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MAGNETIC FIELD TRACKING WITH MCNP5

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Abstract

With the introduction of continuous-energy heavy charged particle transport in MCNP5, the need for tracking charged particles in a magnetic field becomes increasingly important. Two methods for including magnetic field effects on charged particles are included in the proton transport version of the code. The first technique utilizes transfer maps produced by the beam dynamics simulation and analysis code COSY INFINITY. This method is fast and accurate; however, its use is limited to void cells only and to ensembles of particles with a fairly small energy spread. The second technique, particle ray tracing, is based on an algorithm adopted from the MARS transport code. This method can be applied to both void and material cells and is valid over a very large range of particle energies. Results from tracking particles in a quadrupole "identity lens" using the two techniques are compared.

INTRODUCTION

Tracking of particles in the presence of magnetic fields is a highly desirable feature for charged particle transport codes. Many codes[(1-3)] transport charged particles in magnetic fields with ray tracing techniques that use numerical integration methods incorporated into the code. The implementation of magnetic field tracking into the proton transport version of MCNP5[(4,5)] is unique in that it not only includes the particle ray tracing method, but also allows for the use of transfer maps produced by a separate beam optics code. In addition, for the ray tracing method, MCNP5 includes an option that simulates third-order aberrations caused by fringe field effects for quadrupole magnets by providing edge kicks for particles entering and exiting the magnet faces. This latter feature is especially important for proper particle transport through proton radiography beam lines and magnetic lenses.

MAGNETIC FIELD TRACKING METHODS

Transfer Maps

A previous version of MCNP was modified to transport charged particles using magnetic field transfer maps generated by the COSY INFINITY code[(6,7)]. COSY INFINITY is a beam optics computer code that utilizes numerical integration and differential algebraic techniques to generate transfer maps based on a Taylor series expansion of a particle's canonical variables. These transfer maps represent the functional relation between the phase-space coordinates of a particle that has passed through a region of magnetic field and its phase-space coordinates before entering the field region.

In the transfer map approach to particle transport, the actual trajectories that the protons follow through the field region do not appear explicitly; in applying pre-computed maps, charged particles are transported from an initial location to a final location in one step by applying the transfer maps to the initial phase space coordinates.

Although the COSY map method provides a fast and accurate method for transporting charged particles in magnetic fields, the transfer map method has several limitations. First, map methods can only be used in void regions. In addition, the Taylor expansions used in applying the maps have a finite volume of convergence in phase space. The convergence volume has a very complicated shape in five dimensions, requiring that the shape of the phase-space volume and the order of the Taylor series needed in order to get a given accuracy in final particle position is not easily predicted in practice and can be checked only by particle tracking. For example, a map to fifth order in energy deviation might be applied with good accuracy to particles with energies within 10% of the reference energy, but not to those with 50% deviation.

Particle Ray Tracing

To overcome these limitations of the use of transfer maps, MCNP5 has also implemented direct magnetic field tracking utilizing numerical integration methods. These routines were adopted from the MARS high-energy particle transport code.(8) Tracking in a void and material is performed by a higher-order numerical integration algorithm, with a maximum step size controlled by the user. Within a step, the trajectory is approximated by a segment of the helical trajectory corresponding to a constant field equal to the field at the midpoint of the step, i.e., the field variation within the step is neglected. A solution of a 3-dimensional equation of trajectory in such a field provides the new direction cosines and new particle coordinates at the end of the step. With appropriate parameters, this algorithm provides extremely high accuracy of tracking.

The magnetic field tracking option is implemented through the use of a new input data card, BFLD. Using this card, the user specifics the type of field (currently only a constant or quadrupole magnetic field), the field (or gradient) strength and direction, the cell(s) that contain the magnetic fields, and the maximum step size and/or deflection angle. Future enhancements planned for MCNP5 include additional built-in models to represent higher order multipole magnets as well as providing a mechanism for the use of a user-defined magnetic field subroutine.

