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Title:	MCNP5-1.51 Release Notes
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memorandum

Computational Analysis and Simulation (X-3)
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MCNP5-1.51 Release Notes

This memo describes the update of the MCNP distribution package from version MCNP5-1.50 to version MCNP5-1.51.

MCNP5-1.50 was released by the Radiation Safety Information Computational Center (RSICC) in December 2008 as part of RSICC package CCC-740. Subsequent to the release, a significant error was found in the photon Doppler broadening routine that can lead to incorrect results for some photon calculations. The error was corrected and the MCNP5 version number was changed to MCNP5-1.51. The new MCNP5-1.51 distribution package was transmitted to RSICC for release to users in January 2009. Users should obtain MCNP5-1.51 RSICC directly from RSICC or the OECD/NEA Data Bank.

These release notes document the error and corrective actions. Except for the corrections and changes noted below, the MCNP5-1.51 release is identical to the MCNP5-1.50 release.

Photon Doppler Broadening Error

A significant error was found in the photon Doppler broadening routine in MCNP5-1.50 that can lead to incorrect results for some photon calculations. The error specifically involved only 1 line of the *dopplerp.F90* routine, where a term was subtracted rather than added during the sampling of the Doppler broadened exit energy of a photon from Compton scattering.

- This error occurs on all computing platforms – Windows, Linux, Mac OS X, and Unix.
- This error does **not** occur in previous versions of MCNP5 (1.40, 1.30, etc.).
- This error does **not** affect any versions of MCNPX.
- The error does **not** affect results for neutron-only criticality calculations, nor any problems that do not include photons.
- The error was corrected and is **not** present in MCNP5-1.51.

Attachment A - "Checklist for Error Notification" – provides details of the error and its impact.

Initial Corrective Action

For users of MCNP5-1.50 who compile the code themselves, a patch was supplied via email to the MCNP Forum. Users can apply the patch themselves if desired, to correct the error and update the code version number to MCNP5-1.51. A listing of the patch file is included in Attachment B – "Patch File for Creating MCNP5-1.51 from MCNP5-1.50."

The email notification to the MCNP Forum also provided guidance for users of MCNP5-1.50 who do not or cannot patch and recompile the code themselves. The photon Doppler broadening treatment can be disabled by adding the following card to the data-cards section of an MCNP5 input file:

```
phys:p     4j     1
```

Further Corrective Action

The MCNP team corrected the error and released the corrected code as MCNP5-1.51. The new release package MCNP5-1.51 is identical to the previous MCNP5-1.50 package except for the following:

- The source coding error was corrected in file `MCNP5/Source/src/dopplerp.F90`
- The code version number was changed from 1.50 to 1.51 in file:
  `MCNP5/Source/config/VC_info.gcf`
  `MCNP5/Source/src/COPYRIGHT_INFO`
  This results in the new version number (1.51) appearing in the printed output from MCNP5 execution.
- New executables were created for Windows, Linux, and Mac OS X systems. These are contained in the DVD directories:
  `MCNP5/bin/Linux`
  `MCNP5/bin/Windows`
  `MCNP5/bin/macosx`
- To help prevent future errors with the photon Doppler broadening and to provide users with a means of verifying the correct photon Doppler broadening treatment, 2 new test problems (#98 and #99) were added to the MCNP5 Regression Test Suite. The files revised or added in directory `MCNP5/Testing/Regression` are:
  `Makefile`
  `Inputs/inp98`
  `Inputs/inp99`
  `Templates/Linux/mctl98`
  `Templates/Linux/mctl99`
  `Templates/Linux/outp98`
  `Templates/Linux/outp99`
  `Templates/Windows_NT/mctl98`
  `Templates/Windows_NT/mctl99`
  `Templates/Windows_NT/outp98`
  `Templates/Windows_NT/outp99`
  Additional cross-section datasets were also added to the files:
  `MCNP5/Testing/xsec_data/testdir1`
  `MCNP5/Testing/xsec_data/testlib1`
  These new test problems will henceforth be run automatically by the MCNP5 installation scripts, for both users and members of the MCNP Team.
- The templates of correct results for the Shielding Validation Suite were regenerated using the corrected MCNP5-1.51 for Linux and Windows systems. These templates are contained in directories:
  `MCNP5/Testing/VALIDATION_SHIELDING/Templates/Linux`
  `MCNP5/Testing/VALIDATION_SHIELDING/Templates/Windows_NT`

- This release note was included in the documentation files for the DVD release of MCNP5-1.51, and various minor changes were made (e.g., updating MCNP5 version numbers and RSICC volume names for DVDs).
- For Windows systems, a new Windows Installer package was created and included on the DVD.

