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Author(s): J.Timothy Goorley, Forrest B. Brown, Lawrence J. Cox

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MCNP5™ Improvements for Windows PCs

Tim Goorley, Forrest Brown, Lawrence J. Cox

MCNP Development Team, X-5, Los Alamos National Laboratory



Abstract

With the release of MCNP 5, much more emphasis has been placed on improving its functionality on PCs running Microsoft Windows® (9X/NT/2000/XP). Enhanced installation and build systems, support for more Fortran compilers, integration with X11 graphics build files, and MPI and PVM parallel capabilities have been implemented in MCNP 5 for Windows PCs, allowing users to utilize dual CPU PCs, clusters of homogeneous Windows PCs, or heterogeneous clusters. MCNP 5 can be installed with an InstallShield® setup programs, similar to other Windows programs, for users who only need to install executables and data libraries. For those users who need to compile the source, the GNU make utility can be used in conjunction with three supported Fortran compilers. Alternatively, Compaq Developer Studio® can be used to compile MCNP 5. The X-Windows plotting capabilities have been improved, and all the appropriate open source X11R6 files for compiling MCNP 5 are bundled with the MCNP 5 source code.

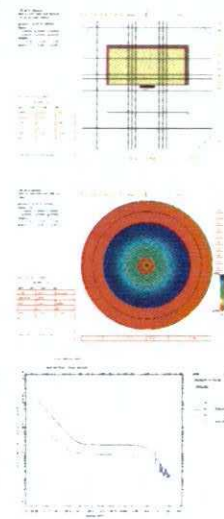
Improved X-windows Graphics



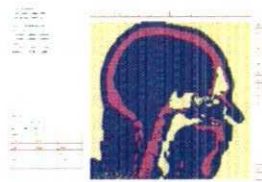
There have been a number of improvements in the X-Windows plotting system, which is the recommended graphics system for all platforms MCNP5 is available on. These improvements include:

- More mouse-driven commands available in plotting screen.
- More MCNP5 capabilities can be plotted:
 - MESH grid plots and importances superimposed over geometry
 - More cell characteristics
 - 64 Color Plotting Scheme
- X-Windows library and include files in MCNP5 distribution.

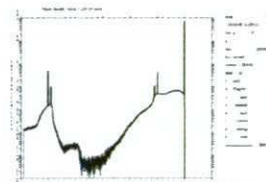
Although X-Windows files are included with MCNP5, an X-server is still necessary to plot. Commercial X-servers which have been tested are: Reflection X (<http://www.wrg.com/products/>), Hummingbird's Exceed_NT (<http://www.hummingbird.com/products/nc/exceed/index.html>), and Starne's X-win32 (<http://www.starne.com/>). The freeware GNU X-server XFree86 has also been tested successfully.



The three plots above show the ability of MCNP5 to plot the MESH tally grid (top), a 64-color mapping of material density (middle), and the neutron cross sections of an element, a material, and a $\Sigma(\alpha,\beta)$ correction to the cross section (bottom).



The screen shot shows the MCNP5 geometry plotter, which is now mostly mouse driven. The model is a 256x256x250 lattice of a human head, which was generated from a 3-D CT digital data set. Air is colored yellow, soft tissue in blue, and bone in magenta. Each individual voxel is roughly cubic and is 1 mm³. This image was generated on a 2.0 GHz Pentium IV with 1 Gigabyte of physical RAM.



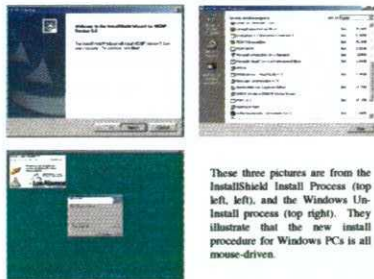
This image from the MCNP5 tally plotter shows the energy spectrum resulting from a 60 keV photon beam incident on a Ge detector with an Al casing. The plot shows the detected energy (in 100 eV bins) vs. number of pulses. Energy bins are 100 eV wide. For each data point, the statistical error bars (1 σ) are also plotted. Doppler photon broadening has been implemented in MCNP5, which is shown by the gradual slope between 10 and 30 keV.

Enhanced Installation and Build Systems

Installing with Install Shield®

Typical InstallShield Process

- Start by opening "setup.exe"
- Boot screen and welcome
- Copyright Agreement
- Name, Co., Serial # (ignore)
- Select Installation Folder
 - (default: Program Files\LANL\MCNP5)
 - (default: Program Files\LANL\MCNPDATA)
- Installer Copies Files
- Option to Modify Environmental Variables
- Summary of Results
- Notice to log off and back on



These three pictures are from the InstallShield install process (top left, left), and the Windows Uninstall process (top right). They illustrate that the new install procedure for Windows PCs is all mouse-driven.

