

Philosophy, Principle, and Method for the CombLayer

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December 8, 2015

Icons

Icons are added to slide to indicate issues



Unexpected/Dangerous code



Legacy Code



Philosophy Driven decisions



Features of MCNP(X)

MCNP(X) is a geometry/physics/variance reduced discrete Monte-Carlo transport code.

Advantages

- World is described in complete volume format using infinite quadratic surfaces.
- Almost every default is best possible result without modification.
- MCNP(X) is tally based meaning that MCNP(X) does not calculate stuff you don't ask for.



Features of MCNP(X)

Consequences

- Complete volume description allows fast simulation but only with small cells [small ⇒ small number of surfaces]
- CVG implies that changing one cell requires the change of ALL cells that it exists directy within
- Cell-to-Cell (C2C) transport is dominated by surface crossing
- Tallys and variance reduction have to be incorperated in build

MCNP(X) is an unforgiving code

MCNP adds a huge number of things to help build geometry. **BUT** All of the following normally result in runtime penaty

- Complementary cells
- Universes require full computation of objects within
- Transform cards / Lattice cards
- Macrobodies
- Boolean invariances



MCNP(X) basics

MCNP(X) allows the definition of quadratic surface types To define a surface the input file has a line :

```
1 IDNumber typeID [values...]
```

Examples

```
2 57 px 3.4 A plane on the x=3.4 surface
3 1782 p 0.5 0.5 0 3.4 A plane on the x=y plane
4 983 c/x 1.2 3.4 7.0 A cylinder along x axis at y=1.2 and z=3.4 radius 7.0
```



MCNP(X) basics

```
MCNP(X) objects are constructed from a set of boolean operations on quadratic surface
Each object is ALSO numbered (!) and using signed surface numbers (to mean true/false).
Intersection (i.e. all have to be true for a point to be in the object) is denoted by a space
Union (i.e. only one has to be true for a point to be in the object) is denoted by a colon (:)
```



1 objectID MatID Density [surfaces]

MCNP(X) basics: Example of a cube

Making a simple cube of size 8cm in each direction :

Examples

```
8 11 px 4.0

9 12 px -4.0

10 13 py -4.0

11 14 py -4.0

12 15 pz -4.0

13 16 pz -4.0

14 Dz -4.0

15 Dz -4.0
```

These little MCNP units are the main sub-building block of CombLayer

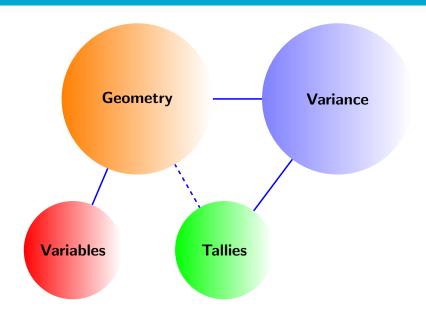


MCNP(X) basics: Placing the cube in a sphere

Placing that cube in a sphere of radius 45 cm. **Examples**

Note the boolean negation of the original cube in the sphere object.

CombLayer Introduction



What does CombLayer provide

- Variable system [fully Turing Complete]
- Boolean level object handler
- Higher level component system
- Variance reduction system
- Error detection

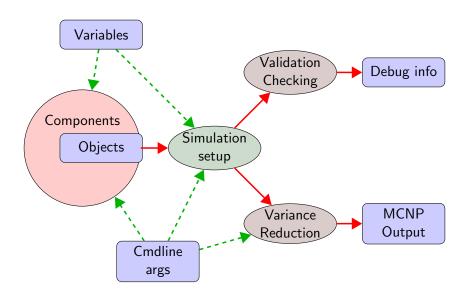


What is NOT in CombLayer

- No minimization routines for variables
- No tally data analysis
- No error correction immediate failure on problem



