Status of TSL data in the new format

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WPEC-SG38: *A modern nuclear database structure beyond the ENDF format*

- In 4th & final year of SG38
- Goal was to develop a “new format” to replace ENDF
- Much bigger job than anyone appreciated ;)
- There will be follow on SG’s
- I am taking notes today, we want your feedback

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Which new format?

- **Generalized Nuclear Data (GND) format is a LLNL in-house format**
  - Version in use at previous WPEC: GND-1.5
  - Current: GND-1.7
  - In development: GND-1.8
- **WPEC/SG-38 is developing a “new format” to replace the ENDF-6 format**
  - Requirements of format finalized, writeups being finalized
  - Specifications very much in development as are specific implementations
  - Specific implementations for XML look an awful lot like GND (and GND keeps getting modified as consensus emerges on what we want from the “new format”). Some would say that they are identical.
- **So, is the “new format” GND?**
  - Reticence from some outside LLNL to use a format named by LLNL
  - ENDF/B is always released in the ENDF format
- **ENDF/B-VIII will be released in the “new format”**

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Competition just started in SG38
for a name that should give the right heavy weight
to a format for data well evaluated
where many scientists will have collaborated
for which they expect to be congratulated
once real progress has been accelerated
and when nobody finally is exasperated.
Proposed were all kinds of well sounding names
a competition timed for winter olympic games,
nice sand, ufo ions have already their claims.
Comprehension, tradition and avoiding confusion
as well as registration and copyright exclusion
they all are shouting aloud to heaven:
It should be “endf-7" — Enrico Sartori

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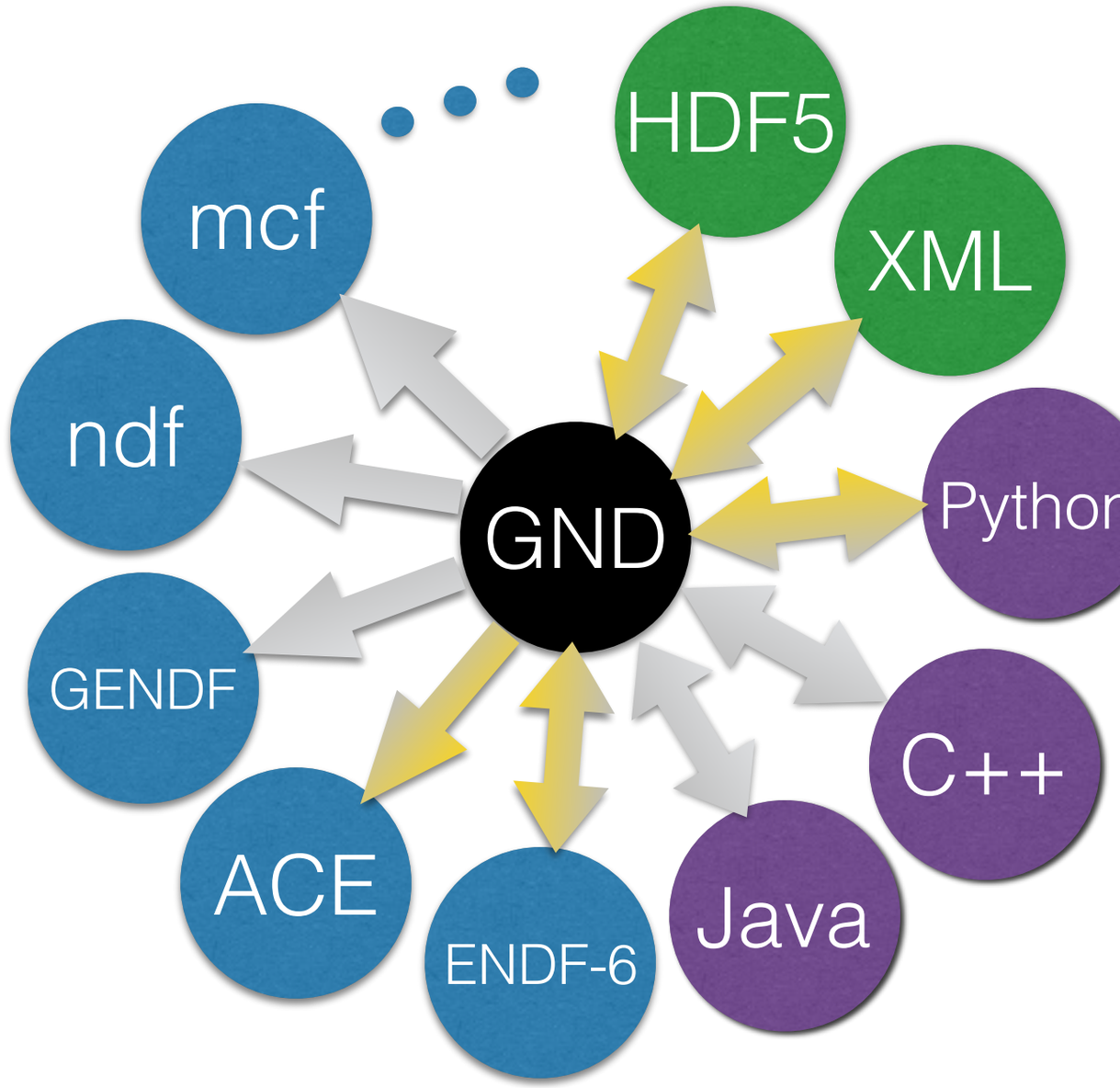
Which “new format”? is the wrong question

