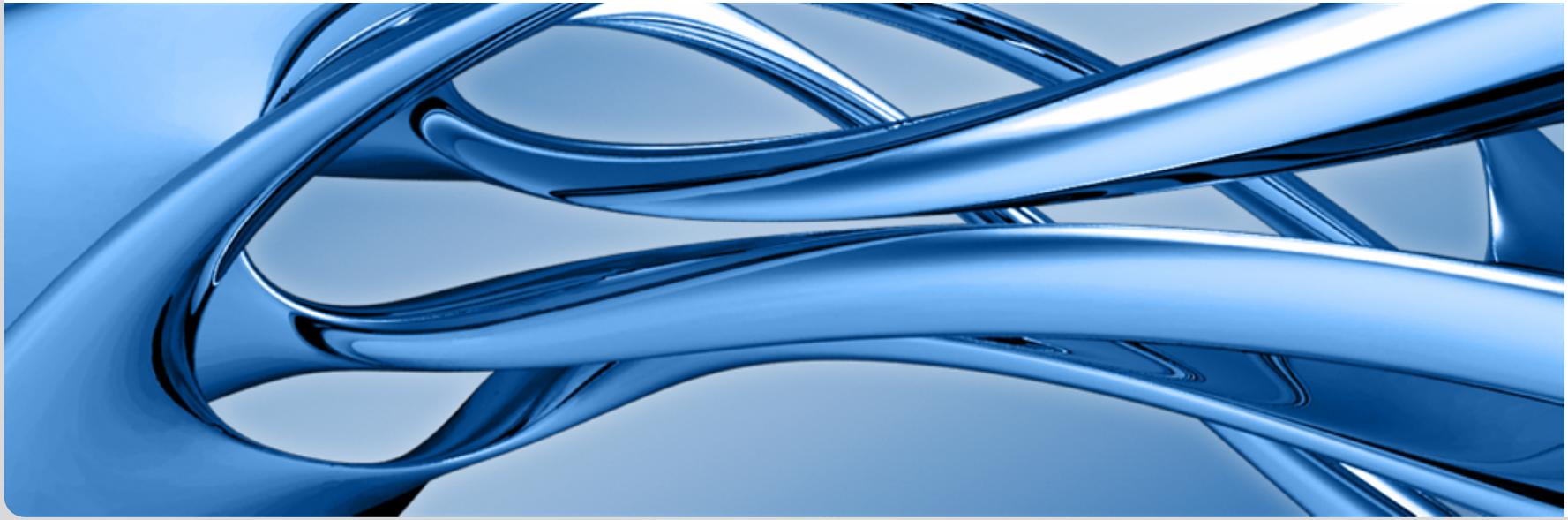
Karlsruhe Institute of Technology

PIRS: Python-based Framework for coupled MC-TH Reactor Calculations

SNA-MC 2013

Institute for Neutron Physics and Reactor Technology



KIT – University of the State of Baden-Wuerttemberg and
National Research Center of the Helmholtz Association

www.kit.edu

Content

- Introduction: what is PIRS, example
- PIRS concept
- Current development status
- Outlook

What is PIRS

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
- OS-independent
- Big community
- Lot of packages

Interaction with code

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

What for?

- Routine preparation of input files
- Framework for coupled calculations
- ...

Example: simplified neutronics model of fuel pin

Geometry:

```
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

Karlsruhe Institute of Technology

Neutronics:

