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Title:	MEMO XCI:MCW-99-17 (U): PHOTONUCLEAR PHYSICS IN MCNP(X) PROGRESS REPORT
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Memorandum

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SUBJECT: Photonuclear Progress Report

Introduction

This memo is a progress report on where the photonuclear patch to MCNP & MCNPX currently stands as well as the work that has been mentioned or discussed and at least tentatively planned. Comments marked TBD are To Be Done though many are outside of what is planned as the first stage for this work.

This memo is being distributed to the following groups: the nuclear data team, parts of the MCNP team, the MCNPX team, my dissertation committee and selected other LANL personnel with an interest in the status of photonuclear simulations.

Executive Summary

MCNP version 4B2 has been modified to allow photonuclear simulations. The first full trial of this ability was performed on February 22. Several other minor modifications need to be made to finish the first cut of what will be available in the package but a working version is running. Verification work is in progress and validation work will begin soon. These modifications currently only work on the Sun Solaris platform; efforts are underway to run on the SGI platform as well. As soon as the MCNP version of the patch is stabilized and tested, the modifications will be applied to MCNPX.

PHOTONUCLEAR DATA FILES

Mark Chadwick (of T-2) has produced (up to now) 8 photonuclear evaluations in the ENDF-6 format. They are Al-27, Ca-40, Fe-56, Cu-63, W-184 and Pb-206, 207 & 208. These files are complete in the sense that they contain full energy/angular emission data for all particles up to alphas and residual yields with energy distributions for all other particles. The data is packaged in the MT5 lumped reaction and extends up to 150 MeV incident photon energy.

Anatoly Blokhin (of IPPE) has provided Mark (and thus me) with several example files from the BOFOD photonuclear data library (also in ENDF-6 format). The evaluations are Th-232 and U-233, 235 & 238. These files contain only neutron emission data. The data is separated into channel reactions, e.g. (gamma, 1n), (gamma, 2n), (gamma, fission), etc. The incident energy range is only up to 20 MeV.

CNDC has provided Mark (and again thus me) with one example file from their photonuclear data library. It is Fe-56. This file contains neutron specific data similar to the BOFOD files except with energy up to 30 MeV incident energy for multiple reaction channels.

The IPPE and CNDC data will be part of the IAEA photonuclear data library which is due to be released sometime early next year. Our early access to some of the data is due to the goodwill of the participating institutes, Mark's graciousness and the fact that he chairs the committee involved.

** TBD: Obtain finalized version of IAEA library, process into ACE format, document and release as package (Time frame February 2000)

** TBD: Determine the distribution path of APT funded T-2 evaluations, process, document and release (Time frame December 2000)

An ACE format (tentatively designated as type 'n', as in photoNuclear even though that will probably get it confused with Neutron) has been developed suitable for storing photonuclear data for use in either MCNP or MCNPX. (It was decided to store photonuclear data separate from photoatomic.) There is a draft of a memo which documents this new format but it will not be finalized and released until such time as the photonuclear physics patch

is finalized. (This is mainly because every time I think I have it right, I discover something else that would be nice to change or add.)

** TBD: Finalized ACE Type ’n’ format and release documentation memo (Time frame May 1999)

I have produced a standalone code called mkpnt which will make an ACE style photonuclear file from an ENDF-6 file. This program consists of three parts: an ENDF file i/o section, an ACE file ’n’ i/o section and an ENDF to ACE converter. The program is currently only documented via comments in the code files.

** TBD: Formalize a test suite for mkpnt to ensure proper conversion of data files (Time frame May 1999)

** TBD: Create an automated data testing procedure to replace the comparisons currently being done by hand (Time frame not determined)

** TBD: Complete documentation of mkpnt and package for use until such time as NJOY handles photonuclear evaluations (Time frame May 1999)

** TBD: Update NJOY to produce ACE type ’n’ files (Outside effort)

** TBD: NJOY processing should include calculation of the photonuclear heating numbers, ie a total heating for complete absorption and partial heating numbers for all particles which might be transported such that they can be subtracted off from the total (Outside effort)

MCNP CODE UPDATES

Input revisions
(Currently only implemented in the sun solaris version of MCNP4B2)

1) Photonuclear data tables can be specified directly on the m card line; material definition of isotope za/fraction remains unchanged.

2) The m card algorithms have been reworked to allow the addition of new library specifiers, e.g. pnlib for specifying a default photonuclear library in a manner analogous to plib for a default photon library.

