MCNP:

Current Capabilities and Future Plans

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MCNP is a Monte Carlo computer code used to solve the linear Boltzmann transport equation in general 3D geometry. The code has been used worldwide for nearly 30 years to analyze neutron, photon, and electron transport in nuclear reactors, medical applications, radiation shielding, oil-well logging, health physics, radiotherapy, nuclear waste disposal, design and analysis of experiments, and many other applications. MCNP has a lineage extending directly back to the original Monte Carlo work by von Neumann and others at Los Alamos in the late 1940s.

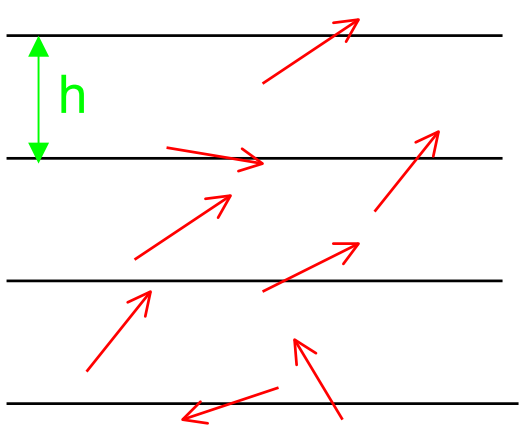
This presentation will briefly describe the history of the Monte Carlos method and MCNP. Several applications of MCNP will be presented, including use in medical treatment planning and shielding calculations. Finally, some current development work in progress will be described.

Outline

- MCNP Overview
- Applications
- New Features
- Research and Development

Monte Carlo methods are algorithms for solving various kinds of computational problems by using (pseudo)random numbers

- **Buffon's needle (1777)**
  - **Determine the value of π experimentally by dropping a needle on ruled paper.**



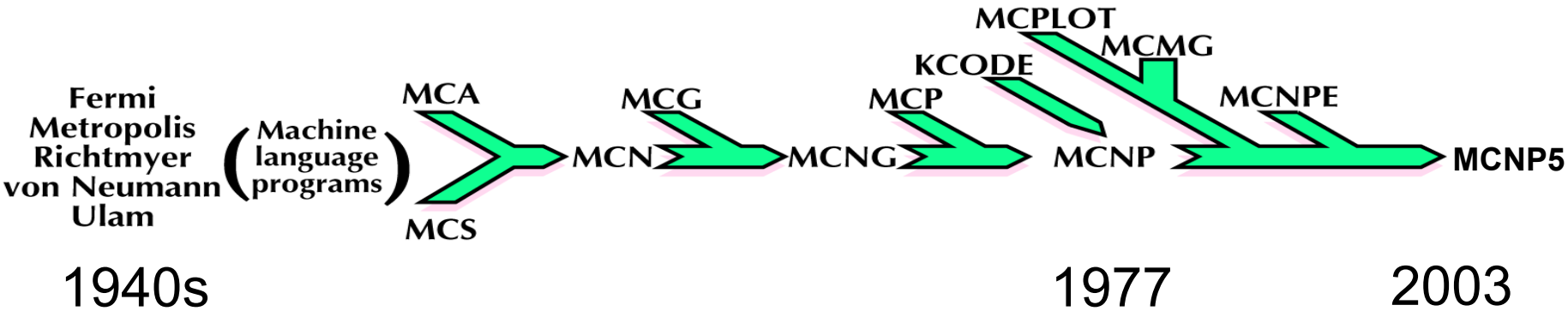
For needle of length l,

$$\pi = \frac{2lN_{tosses}}{hN_{hits}}$$

Simulate neutron, photon, & electron transport using the Monte Carlo method

- Particles
  - Neutrons, n: 10^{-5} eV - 150 MeV
  - Photons, p: 1 KeV - 100 GeV
  - Electrons, e: 1 KeV - 1 GeV
- Problem modes
  - Single particle type: n, p, or e
  - Coupled calculations: n/p, n/p/e, p/e, e/p
- Many code options
  - Fixed source & eigenvalue problems
  - Generalized source & tallies
  - Numerous variance reduction techniques
  - Forward or multigroup adjoint solutions
  - Time dependent

MCNP - History



- **Monte Carlo transport of neutrons, photons, & electrons**
  - **General 3D geometry**
  - **Continuous-energy physical data**
  - **Many code options: Keff, detectors, variance reduction, tallies, …**
- **MCNP = direct descendant of pioneering work by von Neumann, Ulam, Fermi, Richtmyer, & Metropolis**
- **For more than 25 years, MCNP & its data libraries have been developed and supported by the Monte Carlo team in X-Division at Los Alamos**
  - **Continued strong support for MCNP provides funding for R&D activities in many diverse areas of Monte Carlo methods**

General purpose transport

- "Exact" geometry
  - 3D surface-sense geometry, including all 1st & 2nd degree surfaces plus elliptical torus
  - MORSE/KENO-type "macrobodies" (box, sphere, cylinder, etc.)
  - Lattices & repeated structures, can be nested many levels
  - Intersection, union, & complement boolean operators

- Best-available physical data
  - Continuous energy physical data for all reactions, angular distributions, secondary particle production, etc.
  - Extensive list of ENDF/B-V, -VI isotopes
  - Multigroup option available for comparison with deterministic codes

Monte Carlo method for simulating radiation transport - Common sense approach – simulate reality

- Monte Carlo method generates a set of particle tracks and follows them according to the statistical rules of the cross section database.
- **Physics:** Macroscopic cross sections interpreted as the probability that certain interactions occur and the probability that certain outcomes happen after an interaction.
- **Geometry:** Ray-tracing through "exact" model of problem geometry to determine location of interactions.
- **Tallies:** Bookkeeping, record how often certain events occur during the simulation.
- The Monte Carlo simulation is exactly analogous to the experimenter counting particles (if we have the “physics” right.)

MCNP Development Team

- The Diagnostics Applications Group (X-5) continues to develop & support MCNP
  - 12 MCNP code developers in X-5
  - Nuclear Data team also in X-5
  - Two application teams in X-5

X-5 Monte Carlo Development

Jeremy Sweezy (Team Lead)

Tom Booth	Forrest Brown	Jeffrey Bull
Art Forster	Tim Goorley	Grady Hughes
Russell Mosteller	Richard Prael	Avneet Sood
Tony Zukaitis	Marsha Boggs	

X-5 Nuclear Data Team

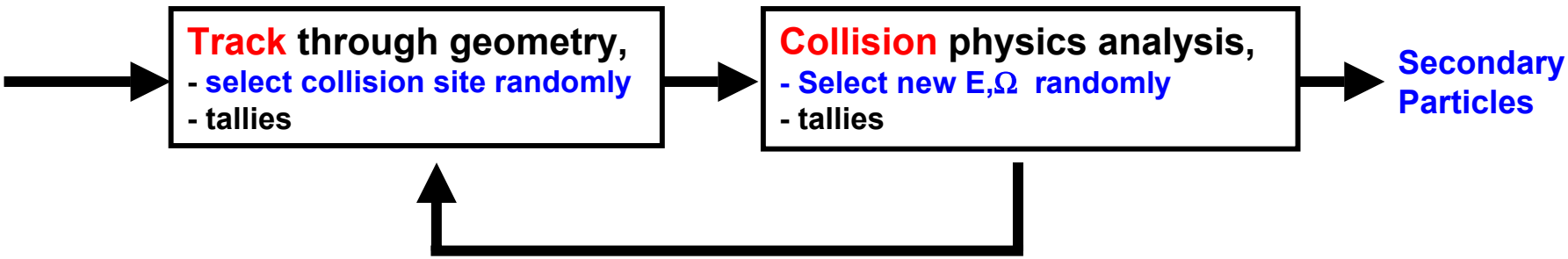
Robert Little	Stephanie Frankle
Morgan White	Stepan Mashnik

University R&D	William Martin	Anil Prinja	Taro Ueki
High-Energy Physics	Nikolai Mokhov	Sergei Striganov	
Visual Editor	Randy Schwarz	Lee Carter	
Manuals & Web Pages	Sheila Girard	Cheryl Royer	

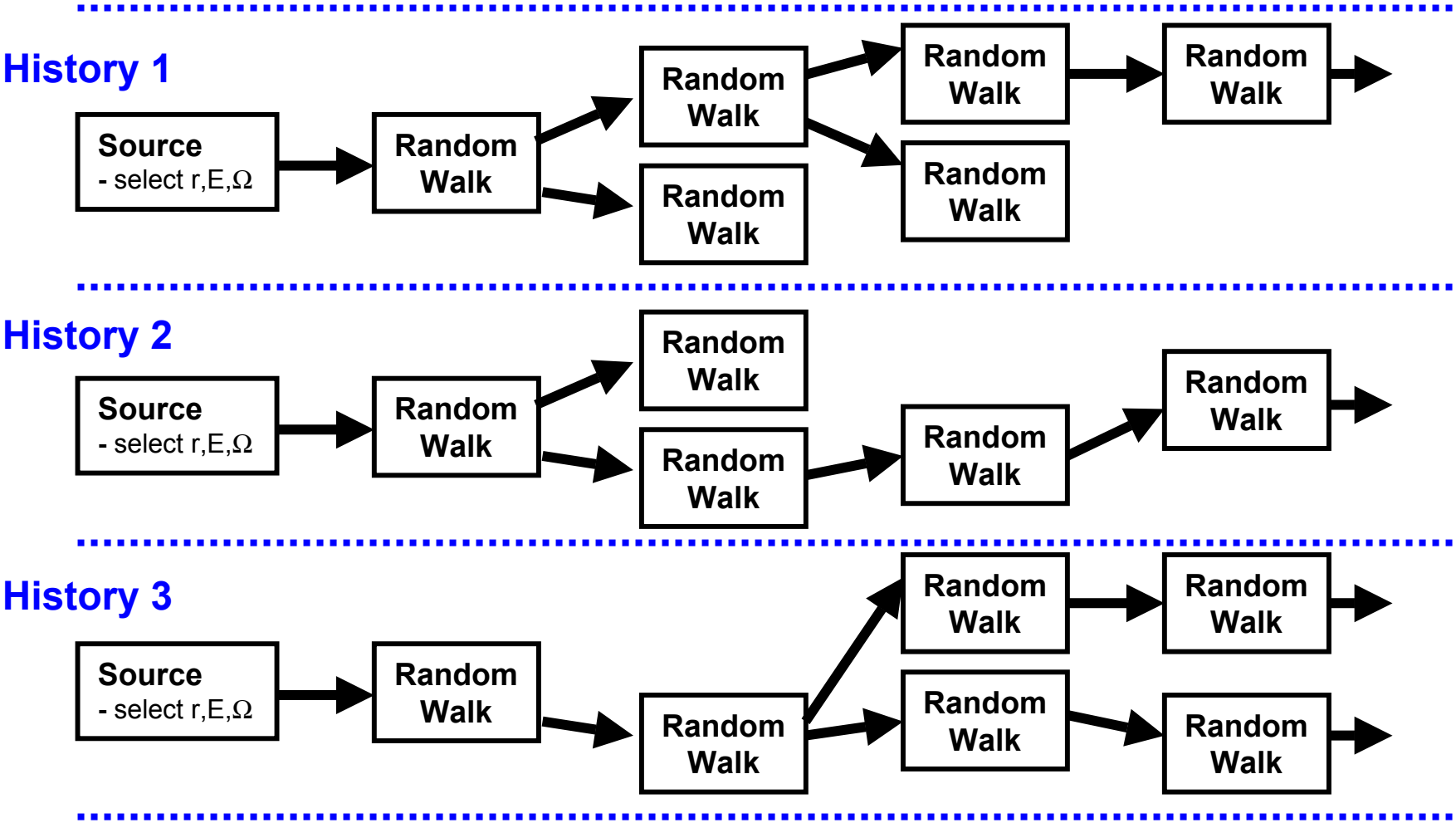
Simulation approach to particle transport:

Faithfully simulate the history of a single particle from birth to death.

- **Random-walk for a single particle**
  - Model collisions using physics equations & cross-section data
  - Model free-flight between collisions using computational geometry
  - Tally the occurrences of events in each region
  - Save any secondary particles, analyze them later



Fixed-source Monte Carlo Calculation



What Can MCNP Do?

Detailed modeling of geometry & physics interactions

- General 3D combinatorial geometry using quadric surfaces
- Repeated structures
- Lattice geometries
- Macrobodies (primitive shapes) with CSG
- Surface sources for large & repetitive problems
- Geometry, cross section, tally plotting
- ENDF/B-VI physics interaction data

Calculate nearly any physical quantity

- Flux
- Current
- Energy deposition
- Charge deposition
- Heating
- Reaction rates
- Response functions
- Radiography images
- Mesh tallies
- K-effective
- Prompt neutron lifetime
- Fission distributions
- η, ν
- $\bar{E}$ of neutrons causing fission
- Neutron balance per cell and nuclide

What Can MCNP Do?

Very general & flexible tallies

1. Surface current
   - number
   - energy
2. Surface flux estimator
3. (not used)
4. Volume flux (track length)
5. Point or ring detector
6. Particle heating
7. Fission heating
8. Pulse height tally
   - Energy deposition spectrum
   - Energy deposition
   - Charge deposition
9. Mesh tallies - flux & reaction rates

Many variance reduction techniques

1. Time, energy, & weight cutoffs
2. Geometry splitting & roulette
3. Weight windows (and weight window generator)
4. Exponential transform
5. Forced collisions
6. Energy splitting & roulette
7. Time splitting & roulette
8. Next-event estimators - Point and ring detectors
9. DXTRAN
10. Implicit absorption
11. General source biasing
12. Secondary particle biasing
13. Bremsstrahlung energy biasing

What Can MCNP Do?

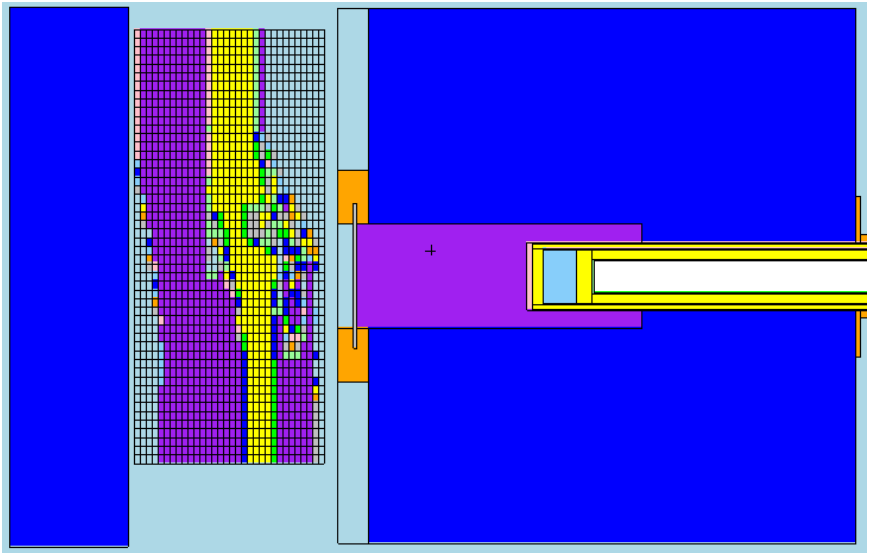
Applications

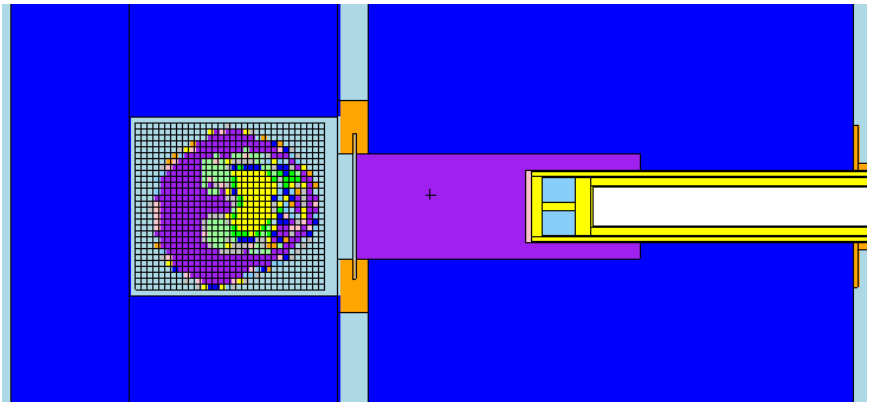
- Nuclear Criticality Safety
- Radiation Shielding
- Detector Design and Analysis
- Nuclear Well Logging
- Personnel Dosimetry
- Health Physics
- Medical Physics and Radiotherapy
- Accelerator Target Design
- Fission and Fusion Reactor Design
- Waste Storage/Disposal
- Radiography
- Aerospace Applications
- Decontamination and Decommissioning
- Nuclear Safeguards

About 3,000 users around the world

Calculate Dose - Investigate Therapies

- Patient-CT based model of **knee & end of accelerator**
- **Calculate dose throughout knee**
- Study impact of moderating/ shielding materials & B^{10} conc. in knee
- Need other code to determine neutron production in accelerator target





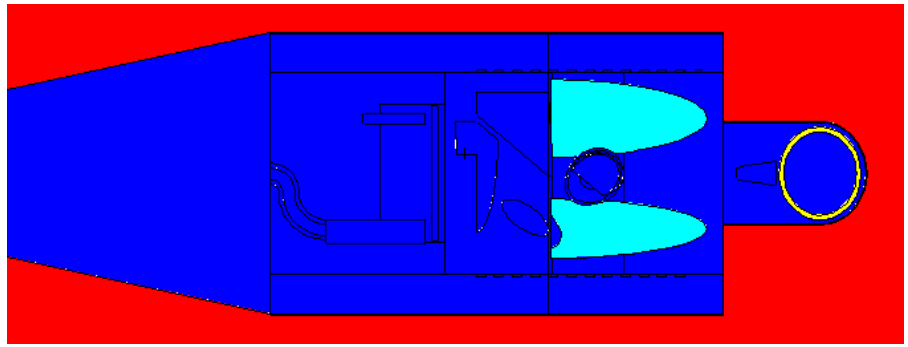
Pictures from mcnp plotter

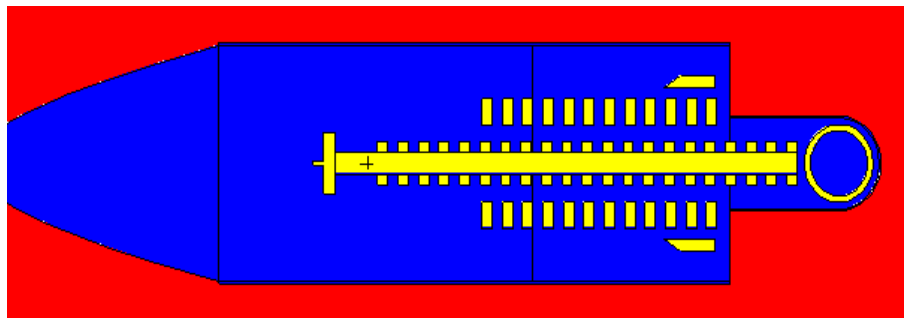
J. R. Albritton, ‘‘Analysis of the SERA treatment planning system and its use in boron neutron capture synovectomy,’’ M. S. thesis, Massachusetts Institute of Technology, 2001.