```
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
```

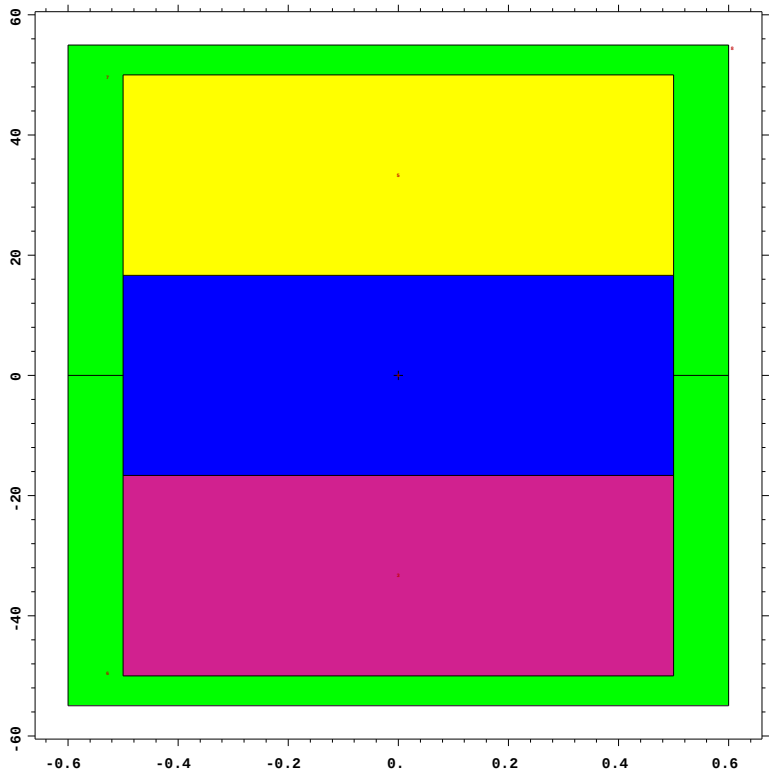
Example: simplified neutronics model of fuel pin

Karlsruhe Institute of Technology

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
```



Concept

Class types

- 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

Concept

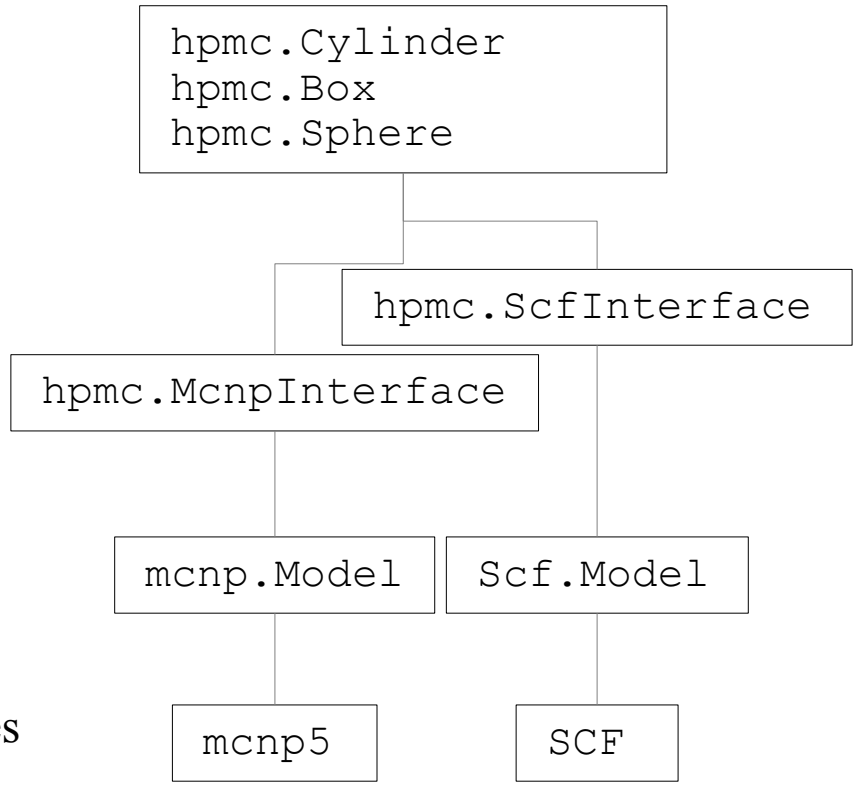
Interaction between classes

Classes to describe geometry:

High-level interfaces

Low-level interfaces

Computational codes



Geometry classes

model dimensions, axial meshes for system variables (temperature, density, heat)

High-level interfaces

code-specific data, e.g. path to xsdir, isotopic material compositions for MCNP

Current development status

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

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
- Reading of meshtal

Means to set up geometry

- Cylinder: vertical cylinder of finite height
- Box: rectangular parallelepiped with facets perpendicular to axes

Interface to SCF

- Only for PWR-like geometries
- Reading of output.txt

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

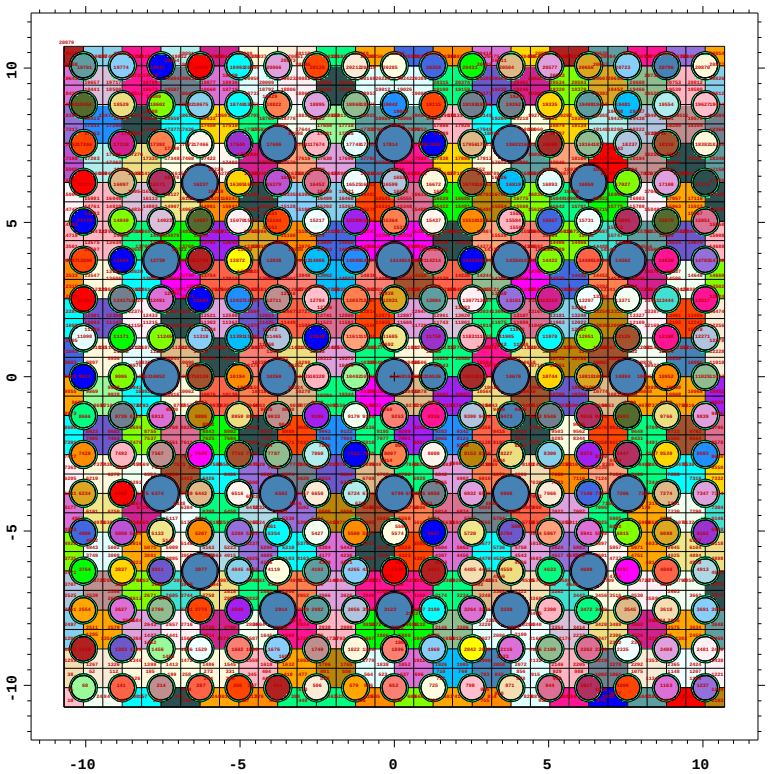
Example: results for coupled MCNP-SCF calculations