3) Photonuclear isotopes maintain a separate ZA list. This list is the same length as the current material list and atomic fractions remain unchanged, e.g. if material m1 has 4 isotopes then the photonuclear ZA list has 4 isotope of the same atomic fractions. However, the ZA may be overwritten using a corresponding mpn1 card. This is useful in two ways: if an isotope does not have a corresponding photonuclear data file it can be ignored by setting the ZA to 0 or a substitute file can be used, e.g. W-184 used for W-186 or even (with appropriate caveats) for Ta-181. This option was implemented to get around what will probably be a lack of photonuclear data for many isotopes for the immediate future.

4) Photonuclear physics is turned on and biasing is set via the 4th entry on the PHYS:p card. The default entry is zero corresponding to no photonuclear physics. Any positive number turns on natural photonuclear physics, i.e. photonuclear events are sampled at their natural frequency, thus emitted particle weights correspond to incident particle weights. A negative number (x) turns on biased photonuclear physics such that a photonuclear event is sampled at every photon collision (above the threshold) and each species of secondary particle is banked with multiplicity abs(x); this implies a corresponding reduction in particle weight.

** TBD: Possibly: Default neutron cutoffs zap the majority of neutrons in a photon-neutron coupled problem; at present the user must turn off the neutron weight cutoffs for photoneutron biasing to work appropriately or tune them by hand once the appropriate weight range has been discovered. A simple algorithm could be implemented to use the first 200

(or appropriate number) histories to gate the weight and then set usable neutron weight cutoffs (Not planned at present)

5) The cross section i/o coding was updated to read and store photonuclear data files.

** TBD: Write the expgpn routine to remove unneeded data from the photonuclear cross sections (Time frame May 1999)

** TBD: Finalize the coding; in particular check warning and fatal error statements to ensure that all appropriate conditions are met (Time frame May 1999)

** TBD: Fully document the photonuclear physics input parameters (Time frame May 1999)

Sampling revisions
(ACE subroutines implemented in both MCNP4B2 and MCNPX 2.1.5 with help and thanks to RCL and HGH)

These changes are due to the expansion of sampling algorithms the ACE routines are now expected to handle. This includes both new angular and energy law data and new and old reaction types, e.g. (from separate routines) neutron in-neutron out, neutron in-gamma out, neutron in-charged particle out, neutron in-delayed fission neutron out, photon in-any particle out and proton in-any particle out.

1) Reworked interface such that all relevant parameters are handed (either implicitly or explicitly) to subroutine acecas (the top level of the particle sampling routines) removing the burden from acecas of "finding" the data for all of the combinations listed above.

2) General clean-up including removing neutron dependencies from sampling laws, separation of redundant code into utility packages, modifications to improve readability and self-documentation, addition of explicit nint/int type conversion, etc.

3) Added generalized center-of-mass to laboratory coordinate transform such that particle emission parameters are always handed back as lab coords.

4) Added tabular angular sampling to acecos angular parameter routines.

5) Added Law 61, Correlated Tabular Energy-Angle, to acecas emisssion parameter routines.

6) Created MCNPX test problems to verify correct functionality of modifications.

** TBD: Finalize documentation of modifications (Time frame June 1999)

** TBD: Create corresponding test problems for MCNP4B2 version of modifications (Time frame June 1999)

Photonuclear Physics Collision Routines
(Added only to MCNP4B2 version)

1) Update photon cross section calculation to include photonuclear in addition to current photoatomic cross section where appropriate.

2) Update photon collision routine to sample photonuclear collision at a natural or a biased frequency.

** TBD: Update sampling routine to handle more than one production reaction. (Mark's current files only use MT5 production but ability to handle multiple production reactions will be needed for other evaluations.) (Time frame April 1999)

3) Update summary tables appropriately:
a) Problem summary - add (gamma,xn) & (gamma,xgamma) production and photon photonuclear absorption
b) Table 130 (Weight balance by event in each cell) - for photons, added photonuclear absorption and (gamma,xgamma) production; for neutrons, added (gamma,xn) production; reoriented the table such that cell data is show in column form with all data for a cell on 1 page; pages list at most 9 cells

c) Table 140 (Nuclide activity by cell and total) - shifted photon production summary out of existing photon table and into neutron table output to correspond to table from which data was sampled; changed existing photon table to be photoatomic table; added new photonuclear table with entries total collisions, collisions * weight, weight lost to capture, total photons produced, weight of photons produced, average energy of photons produced, total neutrons produced, weight of neutrons produced and average energy of neutrons produced