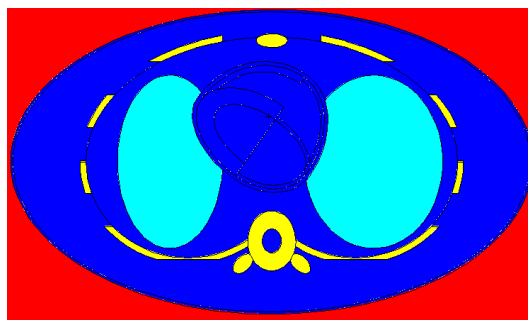
Gierga DP, Yanch JC, Shefer RE, “An investigation of the feasibility of gadolinium for neutron capture synovectomy”, Med Phys. 2000 Jul;27(7):1685-92.

Calculate Dose - Investigate Therapies

- Use of MIRD-like whole body model for accelerator based X-ray or neutron therapies.
- Organ specific doses.
- Vary incident X-ray spectra, shielding.







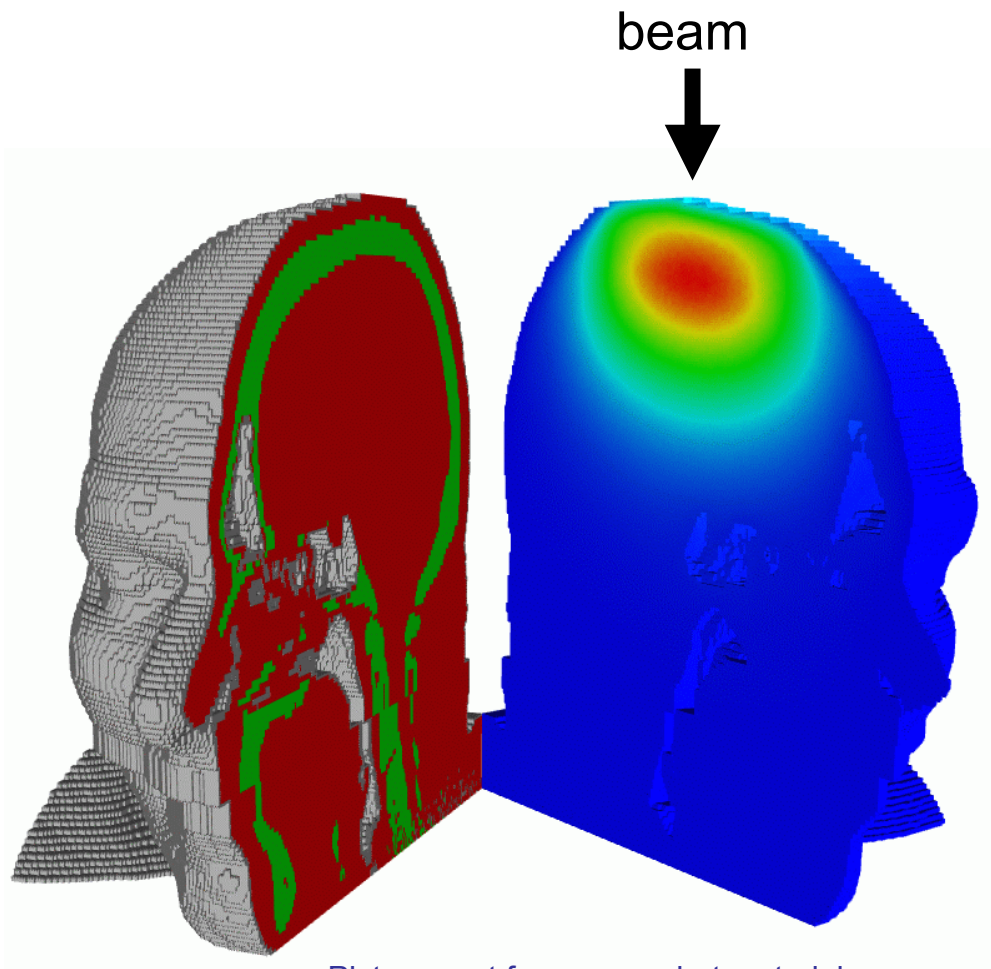
Pictures from mcnp plotter

Lambeth, Melissa. "Development of a computerized anthropomorphic phantom for determination of organ doses from diagnostic radiology." Thesis, B.S., Massachusetts Institute of Technology, Dept. of Nuclear Engineering, 1997.

Gierga DP, Yanch JC, Shefer RE, "An investigation of the feasibility of gadolinium for neutron capture synovectomy", Med Phys. 2000 Jul;27(7):1685-92.

Calculate Dose – Treatment Planning

- Use Patient-based **CT geometry**
- **Calculate dose throughout head, tumor**
- Change beam direction and look at differences in dose distributions

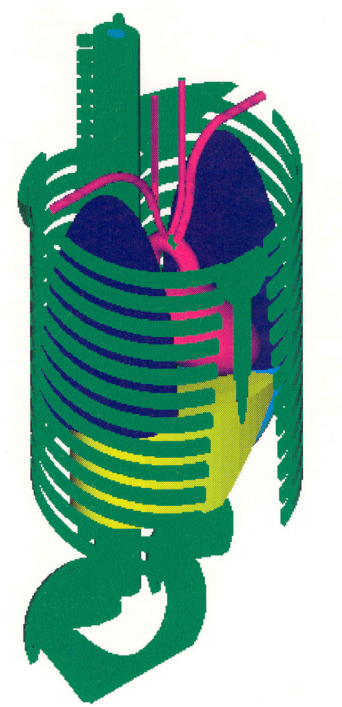


Pictures not from mcnp, but materials (left) and doses(right) from mcnp calculation.

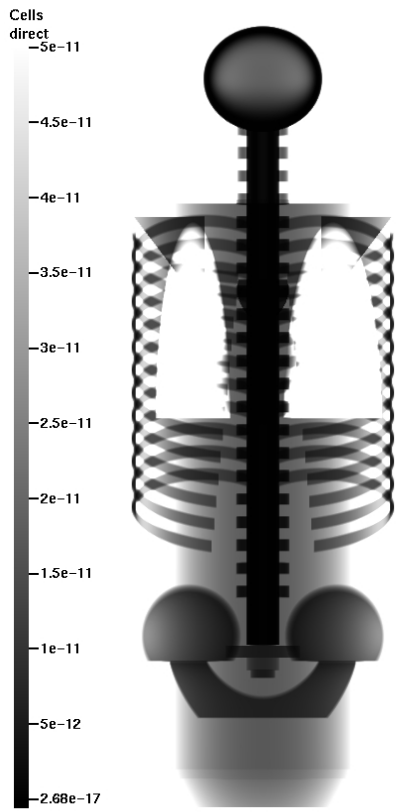
- Larry Cox - Job Queuing & Execution
- Gregg McKinney - Input & Code Modifications
- Robby Russell - Graphics
- Tim Goorley - Input Generation
- ASCI Blue Mountain

Calculate Dose – Simulate Radiograph

- Neutron and photon radiography uses a grid of point detectors (pixels)
- Each source and collision event contributes to all pixels
- **Simulate X-ray, neutron radiographs**
- Investigate role of scatter in image



Picture from Sabrina

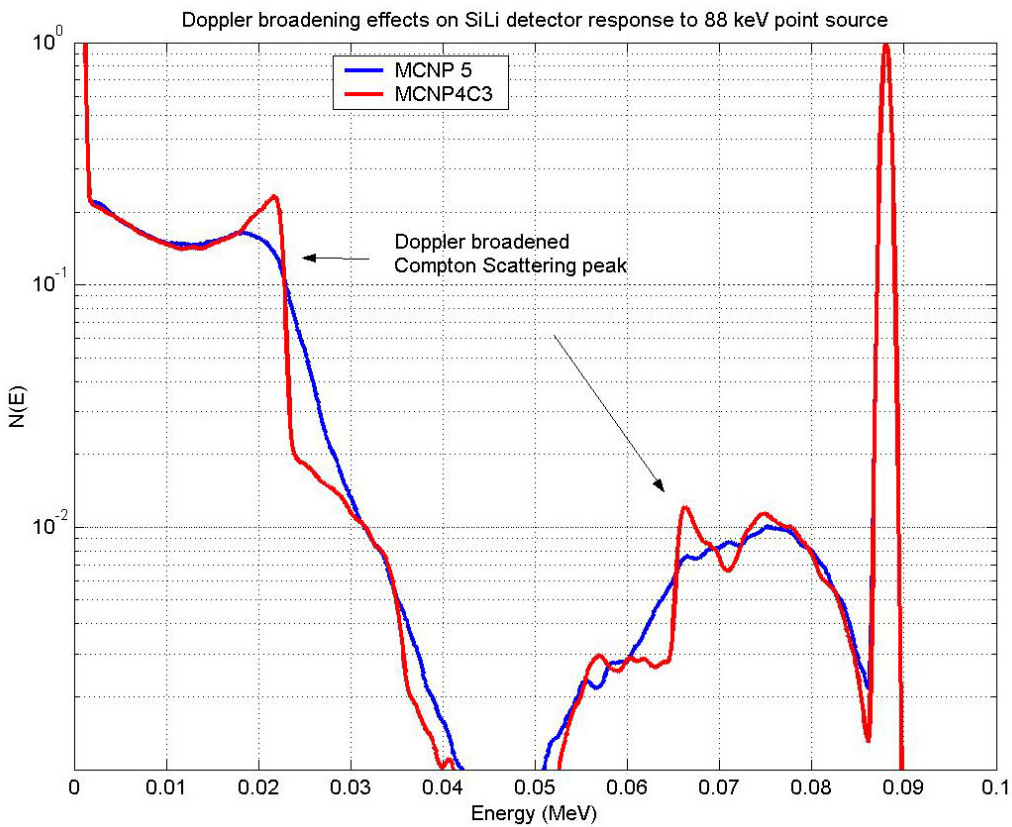


Picture generated with results from MCNP calculation.

Simulated Radiograph
1 M pixels

Calculate Detector Response

- Calculate SiLi **detector response** to 88 keV point source
- Compare to experiment, look at scatter from various portions of geometry
- Other detector response problems in QUADOS comparison. (prob #7)

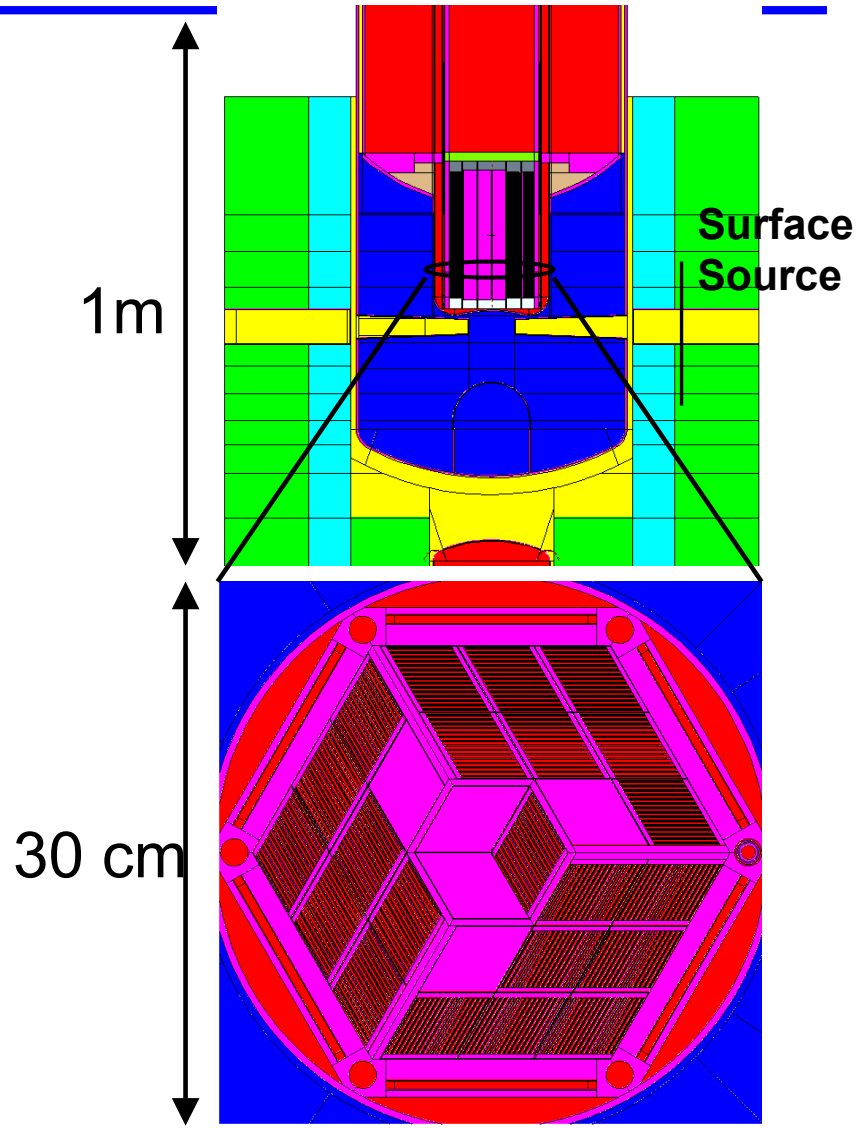


Sood, R. Gardner, "A new Monte Carlo assisted approach to detector response functions", Nuclear Instruments and Methods in Physics Research B, **213** (2004) 100-104.

http://www.nea.fr/download/quados/quados.html

Criticality & Surface Source

- Model **research reactor core**
- Calculate surface source at beam port
- Use surface source for further downstream calculations, like beam port design
- Calculate different K_{eff} from different control rod insertions

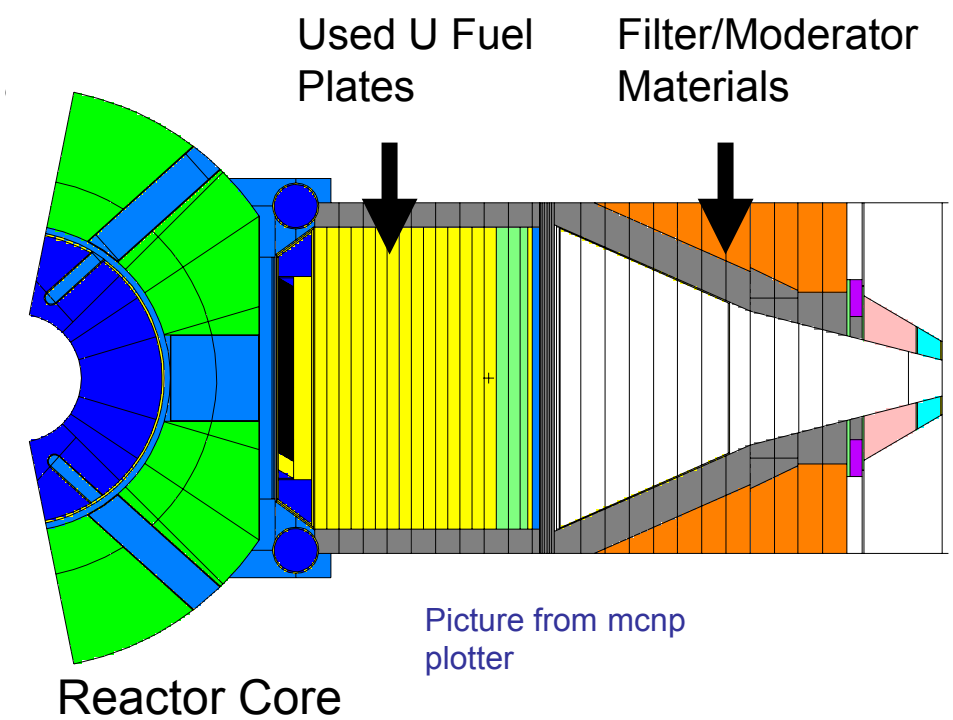


Picture from mcnp plotter

Redmond, E.L., II; Yanch, J.C.; Harling, O.K. “Monte Carlo simulation of the Massachusetts Institute of Technology Research Reactor.” Nuclear Technology; April 1994; vol.106, no.1, p.1-14

Criticality and Flux

- Development of MIT **Reactor Fission Converter Beam**
- Change geometry & materials to find optimal epithermal flux
- Intent: Lower fast n and gamma dose but increase epithermal flux at patient position
- Calculate K_{eff} of U plates



Picture from mcnp plotter

W.S. Kiger III, S. Sakamoto, and O.K. Harling, "Neutronic design of a fission converter-based epithermal neutron beam for neutron capture therapy," *Nuclear Science and Engineering*, **131**, 1-22 (1999).

K.J. Riley, "Construction and Characterization of a Fission Converter Based Epithermal Neutron Beam for NCT," Ph.D. Thesis, Massachusetts Institute of Technology (2001).

