SERPENT-2
- New interface to SCF
- update Documentation, open source
- Geometry plotter
- interfaces to other codes?