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| *Title:* | Doppler Energy Broadening for Incoherent Scattering in MCNP5, Part II |
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| *Submitted to:* | |

# Los Alamos
NATIONAL LABORATORY

# Photon Doppler Energy Broadening for Incoherent Scattering in MCNP5, Part II

## ABSTRACT

The purpose of this research note is to provide details of the modular inclusion of photon Doppler energy broadening from MCNP4C3 into MCNP5. This research note describes the algorithm and data used, defines the interfaces and resources required, and performs software and data quality checks for the new MCNP5 physics feature. This document, coupled with LA-UR-04-0487, summarizes internal MCNP-team documentation and serves as the Eolus software requirements specification and design description. This feature is issue **26** in the Razor database.

# Introduction

A previous X-5 research note (LA-UR-04-0487) reviews the equations and methods for simulating an incoherently scattered photon assuming a bound electron in an orbital shell. The previous work describes the current capabilities of MCNP4C3 and provides the academic background necessary to include Doppler energy broadening to MCNP5. This research note provides the details of the integration of photon Doppler energy broadening from MCNP4C3 to MCNP5, including the algorithm, user interfaces, warning messages, and software and data quality checks. This document serves as the Eolus software requirements specification and design description and is tracked as issue 26 in the Razor database.

# Requirements and Design

## Requirements

The specific requirements to include photon Doppler energy broadening in MCNP5 as a new physics feature are:

1. Create a new set of subroutines containing the required Doppler energy broadening physics to be included as a new module;

2. Incorporate the new Hartree-Fock Compton profile data (Biggs, 1975) for orbital and total atom data for $1 \leq Z \leq 94$;

3. Create a new user interface to neglect photon Doppler energy broadening. Following the Los Alamos tradition of always including the best physics, this feature is to be included by default;

4. Create a new warning if this feature is turned off in any **mode p** problem;

5. Create a new warning if the user-requested data library does not contain Compton profile data.

The new photon data library is to be included with the distribution of this code and the feature is on by default. This new physics feature should be transparent to the MCNP5 user. The user can turn this feature off to allow tracking of previous MCNP versions. This feature must work on all supported computer platforms, compilers and work in both multi-processing and multi-threaded modes.

The capability to plot the Compton profile data using the MCNP5 plotter, mcplot, is a feature for future development.

# Design

## The Algorithm

An algorithm for sampling the scattered energy of a Doppler broadened incoherent (Compton) scatter from an atom has been suggested by Namito et al (1994). This algorithm has been adopted as part of a low-energy extention to the EGSnrc code but differs significantly from the actual coding. The algorithm looks like:

1. Sample $\theta$ from:

$$\frac{d\sigma_{inc}}{d\Omega}(\theta, \phi) \quad = \quad \frac{d\sigma_{KN}}{d\Omega}(\theta, \phi)S(x, Z)$$

where S(x,Z) is the incoherent scattering factor from Hubbell, et al. MCNP4C3 already does this.

2. Pick an electron sub shell $k$ based on the number of electrons per sub-shell. This is done by creating PDF and CDF based on the number of electrons per shell. Randomly select a value from the CDF and find the corresponding electron sub shell corresponding to the selected CDF.

3. Sample the electron momentum, $\frac{p_z}{mc\alpha}$, from 0 to 100 using the Compton profile data for the selected sub-shell. A value of $p_z$ is sampled by:

   (a) First creating a probability distribution function (PDF) from the Compton profile data. Next, create a cumulative probability distribution (CDF) from the previous PDF. Usually, the PDF and CDF have already been created from the original data and are previously stored in the data tables.

   (b) Randomly select a value of the CDF (eg. x=$\xi$ (CDF)).

   (c) Interpolate the corresponding $p_z$ value to the randomly selected CDF value

4. With the sampled value of $p_z$, calculate the scattered photon energy, E', by solving Eqn. 36 for E'.

5. Reject selected momentum if $p_z > p_{z_{max}}$ for the selected sub-shell. The value of $p_{z_{max}}$ is calculated using Eqn. 36 with E'=E-E$_b$. Accept scattered photon energy or go to step 2.

6. If photon linear polarization is not considered (as with MCNP), sample the azmuthal angle, $\phi$, randomly on $[0, 2\pi]$.

The algorithm can be modularized to easily be included in the newest version of MCNP4C3. The algorithm would be inserted as a subroutine call into the main photon transport subroutine **colidp**. The **call** to the Doppler broadening subroutine would occur just after accepting the calculated photon's scattering angle. Including the **call** statement at this location ensures that the Doppler simulation is only included with the detailed physics treatment and will be skipped when using the simple physics option.

## The Data

The algorithm requires the following collection of atomic data for a 1≤Z≤94:

1. number of electrons per shells,

2. binding energy per shell,

3. probability of interacting per shell

4. precollision momentum per shell

5. shell-wise Compton profile data in PDF and CDF form

The additional data must be stored in the appropriate photon data table blocks of array XSS. The structure of these arrays are defined in Appendix F of the MCNP4C3 manual. New additions to these arrays are discussed below.

### New Data Arrays

There are three arrays associated with each data table. The XSS array contains all of the data. The NXS array contains various counters and flags. The NXS array for photons contains parameters like:

1. length of blocks of data,

2. Z,

3. (NES) number of energy entries,

4. (NFLO) length of fluorescence data.

The inclusion of this new data requires a fifth entry to NXS, (**NSH**)the number of electron shells. The number of electron shells for a given element can be referenced as NXS(5,iex).

The JXS array contains pointers in XSS. The JXS array nominally contains five parameters:

1. (ESZG) the location of the energy table,

2. (JINC) the location of the incoherent form factors,

3. (JCOH) the location of the coherent form factors,

4. (JFLO) the location of fluorescence data,

5. and (LHNM) the location of heating numbers.

The inclusion of the new Compton profile data requires five additional entries to JXS:

1. (**LNEPS**), the location of the number of electrons per shell,

2. (**LBEPS**), the location of the binding energy per shell,

3. (**LPIPS**), the location of the probability of interaction per shell,

4. (**LSWD**), the location of the array of offsets to the shell-wise data, and

5. (**SWD**), the location of the the shell-wise data in PDF and CDF form.

   This new data can be simply appended to the end of *mcplib02*, creating a new data library. This extention of *mcplib02* is considered a *beta* version. These new entries are summarized again in a section of this research note titled **MCNP4C3 Manual Revisions**.
   The *beta* release photoatomic data library, **plib03**, is required to simulate photon Doppler energy broadening. This photoatomic data library contains the library **mcplib02** with the Compton profile data simply appended to the end of the file using the format described above. The **xsdir** file must also be updated to include **plib03**. These files are included in the Razor database. The user must include the **plib03** data library by specifying the material ZAID as: ZZZAAA.12p

## User Interface

   Usage of this new physics feature would be controlled by the fifth entry of the **phys:p** card. A non-zero entry deactivates this feature. The photon Doppler energy broadening would be used automatically if MCNP5's detailed physics option was used. Following the Los Alamos tradition of providing the best physics by default, this new feature is automatically on. Subroutine **nextit** was modified to allow this new entry.