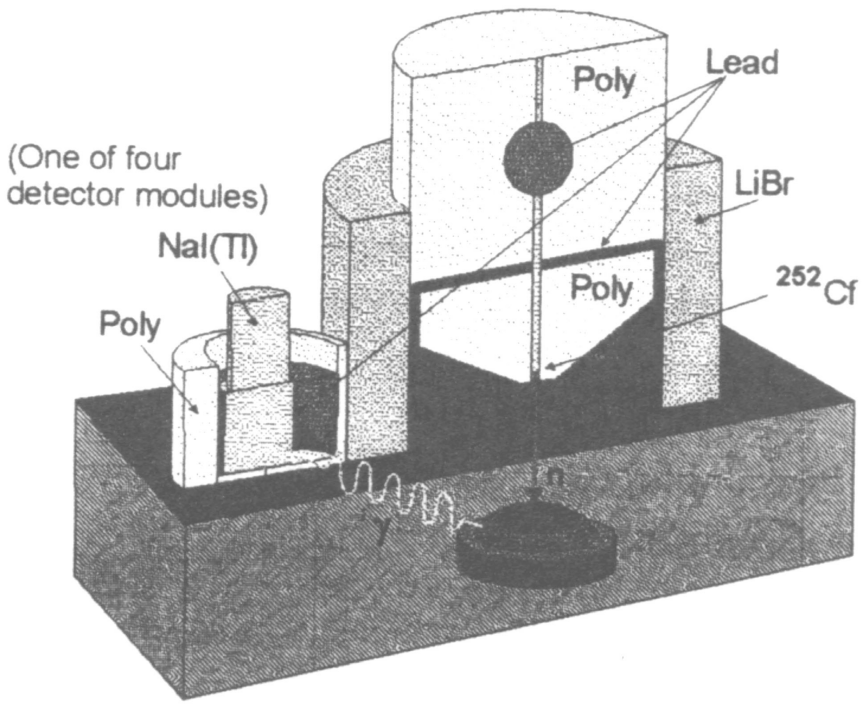
O.K. Harling, K.J. Riley, T.H. Newton, B.A. Wilson, J.A. Bernard, L.-W. Hu, E.J. Fonteneau, P.T. Menadier, S.J. Ali, B. Sutharshan, G.E. Kohse, Y. Ostrovsky, P.H. Stahle, P.J. Binns, W.S. Kiger III, and P.M. Busse, "The Fission Converter Based Epithermal Neutron Irradiation Facility at the MIT Reactor," *Nuclear Science and Engineering*, **140**, 223-240 (2002).

Calculate Flux & Dose

- CDND designed a **landmine detector system**

- Needed to shield personnel and detector from 100 MBq ^{252}Cf source

- Used MCNP to vary shielding materials and dimensions



T. Cousins, T.A. Jones, et. Al. "The development of a thermal neutron activation (TNA) system as a confirmatory non-metallic land mine detector" J. Rad. Nucl. Chem. **235** (1998) 53-58.

Calculate Dose – Health Physics

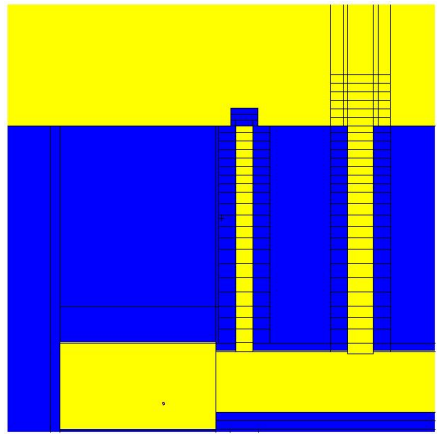
- **Proton Storage Ring at LANSCE accelerator**
- **Investigate dose rates at certain locations**

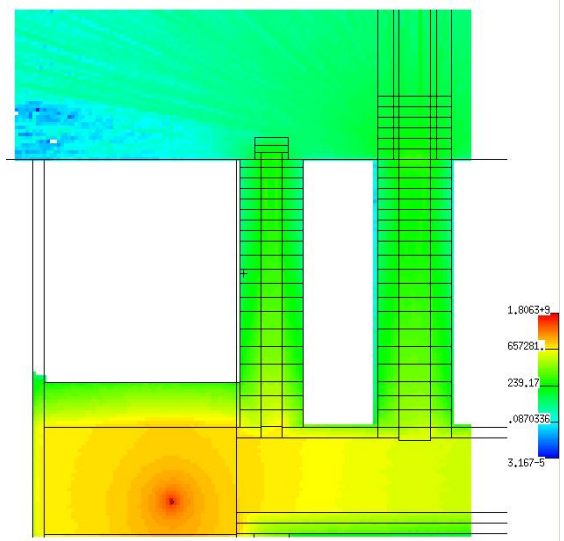
Geometry

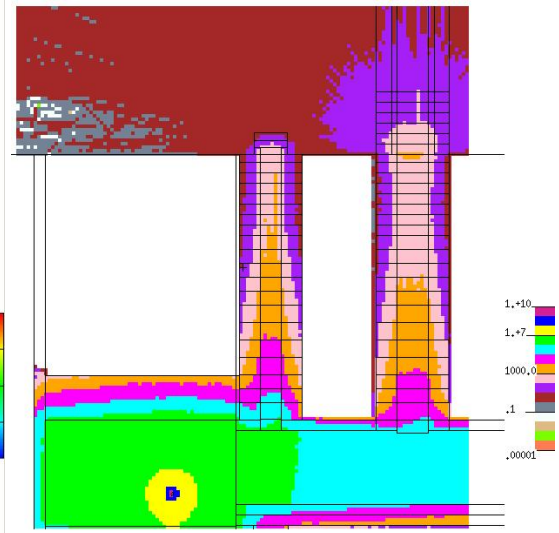
Blue = concrete

Yellow = air

Picture from mcnp plotter







Pictures from mcnp mesh tally plotter

Modernization of MCNP

During 2001-2002, every line of MCNP coding was reworked to produce MCNP5

- Conversion to ANSI-Standard Fortran-90
- Emphasis on code readability & ease of future development
- Standard parallel coding: MPI (message-passing) + OMP (threads)
- Vastly improved modern coding style
- Fortran-90 dynamic memory allocation
- Completely new installation system
- New features & new physics
- Extensive SQA and V&V

MCNP5 released by RSICC in April 2003.

Updates: 1.20- Nov 2003, 1.30- Oct 2004, 1.40- August 2005 (est)

Computer Systems Supported

Serial & parallel (MPI, OMP, MPI/OMP, PVM, PVM/OMP):

- **Unix systems**
  - SGI IRIX64
  - IBM AIX
  - HP/Compaq OSF1
  - Sun SunOS

Serial & parallel (MPI, PVM):

- **Linux systems**
  - with g95 compiler
  - with Absoft compiler
  - with Lahey compiler
  - with Intel compiler
  - with Portland Group compiler
  - with NAG compiler
- **Mac OS X systems**
  - with Absoft compiler
  - with IBMXL compiler

Serial & parallel (MPI, PVM):

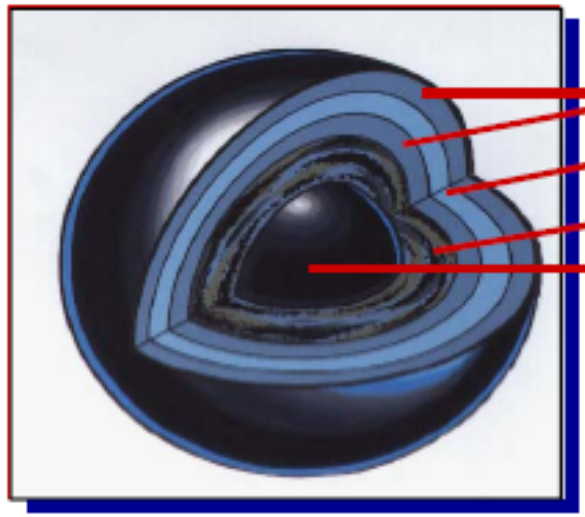
- **Windows PC systems**
  - with CVF compiler
  - with Absoft compiler
  - with Lahey compiler
  - with Intel compiler
- **Itanium systems**
  - with Intel compiler

X11 graphics – all systems

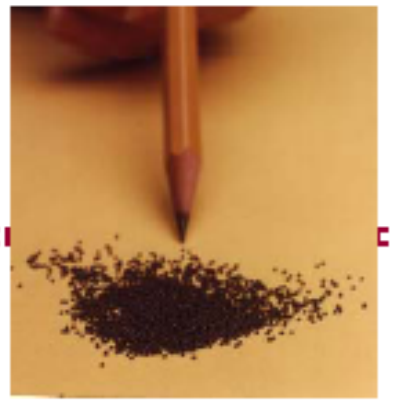
New Features in MCNP5 - 1.40 Update

- **Mesh Tally improvements**
  - Plotting of results
  - Power distributions
  - Cell & surface flagging
- **Stochastic geometry for modeling HTGR fuel kernels**
  - Random, on-the-fly translations of fuel kernels within lattices
- **Electron Transport improvements**
  - On-the-fly sampling from Landau distribution, rather than precomputed
    - Eliminates some significant errors introduced by small geometries
  - Positron sources
- **Relative entropy of fission source distribution**
  - H = relative entropy of fission source distribution
  - Edits & plots of H help assess convergence of source distribution
  - Additional checks on convergence, based on H
- **Bug fixes**
  - Eliminate infinite loop for photon Doppler broadening, …..

Very High Temperature Gas Cooled Reactor



TRISO Coated fuel particles (left) are formed into fuel rods (center) and inserted into graphite fuel elements (right).



PARTICLES

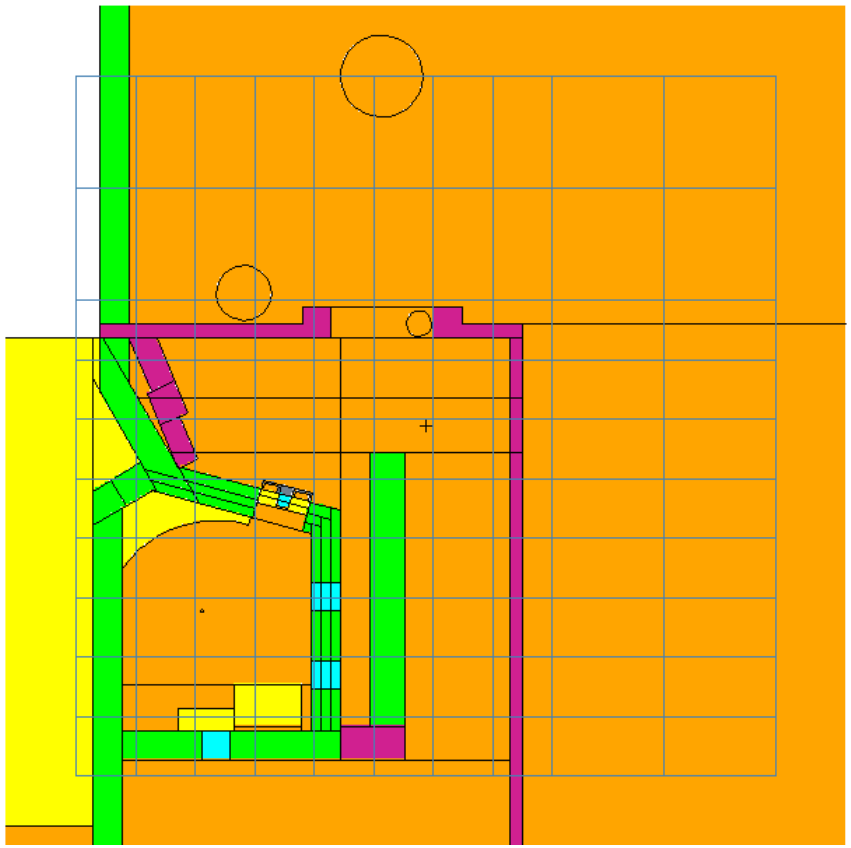
COMPACTS

FUEL ELEMENTS

P. E. MacDonald, et al., "NGNP Preliminary Point Design – Results of the Initial Neutronics and Thermal-Hydraulic Assessments During FY-03", INEEL/EXT-03-00870 Rev. 1, Idaho National Engineering and Environmental Laboratory (2003).

Mesh Tallies

Mesh tallies are track-length tallies that cover 3D regions of space independent of the problem geometry

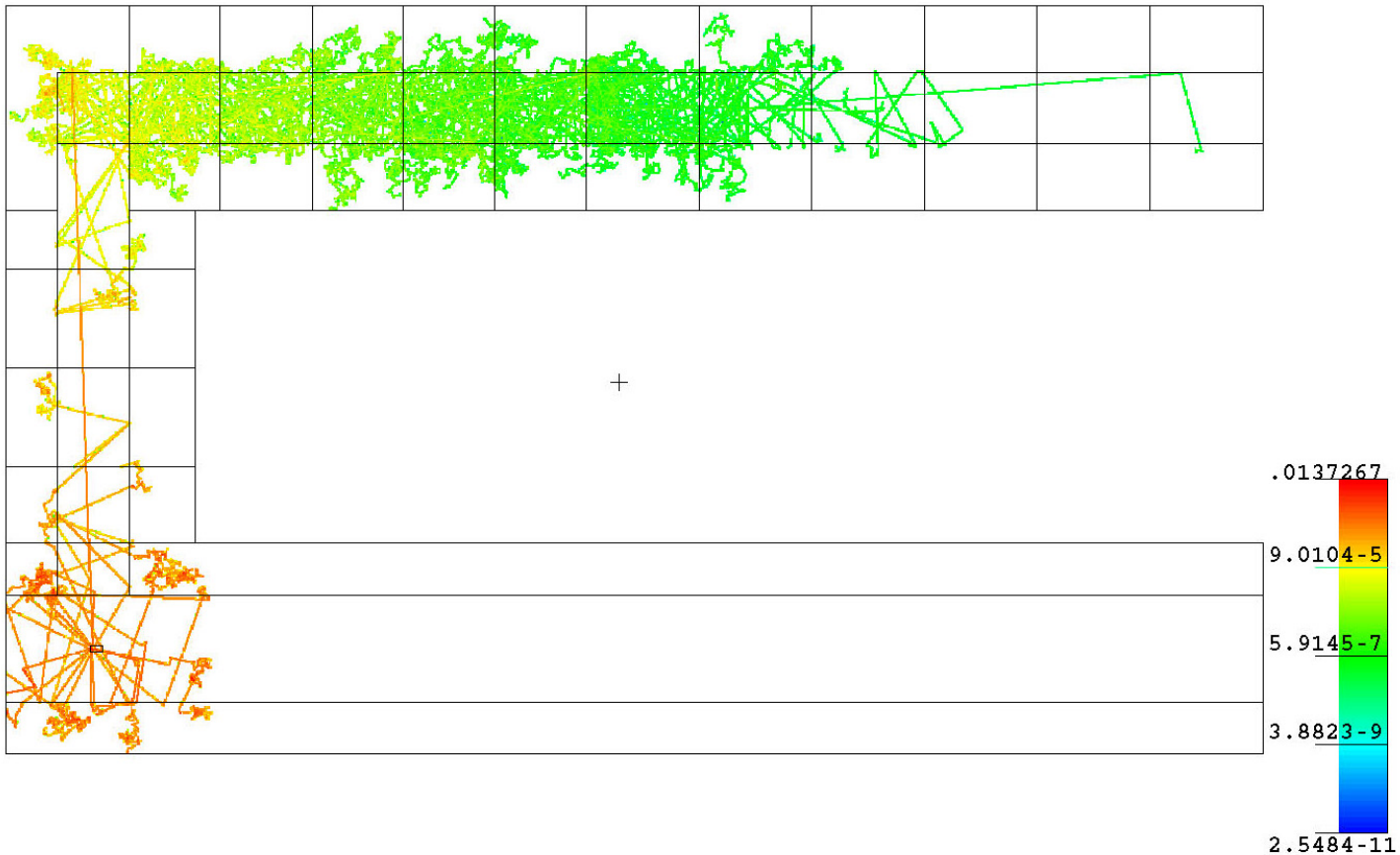


- Both rectangular and cylindrical meshes
- Bin on energy values
- Unlimited number of meshes
- Size of mesh limited by computer parameters
- Rotated by using a TR card
- Modified by DE/DF cards or an FM card
- Plot results in MCNP5_1.40

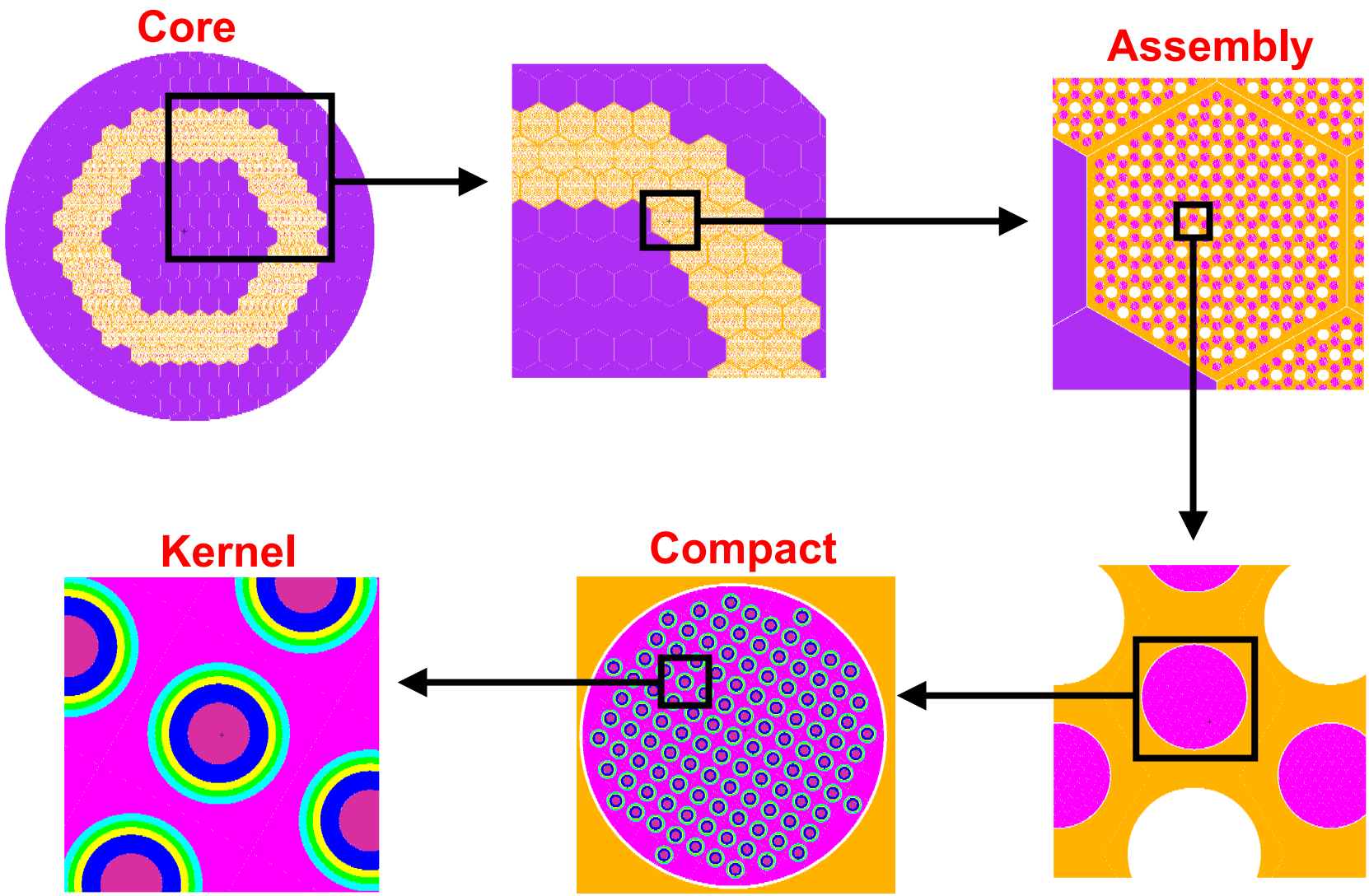
Plotting Particle Tracks

By using a very fine mesh, particle tracks from individual histories can be plotted.

