WPEC SG38 status report

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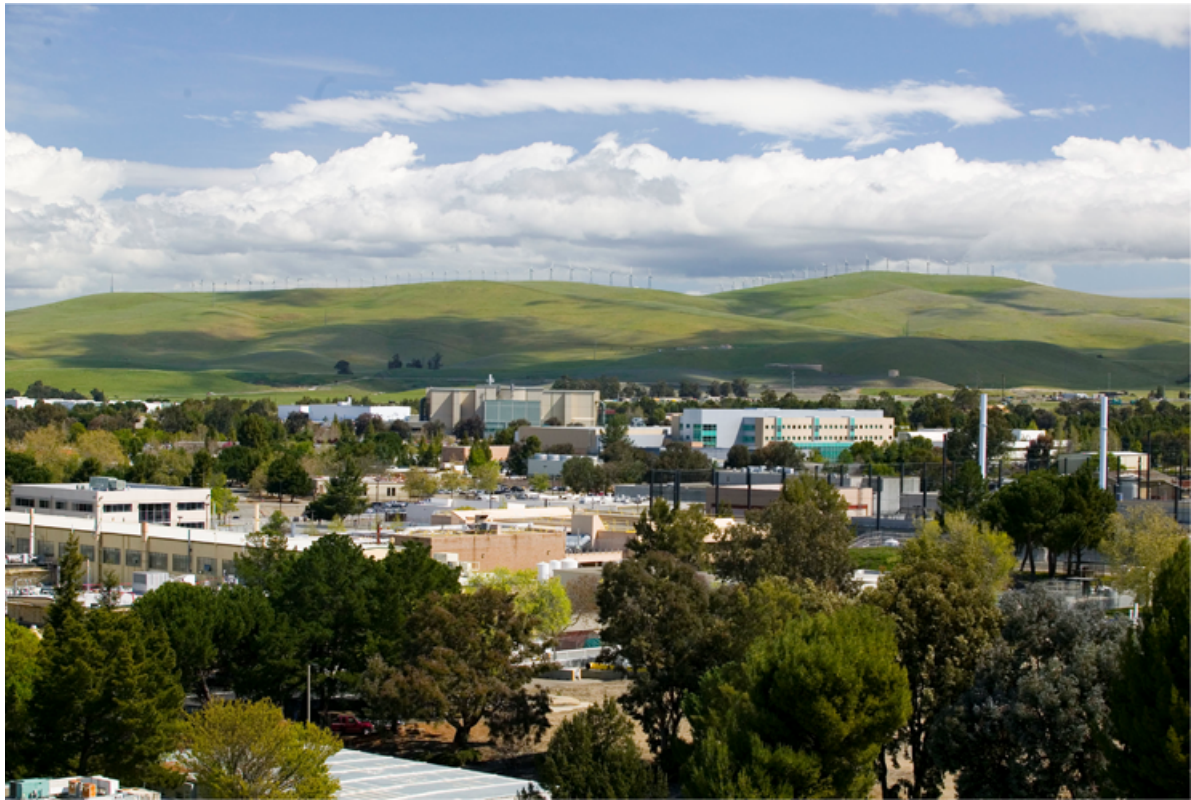

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WPEC Subgroup #38 "Beyond the ENDF format: A modern nuclear database structure"

- Goal: design and document a new structure for storing and exchanging nuclear data, including
  - nuclear reaction evaluations
  - processed (application-ready) data
  - documentation
  - particles
- First meeting November 2012, 7 subsequent meetings. Most recent meeting May 2017
- Nearly complete, but reports still need to be finalized

Final product from subgroup 38: requirements and specifications for storing data in Generalized Nuclear Database Structure (GNDS)

Final SG-38 reports:

- *Detailed Requirements for a next generation nuclear data structure*
  - High-level design decisions, outlines specific data needs addressed by SG38
  - Final version completed June 2016

- *Specifications for the next generation nuclear data hierarchy*
  - Details of how data will be stored. Describes each level of the data hierarchy including allowed sub-nodes, attributes, etc.
  - Estimate 60% complete

Draft and final versions available from https://www.oecd-nea.org/science/wpec/sg38/

Final SG-38 reports:

- *Requirements and specifications for a particle database*
  - Details for storing particle properties like mass, spin, decay data, etc.
  - Estimate 80% complete
- *General-purpose data containers*
  - Describes containers for storing interpolation functions, tables, arrays, polynomial series, etc.
  - Estimate 70% complete
- *Specifications for documentation elements*
  - Containers for documentation, bibliography, storing code input, etc.
  - Estimate 80% complete

Draft and final versions available from https://www.oecd-nea.org/science/wpec/sg38/

GNDS data are organized into 4 types of file:

- **reactionSuite**: contains a full reaction evaluation. Also called a ProTarE (projectile + target + evaluation)
- **covarianceSuite**: collects covariances in a separate file, with links connecting them to the reactionSuite
- **PoPs**: Properties of Particles
- **thermalScattering**: for low-energy neutron scattering including S(α,β)

