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Material Interface Reconstruction for Monte Carlo Particle Tracking

M. J. O'Brien

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Material Interface Reconstruction for Monte Carlo Particle Tracking

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Matthew O'Brien

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1 Introduction

In this project we implement material interface reconstruction into a large, massively parallel Monte Carlo particle transport code. Here we examine the benefit of resolving a material interface for criticality calculations. Input to the code is a mesh with material and density defined on the mesh. For mesh zones that contain more than one material (**mixed zones**), the old approximation made in the code is to homogenize the material properties of all the materials in the zone. The neutron mean free path is a function of the material density that the neutron is traveling through, so for mixed zones, we use the average density of the zone, rather than reconstructing a material interface, determining which material within the zone the particle is in and using the correct density based on the position of the particle within the zone.

In order to get a better answer, here we implement material interface reconstruction and rather than homogenizing the materials in a mixed zone, we have a material interface divide the zone so we can tell which material the particle is in, based on the particle's position and the location of the material interface.

2 Implementation

As a particle tracks through the mesh, the code determines what is the next event that will happen to the particle. Given the particle's position and velocity, will the particle:

1) have a nuclear reaction with the background material,
2) cross into an adjacent cell or
3) reach the end of the time step.

In order for a particle to know what material that it is in, we added a new event:

4) cross a material boundary.

The distance to each of these events is calculated and which ever is the smallest, the particle is advanced that amount. The particle continues to track until it has reached the end of the time step.
As a pre-processing step, a material interface is reconstructed for every mixed zone. Given the volume fraction information for each mixed zone, and the neighboring cell's volume fraction information, we reconstruct a material interface that has a reasonable shape according to the neighboring volume fractions, and the material interface must preserve volume fraction.

Then as the code is tracking particles, we have a routine to calculate the distance to the next material interface. For zones that have exactly one material (clean zones, a.k.a. pure zone), the routine returns infinity. This is so that this event does not turn out to be the next event to advance the particle. Since the zone is clean, we know the particle must first cross a cell boundary before it crosses a material boundary. For mixed zones, we find the distance from the given particle traveling a give direction to the material interface within the cell. If an intersection is impossible, we return infinity.

We also have implemented a routine that tells you what material within a mixed zone a particle is in. This routine examines the location of the interface and the position of the particle and returns which side of the interface the particle is on.

2.1 Material Interface Reconstruction

In 1D spherical geometry, the interface reconstruction is trivial and we can exactly reproduce the position of the material interface, given only the volume fraction information of the two materials. Let v_f be the volume fraction of the material that is father out radially, let r_0 and r_1 be the inner and outer radial positions of the boundary of the zone. Then the postion of the material interface, r_m, is just the volume weighted average of the radial positions:

$$r_m = [(1 - v_f)r_1^3 + v_f r_0^3]^{1/3}$$

In 2D cylindrical geometry, the material interface reconstruction is non-trivial. The process is divided into 2 steps. First calculate the slope of the material interface segment through a zone. Next, calculate the position of the line, such that it conserves volume.

The slope of the material interface line segment is calculated by taking the gradient of the volume fraction, which gives us the normal of the interface line. We use the method of Parker and Youngs, which uses a 3 by 3 stencil of zones. It first calculates a node-centered gradient, then then 4 nodal values are averaged to a zone centered gradient which is used to define the slope of the line.

The "forward" problem of given a line segment through a zone, find the volume fraction of the two peices that the interface divides the zone into is easier than the "inverse" problem, which is: given the volume fracation and slope of the line, find the position of the line that preserves volume fraction. We use the method described in Scardovelli [2], but instead of using planar area, we must use cylindrical volume.

2.2 Which Material is a Particle In?

We needed to write a routine that determines on which side of the material interface a particle is on. In 1D spherical geometry this is trivial, we just check if the point in question is inside of or outside of the material interface sphere. Given a point a (x, y, z) and a material interface with radius r, to answer if the point is inside the surface, the function returns:

$$x^2 + y^2 + z^2 < r^2$$

Here the $<$ operator returns 1 if the expression is true and 0 if it is false.

