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General Tally Support and Post Processing in a Modern Monte Carlo Transport Code

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ABSTRACT

MERCURY is a modern Monte Carlo code under development at Lawrence Livermore National Laboratory. New tally capability has been implemented. While standard tallies are supported by the code, a new general tally has been developed. General tallies react to particle events, are filtered by response functions and are accumulated into a user defined phase space. The post processing tool, CALORIS, has been developed to work with MERCURY's tallies. In addition, the graphical tools, ULTRA II and VisIt are also available to graphically visualize the MERCURY tallies.

Key Words: Mercury, Monte Carlo, General Tally

1. INTRODUCTION

MERCURY[1] is a modern Monte Carlo particle transport code developed at Lawrence Livermore National Laboratory (LLNL) that will replace the older codes TART[2] and COG[3] as the next generation, general purpose radiation transport code at LLNL. MERCURY can transport neutrons, gamma rays and light charged particles through a 1-D spherical, 2-D R-Z or unstructured mesh, 3-D Cartesian or unstructured mesh and/or 3-D combinatorial geometry. Cross sections are treated as either multigroup or continuous energy. MERCURY can perform static and dynamic source calculations and k_{eff} and α eigenvalue calculations.

Standard tallies, which is MERCURY's name for the results that are routinely computed by particle transport codes, have been available from the outset. These tallies include particle flux, energy deposition, isotopic depletion/accretion, particle balance and leakage. Several controls have recently been added to MERCURY to help a user modify the memory and output of the *standard* tallies.

In many instances, a user would like to request new or different information than that which is computed by *standard* tallies. These results may be highly specialized or costly to compute. Several Monte Carlo codes "solve" this problem by having additional pre-defined tallies that can be requested by the user. This approach lacks flexibility in the long term and requires additional post-processing codes in order to gain some level of flexibility. The approach taken in MERCURY has been to develop a mechanism for defining *general* tallies which permits the user to request that almost any type of information may be accumulated while the problem is running.

General tallies have quite a large number of input / output options (such as compact and verbose text, binary file, a particle record file and a plot file for 1-D graphics) and can represent a small or huge phase space in the problem.

CALORIS is the tally post processing code that has been developed for use with MERCURY. CALORIS has the same general tally features as found in MERCURY, but it can be used just to process *general* tally information. Its main purpose is to manipulate particle records or *general* tallies and then re-tally them into a different phase space.

Another useful tally analysis tool is VisIt[4], a parallel, visualization code that has also been developed at LLNL. *Standard* and *general* tally information may be visualized with VisIt as screen images. VisIt has many additional capabilities to assist the user in analyzing the complete set, or relevant sub-set, of the tally data produced by MERCURY or CALORIS.

2. STANDARD TALLIES

The *standard* tallies include eigenvalue information, material flux, particle balances, particle leakage, particle spectrum, material & energy deposition, scalar flux and sampled cross sections. The *standard* tallies may be made inactive to reduce computational and memory costs. Their output may be sent to a standard text output or a special plot file. The plot file is a series of space delimited data that can be plotted with most plotting software.

3. PHASE SPACE

A tally *phase space* can be used to define how to respond (filter or weight) to an event, and/or how to bin the results. A phase space can be defined by any set of attributes that describe a particle. The attributes may be further broken down into *discrete* and *binned* attributes. Discrete attributes include particle type (neutron, proton, etc.), reaction type (if applicable), current cell adjacent cell, particle purpose and event type. Binned attributes are used to specify the range and resolution of a set of bins that constitute one dimension of the phase space. They include time, energy, spatial coordinates, angle, particle weight, creation time and number of collisions. The complete tally space is the union of the discrete and binned attributes.

4. GENERAL TALLIES

General tallies are highly versatile due to their ability to be customized for almost any query. This level of generalization is achieved by allowing this new type of tally to respond to specific particle *events* which are user selectable. A *response* function *phase space*, such as a filter or weighting scheme, can be applied at the specified events, and the *quantity of interest* is then accumulated (tallied) in the *result phase space* specified by the user. For example, a user may be interested in counting the number (*quantity of interest*) of neutrons (first *response phase space*) with energies between two limits (second *response phase space*) that crosses from one cell to another (*event*). Furthermore, the user would like to bin the cell crossings by their X and Y coordinates of the particle (*result phase space*).

This rather complicated tally is simple to set up using the MERCURY or CALORIS input syntax as shown below:

```
start_tally
   tally Tally_Name
# Quantity of interest
     category Count
     events Facet_Crossing_Enter end_events
# Filter out all but neutrons
     response
       set Set_Name
         space Species
         domain Neutron Gammas Alphas end_domain
       end_set
       range 2 0 0 end_range
     end_response
# Ignore particles that are not within energy bounds
     response
       boundary_set Boundary_Set_Name
         space Energy
         interpolation None
# Energy is in MeV
         domain 10 20 end_domain
       end_boundary_set
       range 1 Ignored end_range
     end_response
# See results based on X and Y coordinates
     result
       boundary_set Boundary_Set_Name_2
         space X_Axis
         domain 0.0 0.5 1.0 1.5 2.0 2.5 3.0 end_domain
       end_boundary_set
       boundary_set Boundary_Set_Name_3
         space Y_Axis
         domain 0.0 0.5 1.0 1.5 2.0 2.5 3.0 end_domain
       end_boundary_set
     end_result
  end_tally
stop_tally
```

5. POST PROCESSORS

CALORIS is the tally post processing tool that has been developed for use with the Mercury Monte Carlo code. CALORIS can interpret several of the tally output formats, including compact text, binary and particle records. It can manipulate the particles and tallies, and re-output them in whatever manner the user desires. CALORIS has no additional tally capability beyond those available in MERCURY. Its main purpose is to manipulate particle records or tallies, and re-tally them into a new phase space. For example, a MERCURY calculation may write all leaked particles out to a particle record file. CALORIS may read in this file, move the particles to an image plane, and re-tally the particles in this new phase space. This tally could then be written out to a graphics dump as an image. The user may then decide to repeat this process but change the location of the image plane.

ULTRA[5] is a program for the presentation, manipulation, and analysis of 1-D data sets (i.e., x-y data pairs), and works on text and binary files. The MERCURY code outputs a plot file that may be directly imported into ULTRA. Another tool that is useful for analyzing the tallies is VisIt, a parallel visualization tool that has been developed at LLNL. Both tally output data and particles may be visualized with VisIt, which renders the tallies as images. VisIt has many additional capabilities to assist the user in analyzing the complete set, or relevant subsets, of the tally data produced by MERCURY or CALORIS.

The use of VisIt to analyze tallies is demonstrated in the figures below. Figure 1, presents the geometry for a simple problem. The material in red is high density uranium and the material in blue is a low density water shield. A few neutrons are injected into the uranium and particles are tallied as they leave the back wall of the shield. A biasing method was then applied and tallied as well. Fig 2 shows the comparison of the two images produced by the tally. The biased method is shown on the bottom. This is representative of the many possible uses of tallies and the post processing tools.

