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SUPERIMPOSED MESH PLOTTING IN MCNP

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ABSTRACT

The capability to plot superimposed meshes has been added to MCNPTM. MCNP4C featured a superimposed mesh weight window generator which enabled users to set up geometries without having to subdivide geometric cells for variance reduction. The variance reduction was performed with weight windows on a rectangular or cylindrical mesh superimposed over the physical geometry. Experience with the new capability was favorable but also indicated that a number of enhancements would be very beneficial, particularly a means of visualizing the mesh and its values. The mathematics for plotting the mesh and its values is described here along with a description of other upgrades.

1. INTRODUCTION

MCNP is a general-purpose Monte Carlo N-Particle radiation transport code that models neutrons from 0–100 MeV and photons and electrons from 1 keV to 100 GeV. MCNP (Briesmeister, 2000) is used for nuclear engineering applications such as nuclear criticality safety, oil-well logging, radiation shielding, medical radiation modeling, aerospace, and more. MCNP features detailed continuous-energy physics to provide a near-predictive model of how radiation interacts with matter. MCNP has been continuously developed for over 55 years and has been widely used internationally for over 20 years.

Like all other statistical solution methods, a large number of statistical trials (particle histories) are required to converge to an acceptable problem solution. Variance reduction methods are used to sample important parts of phase space at the expense of less important ones. In particular, the weight window method populates important space, time, and energy regions by splitting particles into many low-weight samples and depopulates unimportant regions by Russian rouletteing them into fewer high-weight samples.

The weight window variance reduction method was limited to specifying weight windows in geometric cells until MCNP4C (Hendricks, McKinney, and Cox, 2000) and (Hendricks, 2000) which featured a superimposed importance mesh (Liu and Gardner, 1997), (Gardner and Liu, 1999), and (Evans and Hendricks, 1998). The mesh could be

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either rectangular (XYZ Cartesian geometry) or cylindrical (RZθ geometry). Weight windows could be generated by a “forward adjoint” method known as the “weight window generator” (Booth and Hendricks, 1984) in the phase space of the mesh which was superimposed over the problem geometry. The superimposed mesh eliminated the need to specify the problem geometry in many superfluous finely divided geometric regions for variance reduction purposes (Culbertson and Hendricks, 1999) and (Hendricks and Culbertson, 2000). Particles are transported in the physical geometry, but their variance reduction weight window parameters are taken from the superimposed mesh. Experience with the superimposed mesh weight windows has been very favorable but also indicated that a number of enhancements would be very beneficial, particularly a means of visualizing the mesh and its values. The mathematics for plotting the mesh and its values is described here along with a description of other upgrades.

2. PLOTTING SUPERIMPOSED MESHES

Plotting of the superimposed rectangular mesh is straightforward, but plotting the cylindrical mesh is complicated by the fact that the cylindrical mesh can have any skew orientation in space. Further, the plot view can have a different skew orientation in space. So the cylindrical mesh must be transformed from its RZθ coordinate system to the XYZ Cartesian system to the ST system of the plot frame. And then, to take advantage of the machinery already in the MCNP plotter, it must be transferred a fourth time to the “convenient parameter space” of the one-dimensional P coordinate system of “conic invariants.” Following is the mathematics of plotting the superimposed weight window mesh.

MCNP is in the x,y,z (Cartesian) coordinate system. The MCNP surfaces are conics of the form

$$Ax^2 + By^2 + Cz^2 + Dxy + Eyz + Fxz + Gx + Hy + Jz + K = 0 \quad (1)$$

These surfaces may be written in matrix form as

$$\begin{bmatrix} 1 & x & y & z \end{bmatrix} \begin{bmatrix} K & \frac{G}{2} & \frac{H}{2} & \frac{J}{2} \\ \frac{G}{2} & A & \frac{D}{2} & \frac{F}{2} \\ \frac{H}{2} & \frac{D}{2} & B & \frac{E}{2} \\ \frac{J}{2} & \frac{F}{2} & \frac{E}{2} & C \end{bmatrix} \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} = 0 \quad (2)$$

or

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = 0 \quad (3)$$

The superimposed mesh is in either the x,y,z rectangular mesh coordinate system or the r,z,θ cylindrical mesh coordinate system.