In 2D cylindrical geometry we want to know if the particle (x, y, z) is below the line segment $\mathbf{a} = (r_a, z_a)$ to $\mathbf{b} = (r_b, z_b)$. We first "project" the 3D particle to 2D cylindrical coordinates: $\mathbf{p} = (r, z) = (\sqrt{x^2 + y^2}, z)$, now we just check the sign of the cross product of the face segment and the particle position:

$$(\mathbf{b} - \mathbf{a}) \times (\mathbf{p} - \mathbf{a}) > 0$$

2.3 Tracking to a Material Interface

We must write a routine that takes as input the particle position (x, y, z) and normalized direction it is traveling in (α, β, γ), the output of the routine is the distance to the next material interface. In 1D spherical geometry, the distance to a material interface at radius r is attained by solving the following quadratic equation for t:

$$r = \sqrt{(x + \alpha t)^2 + (y + \beta t)^2 + (z + \gamma t)^2}$$

Which is simplified to

$$t^2 + 2(x\alpha + y\beta + z\gamma)t + x^2 + y^2 + z^2 - r^2 = 0$$
$$At^2 + Bt + C = 0$$

This is just a matter of finding the largest positve root, t, of this quadratic equation.

In 2D we represent the material interface as a line segment in cylindrical r-z coordinates. You can think of tracking a 3D particle to a conical surface defined by revolving the line segment around the z-axis, or you can think of projecting the 3D coordintes of the particle to 2D cylindrical coordinates and tracking to a line segment (using the "projection" $(x, y, z)_{3D}$ becomes $(\sqrt{x^2 + y^2}, z)_{2D}$). This is a challenging problem to solve robustly and deal with all of the end cases. Luckily the code already has a 2D cylindrical tracking for unstructured meshes, where the face of each zone is exactly the line segment we are tracking to here. So we just modularize out that part of the tracking and created a routine to track to a conical segment.

3 Results

We consider the double density Godiva criticality calculation. The problem is defined by a Uranium sphere of density 37.48 g/cm^3 with radius 8.7407 cm surrounded by air. We run the problem on two different mesh types, 1D spherical and 2D cylindrical.

3.1 1D Results

To exaggerate the effect of the mixed zone homogenization, we test the problem using 1D spherical geometry, defined by 3 zones. The endpoints of the zones are at 0, 1, 11, and 12 cm. So the zone from 1 to 11 cm has the Uranium-Air interface in it at radius 8.7407. The old homogenization approximation will make this a zone of density 18.79 g/cm^3. The new material interface reconstruction method will know the position of the interface and will use the correct material density, based on the position within the zone. As a comparison problem, we introduce a mesh line exactly at the interface, 8.7404 cm so that all zones are clean. Here there is no mixed-zone approximation since all zones have exactly one material in them.

We run this problem 4 different ways, the first one **"Original"** is running the code before we have implemented material interface reconstruction. The next way is **"MIR off"**, this is after we have implemented MIR, but turning the option off. We run these two cases to make sure that we get exactly the same answer to confirm that we haven't changed anything when we have added the code for the model, but turn the model off. The next way we run the problem is **"MIR on"**, which is enabling the MIR model so we should get exactly the same answer as the last way of running the problem which is **"All pure"**, where we have inserted a mesh line at the material interface so all zones have exactly one material in them.

The output of the calculation is two numbers, **Alpha** and **K effective**. Alpha is defined to be a neutron population growth constant. The neutron population as a function of time is $N(t) = N_0 e^{\alpha t}$. The code

finds the alpha value which makes that equation true. A system is super critical if K effective is greater than 1, and it is sub-critical if K effective is less than 1.
Here we present results for this test problem run with 100,000 particles, 1,000,000 particles and 10,000,000 particles. We have asked the code to stop iterating when the standard deviation of K effective is less than 2.0e-3.