## New Warning Messages

   Two new warning messages were included to notify the user if the photoatomic library does not contain the Compton profile data, and if photon Doppler energy broadening was turned off. Doppler broadening is always on following the Los Alamos tradition of including the best physics by default. The two new warning messages look like:

```
warning.   <datalibrary> lacks Compton profile data.

warning.   photon Doppler energy broadening may be needed (phys:p).
```

where *datalibrary* is the photoatomic data library specified by the user. These additional warning messages were added to subroutines **getxst** and **chekit**. Both messages are printed to the screen and to the output file.

# Modified/New MCNP Subroutines

1. Subroutine fixcom:

   ```
   integer :: nodop      != Flag to inhibit Doppler photon scattering.
   ```

2. Subroutine colidp:

   ```
   ...after accepting scattering angle...

       if( nodop==0 .and. jxs(6,iex)/=0 ) then
         call dopplerp(erg,cs,enes)
         t4  = enes/gpt(3)
       endif
   ```

3. Subroutine nextit

   ```
   case( 54 )
     ! >>>>>  physics parameters                          phys
   ...
      elseif( nqp(2)/=0 ) then
        if(nwc==1)emcf(2)=max(ritm,zero+.001)
        if(nwc==3 .and. iitm/=0)nocoh=1
        if(nwc==5 .and. iitm/=0)nodop=1
   ```

4. Subroutine getxst

   ```
   case( 5 )
     ! >>>>>  Photon table.
     ! Print information about the table.
   ...
      if(jxs(6,iex) == 0.and.nodop == 0)call erprnt(1,2,0,0,0,0,0,0,&
        & '38h'//ht//' lacks Compton profile data.')
   ```

5. Subroutine chekit

   ```
   case( 54 )
   ! >>>>>  physics parameters                          phys
   ...
   if( nqp(2)/=0 ) then
     if(nwc==1 .and. ritm<.001)call erprnt(2,2,0,0,0,0,0,0,&
       & ' "photon emcf will be set to .001 mev."')
     if(nwc==4 .and. ritm/=0. .and. kpt(2)==0)call erprnt(2,2,0,0,0,&
       & 0,0,0,' "photonuclear turned off. photons not on mode card."')
     if(nwc==5 .and. iitm/=0) call erprnt(2,2,0,0,0,0,0,0,&
       & ' "photon Doppler energy broadening may be needed (phys:p)."')
   endif
   ```

6. Subroutine dopplerp

   ```
   subroutine dopplerp(ene,amu,esc)

      ! ---------------------------------------------------------------
      !
      !    PURPOSE
   ```

```
!    -------
!        This subroutine calculates Doppler-broadened energy of a
!        scattered photon when incident energy and
!        amu=cos(theta) are given.
!
!    ON ENTRY
!    --------
!        ENE          - photon energy (MeV).
!        AMU          - cos(theta), theta = scattering angle
!
!    ON RETURN
!    ---------
!        ESC          - energy of scattered photon (MeV).
!
! --------------------------------------------------------------
use cm_mod
use mcnp_random, only : rang

implicit real(dknd) (a-h,o-z)

real(dknd), parameter :: asc1 = 1.956934142    !1/rest mass electron
real(dknd), parameter :: asc2 = 137.03605      !fine struct. const.
!--------------------------------------------------------------

! Select index of element
nsh = nxs(5,iex)
do
  ! sample electron subshell to interact with
  rn = rang()

  ! binary search of cdf form of probablility per shell
  if(nsh>1) then
    lp = jxs(8,iex)
    jl = lp
    ju = lp+nsh
    do
      if( ju-jl<=1 ) exit
      jm = (ju+jl)/2
      if( rn<xss(jm) ) then
        ju = jm
      else
        jl = jm
      endif
    enddo
    ishell = jl-lp+1
  endif

  ! binding energy for selected shell
  be = xss(jxs(7,iex)+ishell-1)
  esgmax = ene-be
  if( esgmax<=0. ) cycle

  ! Sample electron momentum pz from Compton profile cdf...
  ! binary search of Compton profile cdf
```

```
      rn = rang()
      lp = jxs(10,iex)+nint(xss(jxs(9,iex)+ishell-1))
      ne = nint(xss(lp))              !ne = number of momentum entries
      jl = lp+1+2*ne
      ju = lp+1+3*ne
      do
        if( ju-jl<=1 )  exit
        jm = (ju+jl)/2
        if( rn<xss(jm) ) then
          ju = jm
        else
          jl = jm
        endif
      enddo
      cdf = xss(jl)
      pdf = xss(jl-ne)    !(lp+1+ne) + (jl-(lp+1+2ne))
      p1  = xss(jl-2*ne)  !(lp+1) +  (jl-(lp+1+2ne))
      ! histogram interpolation scheme
      pzrn =  p1 + (rn-cdf) /pdf

      ! Calculate ESC from sampled pzrn
      xa=(pzrn/asc2)**2-1.-((ene*(1.-amu)*asc1)**2)-2.*ene*(1.-amu)*asc1
      xb=2*ene+2*(ene**2)*(1.-amu)*asc1-2.*(pzrn/asc2)**2*ene*amu
      xc=((pzrn*ene/asc2)**2)-ene**2
      xrad=xb**2-4.*xa*xc
      if( xrad<0. ) cycle
      rn = rang()
      if( rn<0.5 ) then
        esc = (-xb+sqrt(xrad))/2/xa
      else
        esc = (-xb-sqrt(xrad))/2/xa
      end if
      if( esc>esgmax .or. esc<0. ) cycle
      rn = rang()
      if( esc>=esgmax*rn ) exit
    enddo
    return
  end subroutine dopplerp
```

# MCNP4C3 Manual Revisions

## Chapter 2

- Page 2-8, last paragraph beginning with "COLIDP for photons..." needs to modify the statements:

  OLD: *The simple physics treatment...and includes form factors for electron binding effects, coherent...*

  NEW: *The simple physic treatment...and includes form factors and Compton profiles for electron binding effects, coherent...*

  OLD: *COLIDP samples for the collision nuclide..., incoherent (Compton) scatter (with form factors in the detailed physics treatment to account for electron binding)...*

  NEW: *COLIDP samples for the collision nuclide..., incoherent (Compton) scatter (with Compton profiles and incoherent scattering factors in the detailed physics treatment to account for electron binding)...*

- Page 2-21, paragraph beginning with "Photon interaction cross sections..." needs to modify the statement:

  OLD: *There are two photon interaction data libraries: nn=01 and nn=02*

  NEW: *There are three photon interaction data libraries: nn=01, nn=02, and nn=12*

- A new paragraph needs to be inserted after the paragraph on page 2-22, beginning with "The ZAID=ZZZ000.02P library...".