The x,y,z rectangular mesh system is the same as the x,y,z MCNP Cartesian coordinate system. The mesh surfaces are all planes from the mesh input description:

$$\text{MESH} \quad \text{geom} = \text{rec} \quad \text{origin} = x_o \quad y_o \quad z_o \quad (4)$$

$$\begin{aligned} \text{i mesh} & \quad x_1 \quad x_2 \dots \quad x_i \dots \\ \text{j mesh} & \quad y_1 \quad y_2 \dots \quad y_i \dots \\ \text{k mesh} & \quad z_1 \quad z_2 \dots \quad z_i \dots \end{aligned} \quad (5)$$

All elements of the MCNP coordinate system **A** matrix are zero except

$$\begin{aligned} K &= -x_i, \quad G = 1 \quad \text{for imesh planes;} \\ K &= -y_i, \quad H = 1 \quad \text{for jmesh planes;} \\ K &= -z_i, \quad J = 1 \quad \text{for kmesh planes.} \end{aligned} \quad (6)$$

For example, the most negative plane normal to the y-axis would have **A** matrix

$$\mathbf{A} = \begin{bmatrix} -y_o & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (7)$$

The r, z,θ cylindrical mesh system may be in any arbitrary skew orientation and is described by:

$$\text{MESH} \quad \text{geom} = \text{cyl} \quad \text{origin} = x_o \quad y_o \quad z_o \quad (8)$$

$$\text{axs} = a_1 \quad a_2 \quad a_3 \quad \text{vec} = v_1 \quad v_2 \quad v_3 \quad (9)$$

$$\begin{aligned} \text{i mesh} &= r_1 \quad r_2 \dots \quad r_i \dots \\ \text{j mesh} &= z_1 \quad z_2 \dots \quad z_i \dots \\ \text{k mesh} &= \theta_1 \quad \theta_2 \dots \quad \theta_i \dots \end{aligned} \quad (10)$$

This r,z,θ cylindrical geometry may be described by an auxiliary cartesian geometry, $s_c = [s, t, u]$, related to the MCNP $\mathbf{x} = [x, y, z]$ geometry as

$$\mathbf{P}_c \mathbf{s}_c = \mathbf{x} \quad (11)$$

or

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ x_0 & a_1 & v_1 & d_1 \\ y_0 & a_2 & v_2 & d_2 \\ z_0 & a_3 & v_3 & d_3 \end{bmatrix} \begin{bmatrix} 1 \\ s \\ t \\ u \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} \quad (12)$$

where $\mathbf{x} = [x_0 \ y_0 \ z_0]$ is the center of the base of the cylindrical mesh, $\mathbf{a} = [a_1 \ a_2 \ a_3]$ is the axis of the cylindrical mesh, $\mathbf{v} = [v_1 \ v_2 \ v_3]$ is the reference direction of $\theta = 0$, and $\mathbf{d} = [d_1 \ d_2 \ d_3] = \mathbf{a} \times \mathbf{v}$.

The cylindrical mesh surfaces are conics which may be described in the s,t,u coordinate system by the matrix equation:

$$\begin{bmatrix} 1 & s & t & u \end{bmatrix} \begin{bmatrix} K & \frac{G}{2} & \frac{H}{2} & \frac{J}{2} \\ \frac{G}{2} & A & 0 & 0 \\ \frac{H}{2} & 0 & B & 0 \\ \frac{J}{2} & 0 & 0 & C \end{bmatrix} \begin{bmatrix} 1 \\ s \\ t \\ u \end{bmatrix} = 0 \quad (13)$$

or

$$\mathbf{s}_c^T \mathbf{C} \mathbf{s}_c = 0 \quad (14)$$

The mesh surfaces are either z-planes

$$\mathbf{C}_z = \begin{bmatrix} -z_i & \frac{1}{2} & 0 & 0 \\ \frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad (15)$$

or r-cylinders,

$$C_r = \begin{bmatrix} r_i^2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (16)$$

or θ planes passing through the z-axis,

$$C_\theta = \begin{bmatrix} 0 & 0 & \sin\theta_i & \cos\theta_i \\ 0 & 0 & 0 & 0 \\ \sin\theta_i & 0 & 0 & 0 \\ \cos\theta_i & 0 & 0 & 0 \end{bmatrix} \quad (17)$$