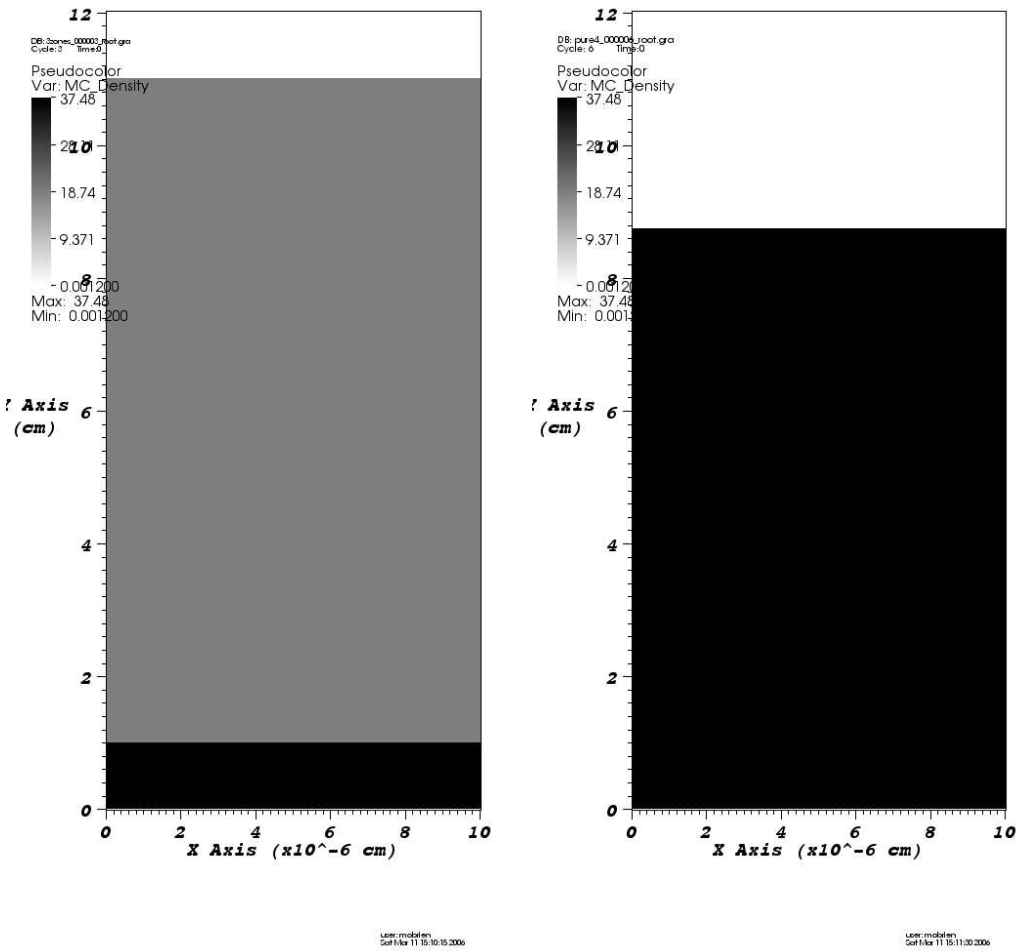

Figure 1: **1D Spherical Double Density Godiva Problem.** These figures show the density as a function of radius for the Double Density Godiva Problem. In the first picture the density of the mixed material zone is homogenized based on the volume fraction and density of each material in the zone. The second picture resolves the material interface and has the correct density everywhere based on the problem definition: a Uranium sphere of radius 8.7407 cm and density 37.48 g/cm^3 surrounded by air of density 1.2e-3 g/cm^3. There are 3 zones in this problem with mesh points at 0, 1, 11 and 12 cm.