2000 x 1100 x 1 mesh

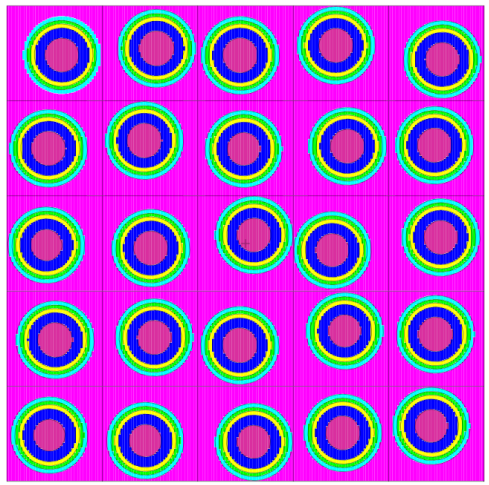


HTGR Modeling with MCNP5



MCNP5 Stochastic Geometry

- Fuel kernels randomly displaced **on-the-fly** within the lattice cells



Fuel kernel displaced randomly within lattice element each time that neutron enters

- **The new stochastic geometry treatment for MCNP5 provides an accurate and effective means of modeling the particle heterogeneity in TRISOL particle fuel**
  - **Same results as (brute-force) multiple realizations of random geometry input with standard MCNP**
  - **Negligible difference from "truly random" multiple realizations**

Work in progress

- **Proton transport**
  - **Continuous-energy physics up to 50 GeV**
  - **Direct tracking through magnetic fields**
  - **COSY-map tracking through magnetic fields**
- **Many additional particle types**

- **ENDF/B-VII** (Data Team)
- **Automated variance reduction, using deterministic adjoint**
- **Criticality**
  - **Automated stationarity testing (using relative entropy)**
  - **Dominance ratio**
  - **Perturbation theory – source shape effects**
  - **Wielandt acceleration of convergence**
- **Continuously varying tallies**
- **Improved electron transport**
- Etc.

Proton Radiography

- For many experiments being conducted now at LANL & BNL, high-energy proton beams are directed at test objects to produce radiographic images
  - LANL: 800 MeV proton beams
  - BNL: 24 GeV proton beams
  - Proposed: 50 GeV proton beams
- Proton beams are collimated & focused by magnetic lenses
- Both the design of the experiments & analysis of results are carried out using MCNP6, the latest LANL development version of MCNP
  - All MCNP5 features plus:
  - Continuous-energy proton physics up to 50 GeV
  - Models for multiple Coulomb scatter, nuclear elastic scatter, etc.
  - Direct tracking of protons through magnetic fields
  - COSY-map tracking of protons through magnetic fields
  - Many additional particle types being added to account for background

Magnetic Field Transfer Maps

- Taylor series expansions of a particles canonical variables
- 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
- 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
- Transfer maps calculated by the beam optics code COSY INFINITY.
- Fast and accurate

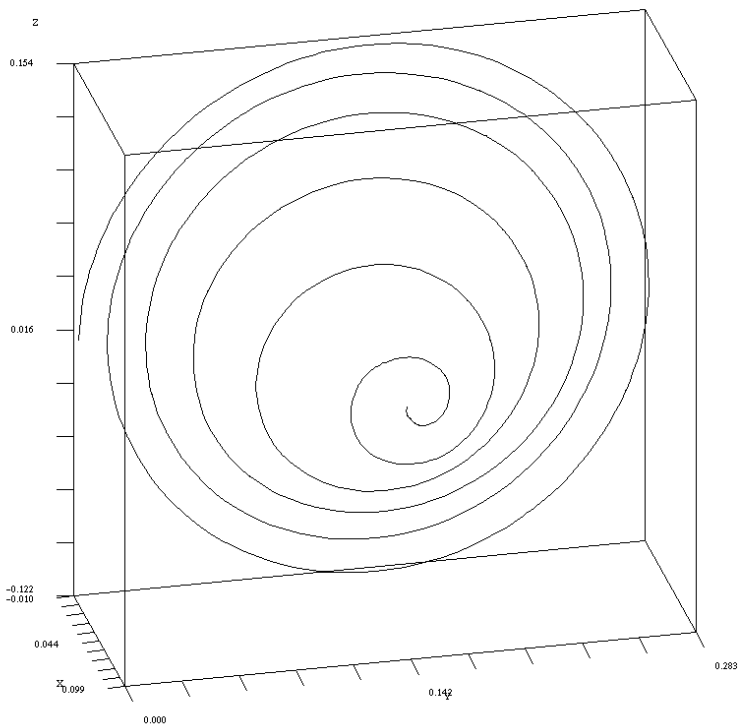
Transfer Map Limitations

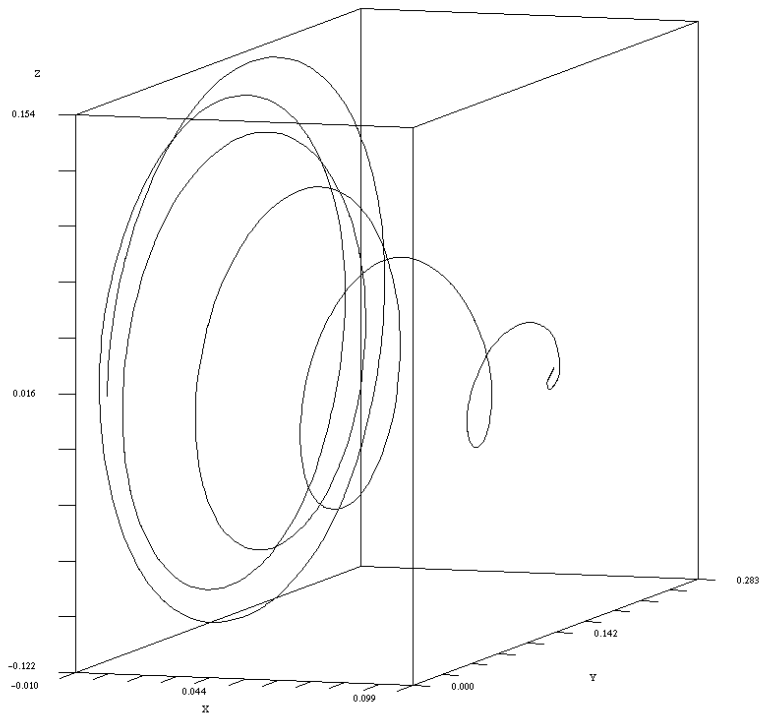
- Can only be used in void regions
- The maps have a finite volume of convergence in phase space
  - The convergence volume has a very complicated shape in five dimensions, requiring that the shape of the phase-space volume and the order of the Taylor series needed in order to get a given accuracy in 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.

Numerical Integration (Direct Tracking)

- Tracking routines adapted from MARS code (N. Mokhov)
- Tracking in a void and material is performed by a higher-order numerical integration algorithm
- The trajectory is approximated by segments of the helical trajectory corresponding to a constant field equal to the field at the midpoint of each step
- 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.
- Maximum step size and deflection angle controlled by the user

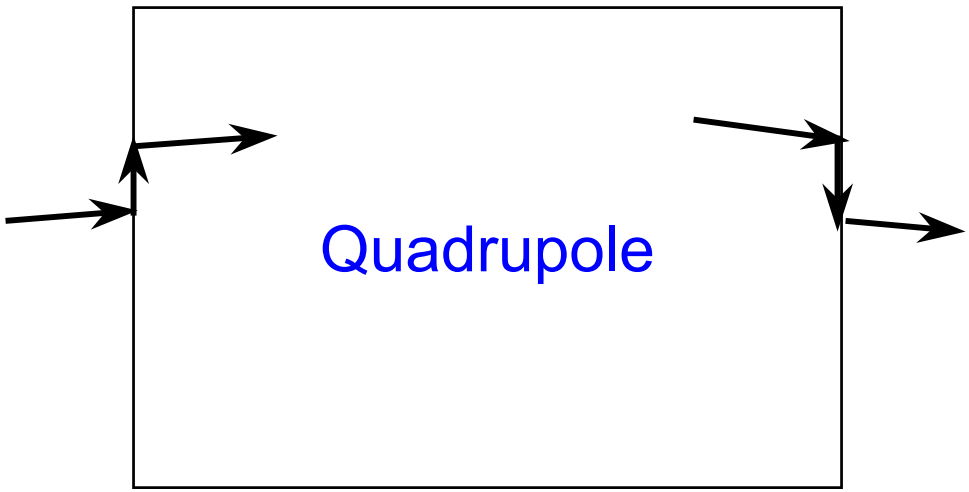
Proton in Air & Constant B Field – With Energy Straggling





Fringe Fields

The effect of quadrupole 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. These edge kicks account for the 3rd order geometric aberrations of the magnetic lens system.



Edge Kicks

For a particle traveling along the *z*-axis, the position and momentum jumps applied to a particle as it enters the upstream fringe field of a quadrupole are

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

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

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

where t_x, t_y, and t_z are the direction cosines of the momentum vector

G is the quadrupole gradient (T/m)

p/q is the particle rigidity (T-m)

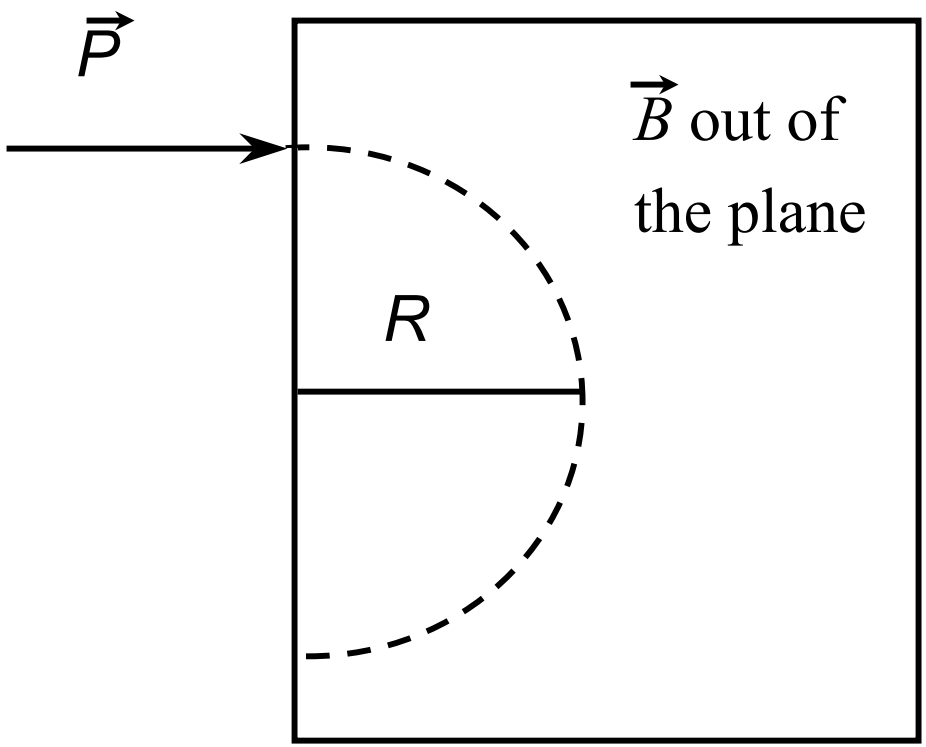
Edge Kicks

For a particle exiting a quadrupole, the expressions are the same except that Gp/q is replaced with $-Gp/q$

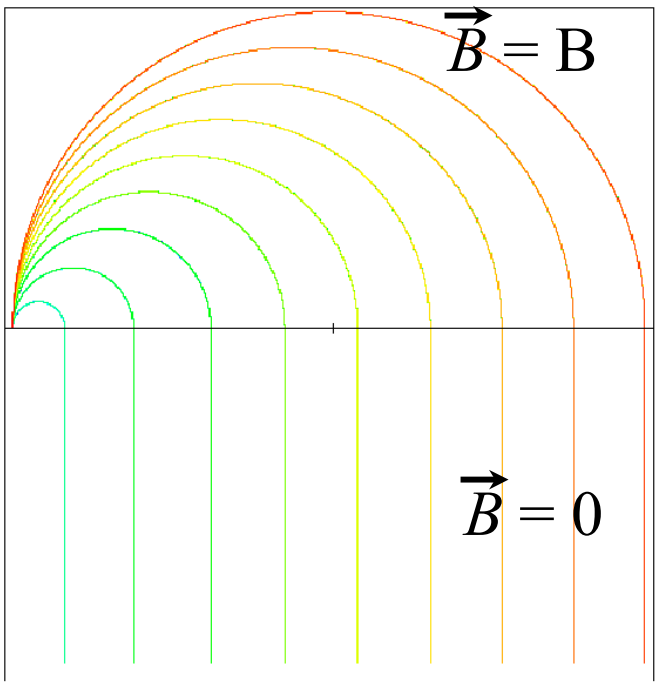
Edge kicks are valid for the bore region of the quadrupole magnet

Testing – Constant Magnetic Field

In a constant magnetic field, a particle will travel in a circle with a radius $R = P/qB$



Testing – Constant Magnetic Field



Energy Range

10 keV – 100 GeV

Field Strength Range

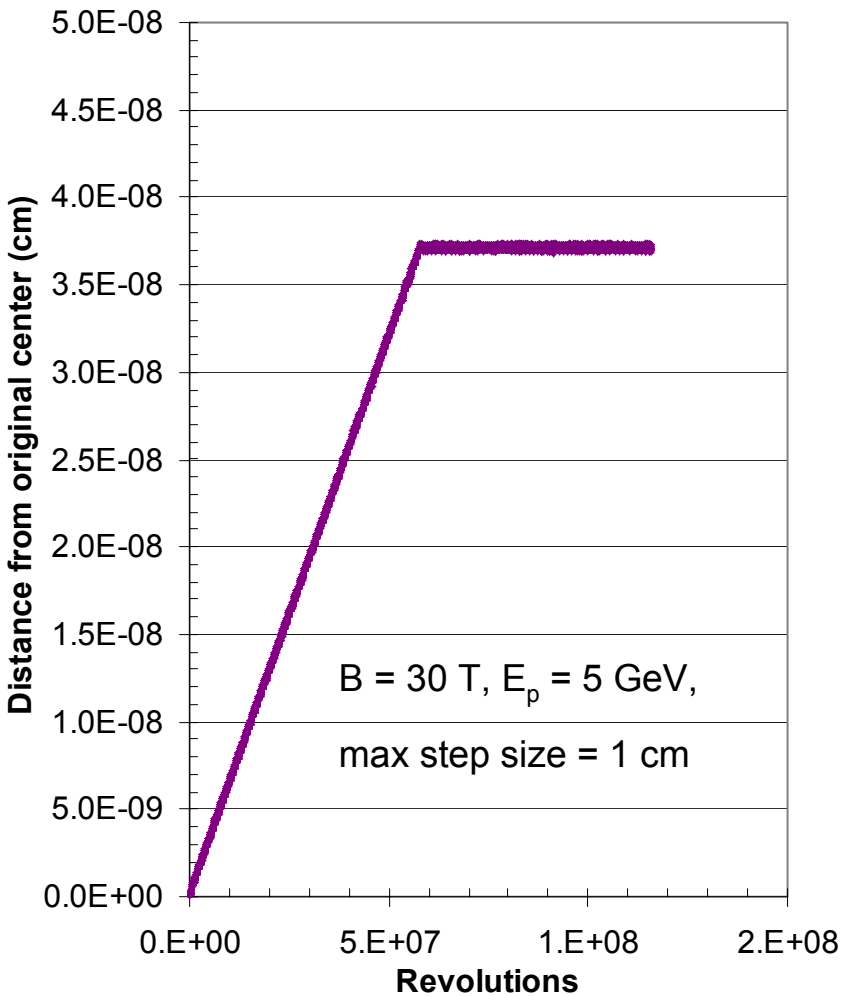
0.01 T – 30 T

Results

$R_{\mathrm{MCNP5}} = R_{\mathrm{analytical}}$

lateral direction cosine ± 10^{-11}

Testing – Constant Magnetic Field



Stability of Orbits

Every 10,000 revolutions, calculate the center of the circular orbit and examine the drift of the orbits against the number of revolutions.

Results

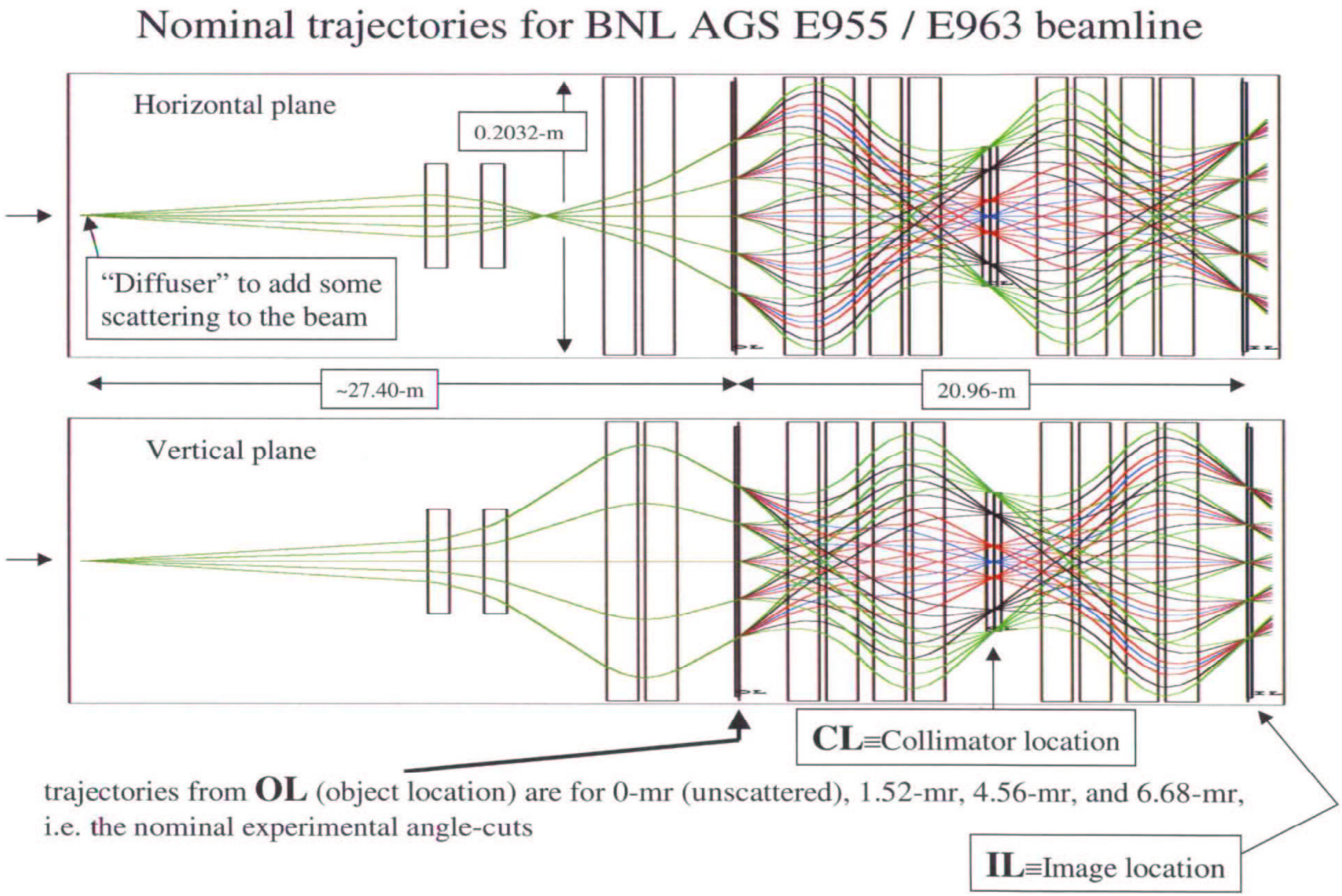
Slope = 6 x 10^{-16} cm/rev

σ@ plateau = 1 x 10^{-10} cm

Drift caused by floating-point limitations.

