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The EPRDATA Format: A Dialogue

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ABSTRACT

Recently the Los Alamos Nuclear Data Team has communicated certain issues of concern in relation to the new electron/photon/relaxation ACE data format as released in the eprdata12 library. In this document those issues are parsed, analyzed, and answered.

I.   INTRODUCTION

The first production-level release of the MCNP6 transport code system[1] included a new ACE-format data library, **eprdata12**, based on the electron, photon, and atomic relaxation data originally released in the EEDL,[2] EPDL,[3] and EADL[4] libraries developed by D. E. Cullen and collaborators, and subsequently adopted into the ENDF/B VI.8 release of the Evaluated Nuclear Data File.[5] The data in **eprdata12** include many more kinds of information than were available in the traditional **mcplib** libraries, so the ACE format of this and future **eprdata** libraries is extended beyond that of the earlier versions. A complete description of the new extended format is given in Reference 6.

The Los Alamos Nuclear Data Team is considering adopting the current **eprdata12** and future versions of **eprdata** libraries into the collection of ACE files for which they assume responsibility for testing, maintenance, and future documentation. As part of this consideration they have undertaken a review of the current **eprdata12** file. From this review they have identified five areas of question or concern. The purpose of this document is to record these issues and report my analysis and evaluation of these matters.

II.   HOW TO READ THIS DOCUMENT

In the next five sections I address each of the five concerns in turn. The titles of the five sections are "**CONCERN 1**" … "**CONCERN 5**". Each section begins with a statement of the particular concern from the review. To make sure that the reader can distinguish the source of all text, these statements from the review, and any quotes therefrom, are printed in italics with a different font size. The concerns are followed by my responses, titled "**Response 1**" … "**Response 5**" and by short conclusions, titled "**Conclusion 1**" … "**Conclusion 5**". At the end of the five Concerns sections, a brief overall summary of the findings will be given.

III.   CONCERN 1

The issue of backwards compatibility is important. We have never updated the ACE format to include a format change that was *not* backwards compatible. Grady's definition as it stands *is not* backwards compatible. MCNP6 and MCNP6.1.1 already understand how to sample this prototype format. Depending on how they test for the presence of the new form factor data, it may or may not be possible to achieve both backwards compatibility and MCNP6 compatibility. If this is the case, this is exceptionally troublesome.

At the moment I lean towards backwards compatibility as the keystone.

Response 1

The phrase "backward compatibility" has at least two different meanings. The first meaning is that new versions of the transport codes should be able to read correctly not only the current new releases, but also all earlier releases of data files that are still endorsed and supported by the data team. This requirement has been generally satisfied. I am unaware of any instance in recent memory when the latest version of MCNP lost or removed the ability to parse correctly any libraries in the supported collection of data released by the data team. Therefore backward compatibility of the first kind is not an issue.

The second meaning of backward compatibility is that any new data library should be designed so that not only the corresponding new version of the transport code, but also all earlier versions will be able to read the new data without ill effect. This is clearly a more difficult requirement. Usually this requirement has been successfully met, but looking back over history we can see the occasional instance in which it has turned out to be impossible. In fact, just two years ago the then-current official release from the data team included data which did not satisfy the requirement of backward compatibility of the second kind. I refer to the new and improved continuous form of the $S(\alpha,\beta)$ thermal neutron scattering data. MCNP6 was taught to read and use these new data, as well as the older data, but the older frozen codes MCNP5 and MCNPX could not do so. (When using the new data, the older codes eventually reach certain rare events, and crash.)

Fortunately a solution to this troublesome situation was worked out by controlling the various codes' access to the data. Specifically, MCNP6 was modified so that it looks by default for a cross-section directory file called "xsdir_mcnp6.1" while the earlier codes, now frozen, continue to look for "xsdir". The new xsdir_mcnp6.1 file includes all data libraries that are not backwardly compatible in the second sense, such as the continuous $S(\alpha,\beta)$ data, and these same libraries are deliberately omitted from the new released version of the xsdir file. In this way users of older versions of MCNP are guided away from libraries that they cannot correctly read, while

MCNP6 users can have the expected access to these new libraries. Additional documentation of this situation can be found in Reference 7.