  *The ZAID=ZZZ000.12P library is also a superset of ZAID=ZZZ000.02P with the inclusion of Hartree-Fock Compton profiles. The Hartree-Fock Compton profiles are used to account for the effects of a bound electron on the energy distribution of the scattered photon. These Compton profiles are a collection of orbital and total atom data tabulated as a function of the projected precollision momentum of the electon. Values of the Compton profiles for the elements are published in tabular form by Biggs, et al (REFERENCE XXX) as a function of $p_z$.*

  The REFERENCE XXX is:

  Biggs, F., Mendelsohn, L.B., and Mann, J.B., 'Hartree-Fock Compton Profiles for the Elements,' Atomic Data and Nuclear Data Tables, Vol. 16, No. 3, pg. 201-309 (1975).

- Page 2-56, the paragraph beginning with "The detailed physics treatment..." needs to be corrected to:

  OLD: *Form factors are used to account for electron binding effects.*

  NEW: *Form factors and Compton profiles are used to account for electron binding effects.*

- Page 2-56, the paragraph beginning with "The simple physics treatment..." needs to be corrected to:

  OLD: *...regarded to be on free electrons (without use of form factors)...*

  NEW: *...regarded to be on free electrons (without use of form factors or Compton profiles)...*

- A new set of paragraphs needs to be inserted after the paragraph on page 2-60, at the top of the page, after the equation.

  *The new energy, E', of the photon accounts for the effects of a bound electron. The electron binding effect on the scattered photon's energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. This effect on the energy distribution of the incoherently scattered photon is called Doppler broadening.*

  *The Hartree-Fock Compton profiles, J($p_z$), are used to account for the effects of a bound electron on the energy distribution of the scattered photon. These Compton profiles are a collection of orbital and total atom data tabulated as a function of the projected precollision momentum of the electon. Values of the Compton profiles for the elements are published in tabular form by Biggs, et al (REFERENCE XXX) as a function of $p_z$.*

  *The scattered energy of a Doppler broadened photon can be calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and calculating the scattered photon energy, E', from:*

  $$p_z = -137 \frac{E - E' - EE'(1 - \cos(\theta))/mc^2}{\sqrt{E^2 + E'^2 - 2EE' \cos(\theta)}}$$

  *The Compton profiles are related to the incoherent scattering function, I(Z,v) by:*

  $$I(Z,v) \quad = \quad \sum_k \int_{-\infty}^{p_z^{max}} J_k(p_z, Z) dp_z$$

  *where k refers to the particular electron subshell, $J_k(p_z, Z)$ is the Compton profile of the k-th shell for a given element, and $p_z^{max}$ is the maximum momentum transferred and is calculated using E'=E-$E_{binding}$.*

## Chapter 3

- Page 3-117, paragraph beginning with "b) Photons"

  OLD:

  ```
   Form:   PHYS:P   EMCPF   IDES   NOCOH

      EMCPF=...
      IDES=...
      NOCOH=...

      Default: ...
  ```

  NEW:

  ```
   Form:   PHYS:P   EMCPF   IDES   NOCOH   NODOP

      EMCPF=...
      IDES=...
      NOCOH=...
      NODOP = 0  Doppler energy broadening occurs. \\
            = 1  Doppler energy broadening will not occur. \\

      Default:  EMCPF=100 MeV; IDES=0; NOCOH=0 NODOP=0.}
  ```

- Change page 3-118, first full paragraph from:

  OLD: *The simple physics treatment, intended...Compton scattering from free electrons without the use of form factors,...*

  NEW: *The simple physics treatment, intended...Compton scattering,...*

- Page 3-118, paragraph beginning with "In the detailed physics treatment..."

  OLD: *...differential cross sections are modified by appropriate form factors taking electron binding effects...*

  NEW: *...differential cross sections are modified by the appropriate form factors and Compton profiles taking electron binding effects...*

- Page 3-118, add the following below the paragraph beginning with "NOCOH is a switch to..."

  *NODOP is a switch to turn off Doppler energy broadening for photons. This feature is automatically turned off when using simple physics. Turning this feature off with the detailed physics treatment results in a warning. Photon data libraries without Compton profile data also results in warning messages.*

## Appendicies

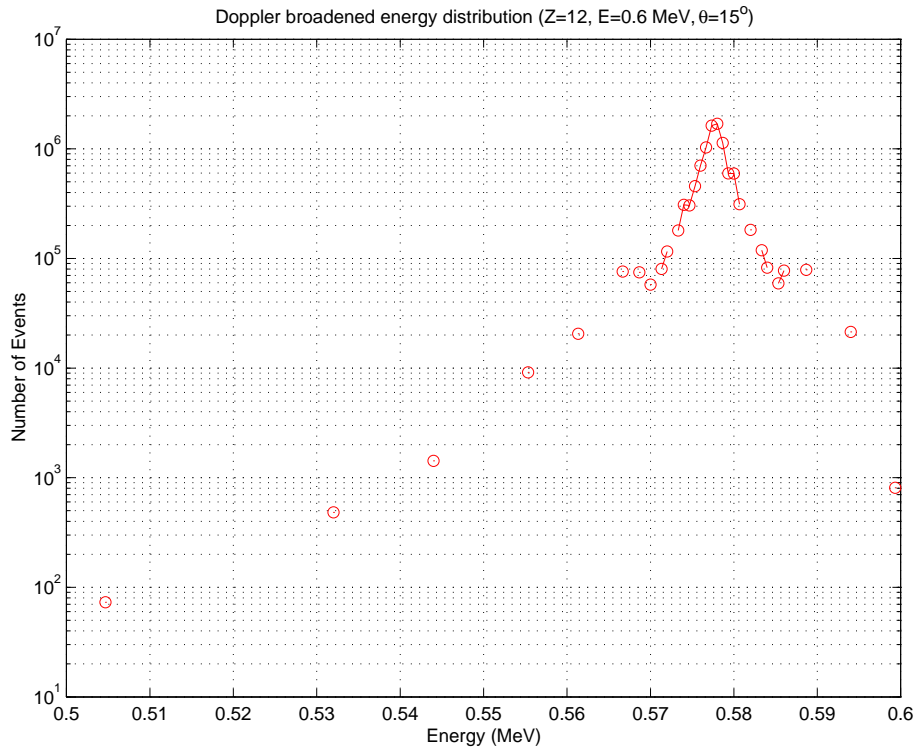Additions to the appendicies will be made later.