- WPEC-SG38 (and LLNL before it) are developing a common hierarchy
- Data arranged in this hierarchy can be serialized into a variety of forms
- Legacy forms (e.g. ENDF-6) may not be as faithful a representation as other more modern ones
- A common hierarchy means you can pick up a file or source code and have a good chance of understanding both



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What is status of processing codes with respect to GND?

- **FUDGE (LLNL)**
  - First code to use GND
  - Open source, under BSD license
  - See https://ndclx4.bnl.gov/gf/project/gnd/
- **NJOY-21 (LANL)**
  - Long term, open source, replacement for NJOY2012
  - In active development, adding GND functionality
  - See https://njoy.github.io/
- **AMPX (ORNL)**
  - Being modernized as part of overall SCALE modernization effort
  - In active development, adding GND functionality
- **TRENDD (CEA)**
  - GND support planned
- **GALILEE (CEA)**
  - Unknown
- **GAIA (IRSN)**
  - GND support planned
- **GRUCON (Kuchatov Inst.)**
  - GND support planned

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Tour of GND-1.7 TSL prototype

- **tsl-SiO2-beta.gnd.xml:**
  - coherentElastic (S),
  - incoherentInelastic (Sab)
- **tsl-ZrinZrH.gnd.xml:**
  - incoherentElastic (DebyeWaller),
  - incoherentInelastic (Sab)

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GND-1.7 has a prototype TSL implementation

- **More or less a literal translation of ENDF-6**
- **Missing many new/proposed features:**
  - Uncertainty/Covariance missing (new)
  - Does not use standard GND reaction hierarchy (new)
  - ENDF MAT numbers far too restrictive, but metaEvaluation markup not fleshed out (proposed)
  - No spot for phonon spectra or structure factors (proposed)
  - Documentation is primitive (proposed)
- **Even in this early stage, many new things evident:**
  - Material name is a string
  - “Unlimited” precision
  - Units on all numbers

