LA-UR- 04-8086

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Title: Release of MCNP5_RSICC_1.30

Author(s): Tim Goorley, Jeff Bull, Forrest Brown, et. al.
MCNP Monte Carlo Team, X-5
Los Alamos National Laboratory

Submitted to: American Nuclear Society Winter Meeting
Washington, D.C.
Nov. 14-18, 2004.

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Form 836 (8/00)

Release of MCNP5_RSICC_1.30

Tim Goorley, Jeffery S. Bull, Forrest B. Brown, Thomas E. Booth, H. Grady Hughes, Russell D. Mosteller, R. Arthur Forster, Susan E. Post, Richard E. Prael, Elizabeth C. Selcow, Avneet Sood, Jeremy E. Sweezy

Diagnostic Applications Group(X-5) Los Alamos National Laboratory, P.O .Box 1663 MS F663, Los Alamos, NM, 87545. mcnp@lanl.gov, http://www-xdiv.lanl.gov/x5/MCNP/

INTRODUCTION

In July of 2004, an updated version of MCNP5™ (MCNP5_RSICC_1.30) was released to the Radiation Shielding Information Computational Center.[1,2] This updated version has three new features, thirteen bug fixes and several minor coding improvements. The new features are: support for 8 byte integers, specialized tally treatment of large lattices, and mesh tally enhancements. Of the thirteen bug fixes, only four resulted in incorrect answers in specific circumstances. In addition to the standard RSICC distribution of the MCNP5 source, executables and patches, the patch file (only) is available on the MCNP website: http://www-xdiv.lanl.gov/x5/MCNP/theresources.html

NEW FEATURES

The three new MCNP5 features are discussed in the following paragraphs. Several new improvements have also been made to the manual and development environment. All of the features, bug fixes, coding improvement issues and related documentation are now maintained in Sourceforge[3]. Fortran and C source code and regression test problems are now under version control with CVS.

8 Byte Integer Support

There have been occasional requests on the mcnp-forum from users who wish to run more than 2.1 billion particles to improve their tally statistics. In the updated version of MCNP5, twenty-five integer variables are now explicitly declared as 8 byte integers. Most of these variables are related to NPS, the number of histories, and allow users to run more than 2.1 billion source particles. Besides the NPS card in the MCNP input deck, the other cards which allow some 8 byte integer entries are: PRDMP, RAND, PTRAC and MPLOT. These entries control how frequently file dumps and parallel communication rendezvous occur, random number parameters, particle track file generation, and tally plot frequencies, respectively. Additionally, format statements in the output files were expanded to print allowed 8 byte integers in fields of twelve characters, or up to 999 billion. Since longer MCNP runs can cause larger ptrac files to be created, ptrac files larger than 250 Gigabytes were created and tested.

Lattice Tally Enhancements

In some medical physics radiation transport applications, lattices, often based on CT images, are used to represent human geometry. These calculations, particularly for large lattices, are very time consuming. Lattice tally enhancements included in this release of MCNP5 reduce wall-clock runtimes by orders of magnitude[4] for these specific problems. MCNP5 also has the capability of determining if the input deck meets stringent requirements necessary to use the lattice speed tally treatment. If so, MCNP5 will issue a warning and will automatically use the enhancement. A new card, SPDTL, can also be used to turn this treatment on or off, and to print out which requirements are not fulfilled, if any.

Mesh Tally Enhancements

The original release of MCNP5 in June 2003 contained support for mesh tallies, or a 3-D grid which calculates volume-averaged fluxes in each voxel in that grid. Included with this feature was the ability to use the tally multiplier card (FM card) in combination with a mesh tally. On the FM card, the user must specify the material whose data are used to calculate the tally values. These data were used over the entire mesh, even if the particle was traveling in a material other than that identified on the FM card. This prevented the calculation of material dependent quantities such as k_{eff} and particle production rates in mesh tallies that range over several materials. This drawback has been rectified in this new version of MCNP5. If zero is entered as the material number on an FM card containing a multiplier set, the reaction data for the material in which the particle is traveling is used to calculate the tally values.