Building with Compaq Developer Studio®

The CVF Developer Studio is a GUI "workspace" where it is easy to edit source text files, control the compile and link options, and compile, link, execute, and debug your application. There is a CVF project for each MCNP5 MPI, PVM, plotting and sequential executable. The appropriate default settings for all of these projects have already been configured.

- Changes in directory locations or libraries are fairly straightforward
- Can build MPI or PVM executables

The image to the left shows a screen shot of the Compaq Developer Studio.



Building with GMAKE

The second build procedure is analogous to the installation procedure used on other platforms (Linux, Unix, etc.)

- Useful for people who want to re-compile the source code, and especially useful for those who re-compile frequently.
- Useful for people who have more experience with Unix
- In the /MCNP5/Source directory, type `make build CONFIG=FCOMPILER CCOMPILER plot`

The gmake utility on Windows PCs can be used to build a MPI executable.

- Work is in progress to allow it to build a PVM executable
- Verify that the path to MPICHINT.h files and library are correct in the Windows_NT_gcf files in /MCNP5/Source/config directory
- In the /MCNP5/Source directory, type `make clean CONFIG=compaq cl mpi`
- In the /MCNP5/Source directory, type `make build CONFIG=compaq cl mpi`

Requires

- Cygwin - A unix shell for Windows
 - <http://www.cygwin.com>
 - <http://www.redhat.com/apps/download/>
 - Should also install gmake, perl, and gcc packages
 - Optional X11 client package - XFree86
- A Fortran 90 Compiler
 - compaq (Compaq Visual Fortran 95 v 6.6B)
 - lahey (Lahey Fortran 95 Professional v 5.70c)
 - absoft (Absoft Fortran 95 v 8.0)
- A C Compiler
 - gcc (GNU gcc v 2.95.2-8 [Cygwin special])
 - icl (Microsoft C/C++ v 12.0.0.8168)
 - fcc (Puytrau C/C++ v 3.0 [only with Lahey])

MPI and PVM Capabilities

With the release of MCNP5, the parallel capabilities of MCNP have been extended to Windows PCs. MCNP5 can run across a cluster of several Windows NT/2000 PCs using the Message Passing Interface (MPI) or Parallel Virtual Machine (PVM) communications protocols. Using either method, the behavior of MCNP is effectively the same:

- For homogeneous clusters or dual/quad PC, mcrp will run an identical number of histories on each "slave" process

```
-mcrp5pvm inp=x tasks -#
-mpirun -np # mcrp5mpi inp=x
```

- For a heterogeneous cluster, mcrp will run 200 particles on each "slave" process and collect the appropriate timing information. Using this information, MCNP will determine how many particles each process should run.

```
-mcrp5pvm inp=x tasks #
-mpirun -np # mcrp5mpi inp=x BALANCE
```

The communication of processes with the "master" process is controlled by the 6th entry on the prdmp card in the mcrp input deck.



Small Laptop Cluster Timing Study

DELL Inspiron B200 - Windows 2000
Pentium IV @ 1.6 GHz, 1024 Mbytes RAM, 512 kbytes L2 Cache

DELL Latitude C800 - Windows 2000

Pentium III@ 1.0 GHz, 512 Mbytes RAM, 256 kbytes L2 Cache

Wall Clock Runtimes (min:sec)	Sequential		PVM tasks 2	PVM* tasks 2	MPI 3 processes	MPI 3 processes BALANCE
	Pentium 4	Pentium 3	P4:Master + Slave P3:Slave	P4:Master + Slave P3:Slave	P4:Master + Slave P3:Slave	P4:Master + Slave P3:Slave
NPS 10,000	9:41	30:25	11:41	10:05	16:33	9:30
NPS 100,000	90:55	298:54	143:32	83:27	153:29	75:34

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MCNP5™ Improvements for Windows PCs

By Tim Goorley, Forrest Brown, Lawrence J. Cox

MCNP Development Team, X-5
X-Division (Applied Physics)
Los Alamos National Laboratory



MCNP Improvements for Windows PCs

With the release of MCNP 5, much more emphasis has been placed on improving its functionality on PCs running Microsoft Windows® (9X/NT/2000/XP).