Figure 1: Incoherent Scattered Doppler Energy Distribution with Various Shells for E=0.6 MeV, $\theta$=15$^o$, and Z=12

# Assessment of Algorithm Performance, Quality of Associated Data, and Regression Testing

Several input decks have been created to test each of the the software requirements listed previously. The results from these input decks are from unit tests of the algorithm and the fully integrated code. The purpose of these tests is to assess the performance of the subroutine **dopplerp** and quality of the Compton profile data. Testing in sequential, multi-processing, and multi-threaded modes have confirmed that the code will automatically include Doppler energy broadening in a **mode p** problem, create a warning if this feature is turned off, or create a warning if the data library does not contain Compton profile data. This feature is turned off automatically when using the simple physics option.

Verification of the coding was done by line-by-line debugging to determine if the resulting code was the intended code of the code developer. Line-by-line verification confirmed that access to the new Compton profile data was as intended by the authors. Variables like **nsh, ishell, be, cdf, pdf, pzrn** were compared with the data table to verify their values.

## Algorithm Performance

The Compton profiles are data tabulated as a function of the projected precollision momentum of the electon on the momentum transfer vector of the photon as described by Eqn. 39 of the previous research note. Figure 3 of LA-UR-04-0487 shows the Compton profile for Z=12 for each shell. Figure 1 shows the scattered photon energy distribution as a function of interaction with various electron shells. This energy distribution would reduce to a single point at 0.5769 MeV (Eqn. 14, LA-UR-04-0487) if Doppler energy broadening was not simulated. The resulting distribution is centered around this value. This figure is a result of unit testing of subroutine **dopplerp** which was sampled using a ten million histories. This was done to test the algorithm's performance.
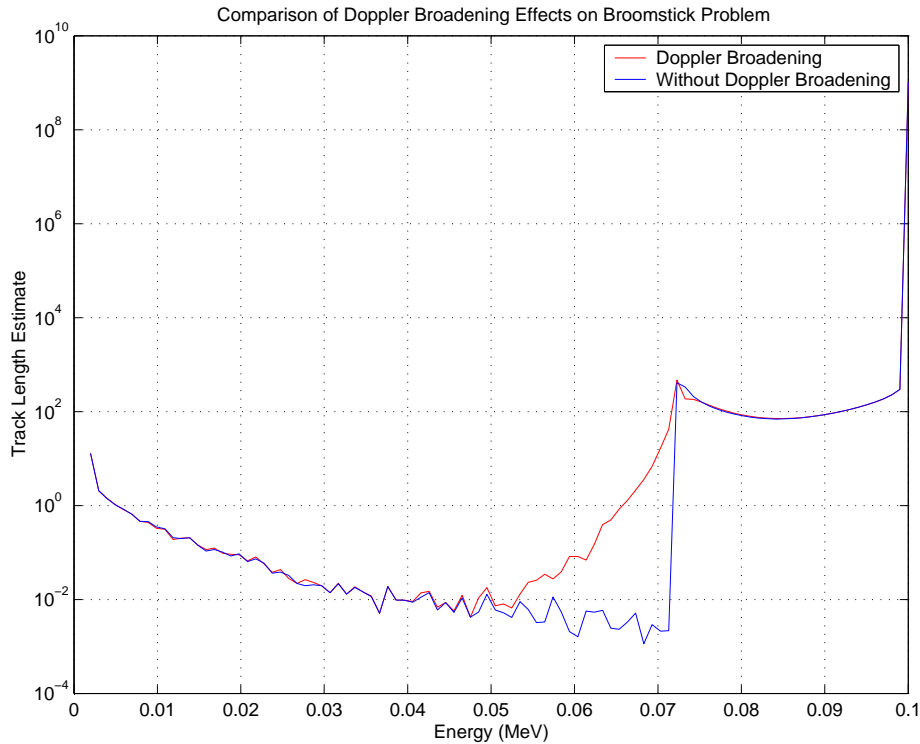
Figure 2: Track Length Comparison with Doppler Energy Broadening for Broomstick Problem (E=0.6 MeV)

A second test was created to see the effect of Doppler energy broadening from single scatter events. An input was created simulating a photon beam of 0.6 MeV incident on a 10 cm cylinder with a $10^{-6}$ cm radius (a.k.a. the broomstick problem). Figures 2 and 3 compares an F4 and F8 tally result with and without Doppler broadening. The Compton distribution is noticeably broadened.

## Compton Profiles

To assess the proper inclusion of the Compton profile data by Biggs with the existing incoherent scattering factor data in MCNP4C3, several checks must be performed. The first check of the Compton profile data was verifying that the shellwise and total Compton profile data for any element satisfies:

$$\int_{-\infty}^{p_z} J_k(p_z, Z) dp_z = 1/2 \text{ for each subshell}$$
$$\int_{-\infty}^{\infty} J(p_z, Z) dp_z = 1 \text{ for the total}$$

As a second check of the data, for any element the shellwise Compton profile will combine to the reported total. The total Compton profile for an element can be reconstructed from the shellwise data by multiplying the shellwise values by the respective number of electrons per shell and summing over each shell. These first two checks are currently being done and are not reported here.
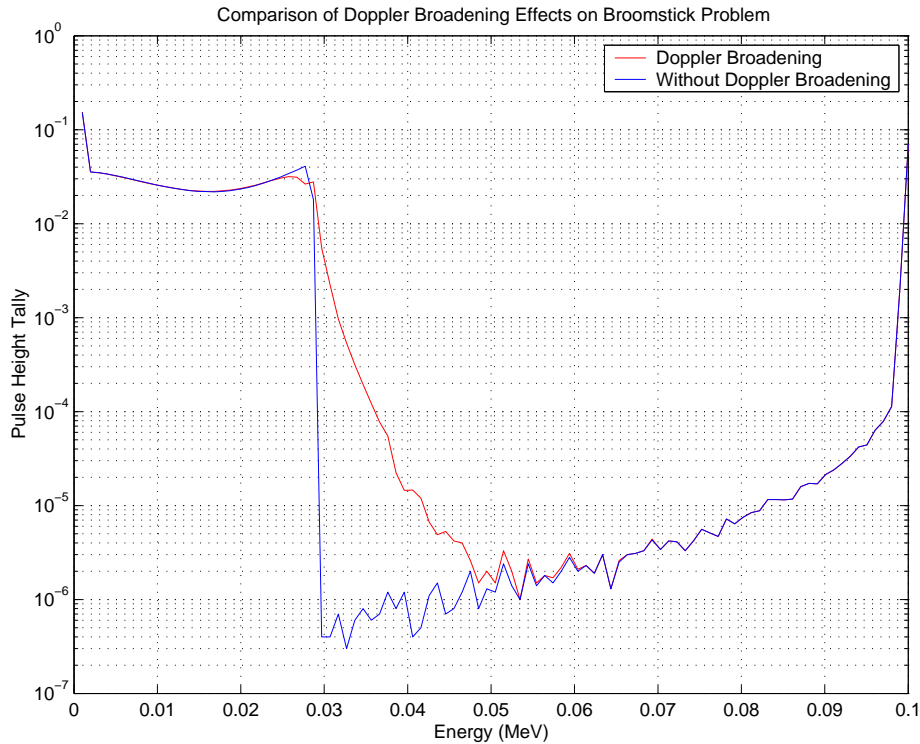
Figure 3: Pulse Height Tally Comparison with Doppler Energy Broadening for Broomstick Problem (E=0.6 MeV)

