Modern Nuclear Database Format and Database Management Tools

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Introduction

- At LLNL we are developing
  - a new structure for nuclear reaction data
    - To Replace ENDF and ENDL formats – more later
  - an infrastructure to read, manipulate, plot, etc. nuclear reaction data
  - an API for the new structure to support Monte Carlo and deterministic transport
- We have been working with the SLAC/GEANT4 team to incorporate the API into GEANT4
  - See Tatsumi Koi talks
- We have “stimulus money” for this project
  - Have released 2 beta version of the new structure
  - Started working with Brookhaven Nat. Lab.

Outline

- Brief review of Low Energy Nuclear Data (LEND)
- Why a new format
  - Legacy formats and access routines
- New structure (format)
  - Structure
  - API for Monte Carlo sampling
- Management tools/infrastructure
- Data we plan to release
- Conclusion

What is low energy nuclear data: Review

- Nuclear data for reaction of projectile hitting a target
  - Example: n + $^{16}O \Rightarrow$ n + p + ^{15}N
- Most data are
  - For neutron as projectile
  - Low projectile energies: 10^{-11} to 20 MeV
  - In legacy formats
    - ENDL (Evaluated Nuclear Data Library)
      - Started at AWE then LLNL ~1960
      - Used only at LLNL
    - ENDF (Evaluated Nuclear Data File)
      - Developed by international committee ~1964
      - Used everywhere but LLNL

The ENDL and ENDF formats are antiquated

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Issues with legacy ENDF and ENDL formats

- Have a fixed number of supported reactions
  - The following reaction is not supported

$$n + {}^{79}Kr \Rightarrow {}^{2}H + n + {}^{3}H + {}^{74}Se$$

- Fixed precision format
  - 1.23456789e-12 ⇒ 1.23456-10
- Very difficult to read – try reading ENDF formatted data
- Formats do not represent physics
- Do not have API

New format and infrastructure are designed to remove many issues

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New structure (format)

- Format being designed is structure based (OO)
  - Defining the structure not the language
    - Plan to support XML and HDF5 languages
    - Have routines that convert ENDF and LLNL's ENDL nuclear data into new format
    - XML to HDF5 converter was written in 1 day and contains < 100 lines of python
- Design is more flexible as well as more unambiguous and explicit for storing nuclear data
- Supports more physics than legacy formats
  - No limit to number or type of reaction channels
  - No limit to the type of particles allowed

Status of new structure

- Rewrite in last year to better handle ENDF data forms
  - Includes adding covariance data for sensitivity studies
    - First release of data used in GEANT was
      ENDF ⇒ ENDL ⇒ new structure
      - Bloated and was not always a faithful representation
    - Next release will be
      ENDF + Others ⇒ new structure
- 2 beta releases of the new infrastructure with direct ENDF conversion for review by international community
  - We have gotten positive feedback from

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API for new format

- Access API
  - Core routines in C
    - Access speed and file size are a concern
- Monte Carlo sampling API
  - Core routines in C
  - GEANT C++ wrappers with prefix "G4GIDI"
    - Tatsumi Koi and Dennis Wright from SLAC
    - See Tatsumi's talks
  - Sample reaction for an isotope and its outgoing products (energy and angle).

API is thread safe after initialization and will support MPI, LLNL codes require this!

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Nuclear reaction data infrastructure

- Data management tool called FUDGE
  - For Updating Data and Generating Endl
  - Can read new structure
  - Makes manipulating data “easy”
  - Can write data
  - Can plot data
  - Converts legacy ENDF or ENDL formatted data into new formats
    - We found many issues with the latest ENDF/B-VII data and reported them to Brookhaven Nat. Lab.

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Differences between ENDF and ENDL databases

$n + {}^{16}O \Rightarrow n + p + {}^{15}N$

Products

ENDF	ENDL
Only requires neutron product data	Requires product data for n, p, d, t, ^{3}He, α and γ
$n + {}^{16}O \Rightarrow n + p + {}^{15}N$	$n + {}^{16}O \Rightarrow n + p + {}^{15}N$
Product data (n)	Product data (n + p)

Many ENDF reactions are missing product data, our data will include all product data for n, p, d, t, 3He, α and γ

We will provide nuclear reaction data in new format

- Data for various projectiles
  - Neutron: over 900 targets (isotopes)
    - Latest release of ENDF has a 418 targets
  - Proton, deuteron, triton, ^{3}He, alpha
  - Gamma

- Product data for each projectile listed above

Getting the latest infrastructure (FUDGE) release

- To retrive fudge-2.0.tar.gz from LLNL do:
  - >ftp gdo142.ucllnl.org
  - When prompted for user name, enter 'anonymous', with your email address as the password. Then
  - >cd pub
  - >get fudge-2.0.tar.gz
  - >bye
- The code is also available on the NNDC website
- We would like feedback on new data structure and infrastructure
- Questions and feedback can be sent to beck6@llnl.gov
- Converted ENDF data will not work with current GEANT API

Conclusion

- We are nearly complete the the first (non-beta) version of our nuclear data infrastructure and new data structure
  - It will be released in 2012
- See Tatsumi's talks
  - Sep. 20th Parallel 4A (Hadronic): Validation
  - Sep. 22th Plenary 8: Ongoing Developments II (Physics)
- Collaborators
  - LLNL: Caleb Mattoon, Neil Summers, Nidhi Patel and Doug Wright
  - BNL: Dave Brown
  - SLAC/GEANT4: Tatsumi Koi and Dennis Wright

Caveat emptor: Sampling only as good as the data

- Two main types of interactions:
  - Two body
    - Examples: Elastic scattering, (n,p), (n,n’)
    - Particle number, energy and momentum are conserved per interaction (not including photons)
  - Uncorrelated N-body:
    - Example: (n,2n), fission
    - Energy and momentum are conserved statistically, not on a per interaction bases.
    - Particle number sometimes only conserved statistically (mainly photons and fission neutrons)
    - product data only guaranteed for neutrons