The r,z, θ cylindrical mesh surfaces can now be put into the x,y,z MCNP cartesian system in **A**- matrix form as follows:

$$\begin{aligned} \mathbf{P}_c \mathbf{s}_c &= \mathbf{x} \\ \mathbf{s}_c &= \mathbf{P}_c^{-1} \mathbf{x} \\ \mathbf{s}_c^T &= \mathbf{x}^T (\mathbf{P}_c^{-1})^T \\ \mathbf{s}_c^T \mathbf{C} \mathbf{s}_c &= \mathbf{x}^T (\mathbf{P}_c^{-1})^T \mathbf{C} \mathbf{P}_c^{-1} \mathbf{x} \\ \mathbf{A} &= (\mathbf{P}_c^{-1})^T \mathbf{C} \mathbf{P}_c^{-1} \end{aligned} \quad (18)$$

The inverse of the \mathbf{P}_c matrix is

$$\mathbf{P}_c^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ \mathbf{x} \cdot \mathbf{a} & a_1 & a_2 & a_3 \\ \mathbf{x} \cdot \mathbf{v} & v_1 & v_2 & v_3 \\ \mathbf{x} \cdot \mathbf{d} & d_1 & d_2 & d_3 \end{bmatrix} \quad (19)$$

Once all the superimposed mesh surfaces are in **A**-matrix form in the MCNP coordinate system, they are plotted using the MCNP geometry plot algorithms as described in the MCNP manual (Briesmeister, 2000). That is, let the two-dimensional plot frame s,t coordinate be related to the MCNP x y z geometry as

$$\mathbf{P} \mathbf{s} = \mathbf{x} \quad (20)$$

or

$$\begin{bmatrix} 1 & 0 & 0 \\ 0_1 & b_1 & b_4 \\ 0_2 & b_2 & b_5 \\ 0_3 & b_3 & b_6 \end{bmatrix} \begin{bmatrix} 1 \\ s \\ t \end{bmatrix} = \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix} \quad (21)$$

where

$$\mathbf{0} = [0_1, 0_2, 0_3] = \text{the plot origin,}$$

$$\mathbf{b}_1 = [b_1, b_2, b_3] = \text{the first basis vector} \quad (22)$$

and

$$\mathbf{b}_4 = [b_4, b_5, b_6] = \text{the second basis vector of the plot frame .} \quad (23)$$

Then the surfaces to be plotted in the s-t plot coordinate system are conics of the form

$$q_{22}s^2 + 2q_{23}st + q_{33}t^2 + 2q_{12}s + 2q_{13}t + q_{11} = 0 \quad (24)$$

or

$$\begin{bmatrix} 1 & s & t \end{bmatrix} \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{22} & q_{23} \\ q_{13} & q_{23} & q_{33} \end{bmatrix} \begin{bmatrix} 1 \\ s \\ t \end{bmatrix} = 0 \quad (25)$$

or

$$\mathbf{s}^T \mathbf{Q} \mathbf{s} . \quad (26)$$

Whereas

$$\mathbf{P} \mathbf{s} = \mathbf{x} \quad (27)$$

and

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = 0 \quad (28)$$

then

$$\mathbf{x}^T = \mathbf{s}^T \mathbf{P}^T \quad (29)$$

and

$$\mathbf{s}^T \mathbf{P}^T \mathbf{A} \mathbf{P} \mathbf{s} = 0 \quad (30)$$

and

$$\mathbf{Q} = \mathbf{P}^T \mathbf{A} \mathbf{P} \quad (31)$$

These \mathbf{Q} -matrix surfaces are converted to conic invariants (Spain, 1957)

$$\begin{aligned} s &= C_1 + C_2 p \\ t &= C_4 + C_5 p \end{aligned} \quad (32)$$

for straight lines (planes and parallel view to the cylinder). For skew or normal views of the cylindrical mesh cylinder, the conic invariant parametric equation is:

$$\begin{aligned} s &= C_1 + C_2 \sin p + C_3 \cos p \\ t &= C_4 + C_5 \sin p + C_6 \cos p \end{aligned} \quad (33)$$