The following executables for MCNP5-1.51 were recompiled using the CONFIG option strings shown, tested, and included with the new MCNP5-1.51 release package:

- **Mac (Intel, 32-bit) -** OS X 10.4.11, Intel F90 compiler 10.1, gcc 4.0.1

  mcnp5_i386 `CONFIG='intel gcc plot omp'`

- **Mac (PowerPC, 32-bit) -** OS X 10.3.9, IBM XLF compiler 8.1, gcc 3.3

  mcnp5_powerpc `CONFIG='ibm gcc plot'`

- **Linux (32-bit) –** Fedora Core release 3 (Heidelberg), Intel Fortran compiler 9.1.037, gcc 3.4.4

  mcnp5_i386
  ```
  CONFIG='intel plot'
  FOPT="-O1 -mtune=pentium-mmx -i_static"
  MARCH=M32
  ```
  mcnp5_i386_omp
  ```
  CONFIG='intel plot omp'
  FOPT="-O1 -mtune=pentium-mmx -i_static"
  MARCH=M32
  ```

- **Linux (64-bit) -** Red Hat Enterprise Linux ES release 4 (Nahant update 3), Intel Fortran compiler 10.0.023, gcc 3.4.5

  mcnp5_x86_64
  ```
  CONFIG='intel plot'
  FOPT="-O1 -mtune=pentium4 -i_static -no-vec"
  MARCH=M64
  ```
  mcnp5_x86_64_omp
  ```
  CONFIG='intel plot omp'
  FOPT="-O1 -mtune=pentium4 -i_static -no-vec"
  MARCH=M64
  ```

- **Windows (32-bit) -** Windows XP (Service Pack 2), Cygwin 1.5.24-2, Intel Visual Fortran Compiler 10.0.027, gcc 3.4.4, MPICH2 1.0.6p1

  mcnp5.exe `CONFIG='intel plot'`
  mcnp5_threads.exe `CONFIG='intel plot omp'`
  mcnp5_mpi.exe `CONFIG='intel plot mpi'`

The release package for MCNP5-1.51 was then burned to DVDs.

Using the DVDs, the release was tested on Windows, Linux, and Mac OS X systems, including: installation, compilation, the Regression Test Suite, the Shielding Validation Suite, the Criticality Validation Suite, and the Analytic Criticality Verification Suite.

The DVDs for the MCNP5-1.51 release package will be conveyed to RSICC for distribution.

RSICC has provided the following advice for users concerning the CCC-740 package:

> If you do not have an urgent need for MCNP5 1.50, we request that you wait until 1.51 is released before ordering the code from RSICC. Announcement of availability will be posted on the RSICC website and newsletter. RSICC will send replacement DVDs to all recipients of MCNP5 1.50. No additional action is required to get the replacement DVD, which will be the new package containing MCNPX 2.6.0,MCNPDATA and the corrected MCNP5 1.51. Upon receipt of the new DVD, please delete all copies of MCNP5 1.50 and shred the original DVD. The same license and export control restrictions to which you agreed for the initial release apply to the new package.

Installation instructions

Any previous versions of MCNP5 or the nuclear data libraries should be renamed, relocated, or deleted prior to installing the latest versions.

> ***Before installing MCNP5 and the new MCNP Data Libraries on Unix, Linux, and Mac OS X systems, users should make sure that at least 12 GB of free disk space is available.***
>
> ***On Windows systems, additional disk space is required when using the Windows Installer, and users should make sure that at least 25 GB of free disk space is available.***

Installation of the latest release of MCNP-1.51 and the data libraries on Windows systems is the same as described in the PDF file 'MCNP5 Installation Guide' that can be accessed from the file `ABOUT_MCNP5.htm` on the RSICC DVD.

For Linux and Mac OS X systems, there is a new installation script available, also available from the file `ABOUT_MCNP5.htm` on the RSICC DVD.