** TBD Mirror of photons produced from neutron collisions table for both neutrons and photons produced from photon collisions (Except for the emission energy spectrum, this is redundant information and not currently planned for release 1)

** TBD: Tie photonuclear collision routine into point detector and dxtran routines (Time frame April 1999)

** TBD: Tie photonuclear collision routine into weight window routines to prevent banking of undesired particles (Time frame April 1999)

** TBD: Tie photonuclear collision routine into energy importance checking. (It was decided that this functionality is already in the weight window capabilities and it is not planned at present.)

** TBD: Check photonuclear routines for compatibility issues with other MCNP abilities:

- tally multipliers including heating numbers (not planned yet)
- perturbation capability (not planned yet)
- PVM parallel multitasking (not planned yet)
- CRAY multitasking (not planned yet)
- plot (worked without any changes)
- mcplot (not planned yet)

** TBD: Create a test suite for verification of these new abilities (Time frame June 1999)

** TBD: Document the photonuclear physics module (Time frame June 1999)

VERIFICATION, VALIDATION & PACKAGING

Verification: simple slab penetration problem to check functionality of the distance to collision calculation. (Completed March 1999)

Verification: simple secondary particle yield/energy/angle tallying on a small target to ensure accurate sampling of emission parameters (i.e. data in shouldn't equal garbage out) (Completed March 1999)

** TBD: Validation: simple secondary particle yield calculations against published experiments from literature (Time frame May 1999)

**TBD: Validation: flux measurements (experimental versus simulated) for a Phillips SL25 machine (experimental measurements to be made at the University of Florida's Shands Cancer Center) (Time frame May 1999)

** TBD: Application: neutron dose calculation to patient from standard linac treatment beam (Time frame May 1999)

** TBD: Application: neutron shielding calculation for protection of med techs operating standard linac treatment facility (Time frame May 1999)

** TBD: Write up the experience to date and call it a dissertation (Time frame June 1999)

** TBD: Validation: flux measurements (experimental versus simulated) for ESA Microtron (assuming we can find the report giving experimental measurement values or can make new measurements) (Outside effort)

** TBD: Application: neutron contamination as source of background haze in radiography experiments (Outside effort)

** TBD: Tantalum evaluation for detailed comparisons to the wealth of ORNL ORELA experimental photonuclear measurements (of interest but not currently planned)

** TBD: Validation: Time of flight experiments for comparison of neutron energy flux (possibly at the microtron or maybe just data from ORELA)

Conclusions

As stated above, this list is supposed to be a complete update of everything that has been done or is proposed to be done at some point. It contains not only work I will do directly, but hopefully some other projects I can pass on. I expect parts of this effort to be ongoing for a long time to come.

Distribution:
XCI Files
Kenneth J Adams
Samim Anghaie
Phillip C Berry
Frank J Bova
Joann M Campbell
Mark B Chadwick
Jack C Comly
Lawrence J Cox
Skip Egdorf
Guy P Estes
Jeffrey A Favorite
Paul Fishwick
Arthur R Forster
Stephanie C Frankle
Robert J Hanrahan
Alexandra R Heath
John S Hendricks
H Grady Hughes
Todd J Kauppila
Charles F Lebeda
Robert C Little
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Gregg W McKinney
Karl H Meuller
Jatindar R Palta
Richard E Prael
Donald G Shirk
Edward Snow
Wolfgang Tome
Bill T Urban
Laurie S Waters
Scott A Watson
Christopher J Werner
Morgan C White

Photonuclear Physics In MCNP(X)

Executive Summary

- Evaluated photonuclear data now exists as ENDF files
- A standalone data processing code has been written to process the ENDF data into a new ACE format for use in MCNP(X)
- Verification work has been done to show that the ACE data from the processing code matches the original ENDF data
- A developmental version of MCNP4B2 has been written to include photonuclear physics (First simulation run 2/22/99)
- Verification work has been done to show that the MCNP output matches the ACE data
- Validation work is underway and is planned to include at least comparison against several integral benchmarks