3.2 2D Results

A 1D material interface reconstruction method was done first so that we could work out the issues with the infrastructure of the code so that it could deal with the concept of a particle being associated with a particular material within a mixed material zone. The 2D cylidrical geometry exercises the challenges of

Description	Alpha +/- stddev	K effective +/- stddev
Original	3.278799e+07 +/- 3.0302e+05	1.251037e+00 +/- 2.2178e-03
MIR off	3.278799e+07 +/- 3.0302e+05	1.251037e+00 +/- 2.2178e-03
MIR on	1.486620e+08 +/- 5.4121e+05	1.865066e+00 +/- 2.5711e-03
All pure	1.486620e+08 +/- 5.4121e+05	1.865066e+00 +/- 2.5711e-03

Table 1: **1D MIR on vs. MIR off comparison.** Results for double density Godiva 1D spherical test problem. All of these problems were run with 100,000 particles. Note that "Original" and "MIR off" match exactly which means that the new coding introduced does not affect the answer when the MIR model is turned off. Note that "MIR on" and "All pure" give exactly the same answer, which means that we have correctly implemented a MIR algorithm so that a particle knows which material it is in, when it is in a mixed-material zone. The Original model which homoginizes mixed zones does not give you the correct Alpha or K effective value. But when when enable the MIR feature, we get the correct Alpha and K effective values.

Description	Alpha +/- stddev	K effective +/- stddev
Original	3.284098e+07 +/- 1.4022e+05	1.251507e+00 +/- 9.4127e-04
MIR off	3.284098e+07 +/- 1.4022e+05	1.251507e+00 +/- 9.4127e-04
MIR on	1.500315e+08 +/- 5.2192e+05	1.873261e+00 +/- 3.0796e-03
pure	1.500315e+08 +/- 5.2189e+05	1.873260e+00 +/- 3.0800e-03

Table 2: **1D MIR on vs. MIR off comparison.** Results for double density Godiva 1D spherical test problem. All of these problems were run with 1,000,000 particles. The same comments apply here as did in the 100,000 particle caption.

reconstructing a material interface.

Description	Alpha +/- stddev	K effective +/- stddev
Original	3.288469e+07 +/- 5.0221e+04	1.251864e+00 +/- 3.4762e-04
MIR off	3.288469e+07 +/- 5.0221e+04	1.251864e+00 +/- 3.4762e-04
MIR on	1.498710e+08 +/- 3.8049e+05	1.871273e+00 +/- 2.3993e-03
pure	1.498710e+08 +/- 3.8048e+05	1.871273e+00 +/- 2.3993e-03

Table 3: **1D MIR on vs. MIR off comparison.** Results for double density Godiva 1D spherical test problem. All of these problems were run with 10,000,000 particles. The same comments apply here as did in the 100,000 particle caption.

Description	Alpha +/- stddev	K effective +/- stddev
Original	1.465474e+08 +/- 4.8169e+05	1.824163e+00 +/- 1.9888e-03
MIR off	1.465474e+08 +/- 4.8169e+05	1.824163e+00 +/- 1.9888e-03
MIR on	1.500416e+08 +/- 7.5244e+05	1.832684e+00 +/- 2.5128e-03

Table 4: **2D MIR on vs. MIR off comparison.** Results for double density Godiva 2D test problem. All of these problems were run with 100,000 particles. This problem was run 3 ways. "Original" means run with homoginized mixed zones, before we ever implemented a MIR model. This is used as a baseline calculation to compare "MIR off" to so that we know that we did not introduce and bugs or changes in the coding added for the MIR model, but when the model is turned off. Note that these two results are identical. Then we ran "MIR on" which is when we reconstruct the material interface and particles know which material they are in when they are in mixed material zones. Note that get we a larger Alpha value and a large K effective value which is what you would expect since the Uranium is more concentrated, rather than being averaged with the surrounding air to end up with a low density "layer of fuzz" around the Uranium sphere. Note that the improvement we see with MIR on vs. MIR off is a much smaller affect here than in the 1D case since our zones size is smaller here, so we are homoginizing over a smaller volume.

References

[1] Cullen, D., Clouse, C., Procassini, R., and Little, R. *Static and Dynamic Criticality: Are They Different?.*
LLNL Report, Novemer 2003.