The intersection of two straight lines

$$\begin{aligned} s_a &= C_{1a} + C_{2a} p \\ t_a &= C_{4a} + C_{5a} p \end{aligned} \quad (34)$$

and

$$\begin{aligned} s_b &= C_{1b} + C_{2b} p \\ t_b &= C_{4b} + C_{5b} p \end{aligned} \quad (35)$$

is at

$$p = \frac{C_{5b}(C_{1b} - C_{1a}) + C_{2b}(C_{4a} - C_{4b})}{C_{5b}C_{2a} - C_{2b}C_{5a}} \quad (36)$$

The intersection of a straight line and ellipse is found from the parametric equation of the line,

$$\begin{aligned} s &= C_1 + C_2 p \\ t &= C_4 + C_5 p \end{aligned} \quad (37)$$

and the \mathbf{Q} -matrix equation of the ellipse

$$q_{22}s^2 + 2q_{23}st + q_{33}t^2 + 2q_{12}s + 2q_{13}t + q_{11} = 0 \quad (38)$$

which gives the quadratic

$$Ap^2 + Bp + C = 0 \quad (39)$$

where

$$\begin{aligned} A &= q_{22}C_2^2 + q_{23}C_2C_5 + q_{33}C_5^2 \\ B &= 2[q_{22}C_1C_2 + q_{23}(C_4C_2 + C_1C_5) + q_{33}C_4C_5 + q_{12}C_2 + q_{13}C_5] \\ C &= q_{22}C_1^2 + 2q_{23}C_1C_4 + q_{33}C_4^2 + 2q_{12}C_1 + 2q_{13}C_4 + q_{11} \end{aligned} \quad (40)$$

To make the plot, lines are drawn between the intersections in p-space with points added between the intersections if the curve is an ellipse rather than a straight line.

3. PLOTTING MESH VALUES AND EXAMPLES

Providing the weight window values in the superimposed mesh is straightforward. When drawing the MCNP problem geometry, the particle tracking routines are used to march through the geometry in the plane of the plot frame and put cell numbers or any other specified information in a 100 x 100 grid on the plot frame. In each of these plot grid points, the plotting algorithm simply calls for the weight window value for a specified time or energy at that geometrical point.

Figure 1 provides an illustration of the superimposed mesh plot with weight window values. The underlying problem is an oil-well logging tool benchmark problem. Prior to the superimposed mesh capability, this problem required 277 cells to subdivide the geometry for geometric importances. But here the weight window importance function is superimposed with a cylindrical mesh, and the problem setup requires only 7 geometric cells for the highly-simplified benchmark. Furthermore, the superimposed grid makes it easy to change the geometric specification of the importance function without having to respecify the entire geometry.

Figure 1 shows the well-logging plot with the new MCNP interactive geometry plot point-and-click toggles (Hendricks, 2000). The mesh is controlled by the WW MESH toggle. In Fig. 1 both the cylindrical mesh and well logging tool are in the y-direction and so the superimposed mesh is simply straight lines.

Figure 2 shows a macrobody cylinder (center) in a box with the superimposed cylindrical mesh overlapping it. Figure 3 shows the same problem from a skew orientation. The box still has straight sides and the cylinder now looks like an ellipse. The superimposed mesh also has elliptical surfaces in the R-direction, straight lines for the planes in the Z-direction (which is the Y-direction in the MCNP coordinate system) and a straight line from the center which is the plane defining the start and end of the single mesh in the θ direction.

4. OTHER RELATED CAPABILITIES

In the process of adding the superimposed mesh plotting capability, a number of related upgrades were developed for the next MCNP release version. These are:

Add a weight window scaling factor. Sometimes the generated weight windows that are used in a subsequent problem need renormalization which is now an input feature.

Allow 1 coarse or fine mesh per direction. The MCNP4C weight window mesh requires at least two mesh bins in each XYZ or RZ θ direction. Also, the default is now 1 fine mesh per coarse mesh.

Enable the exponential transform to work correctly with the weight window generator utilizing the superimposed mesh. The exponential transform is a powerful independent variance reduction method which can be used to populate phase space in order to get an initial mesh-based weight window importance function.