BUG FIXES

Thirteen bugs were fixed in the new update. Only four of these bugs caused incorrect answers in specific circumstances. These four bugs apply to the use of

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DXTRAN spheres in lattices, incorrect interpolation in DE DF cards applied to mesh tallies, incorrect material usage for FM cards with mesh tallies, and attenuator or special multiplier sets with the FM card and mesh tallies. Other bug fixes correct crashes resulting from transforming macrobodies, reading runtpe files incorrectly, and incorrect allocation of the variable ibnk. Two warning messages have also been corrected. A full bug fix list is in the patch documentation[2].

CODING IMPROVEMENTS

Slight changes have been made to the code and build system to continue to modernize MCNP. Support for outdated Windows graphics interface, Winteracter, has been removed. Plotting on all platforms is now only supported with X11 graphics. More named constants have been added and more real number constants have been forced to double precision. Support for the Intel 7.1 compiler in sequential plot mode on Windows PCs was also added.

FUTURE RELEASES

Currently under development is the next version of MCNP, MCNP6. This version will contain charged particle transport, magnetic field tracking, and other new features. This version is not expected to be released for at least another year. Patches with bug fixes and possibly new features for MCNP5 will be released in the meantime.

REFERENCES

1. X-5 Monte Carlo Team, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Vol. 1" Los Alamos National Laboratory, LA-UR-03-1987 (April 2003).
2. X-5 Monte Carlo Team, "Patch to Update MCNP5 version MCNP5_RSICC_1.20 to version MCNP5_RSICC_1.30," Los Alamos National Laboratory, LA-UR-04-5921 (August 2004).
3. http://sourceforge.net/index.php
4. T. GOORLEY, "MCNP5 Tally Enhancements for Lattices," Los Alamos National Laboratory, LAUR-04-3400 (May 2004).

Release of MCNP5_RSICC_1.30

X-5 MCNP Team

Speaker: Tim Goorley

Release of MCNP5_RSICC_1.30

- Introduction
- New Features
  - 8 byte Integer Support
  - Lattice Tally Enhancements
  - Mesh Tally Enhancements
- Bug Fixes
- New Data Library
- Future Work

Introduction

- MCNP – Monte Carlo N Particle – General purpose radiation (n,γ,e) transport code.

- MCNP5 released April 2003
  - Initial Release RSICC_1.14
  - 1st Patch – RSICC_1.20 (Dec 2003)
  - 2nd Patch – RSICC_1.30 (Sept 2004)

New Features

- 8 Byte Integer (> 2.14 Billion) Support
  - 25 variables in code changed to 8 Byte
  - More histories
  - More infrequent rendezvous (for parallel calc.)
  - More events in ptrac file (> 250 Gigabytes)
  - Input Cards:PRDMP, RAND, PTRAC, & MPLOT
- Support for Mac OS X
  - Include LAM-MPI compiling options

New Features

- Lattice Speed Tally Enhancements
  - For problems with hexagonal geometric lattices & F4 tallies, exchanges capabilities for speed.
  - Typically used for medical physics voxel models.
  - Wall Clock speedups of ~500x possible.
  - Autodetect if possible, warning if used.

T. Goorley, MCNP5 Tally Enhancements for Lattices, LA-UR-04-3400.

W.S. Kiger, et al., Performance enhancements of MCNP4B, MCNP5, and MCNPX for Monte Carlo Radiotherapy Planning Calculations in Lattice Geometries, 11th International Symposia for Neutron Capture Therapy, Boston USA, Oct 12-15.

New Features

- Mesh Tally Enhancements
  - A geometry-independent user defined grid on which volume averaged fluxes are calculated.
  - Original release in MCNP5.
  - Could be used in conjunction with FM card to calculate reaction rates for a single material.
  - Now whatever material the particle is in can be used, important when mesh tally covers multiple materials.

Bug Fixes

- 13 Bugs fixed
- Only 4 bugs caused incorrect answers
  - DXTRAN spheres in lattices
  - Incorrect DE DX interpolation for mesh tallies
  - Incorrect material usage for FM & mesh tallies
  - Incorrect atten/mult sets for FM & mesh tallies
- Others: crash w/ transform macro, problem with reading runtpe files.