CombLayer Process



MCNP Layout

Object Section

Boolean Rules

index lists

Surface Section

Quadratic types

IDnum : type : values

Remainder Section

weights

IDnum: type: values

Materitals

IDnum: type: values modification lines

Physics

 $type: \ flagNumbers$

Source

type : values subtype : values

tallies

type : values



MCNP Layout

```
221 5 0.0582256 -244 245 ( -305 : 306 : 204 : 206 : ( -212 209 )
          223 : -220) -308 307 -215 -217 tmp=1.72346844e-09
25
  222 5 0.0582256 3 -245 ( -305 : 306 : 205 : 206 : ( -214 211 ) )
          : -222 ) -308 307 -216 -217 tmp=1.72346844e-09
27
28
  49 c/z 59.35095759 94.98138677 20
30 150 c/z 59.35095759 94.98138677 22
31 151 p 0.891006524 -0.4539905 0.0 9.26144319
32 152 p 0.891006524 -0.4539905 0.0 10.2614432
                                      -118.7019152 -189.9627735
33 142 gq 1 1 23.01803079 0 0 0
  0
          -4135.732457
34
```

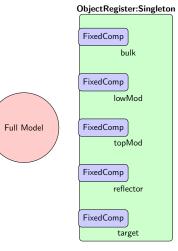
Arrh.....

CombLayer objective

- Consider the model as a whole set of mini-models
- Provide simple interaction between the models
- Avoid the need to use global identifier numbers
- Help out on the service level (variance/tallies)



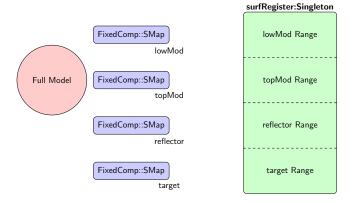
Geometry: Objects [After Construction]



- Each component is a seperate and independent
- Components know everything about themselves (materials / surfaces / position etc.) and nothing about anything else
- Components all stored in a singleton objectRegister.



Geometry: Surfaces [After Construction]



LOCAL surface map for each Component with global surface access.



Output Logging System

std::cout output is expected to be replaced with a managed stream:

ELog::EM

std::endl is replaced by of choice of

- ELog::endDiag
- ELog::endCrit
- ELog::endErr
- ELog::endTrace
- ELog::endBasic

Example:

```
for(size_t i=0;i<10;i++)
ELog:EM<<"test "<<i<" "<<sin(i*3.0)<<ELog::endDiag;</pre>
```



Output Logging System

Adding instance of ELog::RegMethod to all methods that

- throw exceptions
- write output
- 3 call methods that do 1 or 2.

RegMethod's main constructor that takes two strings. Typically I use that for the class name and the method name.



Example:

```
void BigCave::calculate()
{
    ELog::RegMethod RegA("BigCave","calculate");
    ELog::EM<<"Some info"<<ELog::endDiag;
    // ...
    ELog::EM<<"HARD break"<<ELog::endErr;
}</pre>
```

Output:

Some info HARD break

::main

makeEss::build CSpec::createAll

BigCave::calculate

Bunker::createMainWall

Bunker::createMainWall

Vec3D

Unsurprisingly CombLayer has a Vec3D class. However, it is unusual.

- Vec3D provides typical +,-,*,/ and [] operators
- Vec3D is a valid variable type
- It provides scalar interaction BUT ONLY forwards:

This is valid:

```
const Vec3D Out=Origin+X*7.9; // VALID
const Vec3D OutX=Origin+7.9*X; // ERROR
```



Vec3D

The normal methods stuff you would expect to see

- unit(): return a unit vector
- rebase(const Vec3D& A,const Vec3D& B, const Vec3D& C): express vector in basis set A,B,C
- Distance(const Vec3D& A) : distance to vector
- dotProd(const Vec3D& A) : dot produect



Quaternions

Working with vectors involves rotation: to avoid gimbal-lock quaternion rotation is prefered over Matrix/Eurler rotation.