Correct some errors in the initial implementation of the weight window mesh, specifically theta mesh indexing, roundoff errors, and inconsistencies between rectangular and cylindrical mesh tracking. The new mesh plotting capabilities are applicable to both the new point-and-click geometry plotting and the old MCNP command mode of plotting (which is required when X Windows is not available.)

5. SUMMARY

The capability to plot superimposed meshes has been added to MCNP. The superimposed importance mesh makes it no longer necessary for MCNP users to finely subdivide geometries for variance reduction purposes. The ability to plot the mesh and its weight windows values makes it possible to more effectively use the superimposed importance mesh capability. The mathematics for plotting the mesh and its values is described here along with a description of other upgrades.

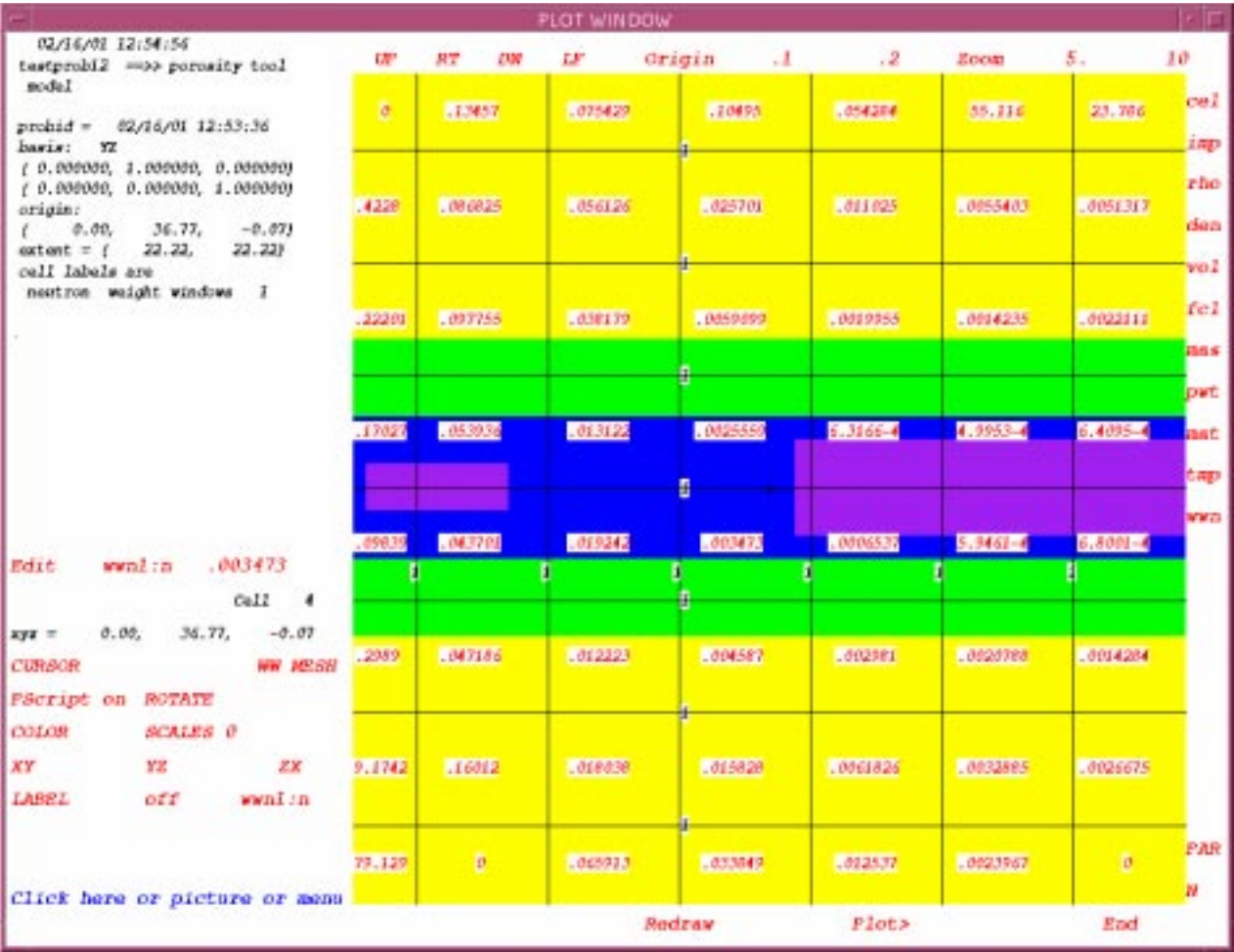


Fig. 1. Superimposed cylindrical mesh overlaying oil-well logging benchmark problem.