The two types of magnetic fields described above, the constant field and quadrupole field, are hard-edge models; the fields abruptly begin and end at the edges of the magnetic field cell with no consideration taken for the effects of the magnet fringe fields. These are idealized models that do not exist in nature. The effect of magnet fringe fields on a particle's motion can be approximated by applying hard-edge kicks to the particle as it enters and leaves the magnetic field cell. An option for edge kicks has been implemented for the quadrupole magnetic field model. For a particle traveling along the *z*-axis, the following equations describe the position and momentum jumps applied to a particle as it enters the upstream fringe field of a quadrupole(9):

$$\delta x = \frac{Gq}{p}\left[\frac{x^3}{12} + \frac{xy^2}{4}\right] \tag{1}$$

$$\delta t_x = \frac{Gq}{p}\left[\frac{xy}{2}t_y - \frac{x^2+y^2}{4}t_x\right] \tag{2}$$

$$\delta y = -\frac{Gq}{p}\left[\frac{y^3}{12} + \frac{x^2 y}{4}\right] \tag{3}$$

$$\delta t_y = -\frac{Gq}{p}\left[\frac{xy}{2}t_x - \frac{x^2+y^2}{4}t_y\right]. \tag{4}$$

In these equations, t_x and t_y are the direction cosines of the momentum vector. The quantity G is the quadrupole gradient (in T/m) and p/q is the particle rigidity (in T-m). In order on conserve energy, t_z is also recalculated using the formula

$$t_z = \sqrt{1 - t_x^2 - t_y^2}\ . \tag{5}$$

For particles passing through the downstream fringe field of a quadrupole, the expressions are the same, except that Gp/q is replaced everywhere by $-Gp/q$.

The quadrupole fringe-field edge-kick model is also implemented on the BFLD card. In addition to specifying the magnetic field cells and the magnetic field parameters, the user must supply the surface numbers of the magnet edges to which the edge kick is applied. The edge kick model is valid for only the bore region of the quadrupole magnet, up to and including the beam pipe.

TESTING

Constant Magnetic Field

A simple and straightforward test of the direct tracking method for magnetic fields is to track a charged particle in a constant magnetic field in a vacuum. In a constant magnetic field, a particle will travel in a circle whose radius is determined by the well-known formula $P = QBr$, with P representing the particle momentum, Q the charge of the particle, B the magnetic field strength, and r equal to the radius of curvature of the particle track.

A test problem was created in which protons were started at the origin along the $+z$-axis and immediately entered a cell with a constant magnetic field in the $+x$ direction. The cell was large enough so that the proton track would complete a half circle and exit the cell at the surface $z = 0$. Protons with several energies and magnetic field strengths were tested. The radius of the circle the particle traveled was compared to the analytical value. In addition, the direction cosines of the proton as it crossed the $z = 0$ plane were examined.

In all cases, the radius of the circle traveled by the proton matched the analytical value to within the expected small numerical integration error. This result was consistent for the proton energy range of 10 keV to 100 GeV and for magnetic fields ranging from 0.01 T to 30 T. Also, the y direction cosine of the particle as it crosses out of the cell was generally within the range $\pm\ 10^{-11}$, very close to the expected value of zero. Several values of the maximum step size and the maximum deflection angle were used, and in all cases, the radius of curvature was the same, although the direction cosine of the y coordinate did vary from -10^{-9} to 10^{-11}, if the maximum deflection angle was set to 10 mrad.

Quadrupole Lens Testing

The main driver for the implementation of magnetic fields into MCNP5 has been to simulate proton radiography experiments. Therefore it is appropriate that the testing of the quadrupole magnetic field tracking routines be performed on a proton radiography beam line. For this work, the beam line and quadrupoles used for Experiment E955 on the Alternating Gradient Synchrotron at Brookhaven National Laboratory was modeled in MCNP5[10]. One aspect of the proton radiography magnetic lenses used to date is that they represent a minus identity lens, in which particles that have been scattered via multiple Coulomb processes in passing through an object are refocused to a point on the image plane with transverse phase-space coordinates that are (to first order) the exact negative of the object-plane transverse coordinates.

The minus-identity lens system used for the Brookhaven E955 experiment consists of a total of eight quadrupole magnets, set up as a pair of repetitive cells. Each cell contains two pairs of quadrupoles, each individual magnet in each pair having the same field gradient, and the two pairs having equal but opposite gradients. The total length of the lens, including drift sections, is 20.964 m. This lens system was aligned along the $+z$-axis. Transfer maps for each individual quadrupole were created using COSY INFINITY. These maps included a soft-edge fringe-field approximation model with up to fifth-order terms.