A third check includes comparison of the shellwise Compton profile data with the pre-existing incoherent scattering function data. This is done by verifying that:

$$S(x, Z) \quad = \quad \sum_k \int_{-\infty}^{p_z^{max}} J_k(p_z, Z) dp_z \tag{1}$$

where k refers to the particular electron subshell, $J_k(p_z, Z)$ is the Compton profile of the k-th shell for a given element, and $p_z^{max}$ is the maximum momentum transferred and is calculated from Eqn. 36 using E'=E-E$_b$. Figure 4 compares the Compton profile and incoherent scattering function for Z=12 as described by Eqn 1.

This can be extended to check the calculation of the differential and integral form of the modified Klein-Nishina.

$$\frac{d\sigma_{inc}}{d\Omega}(\theta, \phi) \quad = \quad \frac{d\sigma_{KN}}{d\Omega}(\theta, \phi) S(x, Z)$$

with analytic, current MCNP5, and Doppler data. A complete check of the data has not been done and is left for future work.

## Regression/Installation Testing

Regression/installation tests have been performed on the SGI (IRIX) system (theta.lanl.gov) in sequential, multi-processing and multi-threaded mode. The results of the regression/installation test suite will be different due to the extra warning messages. The results of the regression/installation test suite of the unmodified sequential and multi-processor/multi-threaded versions of MCNP5 thread 4.5 gives differences in the following files:
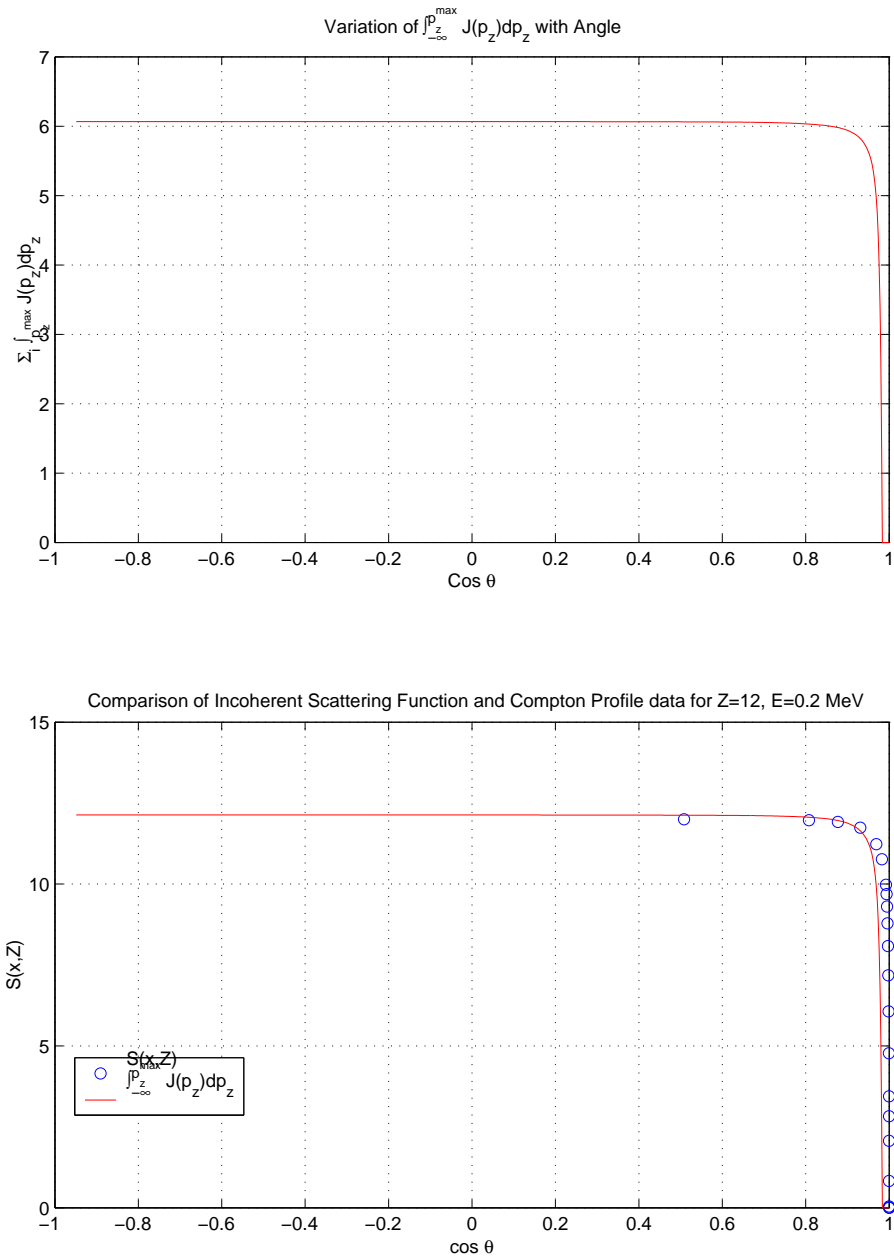
Figure 4: Comparison of Incoherent Scattering Function and Integrated Shellwise Compton profile data for Z=12

```
------- Diff List for Configuration seq debug plot --------
------- MCTAL Diffs --------
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm01
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm02
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm03
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm04
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm05
-rw-------    1 sooda    eolus           0 Jul 26 15:43 difm06
-rw-------    1 sooda    eolus           0 Jul 26 15:44 difm07
-rw-------    1 sooda    eolus           0 Jul 26 15:44 difm08
-rw-------    1 sooda    eolus           0 Jul 26 15:44 difm09
-rw-------    1 sooda    eolus           0 Jul 26 15:44 difm10
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm11
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm12
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm13
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm14
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm15
-rw-------    1 sooda    eolus           0 Jul 26 15:45 difm16
-rw-------    1 sooda    eolus           0 Jul 26 15:46 difm17
-rw-------    1 sooda    eolus           0 Jul 26 15:46 difm18
-rw-------    1 sooda    eolus           0 Jul 26 15:46 difm19
-rw-------    1 sooda    eolus           0 Jul 26 15:46 difm20
-rw-------    1 sooda    eolus           0 Jul 26 15:47 difm21
-rw-------    1 sooda    eolus           0 Jul 26 15:47 difm22
-rw-------    1 sooda    eolus           0 Jul 26 15:47 difm23
-rw-------    1 sooda    eolus           0 Jul 26 15:47 difm24
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm25
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm26
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm27
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm28
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm29
-rw-------    1 sooda    eolus           0 Jul 26 15:48 difm30
-rw-------    1 sooda    eolus           0 Jul 26 15:49 difm31
-rw-------    1 sooda    eolus           0 Jul 26 15:49 difm32
------- OUTP   Diffs --------
-rw-------    1 sooda    eolus       30592 Jul 26 15:43 difo01
-rw-------    1 sooda    eolus       21161 Jul 26 15:43 difo02
-rw-------    1 sooda    eolus        5449 Jul 26 15:43 difo03
-rw-------    1 sooda    eolus       15497 Jul 26 15:43 difo04
-rw-------    1 sooda    eolus        3785 Jul 26 15:43 difo05
-rw-------    1 sooda    eolus        9304 Jul 26 15:43 difo06
-rw-------    1 sooda    eolus       80018 Jul 26 15:44 difo07
-rw-------    1 sooda    eolus       14864 Jul 26 15:44 difo08
-rw-------    1 sooda    eolus        4609 Jul 26 15:44 difo09
-rw-------    1 sooda    eolus       16664 Jul 26 15:44 difo10
-rw-------    1 sooda    eolus       30535 Jul 26 15:45 difo11
-rw-------    1 sooda    eolus        6329 Jul 26 15:45 difo12
-rw-------    1 sooda    eolus       15388 Jul 26 15:45 difo13
-rw-------    1 sooda    eolus        3717 Jul 26 15:45 difo14
-rw-------    1 sooda    eolus        7570 Jul 26 15:45 difo15
-rw-------    1 sooda    eolus        7412 Jul 26 15:45 difo16
-rw-------    1 sooda    eolus       10949 Jul 26 15:46 difo17
-rw-------    1 sooda    eolus       18932 Jul 26 15:46 difo18
-rw-------    1 sooda    eolus        4405 Jul 26 15:46 difo19
```

```
-rw-------    1 sooda      eolus        16806 Jul 26 15:46 difo20
-rw-------    1 sooda      eolus         3255 Jul 26 15:47 difo21
-rw-------    1 sooda      eolus         3547 Jul 26 15:47 difo22
-rw-------    1 sooda      eolus         8130 Jul 26 15:47 difo23
-rw-------    1 sooda      eolus         3762 Jul 26 15:47 difo24
-rw-------    1 sooda      eolus         4595 Jul 26 15:48 difo25
-rw-------    1 sooda      eolus         4155 Jul 26 15:48 difo26