New Data Library

- t16_2003
  - pre ENDF/B-VII evaluations from Los Alamos Group T-16 for 15 isotopes:
  - H-3
  - U-232, U-233, U-234, U-235, U-236, U-237, U-238,
  - U-239, U-240, U-241
  - Np-237
  - Pu-239
  - Am-241, Am-243
- http://laurel.lanl.gov/PROJECTS/DATA/nuclear/nuclear.html

Crit Validation Suite w/ new data

Range	Pre-ENDF/B-VII	ENDF/B-VI
$\lvert k \rvert \leq \sigma$	19	13
$\sigma < \lvert k \rvert < 2\sigma$	7	9
$\lvert k \rvert > 2\sigma$	5	9

Substantial improvements for bare metal spheres (Jezebel-233, Godiva, and Jezebel), BIG TEN, HEU and Pu metal spheres in water (Godiver and Pu-MF-011, respectively), and LEU lattice (B&W XI (2))

ORNL resonance parameters improve results for Godiver, ORNL-10, IEU-CT-03, STACY (36), B&W XI (2), and LEU-ST-02 (2)

R. D. Mosteller, "Comparison of Results from the MCNP Validation Suite Using ENDF/B-VI and Preliminary ENDF/B-VII Nuclear Data," presented at the International Conference on Nuclear Data for Science and Technology, Santa Fe, NM, Sept 27 - Oct 1, 2004 (LA-UR-04-6489).

RSICC Distribution

- 3 CDROMs
  - Unix
    - data_new, data_webpages, source & executables
    - patch & patch description, readme files
  - Windows Data Installer
    - InstallShield® installer for new data
  - Windows Executables Installer
    - InstallShield® installer for source, executables
    - data_webpages, patch & patch description,readmes

Updated MCNP Homepage

- http://laws.lanl.gov/x5/MCNP/index.html
  - MCNP5_RSICC_1.30 patch & description
  - 2005 MCNP Workshops
  - MCNP5 discussion and description
  - Volume I (Overview and Theory) of MCNP5 Manual
  - Publications – 40 recent LAUR reports

Future Work

- Mesh Tally plotting (done)
- Distribution of n emitted from fission [$\overline{\nu}$] (done)
- Plot tallies as a function of lethargy (done)
- Log interpolation [ilog] in input deck (done)
- Expanded Large Lattice Capability
- Stochastic Geometry

Fission Neutron Distribution

- Currently, one of two integer values are selected for neutrons emitted from fission
- Ex. U-235, $\bar{\nu}$ = ~2.43, 2 neutrons are selected with p=0.47 and 3 neutrons are selected with p=0.43
- Now, an isotope specific, E-dependant (~Gaussian) distribution of neutrons can be selected on phys card.

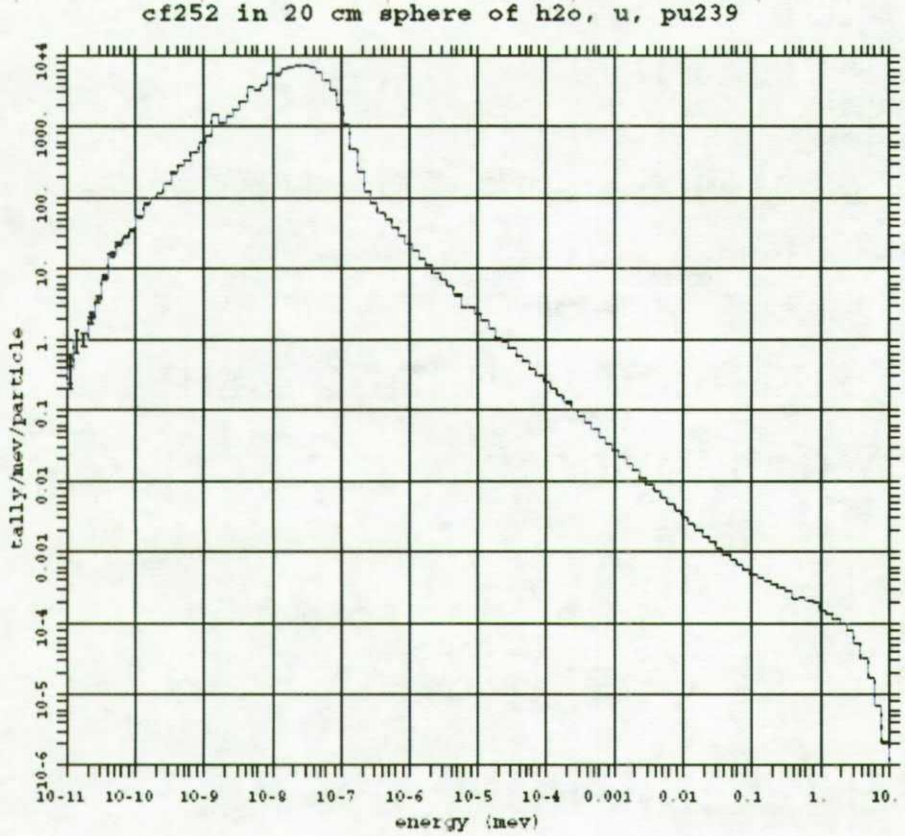
# n's emitted	# fraction	error
nu = 0	0.03894	0.03894
nu = 1	0.15930	0.19823
nu = 2	0.32711	0.52534
nu = 3	0.31159	0.83693
nu = 4	0.13479	0.97172
nu = 5	0.02588	0.99760
nu = 6	0.00230	0.99990
nu = 7	0.00009	0.99999