Karlsruhe Institute of Technology

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
```

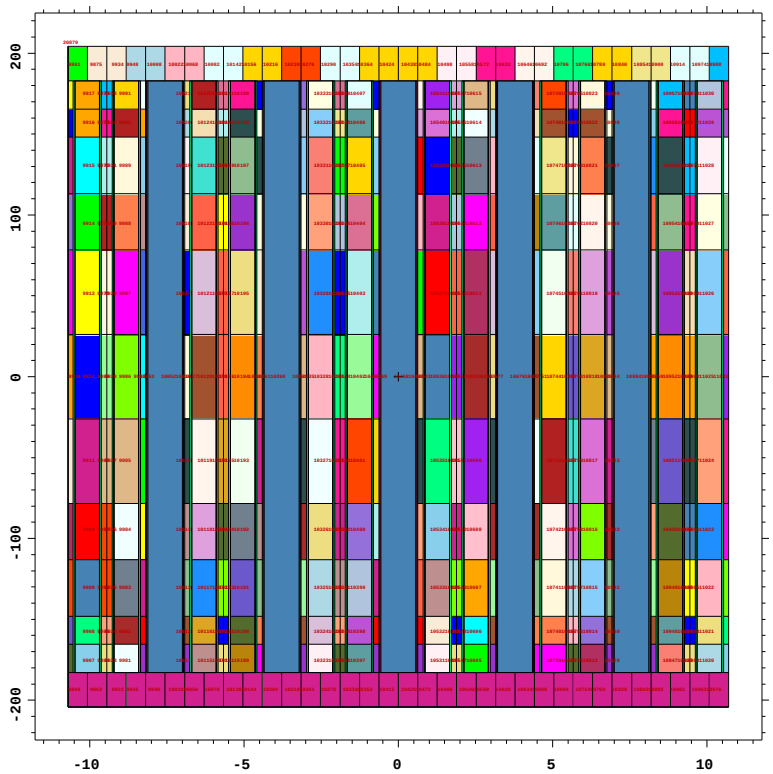


Example: results for coupled MCNP-SCF calculations

Vertical cross-section of MCNP model:

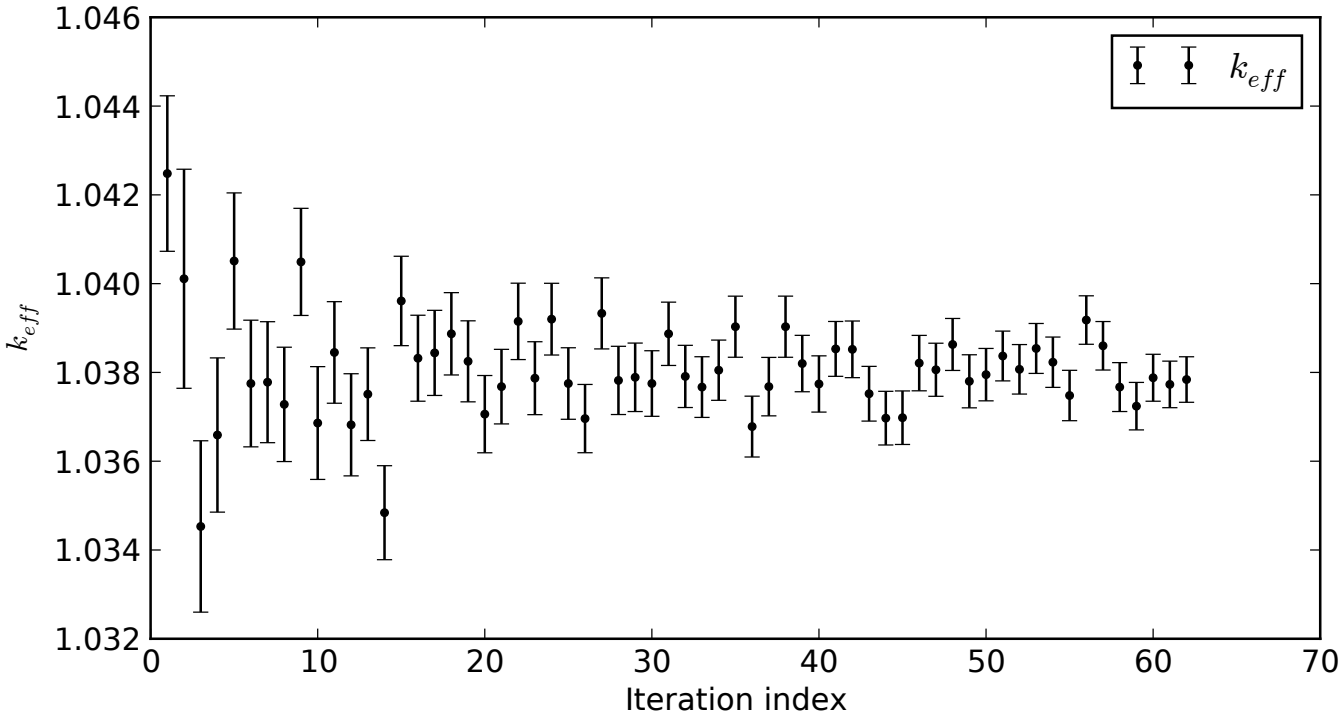
```
 09/10/13 17:32:58
c title