File type #1: reactionSuite

- Contains all reactions between specified projectile and target, organized in following nodes:

• styles	*'evaluated', 'heated', etc.*
• documentation	
• externalFiles	*files linked to by this reactionSuite*
• PoPs	
• resonances	*resolved, unresolved, scattering radius*
• reactions	*all reactions that sum to total*
• orphanProducts	*e.g. gammas of unknown origin*
• sums	*summed cross sections & multiplicities*
• productions	*production cross sections*
• incompleteReactions	*designed to handle sub-actinide fission*
• fissionComponents	*1st-chance, 2nd-chance, etc.*
• applicationData	

reactionSuite overview:

- Contains all reactions between specified projectile and target, organized in following nodes:

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Contents of many nodes are very similar

reactions, orphanProducts, etc. have similar layout:

- reactions:
  - reaction
    - crossSection
    - outputChannel
      - Q
      - products
    - availableEnergy — *derived from incident energy + Q during processing*
    - availableMomentum — *''*
  - reaction
  - …
- orphanProducts
  - reaction
  - …
- productions
  - production — *different name, but same contents as the reaction node*
  - …
- incompleteReactions
  - reaction
  - …
- fissionComponents
  - fissionComponent — *also looks like a reaction inside*
  - …

Contents of resonances node:

- scatteringRadius

  required, may be constant or energy-dependent

- resolved
  - BreitWigner *LRF=1 or 2 equivalent*

    or
  - RMatrix *LRF=3 or 7 equivalent*

  parameters stored as tables, one row per resonance

- unresolved
  - tabulatedWidths

    average parameters stored as interpolation functions:

    interpolate parameters, not cross sections

File type #2: covarianceSuite

- Covariances can be stored inside the reactionSuite, or gathered together in the covarianceSuite. Contents:

  - styles — *similar to reactionSuite*
  - documentation — ‘’
  - externalFiles — ‘’
  - covarianceSections — *handles MF31, 33, 34, 35, 40*
    - *List of ‘covarianceSection’ nodes.*
  - parameterCovariances — *MF30, 32*
    - *List of ‘parameterCovariance’ and ‘averageParameterCovariance’ nodes.*

Most ENDF-6 covariances fit into the GNDS 'covarianceSection'

- covarianceSection label="…" crossTerm="true"
  - rowData href="…"
  - columnData href="…"

rowData/columnData may contain additional metadata, such as Legendre L-value (for MF34), incident energy range (MF35), etc.

columnData only required for cross-terms

rowData/columnData tell what data the covariance applies to. Actual data is stored in one of the following:

- covarianceMatrix

has various compression options to support symmetric, diagonal, sparse and full arrays

- weightedSumOfCovariances
- sandwichProduct

File type #3: PoPs

- Particle properties are collected inside the PoPs node. May be a stand-alone file, or stored inside a reactionSuite. Contents:

• documentation	*similar to reactionSuite*
• aliases	*supports multiple names for the same particle*
• gaugeBosons	*i.e. photon*
• leptons	*electron, neutrinos, etc.*
• baryons	*neutron, proton*
• chemicalElements	

chemicalElements is the largest section inside PoPs:

- Each chemicalElement has a symbol, name and atomic number Z, plus child nodes:

  - documentation *optional*
  - isotopes
    - isotope *defines symbol and A (Z inherited from chemicalElement)*
      - nuclides
        - nuclide *stores properties of the neutral atom with ground or excited-state nucleus*
          - nucleus *properties of the bare nucleus*

File type #4: thermalScattering

- Thermal neutron scattering law data representation, still subject to change (suggestions welcome)
  - documentation
  - reaction
    - doubleDifferentialCrossSection
      - elastic (coherent using cumulative S-factor or incoherent using Debye-Waller)
  - reaction
    - doubleDifferentialCrossSection
      - incoherent inelastic
        - S(α,β) stored as 3-d array or list of 2-d arrays (to support temperature-dependent α,β grids)
- Currently only supports MF7 equivalents, no phonon spectra or other representations

Remaining work: documentation!

- Thanks to Dave for pushing through the main requirements document!
- Working through remaining documents
  - Moving slowly due to other priorities
- Any help with reading / editing documents would be appreciated!

- All documents need to be delivered as part of final SG38 report

GNDS specification is nearing completion

- FUDGE is still being modified to match GNDS specifications

- U.S. nuclear data community plans to release ENDF/B-VIII in both ENDF and GNDS
  - Estimated release date is ~~mid-December 2017~~ early February 2018
  - ENDF ⇔ GNDS translation needs to be nearly one-to-one
    - Still a few types of data to support
  - New version of Fudge will be released at the same time as ENDF/B-VIII
    - same version used to translate ENDF-VIII into GNDS
  - After the release, further changes to GNDS specifications will need to be approved by new format governance board, EG-GNDS.