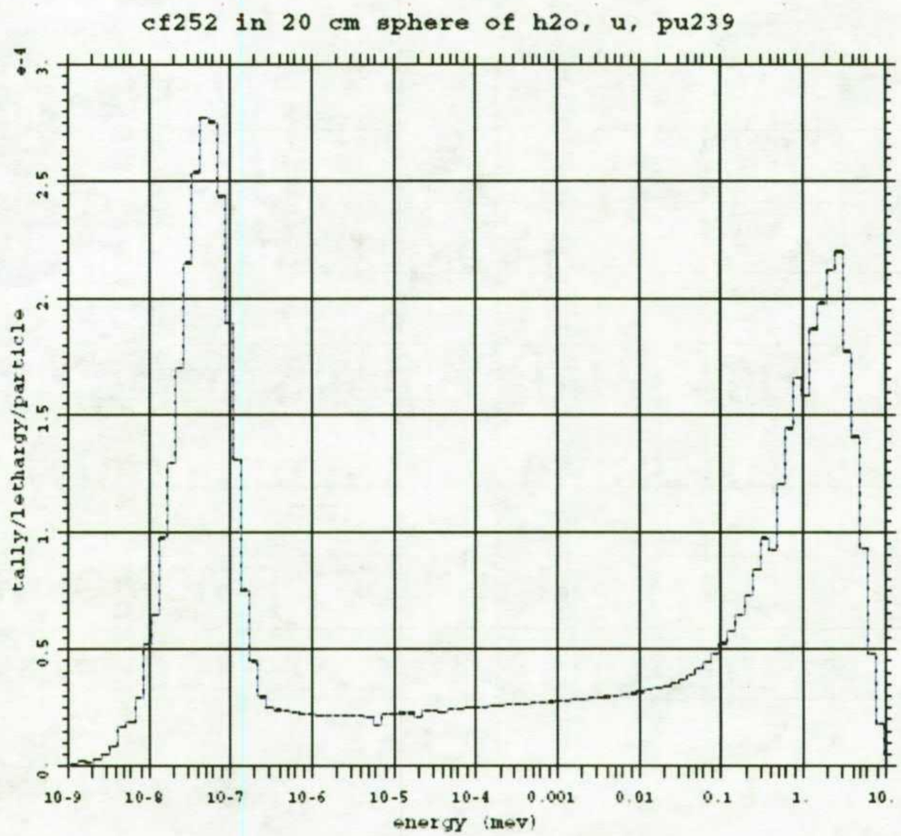
Print Table 115

James Terrell, "Distribution of Fission Neutron Numbers," Phys. Rev. 108, 783 (1957).

John Lestone, X-5 research note.