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
```



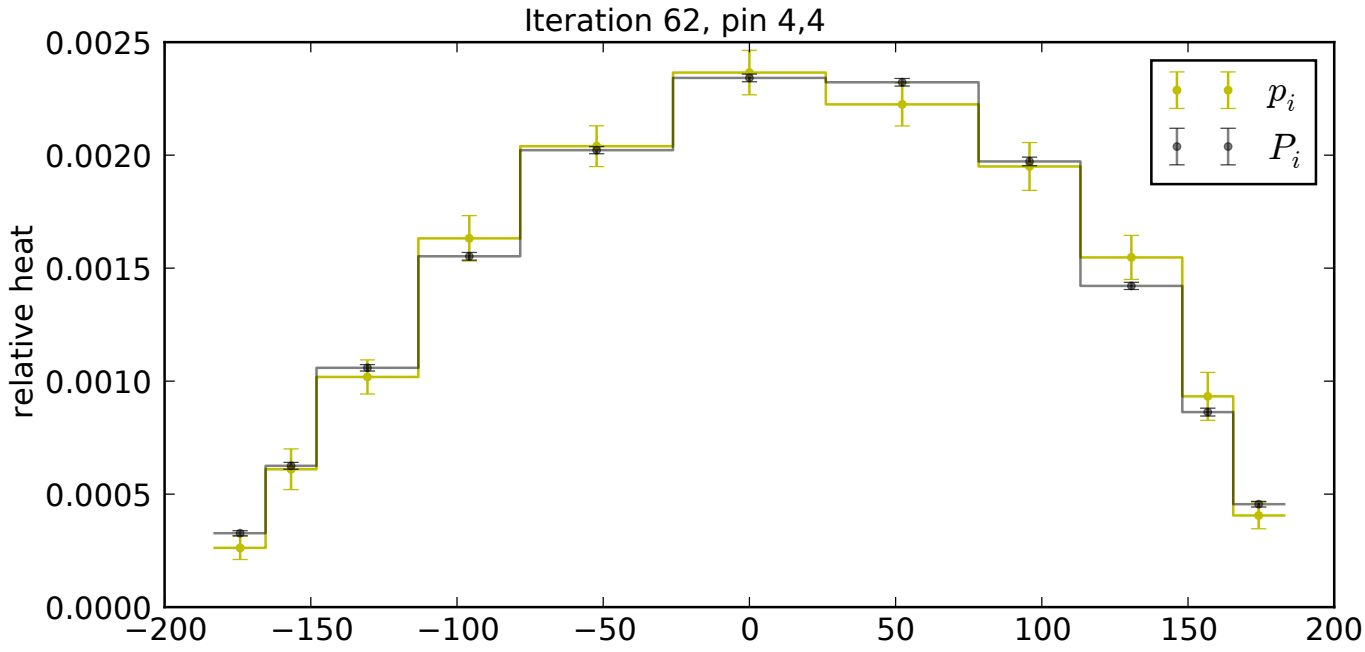
Example: results for coupled MCNP-SCF calculations

Behaviour of k_{eff} with N–TH iterations



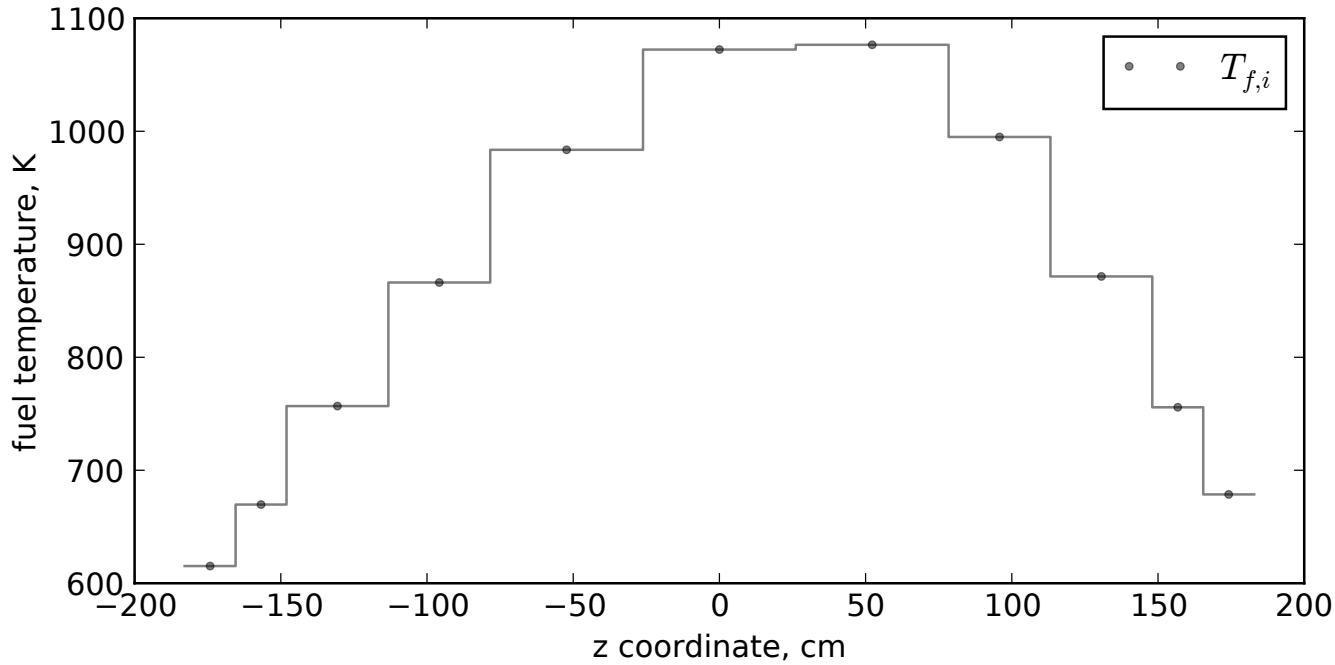
Example: results for coupled MCNP-SCF calculations

Axial distribution of heat deposition in one fuel pin



Example: results for coupled MCNP-SCF calculations

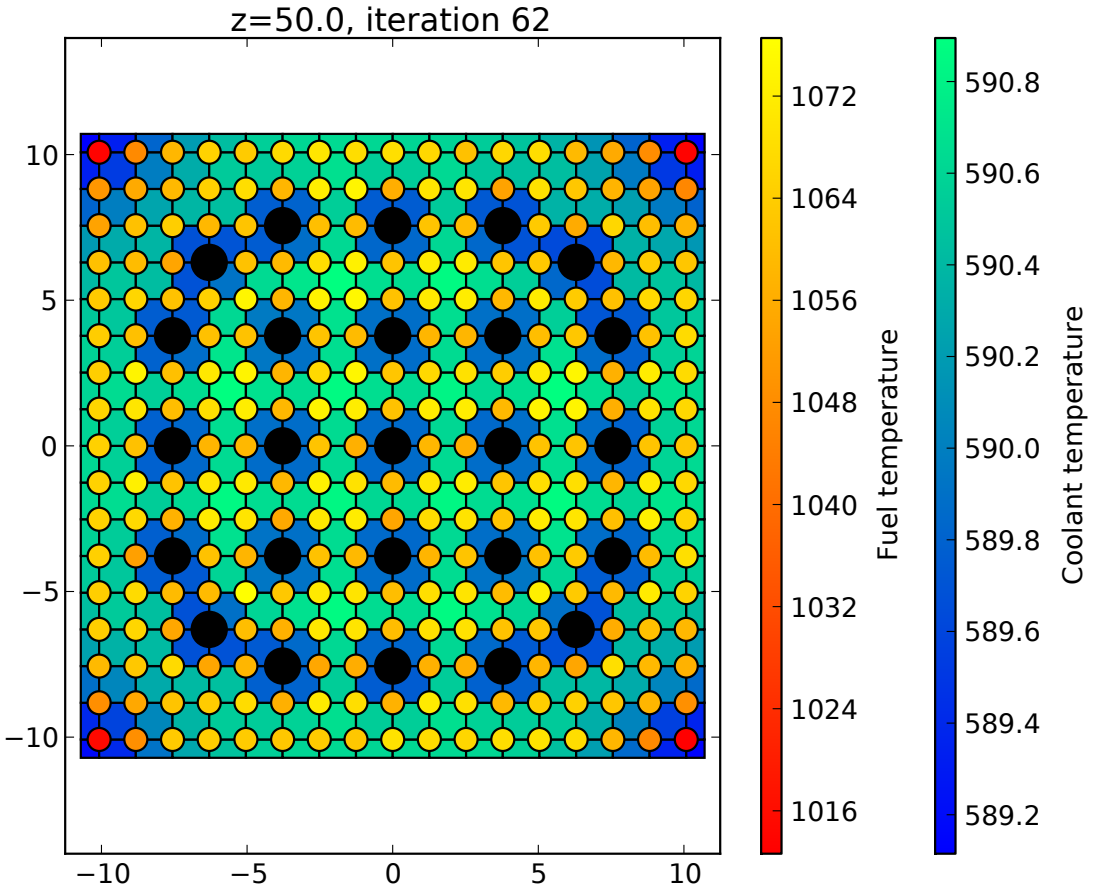
Axial distribution of fuel temperature in the same pin



Example: results for coupled MCNP-SCF calculations

Karlsruhe Institute of Technology

Temperature map



Ongoing work

Curent

- Interface to SERPENT-2
- Interaction with job submission system at Juelich Supercomputer
- Writing documentation
- Extension of SCF interface to represent cluster of assemblies, calculation of a minicore

Plans

- New interface to SCF
- Geometry plotter