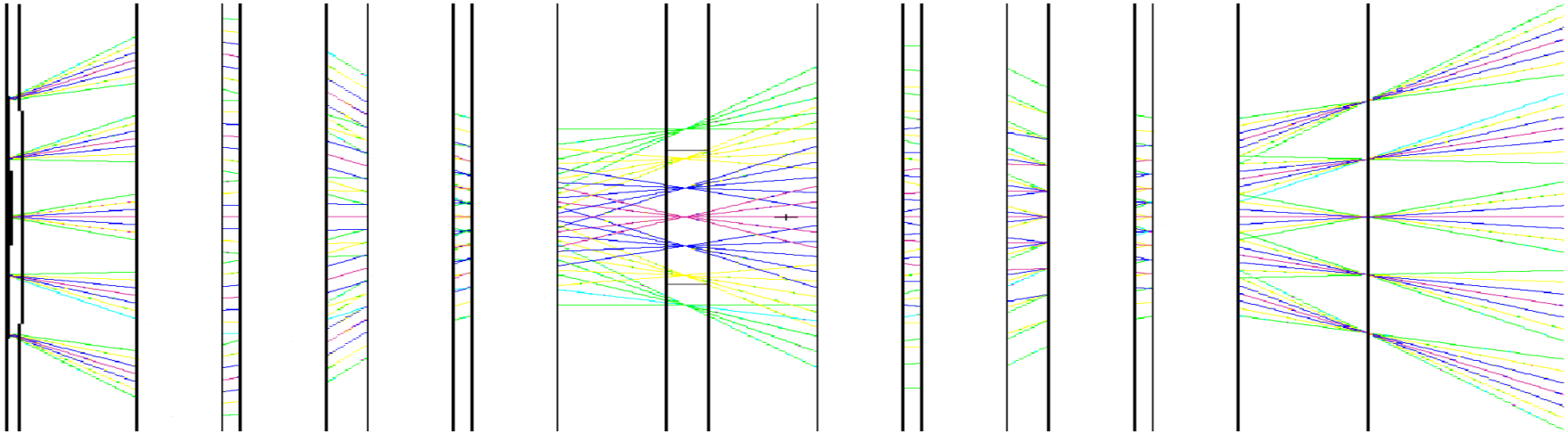
Testing – Quadrupole Field

- Brookhaven E955 Proton Radiography Beam Line

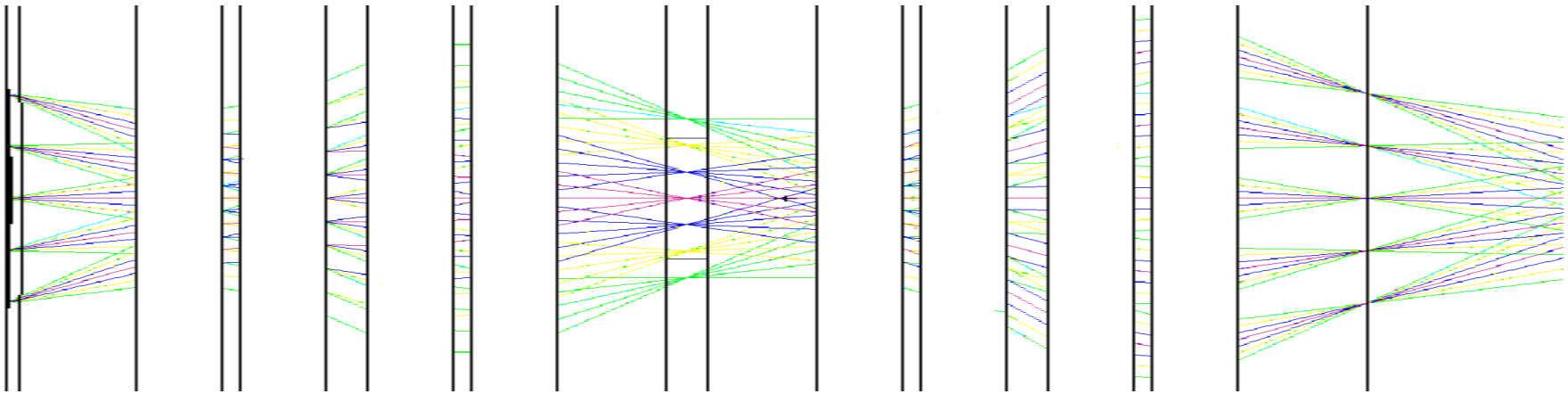


Testing – Transfer Maps

Horizontal Plane



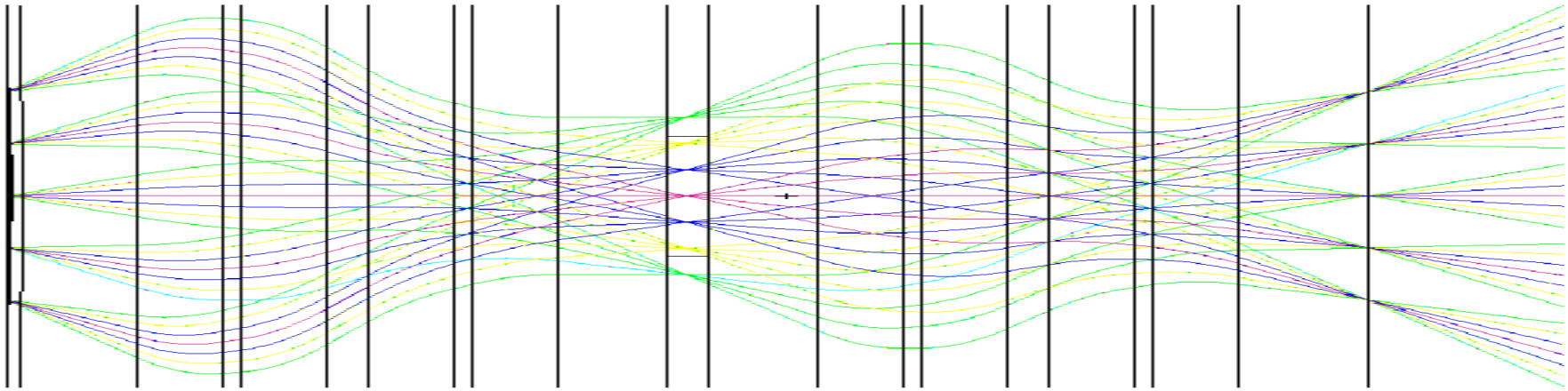
Vertical Plane



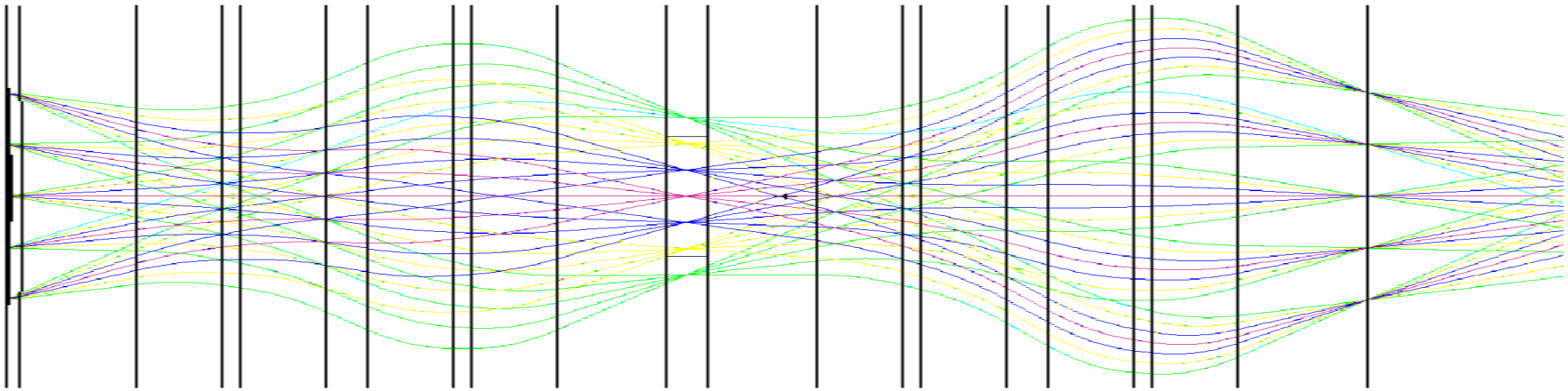
Object Collimator Image

Testing – Direct Tracking

Horizontal Plane

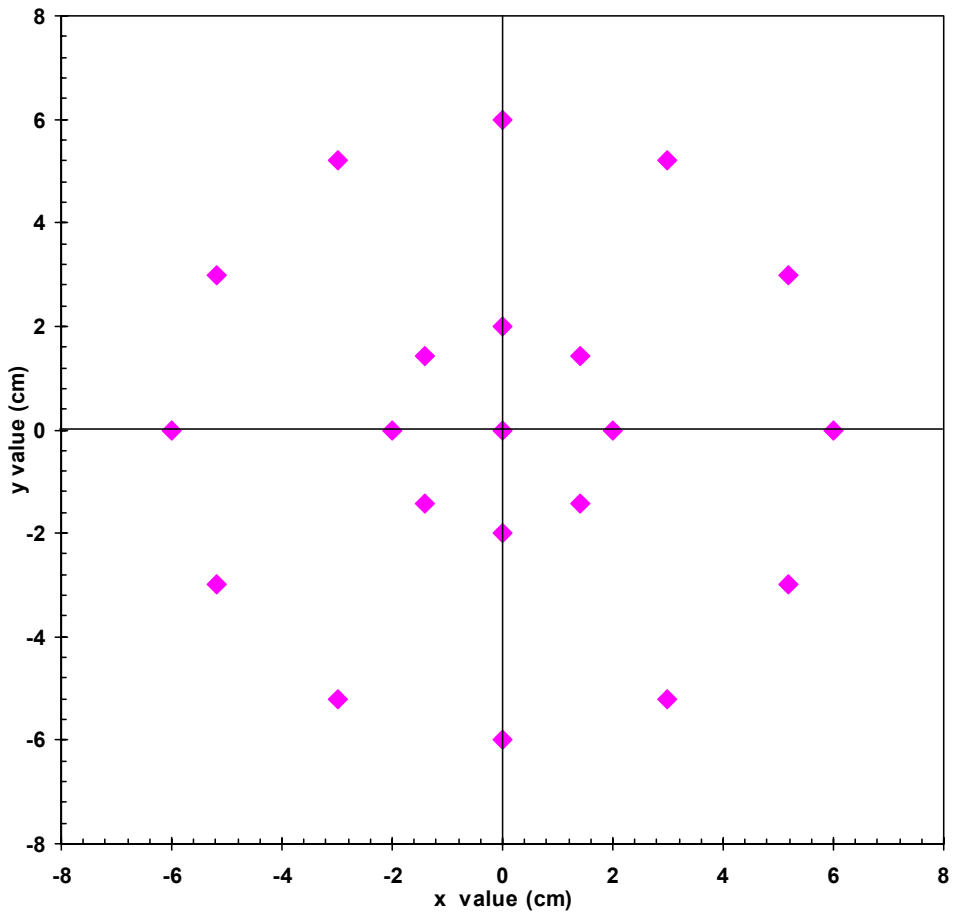


Vertical Plane



Object Collimator Image

Testing – Quadrupoles



Starting locations for matched rays on the object (z = 0) plane

Particle Parameters

E_p = 23.08 GeV

z = 0 (object plane)

$\theta_x = kx$

$\theta_y = -ky$

k = 0.17500935 radians/cm

Transfer maps

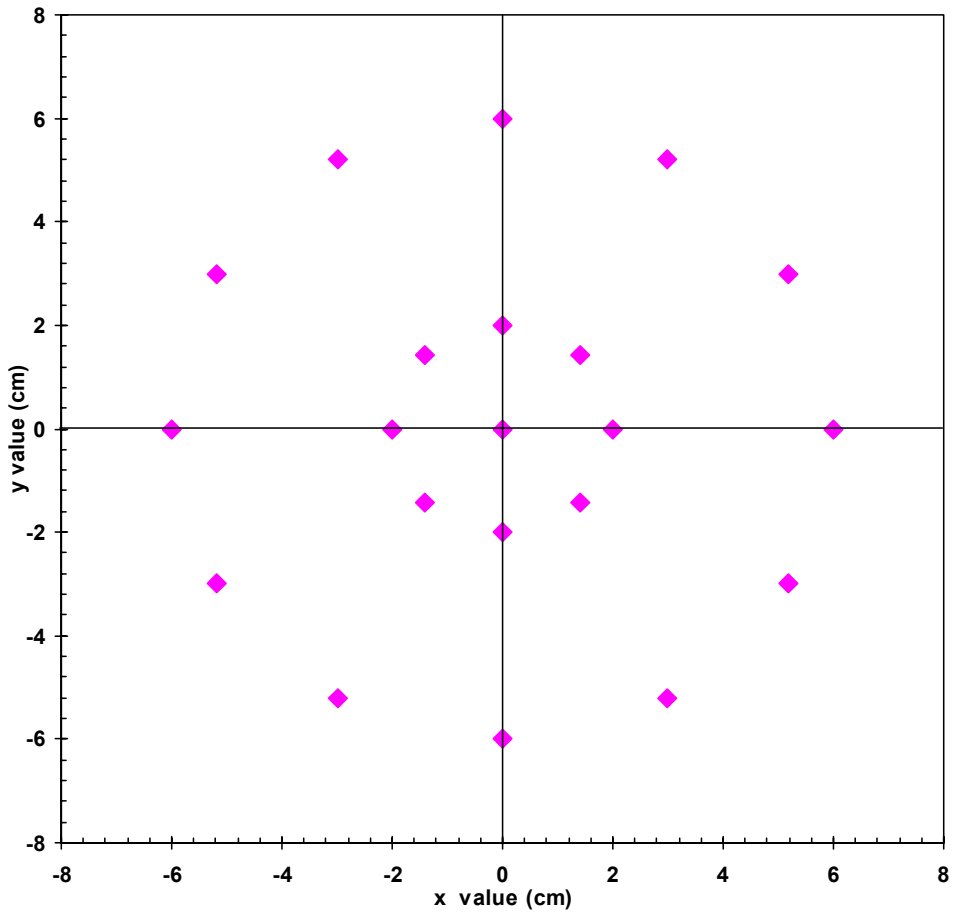
– 5th order w/ fringe-field model

Numerical Integration

– Gradient = 11.633412 T/m

– Edge-kick model

Testing – 0 mrad Cone Angle



Average Distance Between Expected and Actual Image Locations

Source Location	Transfer Map	Direct Tracking
0 cm	0 μm	0 μm
2 cm	0.54 μm	0.58 μm
6 cm	16 μm	18.1 μm

Image Plane Locations for matched rays with a 0 mrad cone angle.

Testing – 5 mrad Cone Angle

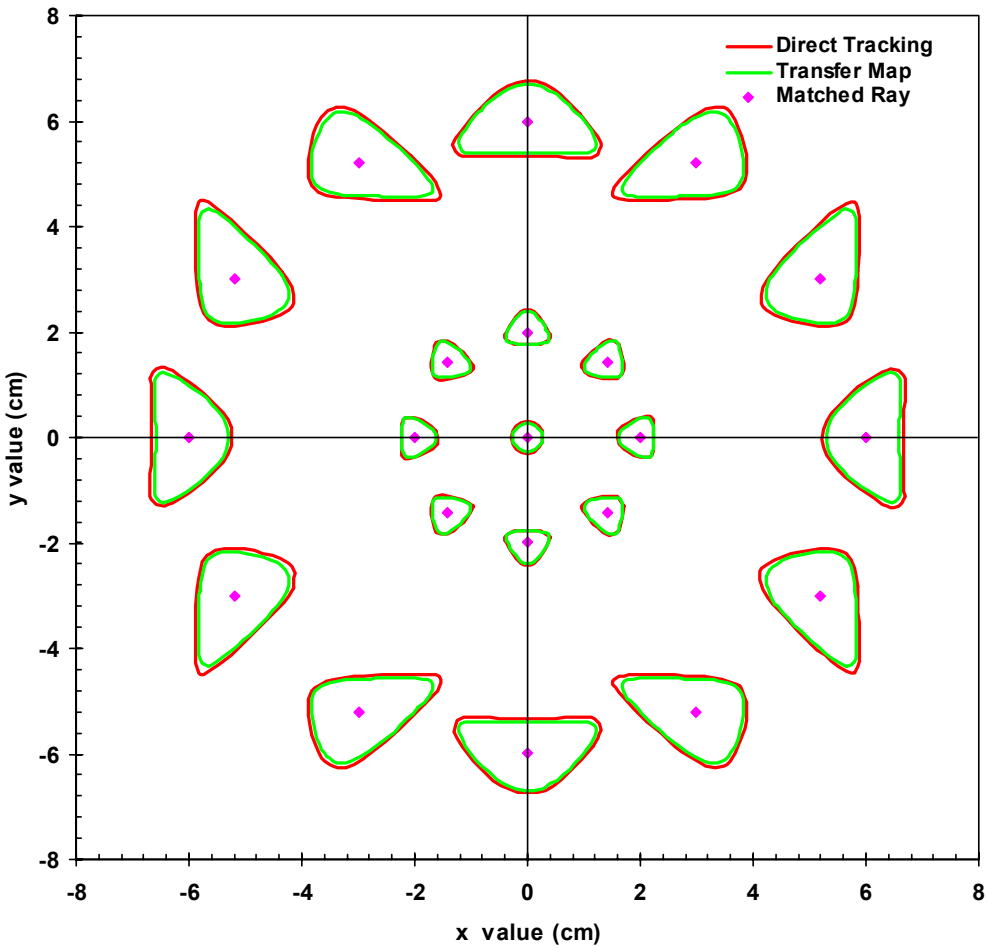


Image Plane Patterns for matched rays with a 5 mrad cone angle. The actual patterns have been enlarged by a factor of 100.