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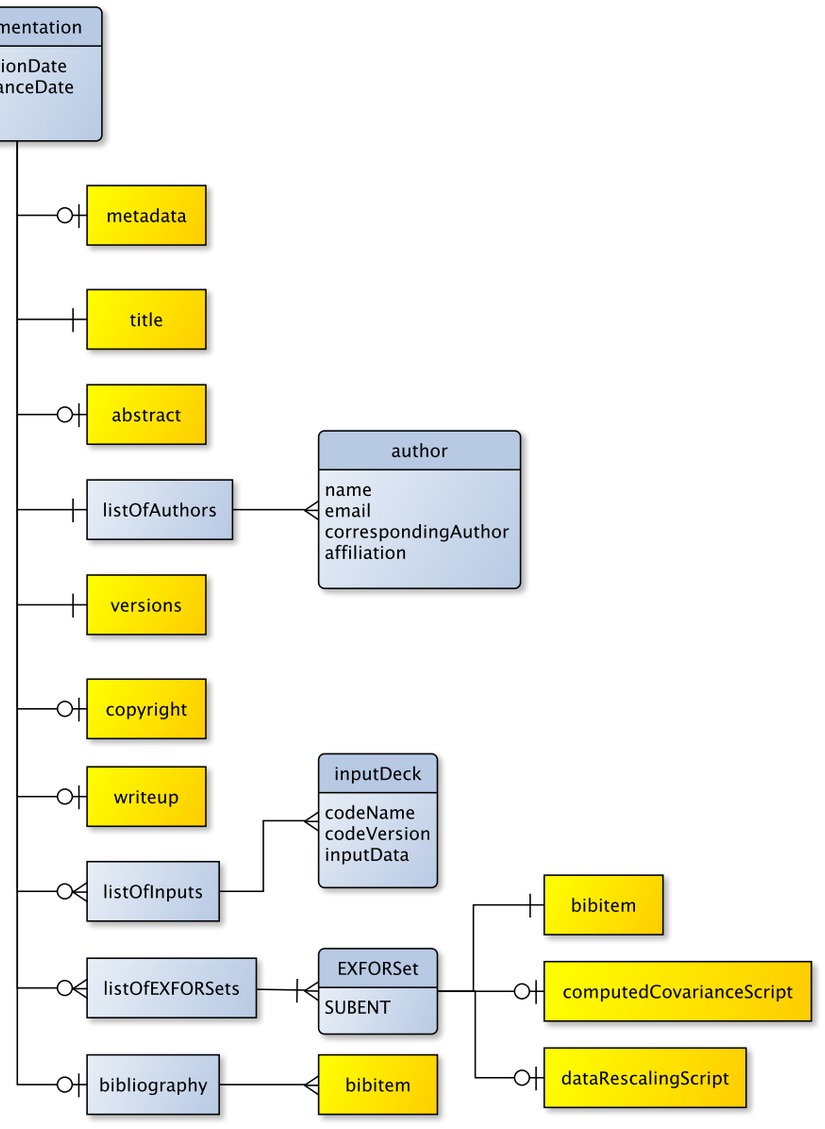
Proposed, but not implemented GND features

- **Phonon spectra & structure factors**
  - This is a simple addition (they are just xy pairs)
  - Need LEAPR like support in processing code(s)
  - Enables UQ ala' Holmes & Hawari
- **Enhanced documentation**
  - Unicode
  - Structured markup (embed HTML or LaTeX)
  - Documentation can be put directly on data structure rather than up at the top of the file
- **metaEvaluation**: a proposed scheme for getting around stoichiometric problems while allowing for more accurate descriptions of material EOS (ask me later)



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Missing feature: Does not use standard GND reaction hierarchy

- evaluation
  - reactions
    - reaction
      - cross section
      - products
        - product #1
          - multiplicity
          - distributions

this is all that's really needed for TSL data

(although "cross section" means dCrossSection_dOmega_dE and "products" are not needed)

Remember: common hierarchy means opportunity for code-reuse, plus users will know where to find stuff

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Missing feature: Uncertainty/ Covariance missing

- **GND covariance unchanged since version 1.5**
  - We are not happy with it
  - …but haven't had time to do anything about it
    - Underlying data containers have changed dramatically so in Fudge-v4.2.1 they are broken (can read/write covariance, but nothing else), being fixed in development version
- **SG38 has many covariance/uncertainty requirements that remain unimplemented**
- **There is no TSL covariance data to use for prototyping!!!**

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Tour of GND-1.7 Covariances

- **n-092_U_235.gndCov.xml**

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Things to note in covariance implementation

- Almost a direct translation of ENDF, but…
- Hyperlinks
- Reaction labels
- Cross-covariance and self-covariance have same format
- In fact, ALL covariances have same format
- Relative or absolute

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What's missing from covariance implementation?

- **Various esoteric covariance composition schemes (ask me later)**
- **Support for log-normal distributions**
- **Parameter covariances (e.g. in resonances)**
  - In development currently
- **Just plain uncertainties**
  - Most requested missing feature is XYdY triplets
  - Handy for plotting
  - Need correlation matrix for use in UQ
- **Option to put the covariances with the data**
  - Second most requested missing feature
  - Sometimes covariance is too big to put with data, other times it makes sense to put it nearby
  - Supported in development version, but ENDF-GND translator assumes you want separate files + links
- **Higher dimension covariance than e.g. cross section or nubar**
  - "Just a question of packing"
  - The fact that GND puts covariance in separate file resolves file size troubles

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WPEC-SG38 has a lot more to do, but we've done a lot already

- **Prototype TSL implementation**
  - Need your feedback: what's good? what's bad? what's missing?
- **Covariance implementation**
  - Need your feedback: what's good? what's bad? what's missing?

We need data to play with, especially covariance data!

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