- Interface to NMC, parts of KANEXT

Appendix

Relaxation scheme

Based on J.Dufek, W.Gudowski, "Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors", *Nucl. Sci. Eng.*, Vol. 152, 2006, pp. 274.

Declared quantities

The following quantities are declared:

- i - the index of an iteration step of the coupling scheme,
- s_i - number of neutron histories simulated by a Monte Carlo criticality code in ith iteration step,
- S_i - combined number of neutron histories simulated in all iteration steps $1, \ldots, i$,
- $\vec{\rho}^{(i)}$ - distribution of the coolant density computed according to relaxed power distribution $\vec{P}^{(i)}$ (see below),
- $\vec{p}^{(i)}$ - power distribution computed by the MC criticality code in ith step
- α - stepsize for the relaxation scheme,
- $\vec{P}^{(i)}$ - relaxed power distribution, computed in ith step,
- c_i - the number of active cycles (generations) simulated by the MC code at ith iteration step.

Description of the coupling scheme

Algorithm 1 Basic scheme for coupled NK-TH calculations

input: s_1, b, $\vec{\rho}^{(0)}$
$S_0 \leftarrow 0$
for $i \leftarrow 1, 2, \ldots$ **do**
  $s_i \leftarrow (s_1 + \sqrt{s_1^2 + 4 s_1 S_{i-1}})/2$
  $c_i \leftarrow integer(s_i/b)$
  $\vec{p}^{(i)} \leftarrow$ power distribution in a system with coolant density $\vec{\rho}^{(i-1)}$
    distribution based on MC crit. simulation with c_i active cycles
  $S_i \leftarrow S_{i-1} + s_i$
  $\alpha_i = s_i / S_i$
  $\vec{P}^{(i)} \leftarrow (1 - \alpha_i)\vec{P}^{(i-1)} + \alpha_i \vec{p}^{(i)}$
  remormalize $\vec{P}^{(i)}$ so that the system gives required power
  $\vec{\rho}^{(i)} \leftarrow$ calculation of the steady-state coolant density distribution
    based on power distribution $\vec{P}^{(i)}$
end for