Comments on an API for GND

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Statement of work

Document APIs to read and write the new structure in C, C++, Fortran, and Java. Implement a substantiation of an API that is tested by relevant stakeholders of Product Teams 1&2 above and the developers of processing and testing codes.

API outline

- Initial comments
  - Language comment
  - Writing/reading
  - Unit conversion
- Useful methods (functions)
- Belong the reactionSuite
- A comment on reaction matching/searching
- Issues from Fudge work
  - Floating point
  - Zipped files

Initial comments

- Structures and infrastructure/API are entwined
  - Care must be taken when designing the structure so as not to
    - Make the infrastructure/API too complex
    - Make the infrastructure/API consume too much computational
      - memory
      - time

- Definition of a "code group":
  - A class or classes in Object Orientated Programming (OOP) or set of functions (procedural) for handling a task
  - Examples:
    - Reading/writing
    - Unit conversion Discussed during infrastructure session.
    - Reaction matching. Discussed during infrastructure session.

- Indexing should be 0 based
  - Note, in Fortran can define arrays as "(0:n-1)"
    - Example: real x(0:n-1)

Language comments

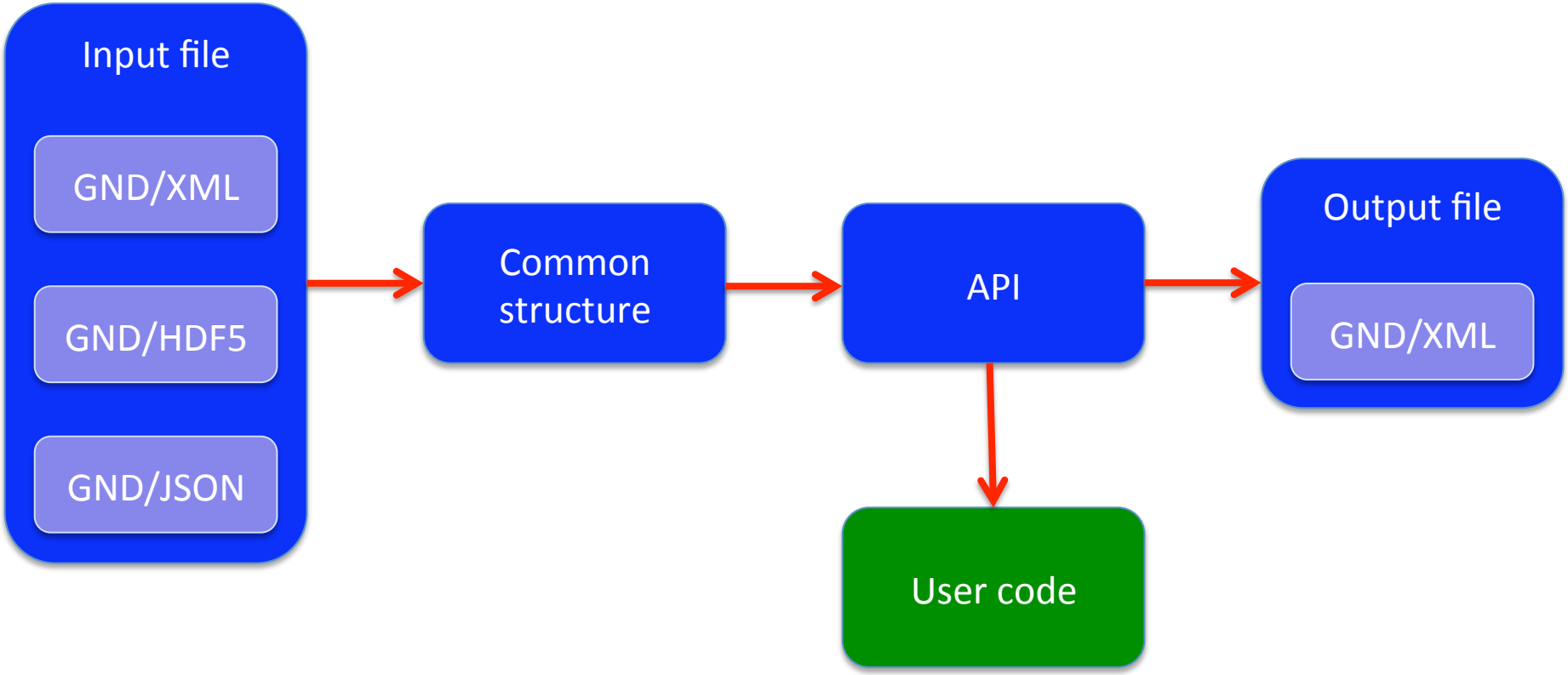
- Procedural languages (e.g., C, FORTRAN-90)
  - Need to define prefixes for all “code groups”
    - That is, all functions (and probably data types) for a code group should have a common prefix
    - Examples: prefixes like gapi_r_, gapi_cs_ and gapi_mul_ for reaction, cross section and multiplicity types and functions.
- Object oriented languages (e.g., C++, FORTRAN-2003)
  - Only need to to define prefixes for classes as each class name prefix its members and methods.
    - C++ example: GOOP_XYs::plot( )
- I think we should write some core groups in C and write wrappers for the other languages.
  - Possible examples: unit conversion and reaction matching.