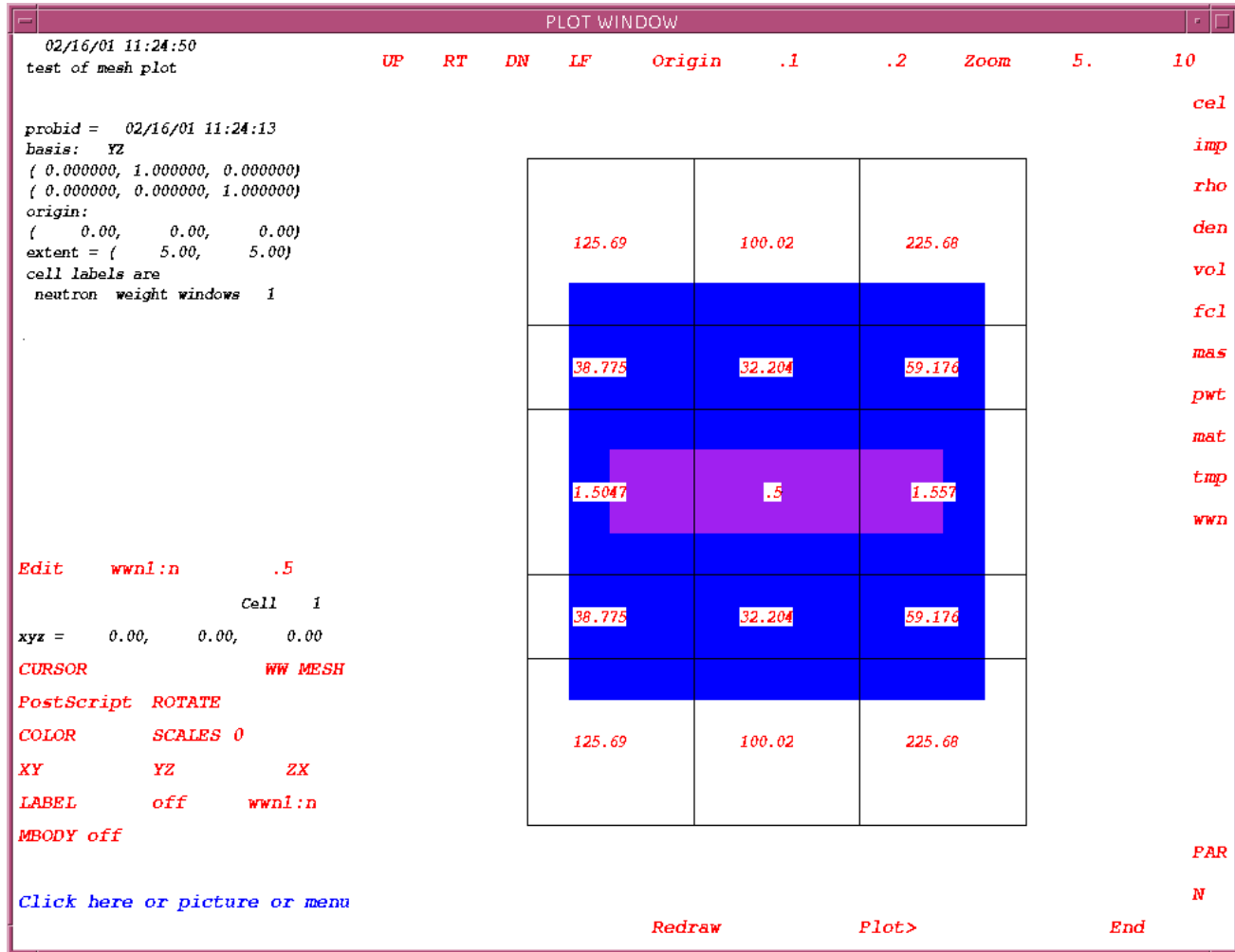


Fig. 2. Can within a box geometry with superimposed cylindrical mesh.