Attachment A. Checklist for Error Notification

Item	
Software Identification	MCNP5, version 1.50 (Previous versions are not impacted) RSICC Package Number CCC-740 Note: this bug does not occur in MCNPX 2.6.0, which is also part of this RSICC package.
Data Library	N/A
Computing platform	All computing platforms
Description of the error	A section of the photon Doppler broadening routine was rewritten to replace the use of the quadratic formula to solve a second degree polynomial equation. During this rewrite a subtraction operation was used instead of addition, causing a miscalculation of the photon energy due to Doppler broadening.
How was the error identified?	The error was identified by a user who compared MCNP5 1.40 to MCNP5 1.50 and obtained significantly different results
When does the error occur?	This error occurs for all photon transport problems for which photon Doppler broadening is enabled. This is the default setting for MCNP5
Potential impact of error	This error causes the incorrect particle energy to be calculated for photons undergoing incoherent scattering if Doppler broadening is enabled.
Frequency / likelihood of error occurring	The error occurs for all problems transporting photons in which photon Doppler broadening is used. The error is most noticeable for photons in the energy range in which Compton scattering contributes significantly to the total photon cross section.
How can users determine if error affects their calculations?	Users should assume that all results are incorrect for photon transport problems which use photon Doppler broadening.

What action should users take if error affects them?	Users can 1) disable photon Doppler broadening by setting the 5th entry of the PHYS:p card to 1. PHYS:p 4j 1 For more information, see p. 3-132 of the MCNP manual, Vol 2, or 2) apply the patch provided in this notification and recompile the code.
Is correction to code/data available?	A patch has been included in this notification.
How to obtain/install correction	RSICC will send replacement DVDs to all recipients of MCNP5 1.50. The replacement DVDs will include the corrected source and executables, MCNP5 1.51.

Attachment B. Patch File for Creating MCNP5-1.51 from MCNP5-1.50

```
# patch-MCNP5_RSICC_1.50_to_1.51
#
# Patch to create MCNP5_RSICC_1.51 from MCNP5_RSICC_1.50
#
# USAGE
# ------------------------------------------------------------------------------
# To apply this patch to an unmodified copy of the RSICC release of
# MCNP5 (CCC-740), MCNP5_RSICC_1.50, follow the directions below.
#
# From a unix/linux/mac command shell window, or from a Cygwin
# command window on a Windows system:
#
# 1) Verify that you have the GNU patch utitity installed by issuing the command
#    "patch -v".  You should see output that looks similar to the output below.
#    Note that the version may be different.
#
#    $ patch -v
#    patch 2.5.4
#    Copyright 1984-1988 Larry Wall
#    Copyright 1989-1999 Free Software Foundation, Inc.
#
#    This program comes with NO WARRANTY, to the extent permitted by law.
#    You may redistribute copies of this program
#    under the terms of the GNU General Public License.
#    For more information about these matters, see the file named COPYING.
#
#    written by Larry Wall and Paul Eggert
#
# 2) Save the patch file "patch-MCNP5_RSICC_1.50_to_1.51" to the MCNP5
#    directory.
#
# 3) Change your working directory to the MCNP5 directory.
#
# 4) Apply the patch with the following command:
#
#    $ patch -p1 < patch-MCNP5_RSICC_1.50_to_1.51
#
# 5) Recompile MCNP5.
#
# Note: This patch may fail if you have modified MCNP5.
# ------------------------------------------------------------------------------
#
Prereq: 1.50
diff -u -r1.34.2.1 -r1.34.2.2
--- MCNP5/Source/config/VC_info.gcf 2 May 2008 17:00:22 -0000     1.34.2.1
```

```
+++ MCNP5/Source/config/VC_info.gcf 15 Jan 2009 01:09:45 -0000    1.34.2.2
@@ -2,4 +2,4 @@
 # --- Thread Name
 THREAD = MCNP5_RSICC
 # --- Thread Version Number
-THD_VERS = 1.50
+THD_VERS = 1.51
diff -u -r1.10 -r1.10.2.1
--- MCNP5/Source/src/dopplerp.F90   25 Feb 2008 18:52:00 -0000    1.10
+++ MCNP5/Source/src/dopplerp.F90   15 Jan 2009 01:09:45 -0000    1.10.2.1
@@ -1,4 +1,4 @@
-!+ $Id: dopplerp.F90,v 1.10 2008/02/25 18:52:00 jsweezy Exp $
+!+ $Id: dopplerp.F90,v 1.10.2.1 2009/01/15 01:09:45 jsweezy Exp $
 ! Copyright LANS/LANL/DOE - see file COPYRIGHT_INFO

 subroutine dopplerp(ene,amu,esc)
@@ -161,7 +161,7 @@
      ! Calculate ESC from sampled pzrn
      xp = (pzrn/fscon)**2

-     xa = xp - xg*(xg-two) - one
+     xa = xp - xg*(xg+two) - one
      xb = two*ene*( xg - xp*amu + one)
      xc = ene**2 * ( xp - 1)
```