The extended electron/photon/relaxation library eprdata12 is in exactly the same situation as the continuous $S(\alpha,\beta)$ data: correctly readable by MCNP6, but not by MCNP5 or MCNPX. And the solution is also exactly the same: eprdata12 can be found in xsdir_mcnp6.1 but not in xsdir.

Conclusion 1

For future code/data releases, the eprdata12 entries need to be kept in xsdir_mcnp6.1 (or its possible successor), and kept out of xsdir. No other action need be taken.

IV.   CONCERN 2

The length of the updated form factor data does not include a value to indicate the number of E/FF pairs. Instead, the number of E/FF pairs is given implicitly by the difference of [JXS(3) - JXS(2)] / 2.

** This is unacceptable. **

There is at least one potential solution that addresses these two issues. Given that we commit to backwards compatibility, the existing space would contain FF data interpolated on the fixed grid. A *new* XSS block would contain the extended FF data with the number of values explicitly given.

Response 2

Historically there have been two ways of deducing the lengths of the data blocks for incoherent and coherent form factors (FF).

(1) The more recent method is the one described above that is objected to with such emphasis. Specifically, the length of the incoherent FF block is found as the distance from its starting location to the starting location of the next block (the coherent FF). Similarly, the length of the coherent FF block is found as the difference from its starting point to that of the next block (the traditional photoelectric fluorescence model). This approach is used in several released versions of MCNPX,[8] and later in the initial production release of MCNP6. For the MCNPX releases, the supporting file mcplib05t provided the FF data; for MCNP6 the file is eprdata12.

There are, of course, reasonable objections to this method. On the practical side, it clearly prohibits the data developer from arbitrarily moving the FF blocks around to other locations within the photon library. I am not especially impressed by this restriction, since the FF blocks have remained in their present positions since the original mcplib library of 1982, and I do not recall ever hearing an argument in favor of moving them.

However the same objection could be restated in other terms, namely that the descriptors of a data structure ought to be installed as an integral part of the structure itself, and not obtained as part of a relation to some other structure. This makes the structure more self-contained, more understandable, and more extensible - more object-oriented so to speak. I find this aesthetic argument more convincing than the relatively minor practical consideration of block mobility.

Nevertheless for the modern FF data, which alters both the length and content of the FF blocks, there really has been no better choice to get the necessary block descriptors.

(2) The older method, going back all the way to mcplib 33 years ago, did not require comparisons to other blocks for the simple reason that the lengths of the FF blocks never changed, either from year to year or from element to element. The length of the incoherent FF block was always the "magic number" 21. For the coherent FF block, it was 110 = 2 * 55. (Besides that, the independent variables for the FF tabulations did not change across elements either, so that the independent variables were not even included in the data files.) Presentation of the data in this form, and use of the magic numbers, preserved the possibility of mobility of the blocks, but at the cost of extensibility, a much more severe restriction. This approach is no longer an option since the data have now been extended both in block length and content, including element-specific changes in the FF independent variables.

Fortunately, there is a relatively easy way out of this conundrum. There are in the eprdata format still four unused NXS() locations. It would be straightforward to devote two of them to holding the lengths of the incoherent and coherent FF blocks. Along with supporting changes to MCNP6, this would restore the minor goal of mobility of the FF blocks, preserve the current support for the ENDF/B VI.8 extended form factors, and facilitate any future extensions of these data that may occur in the future.

I have already begun taking a look at the code to verify the viability and expected simplicity of this potential solution.

Conclusion 2

A straightforward resolution for this issue is available, and a preliminary investigation of its implementation into the forthcoming upgrade of eprdata12 is underway.

V.   CONCERN 3

There are (at least) three (or four) sets of data in play here. There are the evaluated photon cross section data and form factors for each element. There are the evaluated electron cross section data for each element. There are

the atomic relaxation data for an element with one vacancy. [One should keep in mind that there could eventually be photon form factor data for molecules, which are different than for elements. There could be atomic relaxation data for an element with more than one vacancy. Etc...]

There are many ways to encode these data. There are two proposals on the board.

The existing data are given using two tables: one for photon interactions to include their cross sections, form factors and atomic relaxation; and a second for generating condensed history electron data to include their atomic relaxation data. The two sets of data may use different bragg edges, relaxation energies and probabilities (and maybe other issues).