- Installation - InstallShield
- Build system
 - CVF Developer Studio
 - Gmake
- X-Windows
 - More capabilities
 - Library and include files with MCNP5 Source
- Parallel Capabilities
 - Parallel Virtual Machine (PVM)
 - Message Passage Interface (MPI)
- Incorporated into Start Menu
- MCNP Visual Editor

Installing MCNP executables



There are two methods for installing MCNP5 on a Windows PC:

- **InstallShield® Installer** - installs everything needed to start running the sequential MCNP5 executable.
 - It also modifies the environmental variables.
 - No additional software needed to install.
 - Provides parallel executables.
 - Will NOT recompile source.
- **Gmake install** - After the user copies the directory structure to local drive, "gmake install" will compile the source, run the test problems and summarize unexpected differences.
 - Will NOT modify environmental variables.
 - Requires previously installed Fortran Compiler and Unix shell (Cygwin).
 - Will create mpi parallel executables, but not PVM.
 - Will recompile source.

Building MCNP executables - gmake



This method requires that you previously install:

- **Cygwin - A unix shell for Windows**
 - <http://www.cygwin.com>
 - <http://www.redhat.com/apps/download/>
 - Should also install gmake, perl, and gcc packages.
 - Optional X11 client package - XFree86
- **A Fortran 90 Compiler**
 - Compaq Visual Fortran 90 (v 6.6B)
 - Lahey Fortran 95 Professional (v 5.70c)
 - Absoft Pro Fortran 95 (v 8.0)
- **A C Compiler**
 - GNU gcc (v 2.95.2-5 [Cygwin special])
 - Microsoft C/C++ (v 12.00.8168)
 - Fujitsu C/C++ [only with Lahey] (v 3.0)

X-Windows Graphics - Geometry Plotter



- Mouse Driven

```

03/25/03 09:49:12
voxel based on subject 97-4
256-256 images 250 Slices

probid = 03/25/03 09:16:46
basis: YZ
( 0.00000, 1.00000, 0.00000)
( 0.00000, 0.00000, 1.00000)
origin:
( 0.00, 0.00, 0.00)
extent = ( 12.51, 12.51)
    
```

Value for cell 3
in Cell 3

age = 0.10, 0.30, 0.10

CURSOR	Restore	No Lines
PostScript	ROTATE	
COLOR	SCALES 0	LEVEL
ZY	YZ	ZX
LABELS	L1 off	L2 off
BODY		

Click here or picture or menu

X-Windows Graphics - Geometry Plotter



- 64 color plotting for
 - gram density
 - atom density
 - temperature

```

01/28/03 16:53:30
Test for materials and ZHIS for
dchd

probid = 01/28/03 16:50:40
basis: YZ
( 0.00000, 1.00000, 0.00000)
( 0.00000, 0.00000, 1.00000)
origin:
( 0.00, 0.00, 0.00)
extent = ( 3.00, 3.00)
    
```

Value for den 7.5618-4
in Cell 1

age = 0.00, 0.00, 0.00

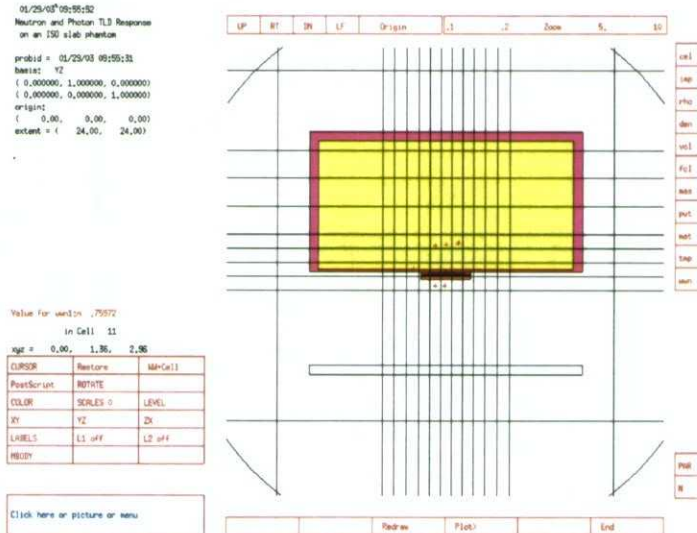
CURSOR	Restore	CellLine
PostScript	ROTATE	
COLOR	SCALES 0	LEVEL
ZY	YZ	ZX
LABELS	L1 off	L2 off
BODY		

Enter Data: color by rho

X-Windows Graphics - Geometry Plotter



- More plotting capability
 - MESH tally grid and importances



MCNP5 Windows Parallel Capabilities



With the release of MCNP5, the parallel capabilities of MCNP have been extended to Windows PCs. MCNP5 can run across a cluster of several Windows NT/2000 PCs using the Message Passing Interface (MPI) or Parallel Virtual Machine (PVM) communications protocols.