Lethargy Plotting





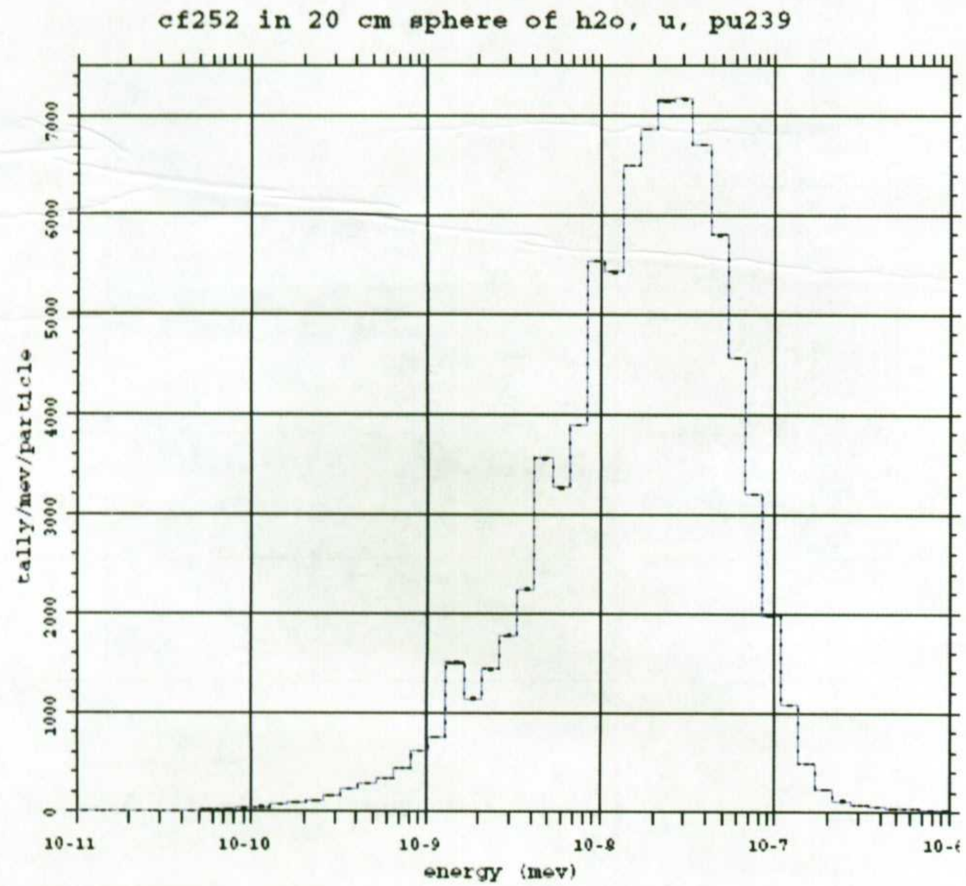
mcnp 5
11/08/04 13:12:51
tally 4
n
nps 5000000
f(e) bin normed
mctal = inpupum