Rotational Quaternions can be created/used directly as :

```
Geometry::Vec3D axis(1,0,0);

// apply rotation about Z axis:
const Geometry::Quaternion Qz=
Geometry::Quaternion::calcQRotDeg(rotAngle,Z);

Qz.rotate(axis);
```

Quaternions (cont)

Most of the time – FixedComp will deal with it for you because you will be rotating a whole object

```
FixedComp::applyShift(xStep,yStep,zStep);
FixedComp::applyAngleRotate(xyAngle,zAngle);
```

Object Component

Object component is a single class that provides a mechanism to produce surfaces and single material cells based on the values of variables.

Examples:

- Moderator
- Jaws
- Sample
- Detector

Composite Component

Composite component is a single class holds a collection of Object components making a more complex object but for some instances wishes to be treated as a single object Examples:

- Target
- Bunker
- Cave
- Chopper system

Basic geometry object

A basic geometry object normally has 2-3 of the public inheritances from the namespace **attachSupport** 1 We are going to cover:

- FixedComp / FixedGroup Mandatory ²
- ContainedComp / ContainedGroup ²
- LayerComp
- CellMap
- SurfMap



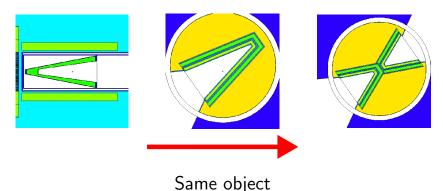
¹Files in System/attachSupportInc

² This class should not be virtually inherited.

CombLayer Component Construction

Models are made of components:

- Local parameters e.g. number of layers
- Containers that allow insertion
- Link points that allow joining



FixedComp

Most geometry components inherrit from FixedComp **It Provides**:

- A unique name [keyName]
- Origin for the object
- X,Y,Z basis for object
- A local name-register for surfaces
- Stores/Accesses link points for the object







Construction of a FixedComp is done as follows:

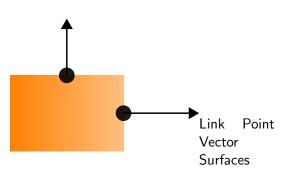
```
class MyBox : public attachSystem::FixedComp
37
     const int boxIndex:
                                  ///< Index of surface offset
38
                                  ///< Cell index
     int cellIndex;
39
40
41
    public:
42
      MyBox(const std::string&);
43
  };
44
45
  MyBox::MyBox(const std::string& Key) :
47
    attachSystem::FixedComp(Key,0),
    boxIndex(ModelSupport::objectRegister::Instance().cell(Key)),
48
    cellIndex(boxIndex+1)
49
50 {}
```



Typical FixedComp object looks like:

```
2
  class MyBox : public attachSystem :: FixedComp ,
    public attachSystem :: ContainedComp
5
6
   private:
7
    const int boxIndex; ///< Index of surface offset</pre>
8
    int cellIndex;
                                ///< Cell index
9
10
    void createUnitVector(const attachSystem::FixedComp&,
11
                            const long int);
12
13
    void createSurfaces();
14
15
    void createLinks():
    void createObjects(Simulation &);
16
17
   public :
18
19
     void createAll (Simulation&,
20
21
         const attachSystem::FixedComp&,
         const long int);
22
```

LinkComp



- Objects are constructed with links
- Other objects are realised relative to these linkages
- The outer Link Surfaces are designated the boundary
- Boundaries are check after construction to allow displacement construction



Definition of a link-point

- A point int space (Geometry::Vec3D)
- An axis direction in space (Geometry::Vec3D)
- A surface(s) rule
- An extra common surface if required



Adding/Defining Link-Points

- The number of expected link-points is defined in the constructor
- Numbers 0-9 are designated outgoing convention.
- Numbers 10-19 are designated in-going convention.

```
25
  class MyBox : public attachSystem :: FixedComp
27
   private:
29
    // this is in most FixedComp derived classes
30
    void creatLinks();
31
32
  };
33
    MyBox::MyBox(const std::string& Key ) :
34
      attachSystem::FixedComp(Key, \tcr{{\bf 6}}),
35
      boxIndex(ModelSupport::objectR egister::Instance().cell(Key)),
36
     cellIndex(boxIndex+1)
37
38 {}
```