Past History of Photonuclear Data

- Meager experimental data available
  - Berman's Atlas was the first compilation of photonuclear data
  - experimental data is generally by integral channel, e.g. (γ,Xn)
  - major gaps in coverage of important isotopes
- Incomplete theoretical models
  - simple fit of Giant Dipole Resonance (GDR) parameters
  - Fermi gas model evaporation spectrum
  - no angular information
- Lack of complete evaluated data
  - accurate simulation requires doubly differential cross section data ($d^2\sigma/dE/d\Omega$) benchmarked to experimental data

Past History Of Photonuclear Simulations

- The multi-step algorithm for transport simulation
  - photon flux folded, either inter- or post- simulation, into experimental cross section data to create a neutron source reaction rate
  - nuclear models used to generate emission characteristics
  - neutron source run as separate simulation
- Limitations of the multi-step algorithm
  - Reaction rate calculations and emission characteristics are approximate unless done inter-simulation on a collision-by-collision basis
  - Energy spectra are typically generated by simplified models that are further degraded by the uncoupled nature of the simulation
  - Angular information has typically been completely ignored
  - The collision density typically ignores photonuclear absorption effects
  - Photophoton information is also typically ignored

Current State Of Photonuclear Data

- LANL T-2 effort in support of the APT project
  - Centered around updating the GNASH code to produce tabulated nuclear data for incident photons, neutrons and protons at energies up to 150 MeV
- International IAEA effort underway to create an evaluated photonuclear data library
  - Effort includes focus on collecting all available experimental data as well as updating nuclear modeling codes to produce evaluated data library files
  - IAEA library scheduled for release around Jan. 2000

GNASH
Nuclear Reaction Modeling

- Statistical Hauser-Feshbach theory with full angular momentum conservation
- Corrections for preequilibrium effects
- Applicable for incident particle energies from 1 keV to 150 MeV
- Relevant experimental data can be input to code
- Has been used heavily to generate ENDF/B-VI data for incident neutrons and protons

GNASH
Photonuclear Modeling

- Applicable for incident photons below 140 MeV (pion-production threshold)
  - Below ~30 MeV, Giant-Dipole Resonance (GDR) is the dominant photonuclear excitation mechanism
  - At higher energies, photoabsorption on a neutron-proton [quasi-deuteron (QD)] becomes important
- Both pre-equilibrium and evaporation models used for characterizing emission parameters
- Pre-equilibrium fraction computed for used with Kalbach correlated energy-angle systematics

Data Availability

- LANL Evaluations
  - ^{27}Al, ^{40}Ca, ^{56}Fe, ^{63}Cu, ^{184}W, $^{206, 207 \& 208}Pb$
- Preliminary BOFOD Evaluations
  - ^{232}Th, $^{233, 235 \& 238}U$
- Preliminary CNDC Evaluations
  - ^{56}Fe
- Other preliminary IAEA files

Photoatomic Versus Photonuclear

Elemental Combined

NXS/JXS	Photoatomic	Photonuclear Isotope 1	…	Photonuclear Isotope M

Isotopic Combined

NXS/JXS	Photoatomic	Photonuclear Isotope 1
NXS/JXS	Photoatomic	Photonuclear Isotope i
NXS/JXS	Photoatomic	Photonuclear Isotope M

Separate

NXS/JXS	Photoatomic
NXS/JXS	Photonuclear Isotope i

Data Processing

- Photonuclear data is stored in separate tables
  - Photoatomic data is specific by element or mixture
  - Photonuclear data is specific by isotopic
  - Provides for easier maintenance of data files
    - Photonuclear evaluators are not necessarily photoatomic evaluators
    - Photonuclear evaluations from many sources
- Photonuclear table provides data by product
  - Cross section and emission data in standard ACE style formats
  - Production cross sections for light and heavy products
- Creation of a new ACE table for photonuclear data
  - ACE ‘n’ format defined
  - Standalone translation code (ENDF->ACE) written
  - Prototype tables processed from LANL, BOFOD & CNDC

ACE Class ‘n’ Photonuclear Data

- Follows the style established for neutron charged particle and proton data
  - Secondary production information is kept for all emission particles with A < 5
- Documented in an unreleased memo (being held in draft due to possible changes as implementation proceeds)

Processing Code mkpnt

- Understands ENDF file 1, ~2, 3, 4, 5 & ~6
  - Minimum needed to process currently available evaluations
- Creates a superset of cross section and yield energy grids
  - Provides ability to do direct comparison of cross sections in ENDF and ACE files
- Keeps all emission particles with A < 5