-rw-------    1 sooda      eolus         2791 Jul 26 15:48 difo27
-rw-------    1 sooda      eolus         4356 Jul 26 15:48 difo28
-rw-------    1 sooda      eolus         4201 Jul 26 15:48 difo29
-rw-------    1 sooda      eolus        14874 Jul 26 15:48 difo30
-rw-------    1 sooda      eolus        17601 Jul 26 15:49 difo31
-rw-------    1 sooda      eolus        20376 Jul 26 15:49 difo32


------- Diff List for Configuration debug ups omp plot --------
------- Tasking: NMPI = 3
------- Tasking: NTRD = 2
------- MCTAL Diffs --------
-rw-------    1 sooda      eolus            0 Jul 29 08:19 difm01
-rw-------    1 sooda      eolus            0 Jul 29 08:19 difm02
-rw-------    1 sooda      eolus            0 Jul 29 08:19 difm03
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm04
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm05
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm06
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm07
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm07a
-rw-------    1 sooda      eolus            0 Jul 29 08:20 difm08
-rw-------    1 sooda      eolus            0 Jul 29 08:21 difm08a
-rw-------    1 sooda      eolus            0 Jul 29 08:21 difm09
-rw-------    1 sooda      eolus            0 Jul 29 08:21 difm09a
-rw-------    1 sooda      eolus            0 Jul 29 08:21 difm10
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm11
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm12
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm13
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm14
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm15
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm16
-rw-------    1 sooda      eolus            0 Jul 29 08:22 difm17
-rw-------    1 sooda      eolus            0 Jul 29 08:23 difm18
-rw-------    1 sooda      eolus            0 Jul 29 08:23 difm19
-rw-------    1 sooda      eolus            0 Jul 29 08:23 difm20
-rw-------    1 sooda      eolus            0 Jul 29 08:23 difm21
-rw-------    1 sooda      eolus         1276 Jul 29 08:24 difm21a
-rw-------    1 sooda      eolus            0 Jul 29 08:24 difm22
-rw-------    1 sooda      eolus            0 Jul 29 08:24 difm23
-rw-------    1 sooda      eolus            0 Jul 29 08:24 difm24
-rw-------    1 sooda      eolus          858 Jul 29 08:24 difm25
-rw-------    1 sooda      eolus            0 Jul 29 08:24 difm26
-rw-------    1 sooda      eolus        15116 Jul 29 08:24 difm26a
-rw-------    1 sooda      eolus            0 Jul 29 08:25 difm27
-rw-------    1 sooda      eolus          698 Jul 29 08:25 difm28
-rw-------    1 sooda      eolus            0 Jul 29 08:25 difm29
-rw-------    1 sooda      eolus            0 Jul 29 08:25 difm30
-rw-------    1 sooda      eolus            0 Jul 29 08:25 difm31
```

```
-rw-------     1 sooda    eolus          0 Jul 29 08:25 difm32
------- OUTP   Diffs --------
-rw-------     1 sooda    eolus      29889 Jul 29 08:19 difo01
-rw-------     1 sooda    eolus      24169 Jul 29 08:19 difo02
-rw-------     1 sooda    eolus       5543 Jul 29 08:19 difo03
-rw-------     1 sooda    eolus      16194 Jul 29 08:20 difo04
-rw-------     1 sooda    eolus       7289 Jul 29 08:20 difo05
-rw-------     1 sooda    eolus       9517 Jul 29 08:20 difo06
-rw-------     1 sooda    eolus      80018 Jul 29 08:20 difo07
-rw-------     1 sooda    eolus      51826 Jul 29 08:20 difo07a
-rw-------     1 sooda    eolus      14864 Jul 29 08:20 difo08
-rw-------     1 sooda    eolus      16371 Jul 29 08:21 difo08a
-rw-------     1 sooda    eolus       4609 Jul 29 08:21 difo09
-rw-------     1 sooda    eolus       5749 Jul 29 08:21 difo09a
-rw-------     1 sooda    eolus      18043 Jul 29 08:21 difo10
-rw-------     1 sooda    eolus      30908 Jul 29 08:22 difo11
-rw-------     1 sooda    eolus       8263 Jul 29 08:22 difo12
-rw-------     1 sooda    eolus      15732 Jul 29 08:22 difo13
-rw-------     1 sooda    eolus       5050 Jul 29 08:22 difo14
-rw-------     1 sooda    eolus      10662 Jul 29 08:22 difo15
-rw-------     1 sooda    eolus       7910 Jul 29 08:22 difo16
-rw-------     1 sooda    eolus      11054 Jul 29 08:22 difo17
-rw-------     1 sooda    eolus      18932 Jul 29 08:23 difo18
-rw-------     1 sooda    eolus       5417 Jul 29 08:23 difo19
-rw-------     1 sooda    eolus      18070 Jul 29 08:23 difo20
-rw-------     1 sooda    eolus       3255 Jul 29 08:23 difo21
-rw-------     1 sooda    eolus       9151 Jul 29 08:24 difo21a
-rw-------     1 sooda    eolus       4210 Jul 29 08:24 difo22
-rw-------     1 sooda    eolus      11092 Jul 29 08:24 difo23
-rw-------     1 sooda    eolus       4748 Jul 29 08:24 difo24
-rw-------     1 sooda    eolus      18068 Jul 29 08:24 difo25
-rw-------     1 sooda    eolus       4155 Jul 29 08:24 difo26
-rw-------     1 sooda    eolus      70560 Jul 29 08:24 difo26a
-rw-------     1 sooda    eolus       2960 Jul 29 08:25 difo27
-rw-------     1 sooda    eolus      10342 Jul 29 08:25 difo28
-rw-------     1 sooda    eolus       5637 Jul 29 08:25 difo29
-rw-------     1 sooda    eolus      15243 Jul 29 08:25 difo30
-rw-------     1 sooda    eolus      53077 Jul 29 08:25 difo31
-rw-------     1 sooda    eolus      20376 Jul 29 08:25 difo32
```

The inclusion of the photon Doppler energy broadening feature into MCNP 5 thread 4.5 creates the following differences:

```
------- Diff List for Configuration seq debug plot --------
------- MCTAL Diffs --------
-rw-------     1 sooda    eolus          0 Jul 26 15:16 difm01
-rw-------     1 sooda    eolus          0 Jul 26 15:16 difm02
-rw-------     1 sooda    eolus          0 Jul 26 15:16 difm03
-rw-------     1 sooda    eolus          0 Jul 26 15:17 difm04
-rw-------     1 sooda    eolus          0 Jul 26 15:17 difm05
-rw-------     1 sooda    eolus          0 Jul 26 15:17 difm06
-rw-------     1 sooda    eolus          0 Jul 26 15:17 difm07
-rw-------     1 sooda    eolus          0 Jul 26 15:17 difm08
```

```
-rw-------    1 sooda    eolus            0 Jul 26 15:17 difm09
-rw-------    1 sooda    eolus            0 Jul 26 15:18 difm10
-rw-------    1 sooda    eolus            0 Jul 26 15:18 difm11
-rw-------    1 sooda    eolus            0 Jul 26 15:18 difm12
-rw-------    1 sooda    eolus            0 Jul 26 15:18 difm13
-rw-------    1 sooda    eolus            0 Jul 26 15:19 difm14
-rw-------    1 sooda    eolus            0 Jul 26 15:19 difm15
-rw-------    1 sooda    eolus            0 Jul 26 15:19 difm16
-rw-------    1 sooda    eolus            0 Jul 26 15:19 difm17
-rw-------    1 sooda    eolus            0 Jul 26 15:20 difm18
-rw-------    1 sooda    eolus            0 Jul 26 15:20 difm19
-rw-------    1 sooda    eolus            0 Jul 26 15:20 difm20
-rw-------    1 sooda    eolus            0 Jul 26 15:20 difm21
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm22
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm23
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm24
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm25
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm26
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm27
-rw-------    1 sooda    eolus            0 Jul 26 15:21 difm28
-rw-------    1 sooda    eolus            0 Jul 26 15:22 difm29
-rw-------    1 sooda    eolus            0 Jul 26 15:22 difm30
-rw-------    1 sooda    eolus            0 Jul 26 15:23 difm31
-rw-------    1 sooda    eolus            0 Jul 26 15:23 difm32
-------  OUTP   Diffs --------
-rw-------    1 sooda    eolus        30592 Jul 26 15:16 difo01
-rw-------    1 sooda    eolus        21161 Jul 26 15:16 difo02
-rw-------    1 sooda    eolus         5449 Jul 26 15:16 difo03
-rw-------    1 sooda    eolus        15863 Jul 26 15:17 difo04
-rw-------    1 sooda    eolus         3785 Jul 26 15:17 difo05
-rw-------    1 sooda    eolus         9304 Jul 26 15:17 difo06
-rw-------    1 sooda    eolus        80018 Jul 26 15:17 difo07
-rw-------    1 sooda    eolus        15302 Jul 26 15:17 difo08
-rw-------    1 sooda    eolus         4609 Jul 26 15:17 difo09
-rw-------    1 sooda    eolus        16931 Jul 26 15:18 difo10
-rw-------    1 sooda    eolus        31018 Jul 26 15:18 difo11
-rw-------    1 sooda    eolus         6329 Jul 26 15:18 difo12
-rw-------    1 sooda    eolus        15388 Jul 26 15:18 difo13
-rw-------    1 sooda    eolus         3717 Jul 26 15:19 difo14
-rw-------    1 sooda    eolus         7570 Jul 26 15:19 difo15
-rw-------    1 sooda    eolus         7412 Jul 26 15:19 difo16
-rw-------    1 sooda    eolus        10949 Jul 26 15:19 difo17
-rw-------    1 sooda    eolus        18932 Jul 26 15:20 difo18
-rw-------    1 sooda    eolus         4405 Jul 26 15:20 difo19
-rw-------    1 sooda    eolus        16952 Jul 26 15:20 difo20
-rw-------    1 sooda    eolus         3535 Jul 26 15:20 difo21
-rw-------    1 sooda    eolus         4028 Jul 26 15:21 difo22
-rw-------    1 sooda    eolus         8477 Jul 26 15:21 difo23
-rw-------    1 sooda    eolus         3762 Jul 26 15:21 difo24
-rw-------    1 sooda    eolus         4595 Jul 26 15:21 difo25
-rw-------    1 sooda    eolus         4155 Jul 26 15:21 difo26
-rw-------    1 sooda    eolus         2791 Jul 26 15:21 difo27
-rw-------    1 sooda    eolus         4356 Jul 26 15:21 difo28
-rw-------    1 sooda    eolus         4536 Jul 26 15:22 difo29
```

```
-rw-------     1 sooda     eolus       15103 Jul 26 15:22 difo30
-rw-------     1 sooda     eolus       17830 Jul 26 15:23 difo31
-rw-------     1 sooda     eolus       20376 Jul 26 15:23 difo32


------- Diff List for Configuration debug omp ups plot --------
------- Tasking: NMPI = 3
------- Tasking: NTRD = 2
------- MCTAL Diffs --------
-rw-------     1 sooda     eolus           0 Jul 29 08:39 difm01
-rw-------     1 sooda     eolus           0 Jul 29 08:39 difm02
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm03
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm04
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm05
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm06
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm07
-rw-------     1 sooda     eolus           0 Jul 29 08:40 difm07a
-rw-------     1 sooda     eolus           0 Jul 29 08:41 difm08