Typicial usage - a box with 6 sides (hence 6 link points)



Adding/Defining Link-Points

Typically I add link points in linkCreate. Not always !!

```
39
40 void
41 MyBox::createLinks()
42 {
43    FixedComp::setConnect(0,Origin+Y*(width/2.0),Y);
44    FixedComp::setLinkSurf(0,-SMap.realSurf(boxIndex+1));
45 }
```

- setConnect :: Defines a point and a direction (Y).
- setLinkSurf :: defines the surface LEAVING the box
- A real surface is required



How to use link-Points [for Geometry]

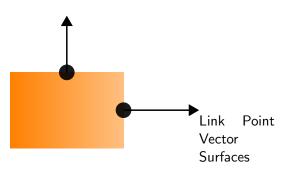
The commonest method is simple orientational construction:

```
46
  void
  MyBox::createUnitVector(const attachSystem::FixedComp& FC,
                            const long int sideIndex)
49
50
  {
    FixedComp::createUnitVector(FC, sideIndex);
51
52
    FixedComp::applyShift(xStep,yStep,zStep);
    FixedComp::applyAngleRotate(xyAngle,zAngle);
53
    return:
54
55
```

Creates a Vec3D Origin to be at link-Point [sideIndex]



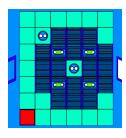
CombLayer Object Construction



- Objects are constructed with links
- Other objects are realised relative to these linkages
- The outer Link Surfaces are designated the boundary
- Boundaries are check after construction to allow displacement construction



CombLayer Component Construction





- Simple connection grid joining at common side surfaces
- Track boundary e.g. for pipe work



ContainedComp

 $\label{lem:many geometry components inherrit from $$\operatorname{ContainedComp}/\operatorname{ContainedGroup}$$$

It Provides:

- A description of the outer boundary
- A description of the inner boundary [optional]
- An approximation to the boundary assuming this is the complete object



ContainedComp

Useage:

- Inherrit into class
- Either register before/after which other objects this object is in
- Define an outerSurface using the command

```
class MyBox : public attachSystem::ContainedComp
     public attachSystem::FixedComp
3
    void createObjects(Simulation&);
6
  };
  void MyBox::createObjects(Simuation& System)
9
  ł
10
    std::string Out;
    // ...
    Out = ModelSupport :: getComposite (SMap, bnkIndex,
12
           " 1 -17 4 -14 5 -6 "):
13
    System.addCell(cellIndex++,matID,0.0,Out);
14
15 }
```





Models are constructed into a data-class called Simulation.

- Simulation is a base clase for the output type required [PHITS/MCNP etc]
- In principle you can have two but... don't
- Joins Physics Geometry Tallies
- Works on a *push-to / pull-from* model

Note: In 99% of the code, I have used this:

```
void MyBox::someFunction(Simulation& System)
```





Example use [Adding a cell]:

```
System.addCell(cellIndex++,matID,300.0," 2 -3 -4 5 6 ");
```

This adds a cell [id number cellIndex] with material type matID and temperature 300K, using the MCNP surface logical format string.





Example use [find cell

```
// Find a cell containing a point:

MonteCarlo::Object* OCell=

System.findCell(Geometry::Vec3D(4,5,6),0);
```





You also used it to do things with everything in the model:

```
15
16 // Global surface replacement:
17 // BE VERY CAREFUL DOING THIS::
18 System.subsituteAllSurface(1082,283);
```

Starting a project

- Copy Main/pipe.cxx to Main/newProject.cxx
- 2 create a directories in Model/projectBuild and Model/projectBuildInc
- Edit CMake.pl
 - Add newProject to masterprog
 - Copy the line**\$gM**-¿addDepUnit("pipe", ...
 - Change pipeBuild to projectBuild



Starting a project (part2)

- Copy Model/pipe/*.cxx to Model/project/
- Copy Model/pipelnc/*.h to Model/projectInc/
- 3 Change each item of pipe to project



Starting a project (part 3)

Consider the Main:

