

# Integrated flux calculations. Comparison of McStas and MCNP

G. Apostolopoulos

October 30, 2007

## 1 Test case calculation

A square shaped monitor of area  $d \times d$  is positioned at a distance  $D$  away from a planar surface source, parallel to the monitor plane and having the same area  $d \times d$ . The total number of particles hitting the detector is to be calculated.

## 2 Analytic calculation

The number of particles  $dN$  hitting the elemental area  $d\sigma_d$  on the monitor surface is

$$dN = I_0 \frac{\cos^2 \theta}{r^2} d\sigma_s d\sigma_d \quad (1)$$

where  $d\sigma_s$  is a surface element on the source area,  $r$  is the vector from  $d\sigma_s$  to  $d\sigma_d$ ,  $\theta$  is the angle between  $r$  and the plane of the monitor/source and  $I_0$  is the constant source brightness in particles per unit area per unit solid angle.

The  $\cos^2 \theta$  term is due to the projection of  $d\sigma_s$  and  $d\sigma_d$  on a plane perpendicular to  $r$ . Some people may argue that only a single  $\cos \theta$  term is proper, so I continue with writing a general  $\cos^n \theta$ .

The total number of particles is found by integrating the above relation. Assuming that monitor and source are parallel to the  $xy$ -plane then

$$r^2 = (x_s - x_d)^2 + (y_s - y_d)^2 + D^2,$$
$$\cos \theta = \frac{D}{r}$$

and

$$N(D) = I_0 D^n \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \frac{dx_s dy_s dx_d dy_d}{[(x_s - x_d)^2 + (y_s - y_d)^2 + D^2]^{1+n/2}}.$$

If  $D \gg d$ , then  $r \approx D$  and the above integral gives just

$$N_\infty \approx I_0 \frac{d^4}{D^2} = I_0 \frac{S_d S_s}{D^2}$$

i.e., the source brightness times the source area times the monitor area times the inverse square of the distance. In this limit the surface source behaves as a point source with intensity  $I_0 \times S_s$  as expected.

In the following we calculate the dimensionless ratio  $R$ :

$$R = \frac{N(D)}{N_\infty} = \frac{D^{2+n}}{d^4} \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \int_{-d/2}^{d/2} \frac{dx_s dy_s dx_d dy_d}{[(x_s - x_d)^2 + (y_s - y_d)^2 + D^2]^{1+n/2}}$$

by three methods:

1. Numerical integration with the aid of Mathematica
2. With McStas
3. With MCNP

### 3 Numerical Integration

The integration is performed in Mathematica in a single command

```
NIntegrate[
  NIntegrate[
    NIntegrate[
      NIntegrate[
        1/((xd - xs)^2 + (yd - ys)^2 + 1)^(1 + n/2),
        {xs, -d/2, d/2}],
      {ys, -d/2, d/2}],
    {yd, -d/2, d/2}],
  {xd, -d/2, d/2}]
```

Note that the  $n = 2$  case can be also done analytically (`NIntegrate` replaced by `Integrate`). In this case it was checked that numerical and analytical integration yield the same results.

### 4 McStas

The following simple instrument definition was used

```
DEFINE INSTRUMENT SourceTest(d,D)

TRACE

COMPONENT Origin = Progress_bar()
  AT (0,0,0) ABSOLUTE

COMPONENT src = Source_simple(
  height = d, width = d, dist = D, xw = d, yh = d, E0 = 25,
  dE = 0)
  AT (0, 0, 0) RELATIVE Origin

COMPONENT mon = Monitor(
  xwidth = d, yheight = d)
  AT (0, 0, D) RELATIVE Origin

END
```

where the “Source\_gen” component was also tested in place of “Source\_simple”.

The output of the Monitor is divided by  $d^4/D^2$  to give the required ratio  $R$ .

## 5 MCNP

The listing of the MCNP input file is

```
Test case
c cells
1 0 1 -2 3 -4 5 -6 imp:n=1
2 0 -1: 2: -3: 4: -5: 6 imp:n=0
c surfaces
1 pz 0
2 pz D
3 px 0
4 px d
5 py 0
6 py d
c source definition
sdef sur=1 z=0 x=d1 y=d2 vec=0 0 1
si1 0 d
sp1 0 1
si2 0 d
sp2 0 1
c tally f1 : particles crossing a surface
f1:n 2
c number of particles histories
nps 1000000
```

where  $D, d$  have to be replaced by the actual values.

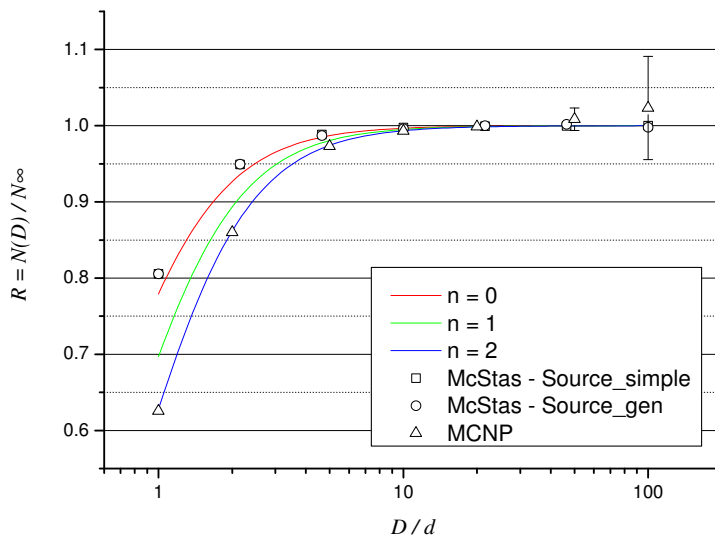
Note that due to the different normalization of MCNP (results are always per source particle), the output of tally f1 has to be multiplied by the total number of particles emitted by the source,  $N_{tot}$ , and then divided by  $d^4/D^2$  to get the same quantity  $R$ .

The value of  $N_{tot}$  may be found by integrating the source probability density of the MCNP planar surface source (as found in the MCNP manual)

$$N_{tot} = \int_S d\sigma_s \int_0^{2\pi} d\phi \int_0^1 2\mu d\mu = \pi d^2$$

where  $\mu = \cos \theta$  in MCNP terminology.

## 6 Results



The results are summarized in the above figure. Solid lines are the numerical integration results for different values of  $n = 0, 1, 2$ . Monte-Carlo data correspond to runs with 1000000 particles and  $d = 1$  cm. Note that MCNP data have greater variance due to the absence direction biasing. The McStas error bars are smaller than the data symbols.

Comments:

- The MCNP results follow the  $n = 2$  curve, i.e. comply with the  $\cos^2 \theta$  term of eq. (1). This is expected since MCNP includes a  $\cos \theta$  weight term in its planar source definition by default. The second  $\cos \theta$  term comes out naturally by the projection of the detector area.
- In McStas the integrated flux is correctly calculated in the far field ( $D \gg d$ ) but in the near field it follows the  $n = 0$  curve, i.e., the  $\cos \theta$  term in eq. (1) seems to be completely ignored. In general this should not be an issue as long as the beam path from source to target component is large compared to source/target dimensions. This is in most cases true in neutron scattering instruments. However, there may be cases where the effect is significant. The discrepancy has to be traced back to the direction focusing routines of the McStas kernel.