Average Distance Between Expected and Actual Image Locations

Source Location	Transfer Map	Direct Tracking
0 cm	27.1 μm	28.7 μm
2 cm	42.5 μm	44.9 μm
6 cm	146 μm	154 μm

Testing – Fringe Field Effects

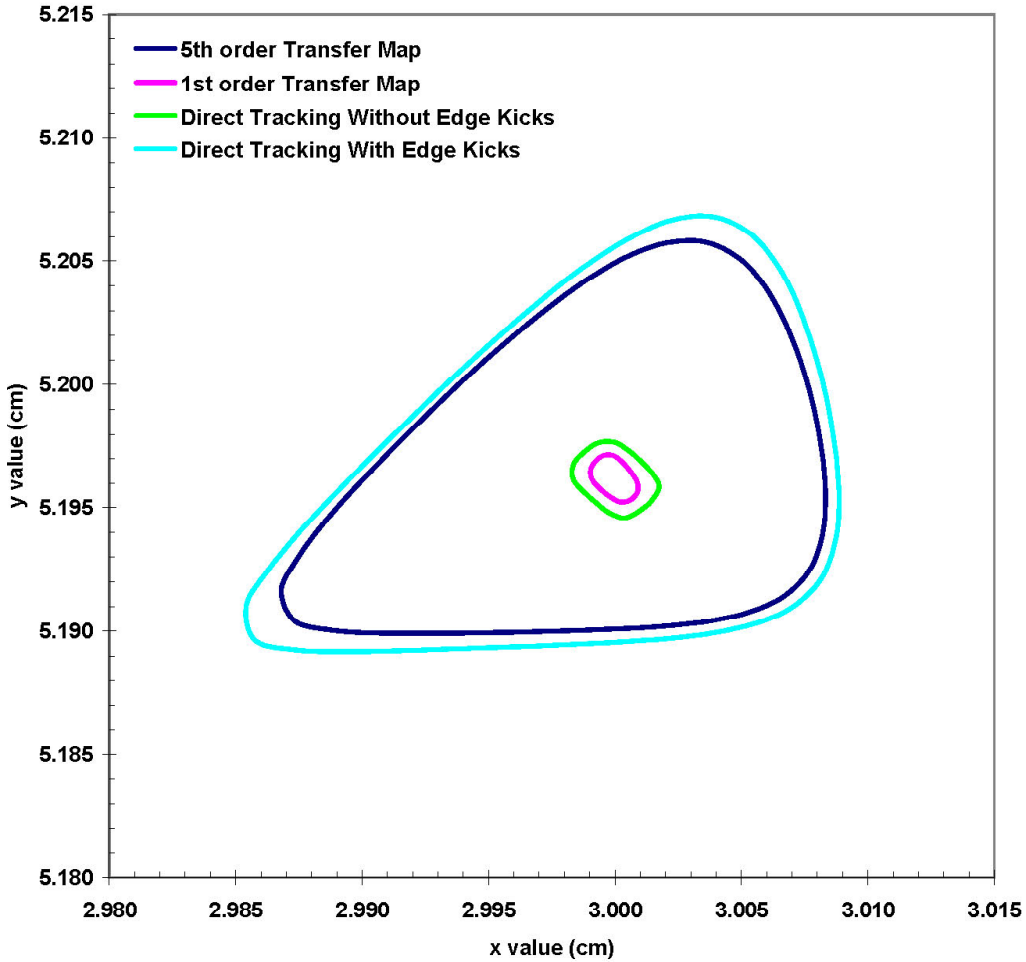
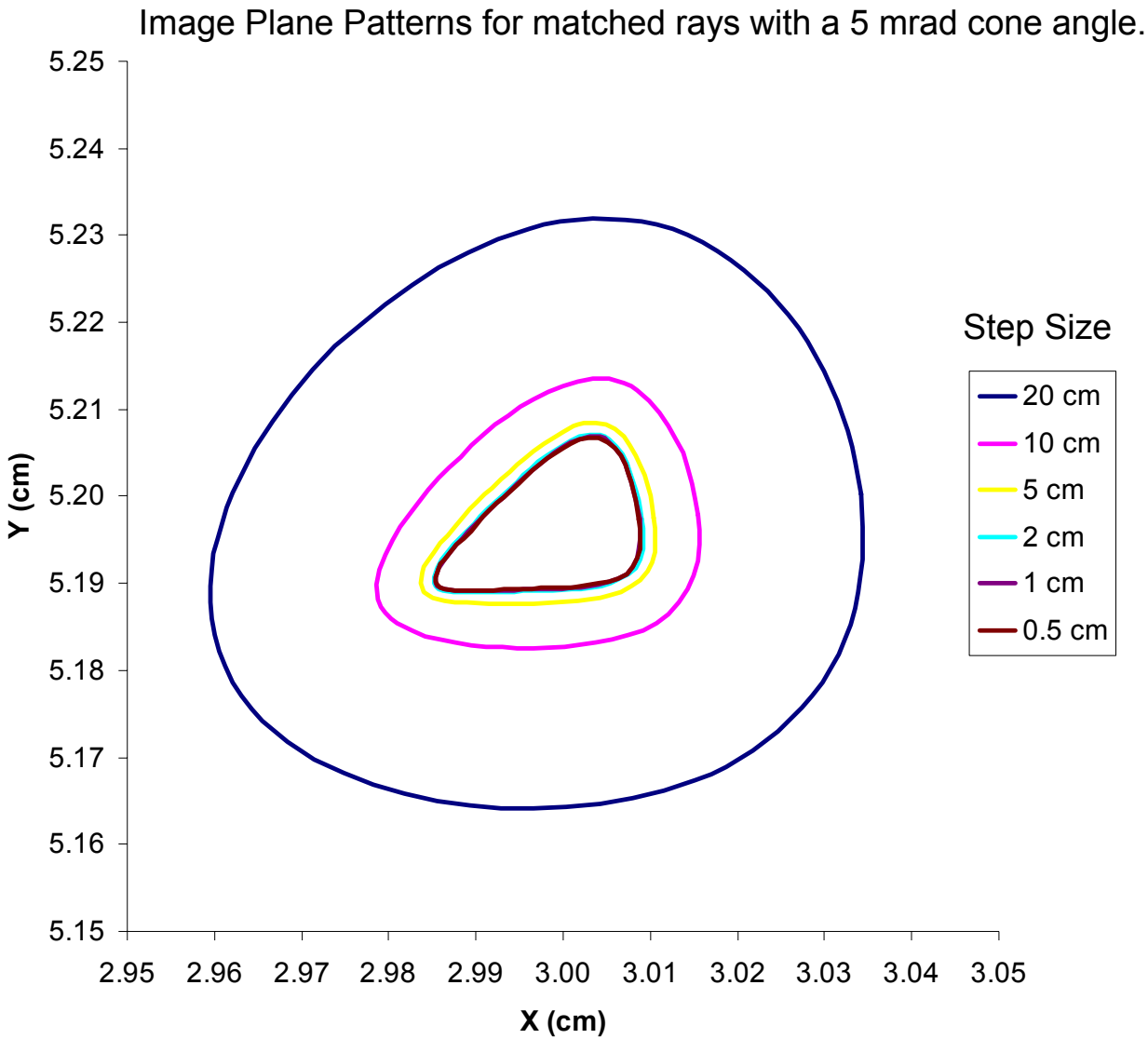


Image Plane Patterns for matched rays with a 5 mrad cone angle.

Fringe field effects can be turned off by

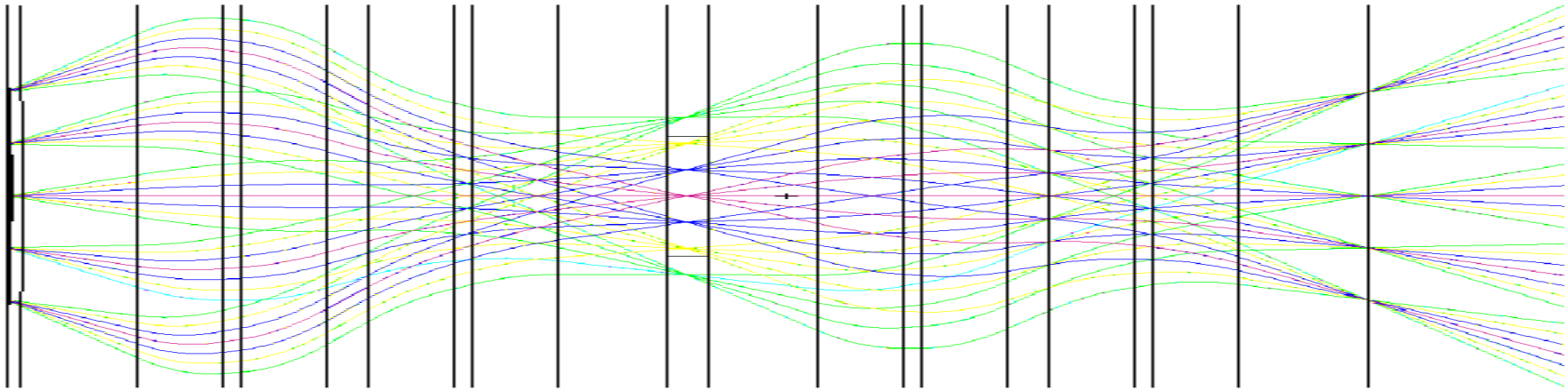
- **Use of only 1st order terms in transfer map**
- **Turn off edge-kick model**