Only need to support writing to GND/XML format?

- API only needs to support writing to XML
  - Format = Structure + meta-language
    - Written as “Structure/meta-language”
    - Examples: “GND/XML”, “GND/HDF5”
  - Conversion to other formats can be done with codes that only need to know a little of the GND structure, as long as the structure is well defined.
    - Example: In fudge, toHDF5.py is a stand alone python script that converts a “GND/XML” file into “GND/HDF5”. toHDF5.py is roughly 110 lines of python and does not import anything from Fudge.

Need to support reading all formats: GND/XML, GND/HDF5, ...

- Best to create common structure that all formats are converted into



"Common structure" is a standard coding practice – see V. Sinitsa's talk on GRUCON during the infrastructure session

Useful methods (functions)

- Read all/write XML
- Iterate over all items in an object or get an item from an object that are list-like or dictionary like
  - This will be different for OOP and procedural APIs
- convertUnitTo
- Methods to add/delete elements to/from structure
- Get data domain
  - Possible arguments:
    - inUnitOf
- Search/Find
  - Reaction, data type (e.g., cross section), product
- Collapsing of deterministic data?

Useful methods (functions) we may not want in API

- Some things may be handled better by the infrastructure
  - Resonance reconstruction
  - Heating cross sections
  - Linearizing data?
    - toLinear – at least for the last two columns for each data type
      - $\sigma(E)$, for both E and σ
      - $P(\mu|E)$, only for μ and P
      - $P(\mu,E'|E)$, only for μ and P
  - Deterministic grouping of the data

Beyong the reactionSuite

- In GND all reactions for a projectile hitting a target is called a “reactionSuite”.

- Users will want to access various reactionSuite’s.
  - Need an MCNP/ACE/xsdir like structure that contains a list of available reactionSuite’s
  - Need to have a unix ‘ls’ like function to allow users to obtain a list of all reactionSuite’s they request
    - Example
      - findReactionSuites(projectile = ‘n’, target = ‘U*’)
    - Should also define a search/matching expression for this

Another comment on reaction searching/matching

- Should define a set of standard types of search patterns
  - Example
    - rsre_two_n
    - rsre_fission
    - rsre_capture
  - I think these would be better than strings like “capture”, for example
    - Word of caution: In LLNL’s ENDL rsre_capture (or “capture”) would often return two reactions
- Similarly for projectile/target matching

Some issues

Floating point precision

- Is ‘a – a’ zero?
- Not always with finite floating-point precision

```
>>> 1e-5 * 1e-6 / 1e-11 - 1
2.220446e-16
```

- We probably need to define fuzzy comparisons
  - For example, a and b are equal if

$$abs(a - b) <= epsilon * max(abs(a), abs(b))$$

  - Example python ‘compare’ method

```
def compare( value1, value2, epsilon = 0 ) :

    epsilon *= sys.float_info.epsilon
    delta = value1 – value2
    if( abs( delta ) <= epsilon * max( abs( value1 ), abs( value2 ) ) ) : return( 0 )
    if( delta < 0. ) : return( -1 )
    return( 1 )
```

zip-a-dee-doo-dah

- Should the API and infrastructure need to read zipped GND files?
- How about reading only sections of a GND file?
- What should be done in the user code and what can also be done in the API?
  - Should deterministic collapsing be supported?

Comment on pointwise/piecewise data structure

- How could we store (x_i,y_i) pairs of data (e.g., cross section or multiplicity data)?
  - How do we define iterating over the data
  - How do we define indexing the data
- For example, the points (1, 1), (2, 2), (3,1) and (4,0).
  - In python we could define the list xys = [(1, 1), (2, 2), (3,1) and (4,0)]
  - For xys Iteration is

```
for x, y in xys :
```

  - For xys indexing is

```
x, y = xys[index]
```

  - This does not tell us how to interpolate between pairs.
  - Take with same points with ENDF interpolation “2 5 4 2”.
    - Between first two points is log-log while the rest are lin-lin

Comment on pointwise/piecewise data structure - continue

- How we store xys = [(1, 1), (2, 2), (3,1) and (4,0)] in GND
  - With ENDF interpolation '4 2'
    - Stored as an instance of XYs class
    - Allows iteration and indexing in a 'natural' way (e.g., x, y = xys[index])
  - With ENDF interpolation '2 5 4 2'
    - Stored as an instance of regionsXYs class.
    - For this example, the regionXYs instance contains two instances of the XYs class
      - First region: xys1 = [(1, 1), (2, 2)] with 'log-log' interpolation
      - Second region: xys2 = [(2, 2) , (3,1) and (4,0)] with 'lin-lin' interpolation
    - Indexing a regionsXYs instance with index = 0 gives the first region, not the first point.
    - regionXYs class has a 'toPointwise_withLinearXYs' method that converts the points into one XYs instance with 'lin-lin' interpolation.

LLNL's current effort

- GIDI
  - General Interaction Data Interface
  - Written in C
  - C++ wrapper for GEANT
  - Status
    - Only read: no writing
    - Also samples from data

The End