Particles were started on the object plane ($z = 0$) at the origin, and from evenly spaced positions on two circles (radii equal to 2 cm and 6 cm) centered at the origin. To simulate the proton radiography experiments, each particle was given an initial direction such that $\theta_x = k_x x$, $\theta_y = k_y y$, $k_x = 0.17500935$ radians per cm, and $k_y = - k_x$ (this correlation greatly reduces the chromatic and geometric aberrations in this lens)[10]. The proton energy was set equal to 23.08 GeV, the energy for which the COSY maps were calculated. For the particle ray tracing tests, the quadrupole field gradient was set to 11.633412 T/m, which was also determined by the COSY INFINITY code. For these runs, the fringe-field edge-kick model was used.

Two series of runs were performed for each of the magnetic field tracking methods. In the first series, the particles were given an initial direction as described above. To simulate multiple Coulomb scattering of protons in an object, in the second series of runs the particles' initial directions were given an additional 5 mrad angle component as compared to the initial directions used in the first set of runs. To obtain a complete picture of the scattering effect, 2000 particles were run with the 5 mrad cone angle for each point.

The location at which the particles crossed the image plane ($z = 20.964$ m) was compared to the location at which they would have crossed the image if the magnetic lens system was a perfect inverting lens. The average distances between the expected and actual locations on the image plane are listed for each circle in Table 1. These results show that the distances from the expected results are greater the further from the origin the particles start, and for particles with the 5 mrad cone angle. These differences from the perfect lens system are due to higher order aberrations caused by the fringe fields of the magnets. The small differences between the two magnetic field tracking methods are caused by the different fringe-field models used. The transfer maps incorporated a soft-edge fringe-field model while the direct tracking used a hard-edge model with edge kicks.

Table 1

	Average Distance Between Expected and Actual Image Locations (μm)			
Source Distance From the Origin (cm)	0 mrad Cone Angle		5 mrad Cone Angle	
	Transfer Map	Direct Tracking	Transfer Map	Direct Tracking
0	0	0	27.1	28.7
2	0.54	0.58	42.5	44.9
6	16.0	18.1	146.	154.

The results of these tests are shown graphically in Figure 1. In order to make the higher order aberrations more visible, the spot sizes have been exaggerated by a factor of 100. Instead of x_{img} and y_{img}, the quantities $x_{scaled} = x_{img} + 100\ (x_{img} + x_{obj})$ and $y_{scaled} = y_{img} + 100\ (y_{img} + y_{obj})$, are plotted, where x_{obj} and y_{obj} are the starting locations of the matched ray on the object plane. Recall that for a perfect lens system, $x_{img} + x_{obj}$ and $y_{img} + y_{obj}$ would equal zero. Also shown is the location of the matched ray (0 cone angle) on the image. This graph not only shows the differences between the transfer map and the direct tracking methods, but the similarity of the shapes between the two methods demonstrate their compatibility.

The effect of the higher-order terms on a particle's motion can be demonstrated by removing these terms from the transfer maps, or by turning off the edge kicks in the particle ray tracing method. Figure 2 is a expanded view of Figure 1, centered on image location x = 5.19615 cm, y = 3.0 cm. For this figure, four separate runs of the matched ray with a 5 mrad cone angle are displayed. Two cases of the COSY transfer map technique are shown, one with the full transfer maps calculated to fifth order, and one using the transfer maps only to first order. Also, two cases of the direct magnetic field tracking are shown, one with and one without the edge-kick model. This figure clearly shows the differences between the hard-edge model with and without edge kicks. As can be seen, the edge-kick model closely tracks with the transfer map method with higher order terms. The differences between the first-order transfer map and the direct tracking methods without the edge-kicks are due to a combination of integration method limitations and differences in focusing effects of the two models. The contribution of the fifth-order terms in the COSY map to the difference between the hard-edge third-order tracking and fifth-order soft-edge COSY model is believed to be small, since a comparison of tracking with fifth-order *vs*. third-order COSY maps with the same soft-edge fringe-field model showed little difference between them.

SUMMARY

Two methods of tracking charged particles in magnetic fields have been implemented into MCNP5. The direct tracking method uses numerical integration techniques to track a particle through the magnetic field. Transfer maps based on Taylor series expansions of the particle's canonical variables provide a quick and accurate method to transport particles down a straight-axis beam line. To include the effects of third-order aberrations caused by fringe fields in the direct tracking method, a hard-edge quadrupole model with edge kicks has been implemented. Comparison studies have shown that the edge kick model produces results similar to fifth-order transfer maps for minus identity quadrupole lens.