[2] Scardovelli, R., and Zaleski, S. *Direct Numerical Simulation of Free-Surface and Interfacial Flow.*
Annu. Rev. Fluid Mech. 1999. 31:567-603

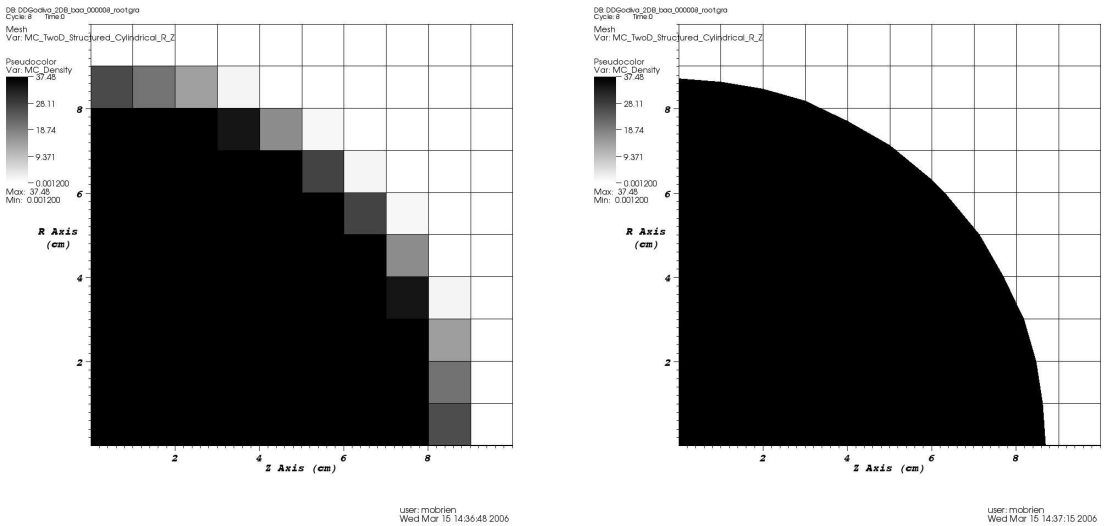

Figure 2: **2D Cylindrical Double Density Godiva Problem.** These figures show the density for the Double Density Godiva Problem. In the first picture the density of the mixed material zones is homogenized based on the volume fraction and density of each material in the zone. The second picture resolves the material interface and has the correct density everywhere based on the problem definition: a Uranium sphere of radius 8.7407 cm and density 37.48 g/cm^3 surrounded by air of density 1.2e-3 g/cm^3. The mesh size is 1cm, and goes from 0 to 10 cm in both the r and z directions.

Description	Alpha +/- stddev	K effective +/- stddev
Original	1.468281e+08 +/- 2.1640e+05	1.826074e+00 +/- 7.3060e-04
MIR off	1.468281e+08 +/- 2.1640e+05	1.826074e+00 +/- 7.3060e-04
MIR on	1.488079e+08 +/- 2.6765e+05	1.826962e+00 +/- 1.1860e-03

Table 5: **2D MIR on vs. MIR off comparison.** Results for double density Godiva 2D test problem. All of these problems were run with 1,000,000 particles. The same comments apply here as did in the 1,000,000 particle caption.