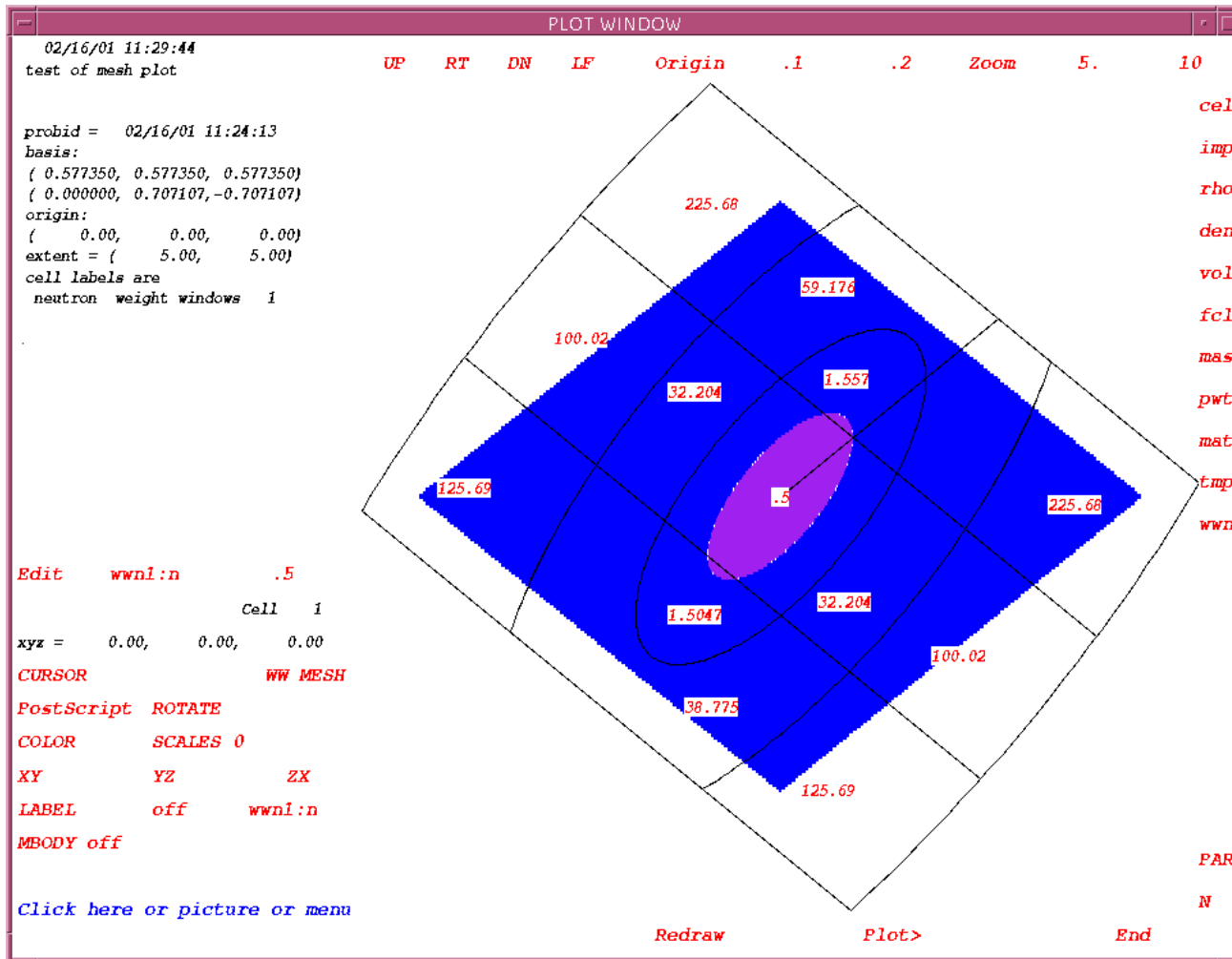


Fig. 3. Plot of Fig. 2 with a skew orientation.

These new capabilities significantly enhance the utility of MCNP.

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