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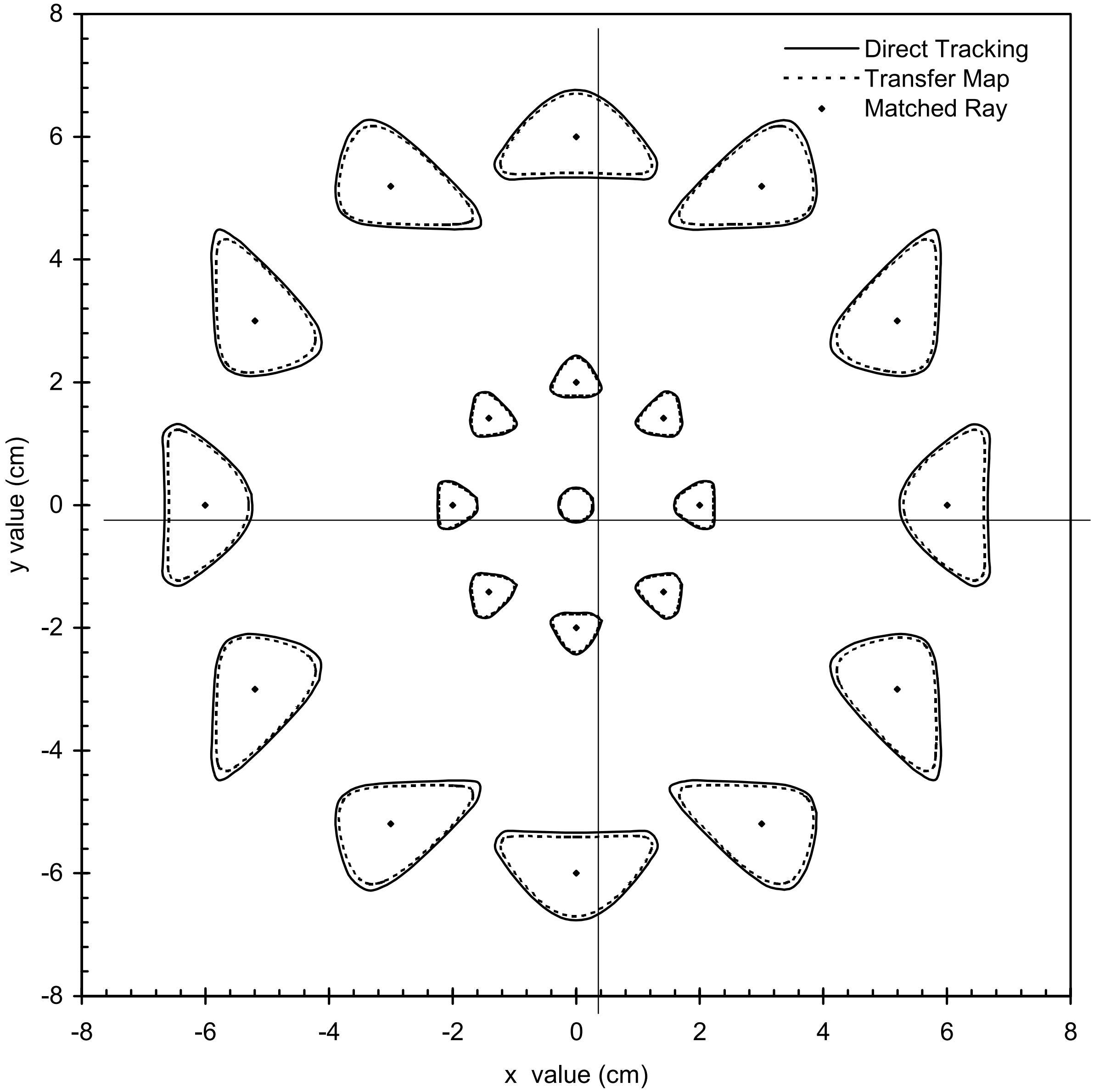
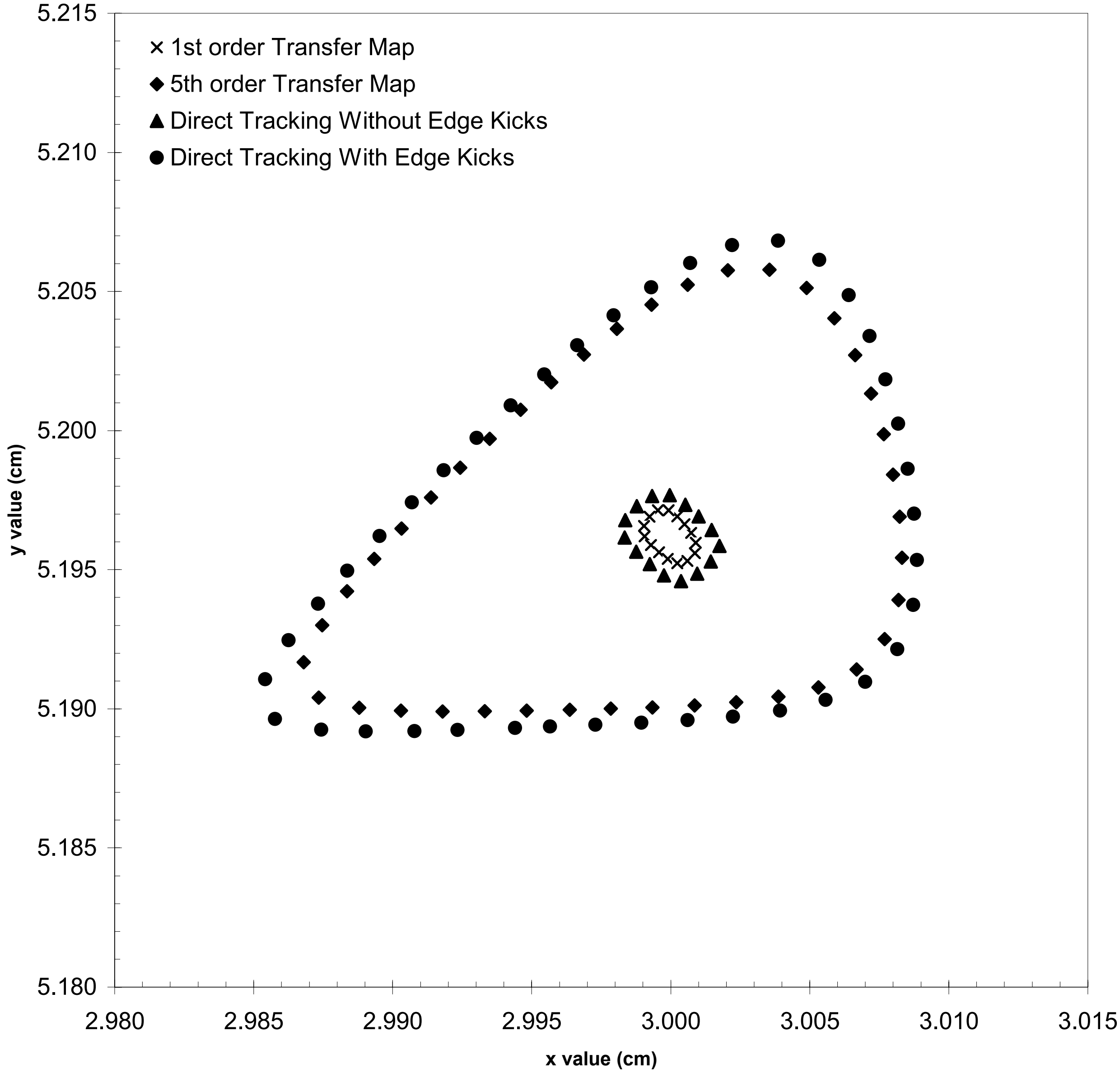
Figure Captions

Figure 1. Plot of scaled image plane patterns for matched rays with a 5 mrad cone angle for the two magnetic field tracking methods. The scaling exaggerates the actual patterns by a factor of 100.

Figure 2. Plot of matched ray locations on the image plane for rays beginning at x = -5.19615 cm, y = -3.0 cm, showing the effects of higher order terms and edge kicks on the magnetic field tracking methods.



Direct Tracking
Transfer Map
Matched Ray
y value (cm)
x value (cm)
8
6
4
2
0
-2
-4
-6
-8



× 1st order Transfer Map
◆ 5th order Transfer Map
▲ Direct Tracking Without Edge Kicks
● Direct Tracking With Edge Kicks
y value (cm)
x value (cm)
5.215
5.210
5.205
5.200
5.195
5.190
5.185
5.180
2.980
2.985
2.990
2.995
3.000
3.005
3.010
3.015