Pros: This is the existing format. People have come to expect to need 'p' and 'e' tables for photon and electron transport. It is

Cons: The two tables can [and often do] led to discrepant data being used.

The proposed format merges these closely coupled data into one table. [But stores electron data only for single event electron transport, not condensed history. See concerns raised in the next issue.]

Pros: Consolidating all the atomic interaction data into one table can help ensure that a fully self-consistent data set is used.

Cons: The format as currently written has issues (as outlines herein).

Response 3

This section, the longest of the Concerns, requires the most careful reading. Paragraph 2 seems to suggest that two different proposals will be discussed. However a close reading of paragraphs 3 and 6 seems to indicate that all discussion is about the existing arrangement with eprdata12 and el03. The statements in the "Pros" and "Cons" categories seem to be consistent with this interpretation as well. Therefore I shall simply address the "Pros" and "Cons".

First Pro: *"This is the existing format. People have come to expect to need 'p' and 'e' tables for photon and electron transport."*

This is a correct recognition of an advantage of continuing the existing formats, which have been already released with the production release and subsequent beta release of MCNP6. I would only add that there are other compelling advantages. For example, the existing data and code methods have been through two releases' worth of testing and checking. Important outcomes of these occasions for review will appear in the forthcoming upgrade of eprdata and in the code within MCNP6 that will support these improvements.

First Con: *"The two tables can [and often do] led to discrepant data being used"*

I believe that the "two tables" referenced here refer to eprdata12 and el03. I agree that gathering data of the same or closely related type into a single table can facilitate consistency, help with the tasks of maintenance and documentation, and enhance extensibility. Indeed, these are the reasons that not only photon data, but also atomic relaxation and single-event electron data are all to be found in the eprdata format. But as I make clear elsewhere in this document, condensed-history data are genuinely different in character from the collision-oriented data of eprdata, and deserve their own separate data format, as the el and el03 files have provided.

Second Pro: *"Consolidating all the atomic interaction data into one table can help ensure that a fully self-consistent data set is used"*

This is simply the other side of the coin of the first Con, and the immediately preceding remarks apply.

Second Con: *"The format as currently written has issues (as outlines herein)"*

The purpose of the original review, and of this response document, was to identify any potential "issues" and to evaluate their significance. I believe that this purpose has been accomplished, and that there are now no outstanding issues from this review. The only issue that has resulted in identifiable action is the providing of form-factor length information in the NXS array. This enhancement is already underway, and will appear in the forthcoming eprdata upgrade for the next release of MCNP6.

Conclusion 3

No action need be taken at the present time.

VI.   CONCERN 4

The proposed update does not address updating the files necessary for running electron transport with the condensed history method. Either we will release these new data libraries where one cannot compare single event versus CH transport using the same data; or, we will need to make an updated 'e' CH data library. [Or we will need to add the necessary information to a end-all, be-all atomic table that includes the data necessary for both single-event and CH transport.]

Response 4

This concern seems to indicate some misunderstanding of the relationship between the single-event and the condensed history methods. To clarify things, I will respond to the various parts of this Concern 4 individually.

(1) "*The proposed update does not address updating the files necessary for running electron transport with the condensed history method.*"

This is a true statement, and is absolutely the appropriate situation. The current work (along with the data in eprdata12 and its forthcoming upgrade) addresses improvements in photon transport, including extension to low energies; improvements in atomic relaxation, including extension to low-energy relaxation processes; and creation of an entirely new model for electron transport, the single-event algorithm. This work does not in any way address the pre-existing condensed-history method nor its supporting data, nor should it do so. Any hypothetical future change or improvement to the condensed-history method or data would be a totally new and separate project. To conflate the two unrelated efforts before there is even a justification for the second would be completely inappropriate.

(2) "*Either we will release these new data libraries where one cannot compare single event versus CH transport using the same data ...*"

We can compare single-event and condensed-history transport at any time we like (and I am doing so as part of V&V efforts). But we cannot, now or in the foreseeable future, compare the two methods using the same data, because the two methods are not based on the same data. For that matter, they are not even based on the same kinds of data. The data that support the condensed-history method are mostly not interaction data in the familiar sense at all. They are ingredients for the production of a variety of data structures needed by the various multiple-scattering theories used by the condensed history algorithm to model the transport of the electron.