Data Issues TBD

- Freeze ACE class ‘n’ format and release documentation
- Freeze mkpnt code, create test suite and document
  - Create verification tools to mimic current hand comparisons
- Update NJOY processing code to supersede mkpnt
- Obtain, process, document and package the IAEA library when released
- Process, document and package the LANL T-2 library
- Create appropriate Appendix G (MCNP Manual) entries
- Determine distribution path for new library packages

Code Implementation

- User interface
  - Materials specification & run-time controls
- Sampling routines
  - Use same laws as neutron emission
  - Revamped ace routines to be particle independent
  - Sampling of photonuclear events in photon collisions
- Summary information
  - Update summary tables and print tables 130 & 140
  - Tally information works as normal

Material Specification

- The material card has been updated to accept photonuclear zaids

```
m1   74186.60c .5  74184.03n .4  75187.02p .1 pnlib=03n
```

- Isotopic substitution is also available

```
mpn1 74184         74184              0
```

Input Options

- Currently defaults to no photonuclear physics
- On/Off/Biasing switch is fourth phys:p entry
  - i.e. **`phys:p EMCPF IDES NOCOH PNPYS`**
- Biasing by collision and by particle splitting
  - e.g. **`phys:p 3j -2`** make particles at every photonuclear interaction and bank them twice
  - e.g. **`phys:p 3j 1`** make particles according to the natural frequency of interaction and bank them once

Possible Runtime Options TBD

- Move particle splitting to a separate card
  - **`BPN n=2 p=1`**
- Allow fractional particle splitting
  - **`BPN n=2 p=0.01`**
- Allow zero particle out
  - **`BPN n=2 p=0`**

Photonuclear Physics

- Tabulated data in standard ENDF file
  - Standard emission laws are valid
  - MT reaction numbers exist for most (γ, x n)
  - Difficult to specify all reactions, e.g. (γ,$\alpha\gamma$n)
- MCNP standard statistical sampling scheme can be applied directly to new physics

Sample Interaction

- Natural collision frequency
  - Compute total photon cross section
  - Compute photonuclear cross section
  - Sample on partial fraction
- Biased collision frequency
  - Create collided and uncollided particles
  - Adjust weight based on partial fraction

Sample Collision Nuclide

- Compute partial photonuclear cross sections for each component nuclide
- Sample specific collision nuclide

Sample Emission Particles

- Compute the total yield for the particle
- Sample an average integer number of particles
- For each emission particle
  - Sample reaction from which to produce
  - Sample emission parameters from reaction tables
  - Bank particle

Updated ACE functions

- Generalization of ace routines
  - Removal of particle specific dependencies
  - Update of center-of-mass transform
- Updates for new sampling functions
  - Included RCL's Law 61 routines
- Modernization of ace routines
  - Formalized front end to ace calls
  - Improved comments to document usage
  - Separation of common routines

Fair Play TBD

- Code sample which reaction
- Verify correct next event estimation
- Tie into weight windows for population control
- Tie into energy importance windows
- Tie into perturbation capability
- Tie into tally multipliers
- Tie into mcplot capability
- Verify correctness with multitasking
- Continue runs and geometry plot capability checked
- Test suite still works

Summary Tables

- Add photonuclear absorption loss summary
  - Particle summary table and print table 130 (weight balance in each cell)
- Add photo-x particle production summary
  - Particle summary table and print table 130
- Update print table 140 (nuclide activity by cell)
  - Add new table for photonuclear nuclide interactions
  - Rearrange neutron-induced photons to correspond to correct neutron table

Other Possible Output TBD

- A course binned particle-x production table, etc., similar to the current neutron-induced photon summary tables

Verification

Cylindrical slab (mono-energetic, mono-directional source with epsilon cutoff in epsilon radius)

- Transmission through slab against escape & mfp
- Creation against yield
- Weight and average energy against computations
- Particle current by energy versus emission bin probability
- TBD: Tallies to match the rest of the summary table information (Courtesy of JXH & the adv. MCNP class)

Validation TBD

- Comparisons against integral production data as documented in various papers
- Comparison against DAHRT shielding calculations (Verification/Validation)
- Comparison against integral gold foil activation measurements to be made at the University of Florida

Future Validation Efforts

- Comparisons against experiments at the ESA-MT Microtron Facility
- Comparison against various ORELA data (will require an evaluated Ta data file)
  - integral and differential data available including time-of-flight angular-energy measurements
- Other user applications upon release