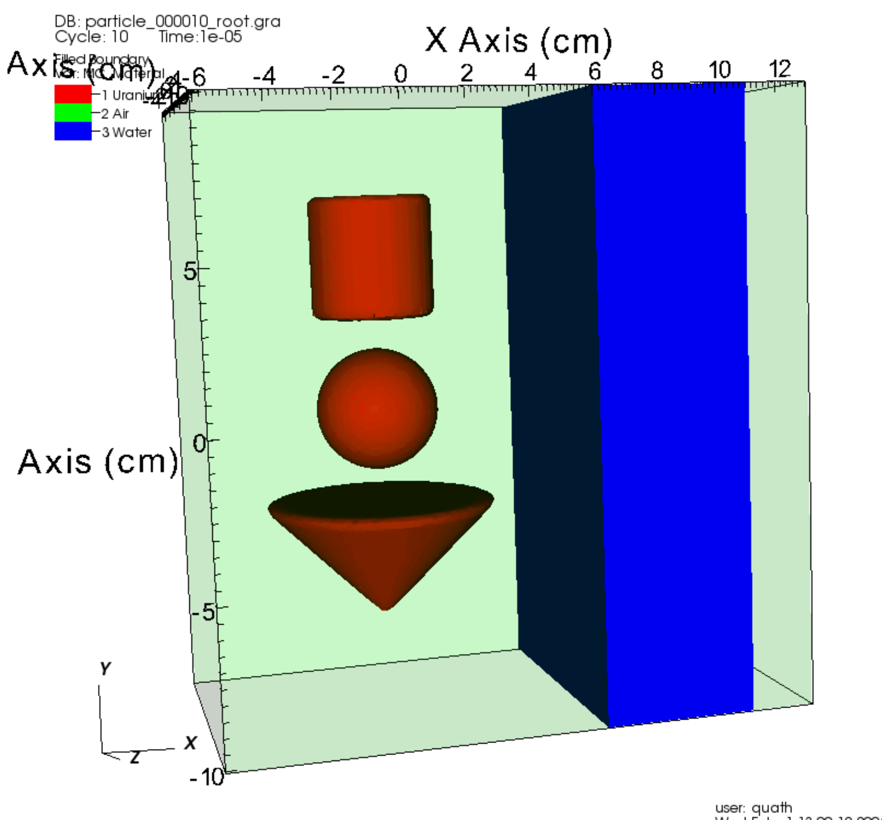

Figure 1. Problem geometry as displayed by VisIt.

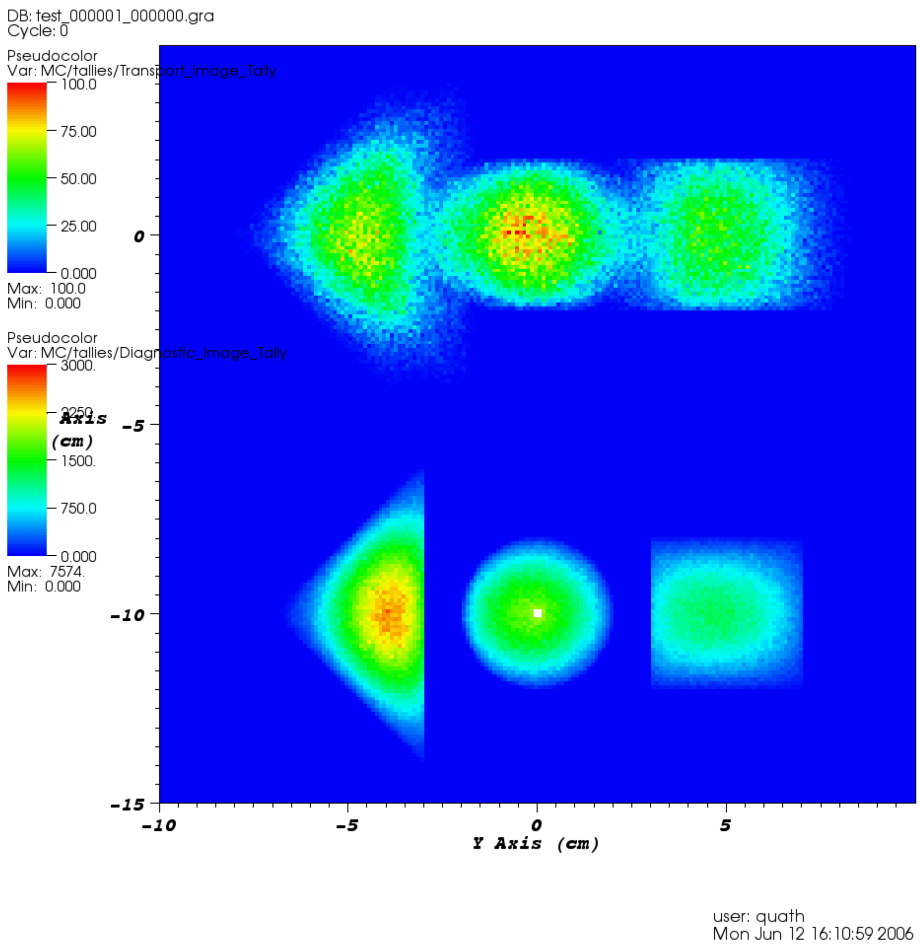

Figure 2. Comparison of a regular transport (top) and biased transport (bottom) tally.

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