- PVM
 - will allow a cluster with Unix, Linux, etc. computers.
 - places some restrictions on mixing Windows 9x with NT/2000 machines.
 - MCNP restrictions on mixing Big Endian with Little Endian Architecture
 - Mcnp5pvm inp=test tasks #
- MPICH.NT
 - will NOT allow a cluster with Unix, Linux, etc. computers.
 - places some restrictions on mixing Windows 9x with NT/2000 machines.
 - Mpirun -hosts x host1 y hosts 2 z ... mcnp5mpi inp=test
- Note clusters can span your desktop (Dual/Quad) or continents.

Running Parallel MCNP5 - Output



Both PVM and MPI MCNP jobs have similar screen output:

```
dump 1 on file loyf3r.r nps = 0 coll = 0
                        ctm = 0.00 nrn = 0
```

xact is done

cp0 = 0.27

master starting 2 tasks with 1 threads each 03/19/03 15:06:03

master sending static commons...

master sending dynamic commons...

master sending cross section data...

master completed initialization broadcasts.

master set rendezvous nps = 200 03/19/03 15:06:20

master set rendezvous nps = 1000 03/19/03 15:06:34

master set rendezvous nps = 2000 03/19/03 15:07:15

master set rendezvous nps = 3000 03/19/03 15:07:57

master set rendezvous nps = 4000 03/19/03 15:08:46

Running Parallel MCNP5



Small Laptop Cluster Timing Study

DELL Inspiron 8200

Pentium IV®, 1.6 GHz, 1024 Mbytes RAM, 512 kbytes L2 Cache

DELL Latitude C800

Pentium III®, 1.0 GHz, 512 Mbytes RAM, 256 kbytes L2 Cache

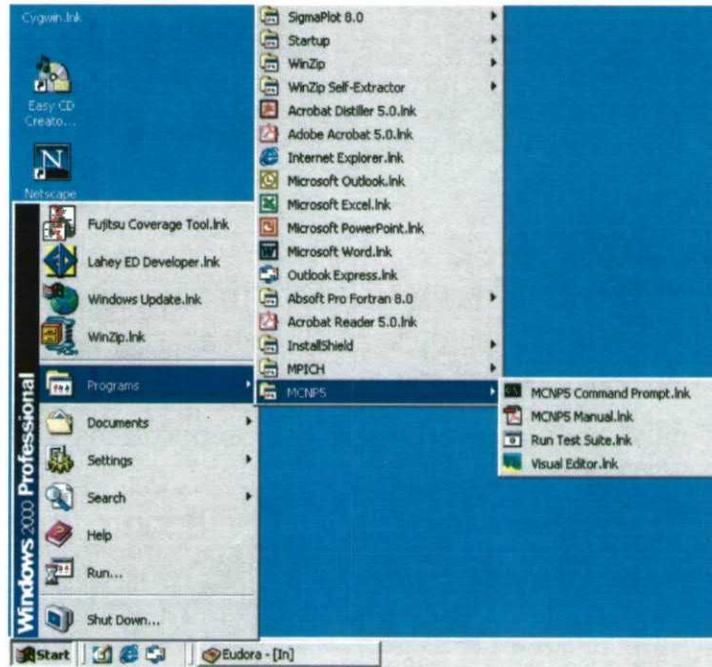
Wall Clock Runtimes (min:sec)	Sequential		PVM tasks 2	PVM tasks 2	MPI 3 processes
	Pentium 4	Pentium 3	P4:Master +Slave P3:Slave	P4:Master +Slave P3:Slave	P4:Master +Slave P3:Slave
NPS 10,000	9:41	30:25	11:41	10:05	16:33
NPS 100,000	90:55	298:54	143:32	83:27	153:29
P4:P3 Ratio	-	-	0.73:1	2.1:1	2.3:1

Integration with Start Menu



From the start menu there are now links to:

- Run the test problems
- Start a command prompt
- Open the MCNP5 Manual
 - (If Acrobat Reader is installed)
- Run the Visual Editor



Visual Editor



MCNP5 Visual Editor now distributed with MCNP