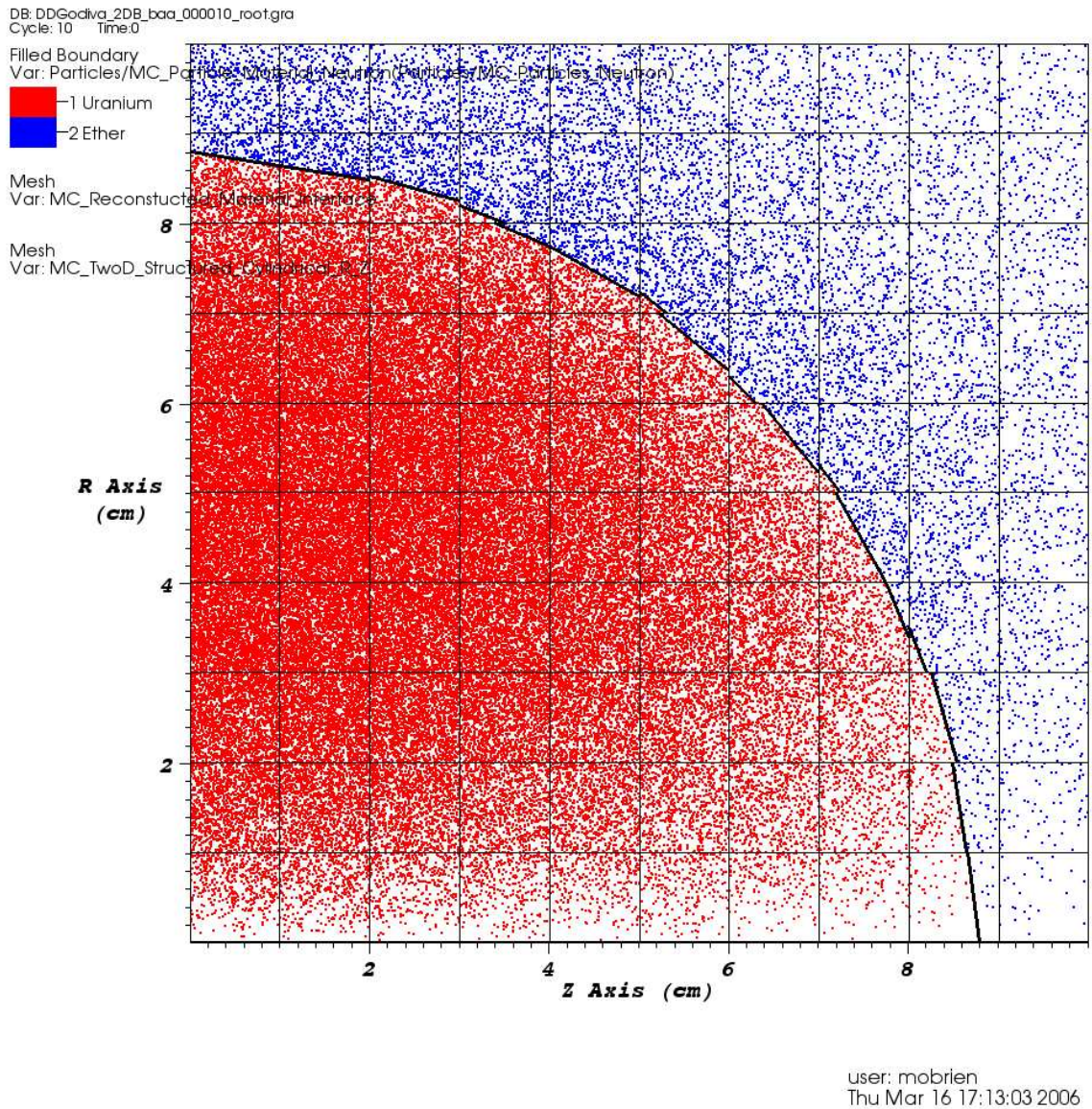

Figure 3: **2D Cylindrical Double Density Godiva Problem.** This figure shows the particle positions colored by which material they are in. Red particles are in Uranium, blue particles are in air. We also see the piecewise linear material interface drawn in a bold black line. This is the material interface that we reconstructed using volume fraction information. The particle now knows which material it is in, when it is in a mixed-material zone, so the code can use the correct material density when determining how far a particle will travel before colliding with the background material.