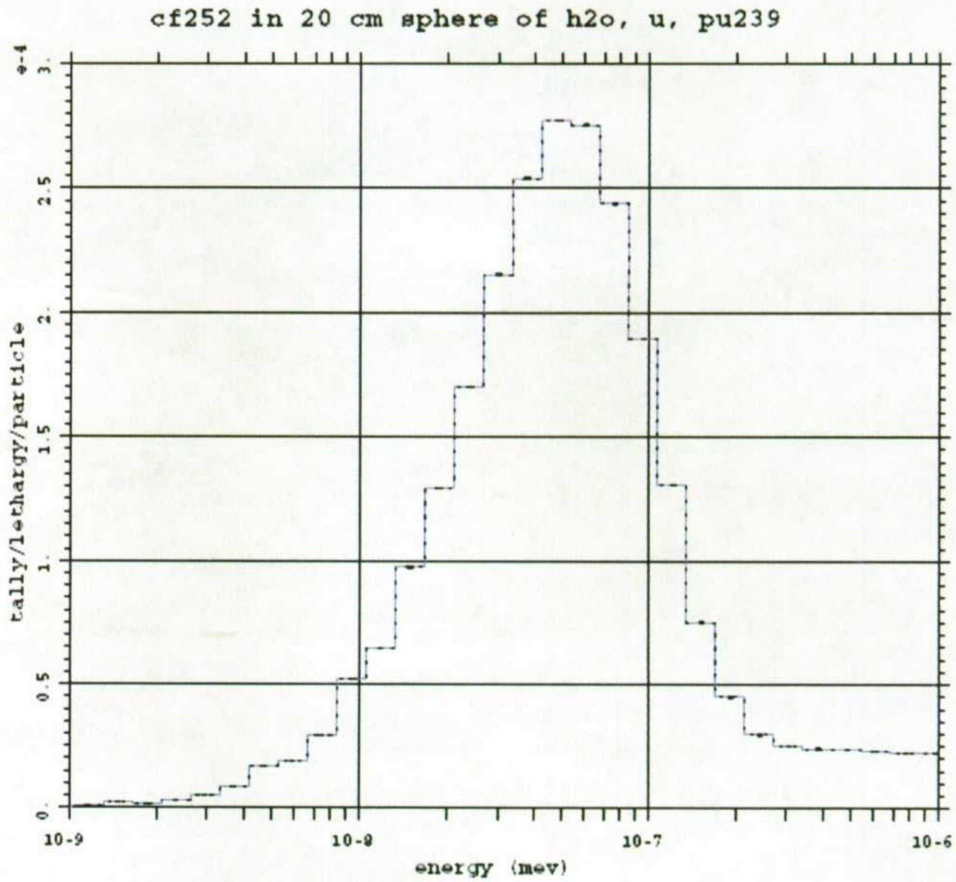
mcnp 5
11/08/04 13:12:51
tally 4
n
nps 5000000
f(u)=ef(e) bin normed
mctal = inpupum

Diagnostics Applications Group (X-5)