(3) "*... or, we will need to make an updated 'e' CH data library.*"

As I hope the previous discussion has made clear, there is at the present time neither need nor justification to make an updated condensed-history library.

(4) "*Or we will need to add the necessary information to a end-all, be-all atomic table that includes the data necessary for both single-event and CH transport.*"

This, on the other hand, would be a bad idea. The pairing of photoatomic libraries (mcplib or eprdata) with electron condensed-history libraries (el03) works very well with the current data-handling infrastructure of MCNP6. To try to combine these fundamentally different formats into one would be a very large task that would require considerable refactoring of the logic and data structures of MCNP, and, I expect, serious changes in ACE formats. I also would not enjoy thinking about the implications for backward compatibility. And, as mentioned at other points, we have no justification for a large project with no discernible gain in capabilities.

Conclusion 4

The content of Concern 4 is basically speculation on possible futures for the condensed-history data libraries. While this is a worthy subject for future planning, it is not relevant to any issues associated with the eprdata libraries. No action need be taken at the present time.

VII.   CONCERN 5

There are redundant data regarding the electron interactions. Specifically, JXS (6) and (12) both point to a list of number of electrons per shell; (7) and (13) both point to a list of electron binding energy per shell; and, (8) and (14) both point to a vacancy probability.

Redundant data are almost always a bad idea. Deliberately releasing a library where these are not consistent would be very questionable. Releasing a library with a format that has them in redundant locations is imprudent.

If the point of updating the library is to help provide more self-consistency between the data, then obviously only one set of data for these values should be given.

If the point of the format is to make it harder to provide or use inconsistent data, then this goes against that laudable goal.

Response 5

To the contrary, this kind of "redundancy" and "incompatibility" is not especially rare, nor generally in urgent need of reconciliation. From a number of possible instances in traditional code and data, one example suffices: mcplib04 contains at JXS(4) a list of shell binding energies and at JXS(7) a different list of the same quantity. These lists, being both of shell binding energies, can certainly be identified as redundant in the sense of Concern 5. In addition, the number of items listed at JXS(4) is generally smaller that the number listed at JXS(7), so these sets of data are also certainly recognizably inconsistent. Note that this situation also obtains for mcplib03 and for the more recent mcplib63 and mcplib84. So, does this mean that the creators of all the recent classical photoelectron libraries are to be criticized for allowing more than one version of physically similar data?

Actually, no. The reason for this situation arising, and the reason that it is not particularly a bad idea, is that these separate sets of data support separate and distinct models of physical processes. The data starting at JXS(4) are part of the traditional MCP (as opposed to MCG) atomic relaxation treatment. They are found already in mcplib from 1982. The data at JXS(7) are part of the much more recent Compton Doppler broadening package first introduced with mcplib03 and its more ENDF-based companion mcplib04. Each package — fluorescence and Doppler broadening — is a self-consistent and reasonably self-contained set of code coupled

with data especially selected and studied for the specific needs of the particular capability.

The purpose of the new cross section libraries at the time of which we speak was the enabling of the new Doppler broadening model, a kind of energy-smearing model for the scattered photons from incoherent scattering. This scattering model had little or nothing to do with fluorescent emission, which in those days could not even occur as a result of Compton scattering. Therefore the developers of the Doppler broadening model had no valid motive to try to reconcile the older fluorescence data with their newer, but unrelated electronic data. In fact, it would have been quite irresponsible to decide to take on a separate complex (and expensive) development effort merely because of a minimalist desire to eliminate loosely associated, but essentially unrelated data in logically separate parts of the transport code system.

Perhaps it is now clear (and if not, then I affirmatively state) that the new electron shell data fall under the same considerations that governed the developers of mcplib04 and its related libraries.

Conclusion 5

The variations on certain data types discussed in Concern 5 are basically harmless. No action need be taken at the present time.

VIII.   SUMMARY

One minor enhancement (the inclusion of form factor block lengths in the NXS array) has been found to be worth implementing into the forthcoming upgrade to **eprdata12**. Its absence in **eprdata12**, as in earlier **mcplib** libraries does not warrant any change in the existing system. Issues raised in other concerns have been found either harmless or actually desirable for the system, and are not found to warrant changes in either **eprdata12** or its immediate upgrade.

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