Effect of Step Size Parameter

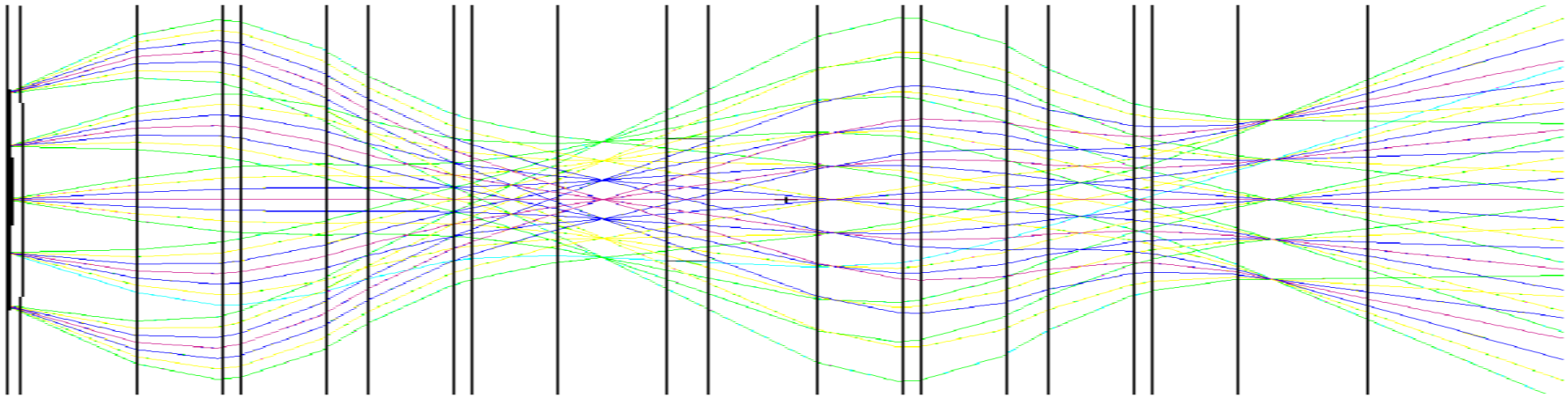


Effect of Step Size on Magnetic Lens Focus

1 cm step size

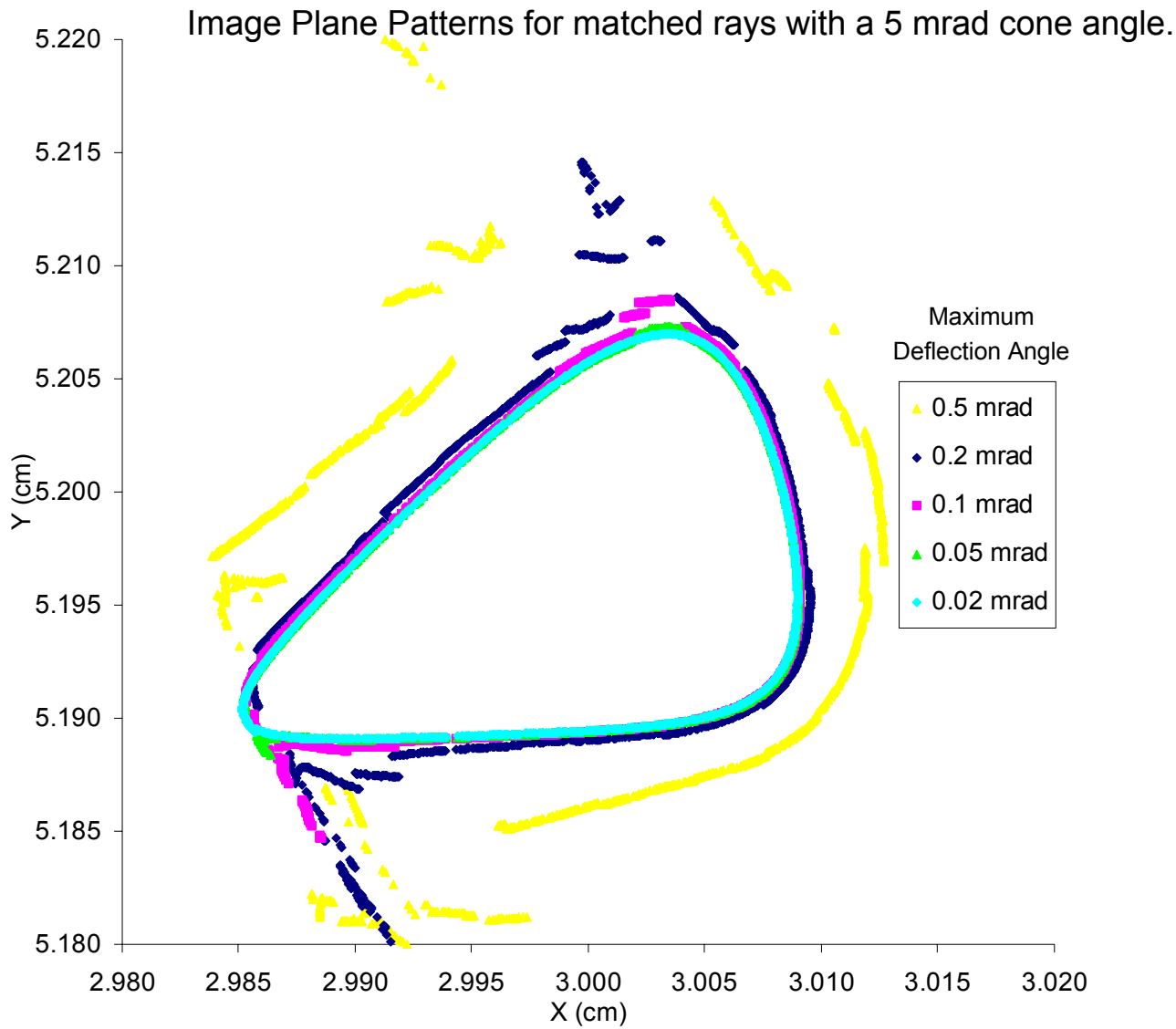


125 cm step size



Object Collimator Image

Effect of the Maximum Deflection Angle



Effect of the Maximum Deflection Angle

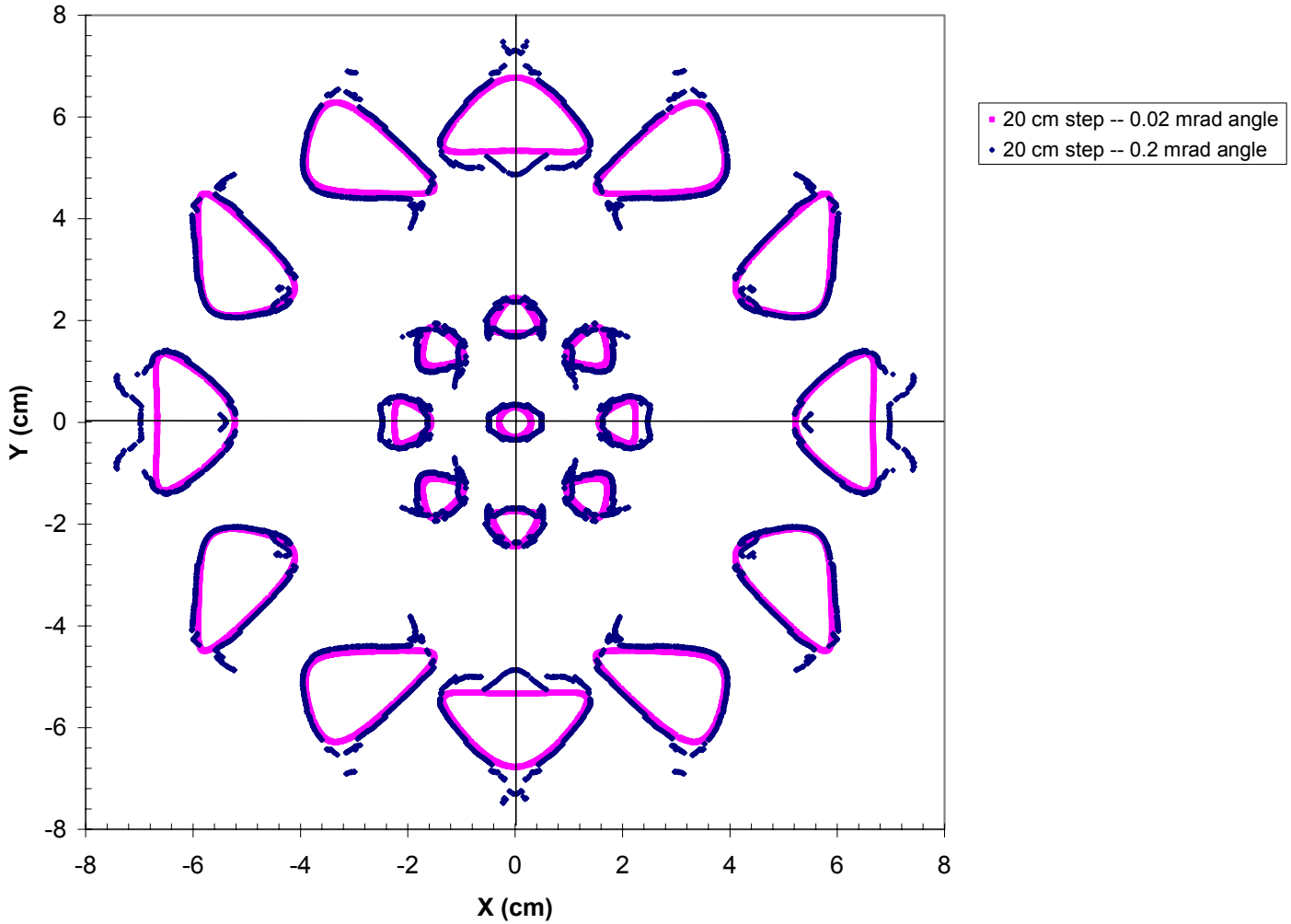
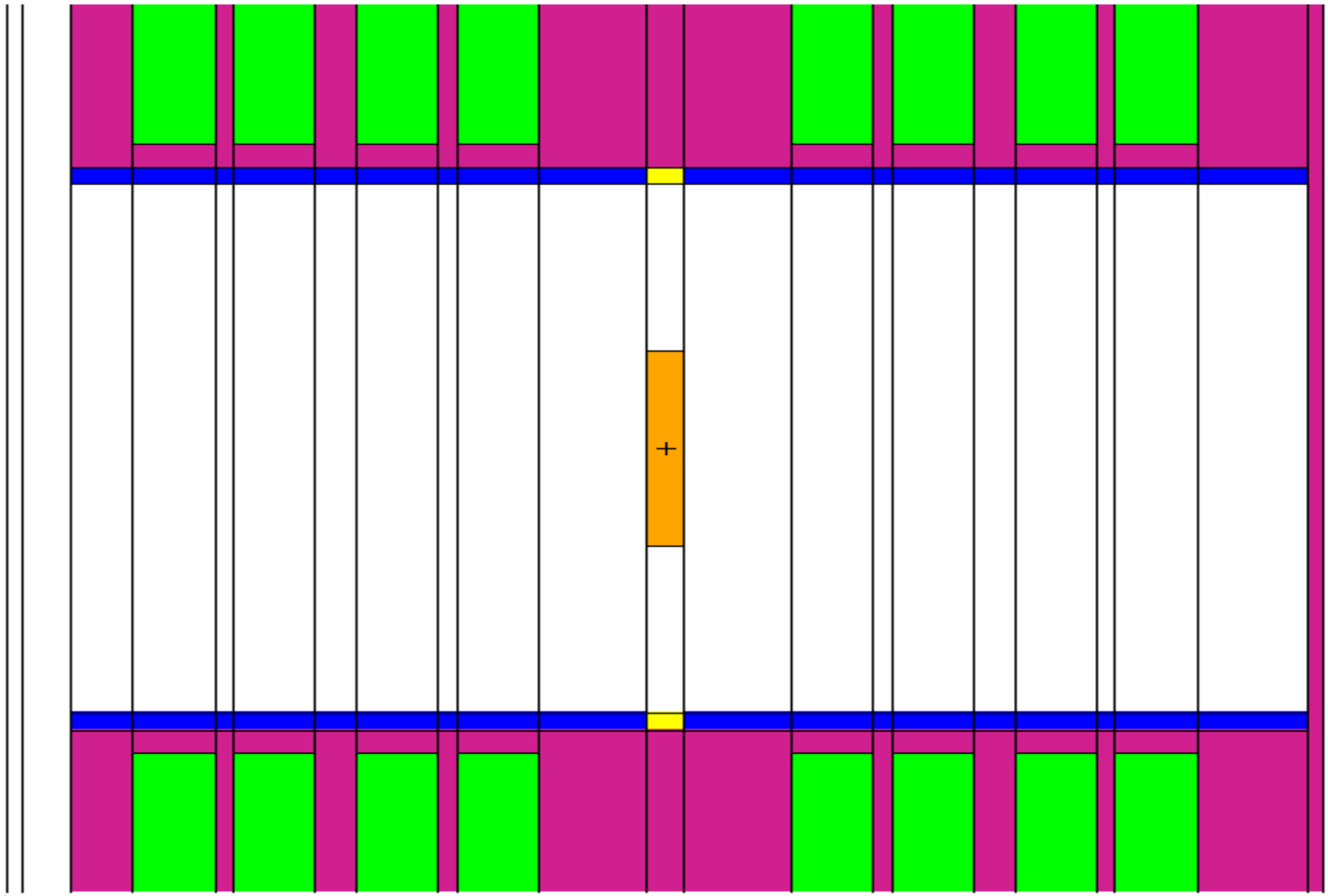
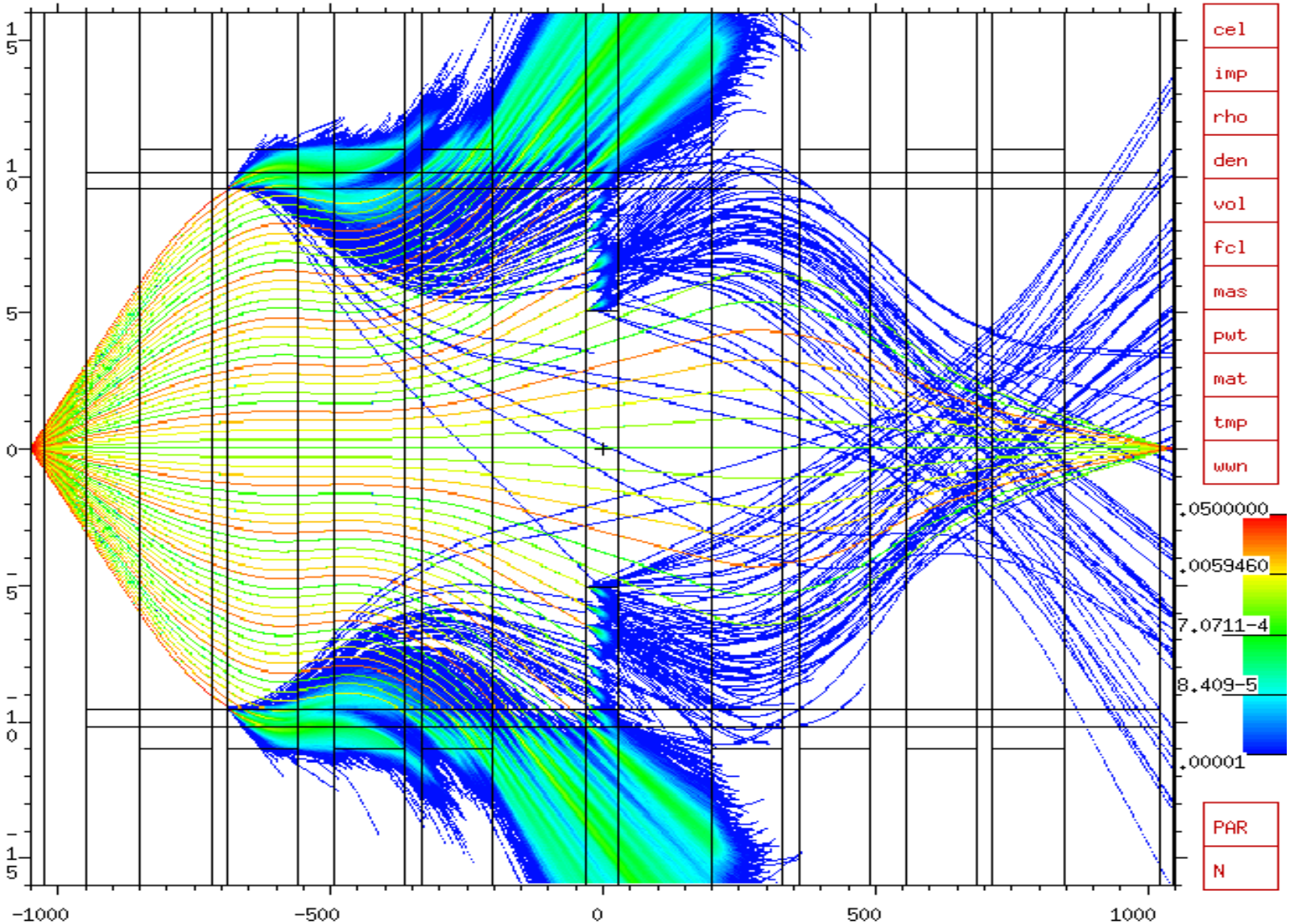


Image Plane Patterns for matched rays with a 5 mrad cone angle.
The actual patterns have been enlarged by a factor of 100.

MCNP Geometry

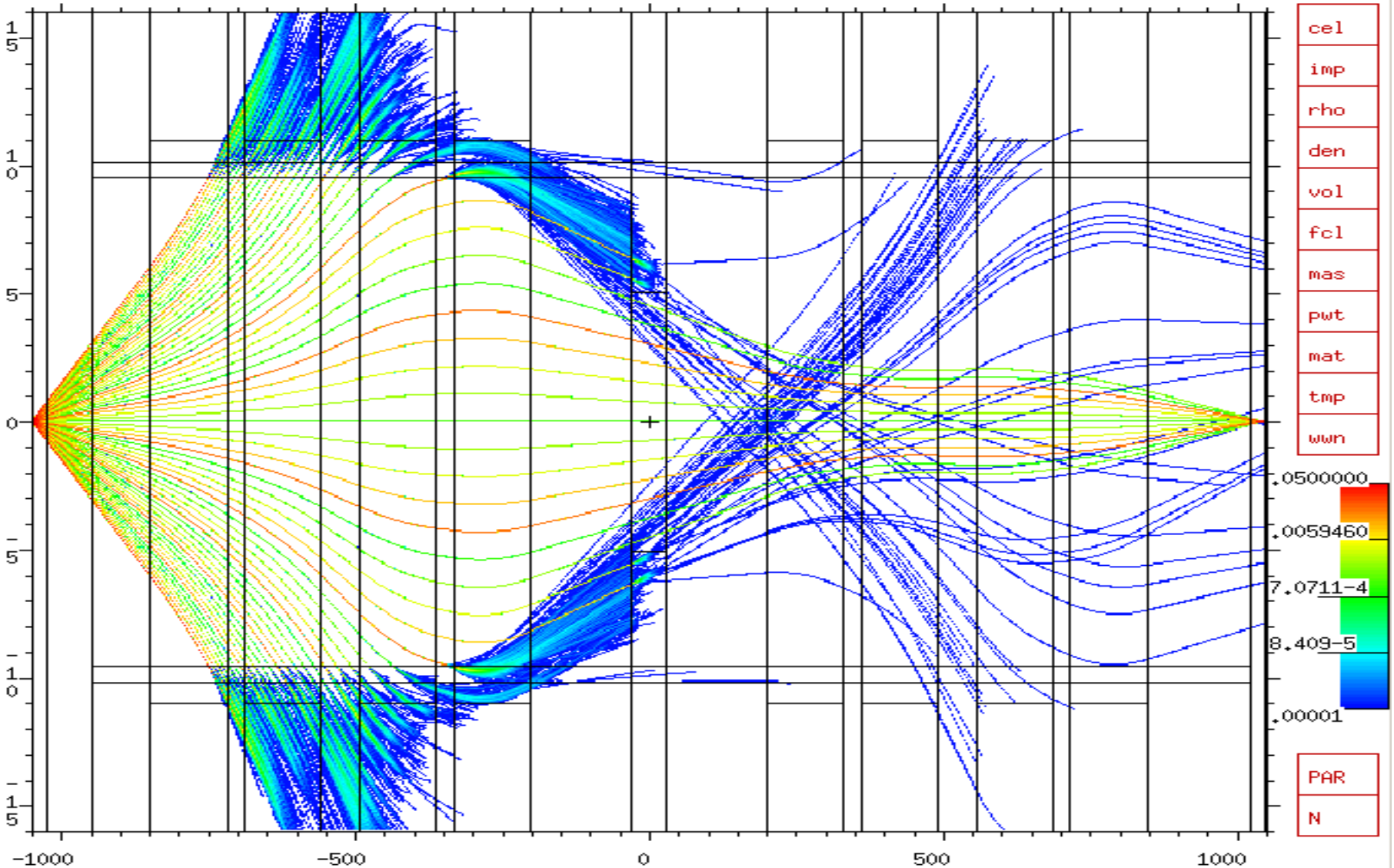


Particle Tracks – Horizontal Plane



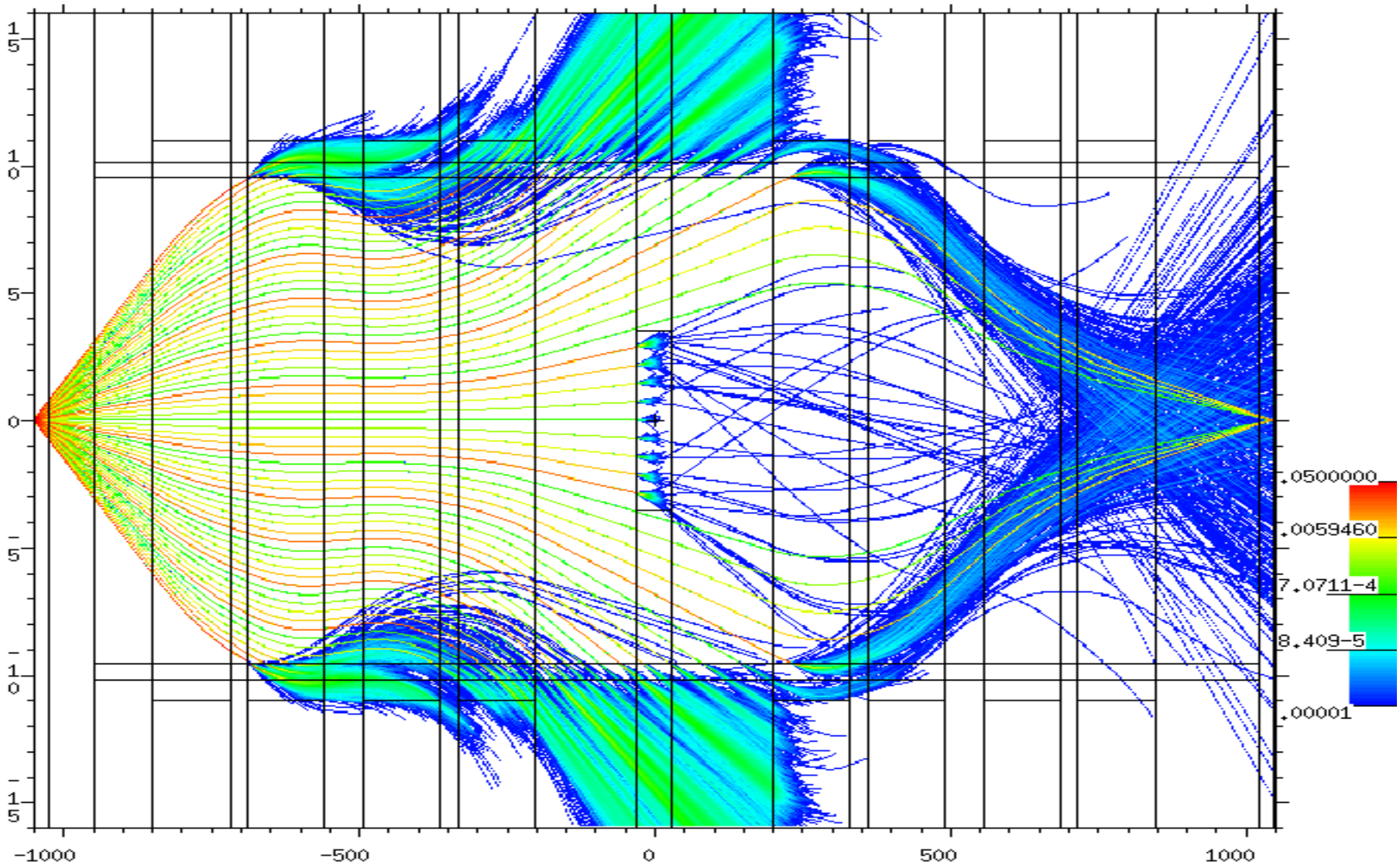
0 – 30 mrads scattering angle, in 1 mrad steps