Los Alamos

Lethargy Plotting

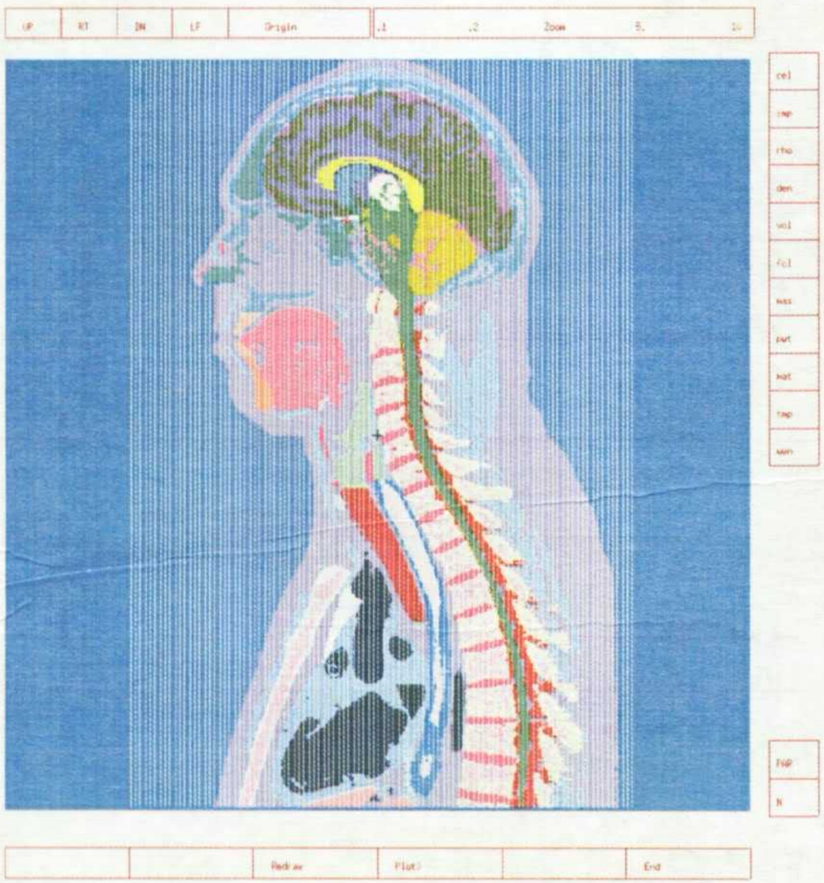


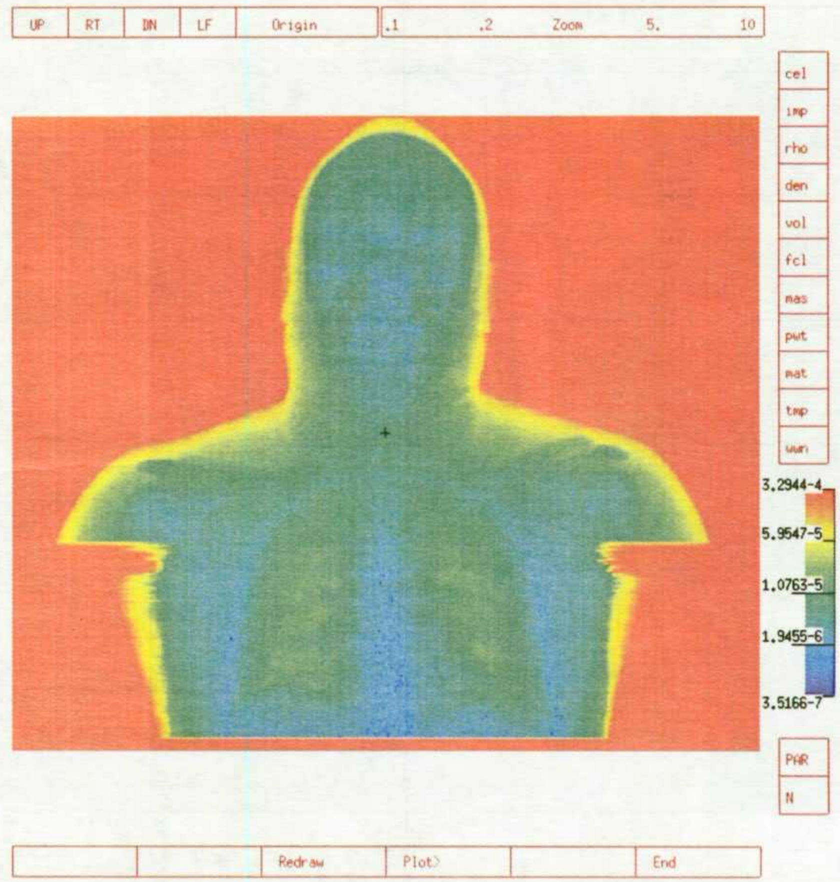


Expanded Lattice Capabilities

100 Million voxel model of VIP-Man, geometry (left) meshtally plot (right)

Collaboration with Prof. George Xu (xug2@rpi.edu), and Brian Wang (RPI)

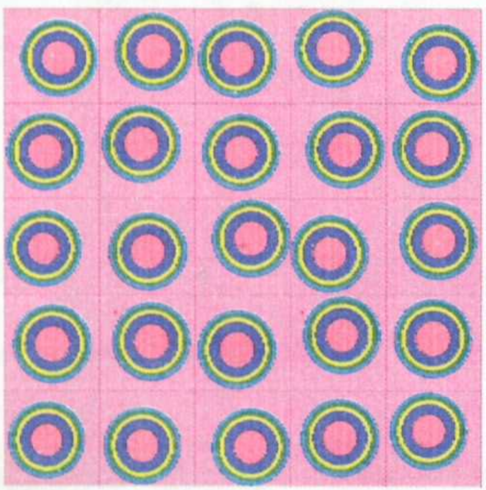




http://www.rpi.edu/dept/radsafe/public_html/home.htm

Stochastic Geometry

- Fixed lattice with random kernels [MCNP stochastic geometry]
  - 5x5x5 cubical lattice
  - Lattice edge chosen to preserve the specified packing fraction.
  - Fuel kernels randomly placed on-the-fly within the cubical cells
  - Reflecting boundaries on the outer surfaces
  - Uses new MCNP5 stochastic geometry



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

Stochastic Geometry for MCNP5, F.B.Brown, W.R. Martin (U. Mich) ANS Winter 2004 (Wed – AM)