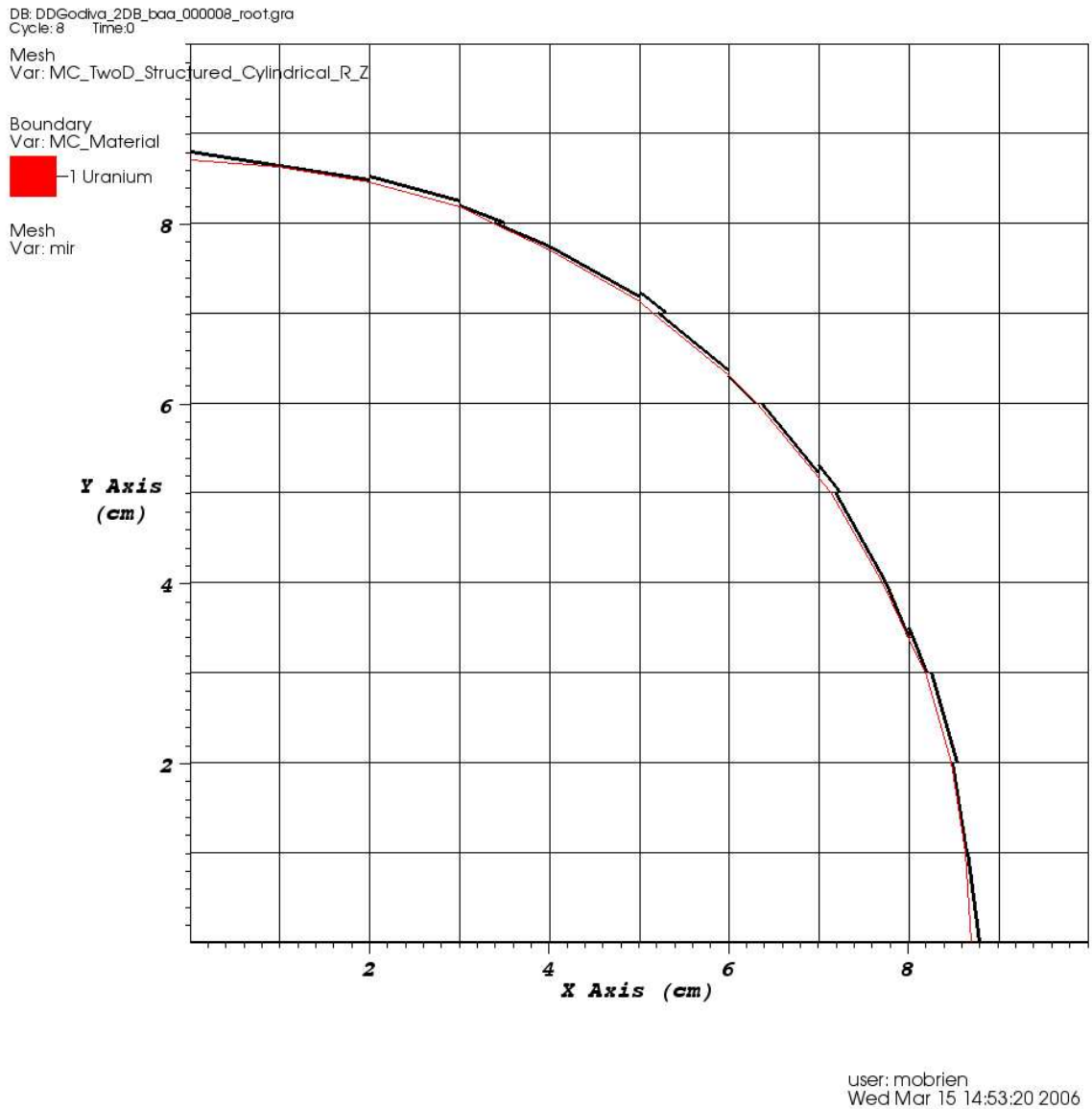

Figure 4: **MIR Comparison.** This figure shows a comparison of the material interface reconstruction method used in the particle tracking code (**bold black line**) with the material interface reconstructed from the Visit graphics program (red line). Note that the interface constructed by the Visit graphics program is continuous. But this method does not preserve volume fraction, this is acceptable for visualization, but unacceptable for physical modeling. The Visit method also uses planar area while the method used for particle tracking uses cylindrical volumes, so the planar area is weighted by a radial factor.