Particle Tracks – Vertical Plane



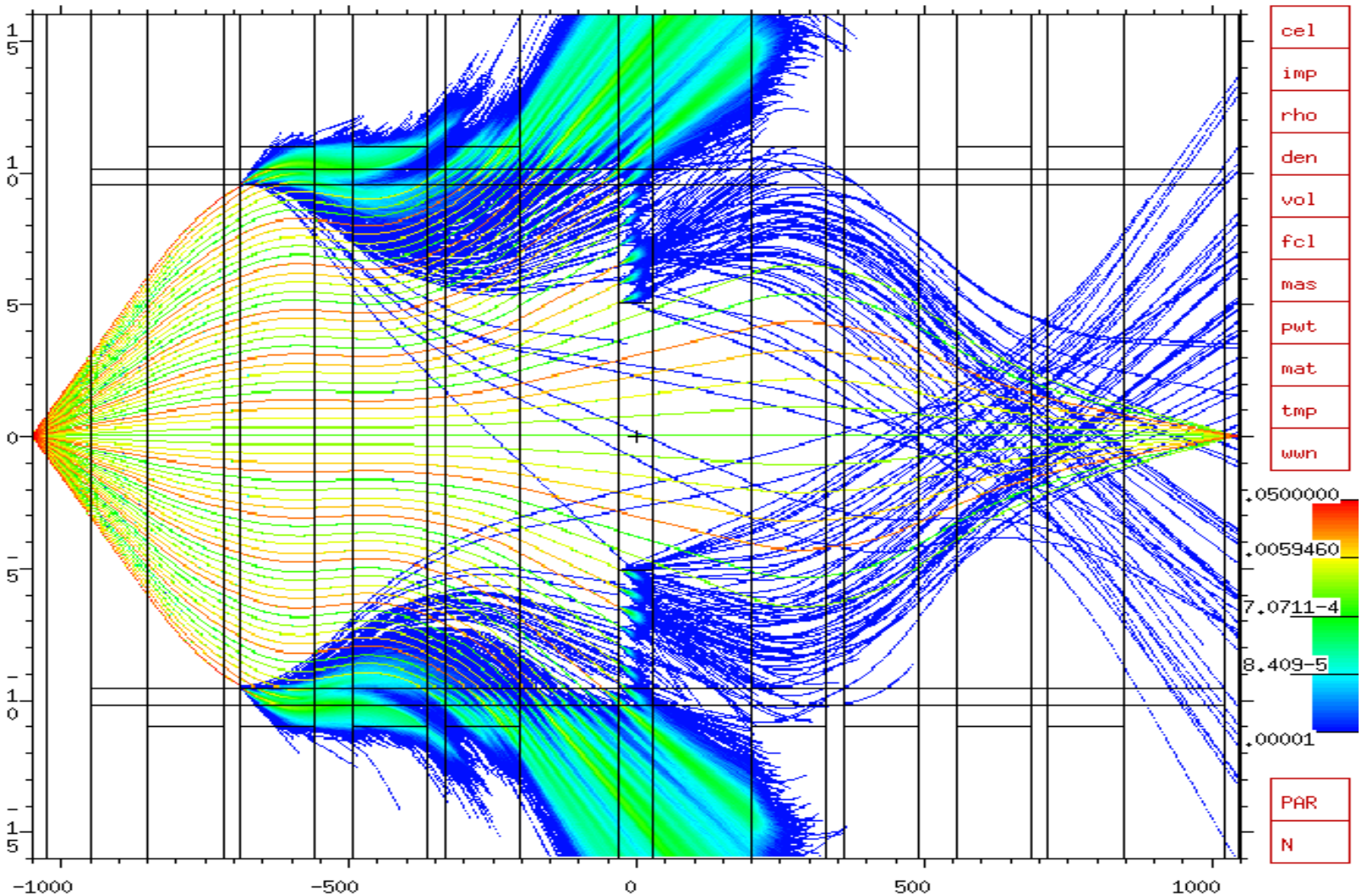
0 – 30 mrads scattering angle, in 1 mrad steps

Anti-Collimator, Horizontal Plane



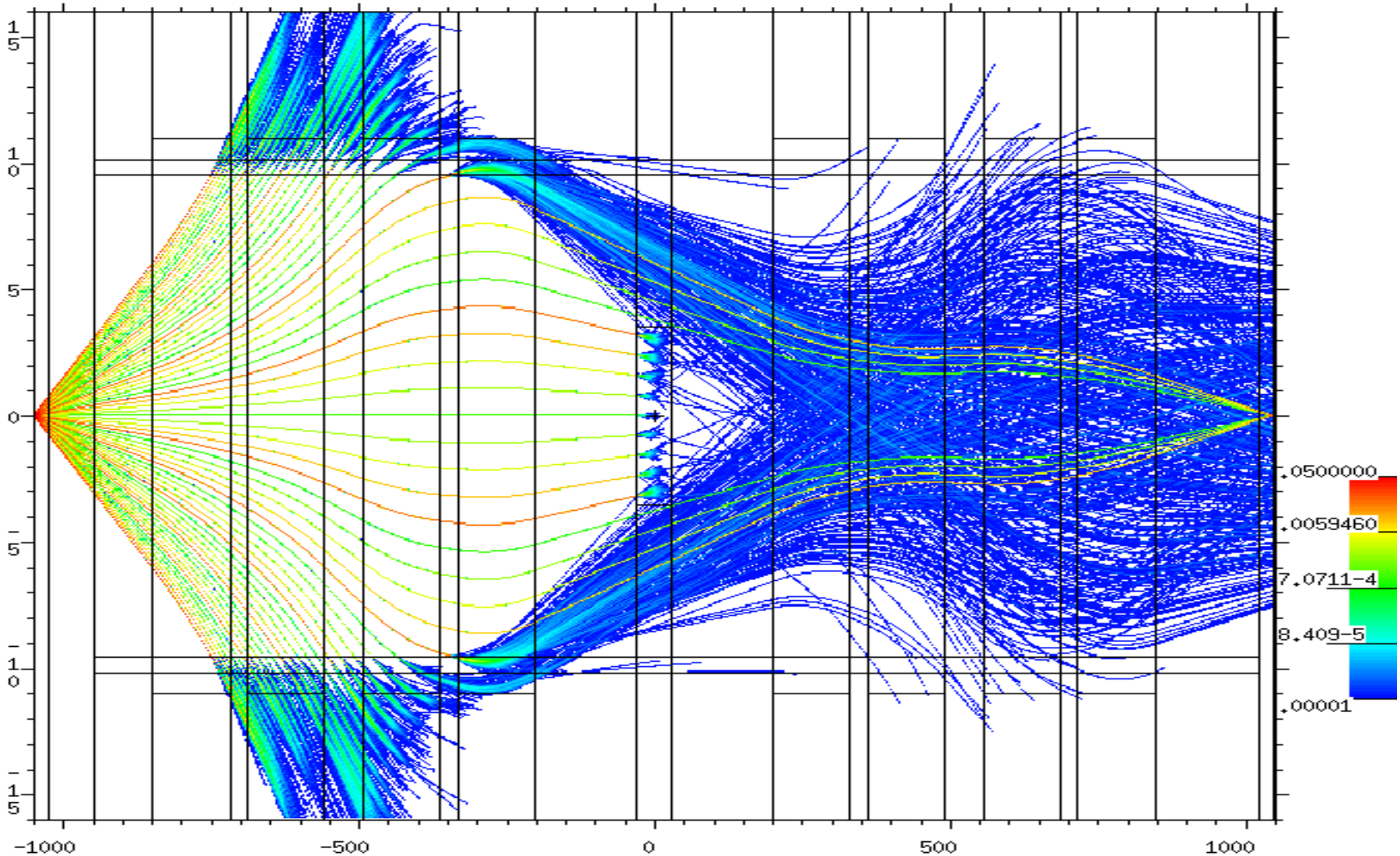
0 – 30 mrads scattering angle, in 1 mrad steps

Particle Tracks – Horizontal Plane



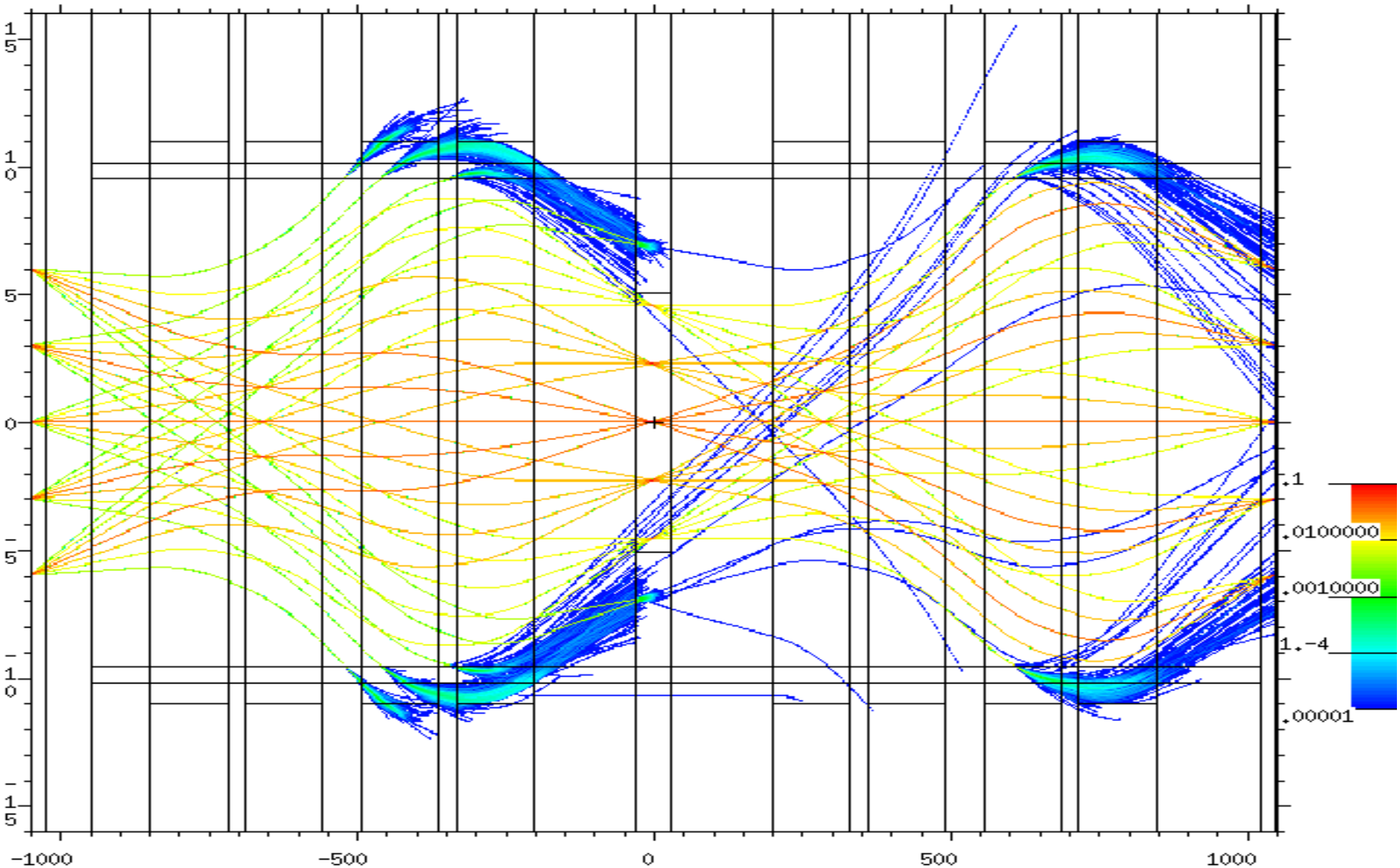
0 – 30 mrads scattering angle, in 1 mrad steps

Anti-Collimator, Vertical Plane

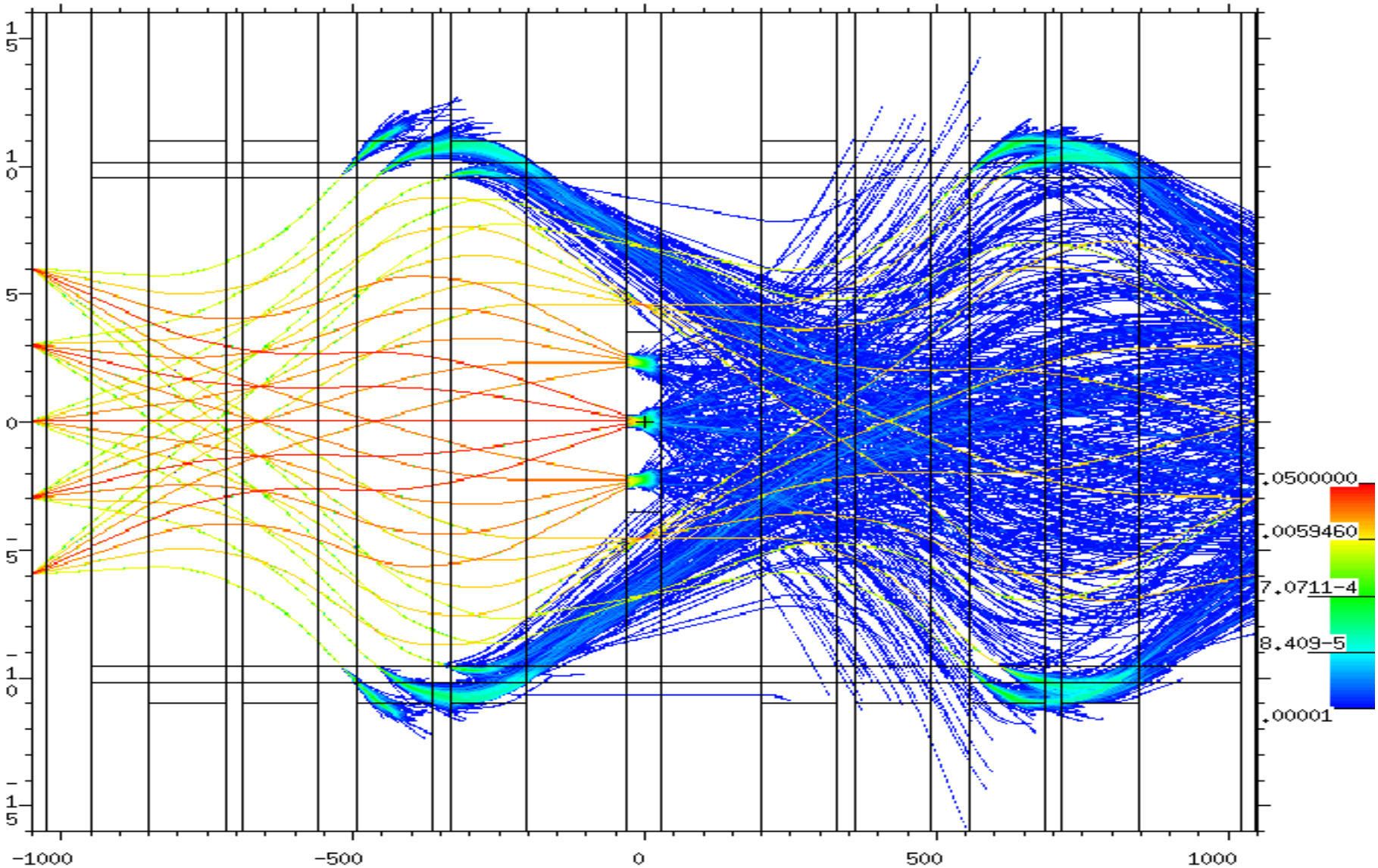


0 – 30 mrads scattering angle, in 1 mrad steps

Vertical axis -- 0, 3, 6, and 9 mrads angles

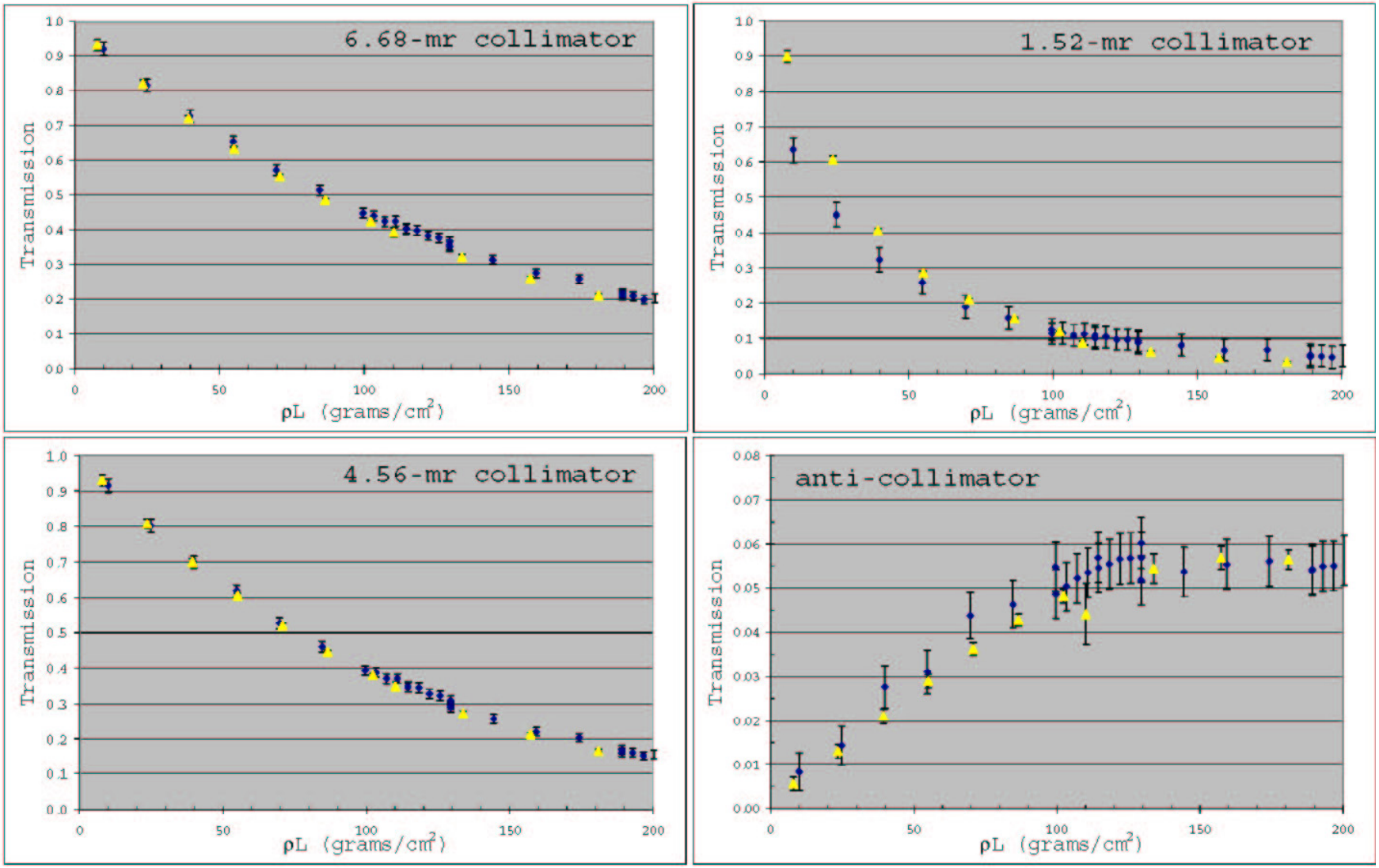


Vertical axis – Anti-collimator



Brookhaven Experiments

Iron target: Blue = data, Yellow = MCNP6 simulation.



Summary

- **Two Magnetic Field Tracking Methods**
  - Transfer Maps
  - Direct Tracking w/ Numerical Integration Techniques
- **Direct Tracking Field Types**
  - Constant
  - Quadrupole
  - Quadrupole w/ Edge Kicks
- **Test Results**
- **Data Results**

Conclusions

- MCNP has a 30+ year history, with continued development, support, and V&V by X-Division at LANL
- MCNP5 is the latest version, with significant improvements & new features
- The MCNP Team in X-Division continues to conduct a wide variety of Monte Carlo R&D work
- Many recent LANL Monte Carlo publications available at:
  http://www-xdiv.lanl.gov/x5/MCNP/index.html