-rw-------     1 sooda     eolus           0 Jul 29 08:41 difm08a
-rw-------     1 sooda     eolus           0 Jul 29 08:41 difm09
-rw-------     1 sooda     eolus           0 Jul 29 08:41 difm09a
-rw-------     1 sooda     eolus           0 Jul 29 08:41 difm10
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm11
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm12
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm13
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm14
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm15
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm16
-rw-------     1 sooda     eolus           0 Jul 29 08:42 difm17
-rw-------     1 sooda     eolus           0 Jul 29 08:43 difm18
-rw-------     1 sooda     eolus           0 Jul 29 08:43 difm19
-rw-------     1 sooda     eolus           0 Jul 29 08:43 difm20
-rw-------     1 sooda     eolus           0 Jul 29 08:44 difm21
-rw-------     1 sooda     eolus        1276 Jul 29 08:44 difm21a
-rw-------     1 sooda     eolus           0 Jul 29 08:44 difm22
-rw-------     1 sooda     eolus           0 Jul 29 08:44 difm23
-rw-------     1 sooda     eolus           0 Jul 29 08:44 difm24
-rw-------     1 sooda     eolus         858 Jul 29 08:45 difm25
-rw-------     1 sooda     eolus           0 Jul 29 08:45 difm26
-rw-------     1 sooda     eolus       15116 Jul 29 08:45 difm26a
-rw-------     1 sooda     eolus           0 Jul 29 08:45 difm27
-rw-------     1 sooda     eolus         698 Jul 29 08:45 difm28
-rw-------     1 sooda     eolus           0 Jul 29 08:45 difm29
-rw-------     1 sooda     eolus           0 Jul 29 08:45 difm30
-rw-------     1 sooda     eolus           0 Jul 29 08:46 difm31
-rw-------     1 sooda     eolus           0 Jul 29 08:46 difm32
------- OUTP   Diffs --------
-rw-------     1 sooda     eolus       29610 Jul 29 08:39 difo01
-rw-------     1 sooda     eolus       24261 Jul 29 08:39 difo02
-rw-------     1 sooda     eolus        6361 Jul 29 08:40 difo03
-rw-------     1 sooda     eolus       36115 Jul 29 08:40 difo04
-rw-------     1 sooda     eolus        7561 Jul 29 08:40 difo05
-rw-------     1 sooda     eolus        9517 Jul 29 08:40 difo06
-rw-------     1 sooda     eolus       80018 Jul 29 08:40 difo07
-rw-------     1 sooda     eolus       52190 Jul 29 08:40 difo07a
```

```
-rw-------    1 sooda    eolus       15302 Jul 29 08:41 difo08
-rw-------    1 sooda    eolus       16638 Jul 29 08:41 difo08a
-rw-------    1 sooda    eolus        4609 Jul 29 08:41 difo09
-rw-------    1 sooda    eolus        5749 Jul 29 08:41 difo09a
-rw-------    1 sooda    eolus       17904 Jul 29 08:41 difo10
-rw-------    1 sooda    eolus       31390 Jul 29 08:42 difo11
-rw-------    1 sooda    eolus        8767 Jul 29 08:42 difo12
-rw-------    1 sooda    eolus       15732 Jul 29 08:42 difo13
-rw-------    1 sooda    eolus        5314 Jul 29 08:42 difo14
-rw-------    1 sooda    eolus       10020 Jul 29 08:42 difo15
-rw-------    1 sooda    eolus        8189 Jul 29 08:42 difo16
-rw-------    1 sooda    eolus       11054 Jul 29 08:42 difo17
-rw-------    1 sooda    eolus       18932 Jul 29 08:43 difo18
-rw-------    1 sooda    eolus        5167 Jul 29 08:43 difo19
-rw-------    1 sooda    eolus       18330 Jul 29 08:43 difo20
-rw-------    1 sooda    eolus        3535 Jul 29 08:44 difo21
-rw-------    1 sooda    eolus       10141 Jul 29 08:44 difo21a
-rw-------    1 sooda    eolus        4611 Jul 29 08:44 difo22
-rw-------    1 sooda    eolus       11275 Jul 29 08:44 difo23
-rw-------    1 sooda    eolus        4498 Jul 29 08:44 difo24
-rw-------    1 sooda    eolus       18068 Jul 29 08:45 difo25
-rw-------    1 sooda    eolus        4155 Jul 29 08:45 difo26
-rw-------    1 sooda    eolus       71742 Jul 29 08:45 difo26a
-rw-------    1 sooda    eolus        2960 Jul 29 08:45 difo27
-rw-------    1 sooda    eolus       10342 Jul 29 08:45 difo28
-rw-------    1 sooda    eolus        6364 Jul 29 08:45 difo29
-rw-------    1 sooda    eolus       15473 Jul 29 08:45 difo30
-rw-------    1 sooda    eolus       55280 Jul 29 08:46 difo31
-rw-------    1 sooda    eolus       20376 Jul 29 08:46 difo32
```

There are no differences in the MCTAL files output for the sequential runs. The increase in the size of the differences in the sequential OUTP files **difo04, difo08, difo10, difo11, difo20, difo21, difo22, difo23, difo30, and difo31** are due to the new warning message included to warn the user that the data library does not contain the Compton profiles.

# Summary

This research note has described the software requirements and design to include photon Doppler energy broadening in MCNP5. The algorithm and data requirements have been documented. Initial testing and data quality checks have been performed. Further testing of the data has been outlined and is strongly suggested. This new MCNP physics feature has been integrated and tested in MCNP 5 beta, thread 4.5.