Implementation of the GNDS format for photo-atomic data

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Definitions

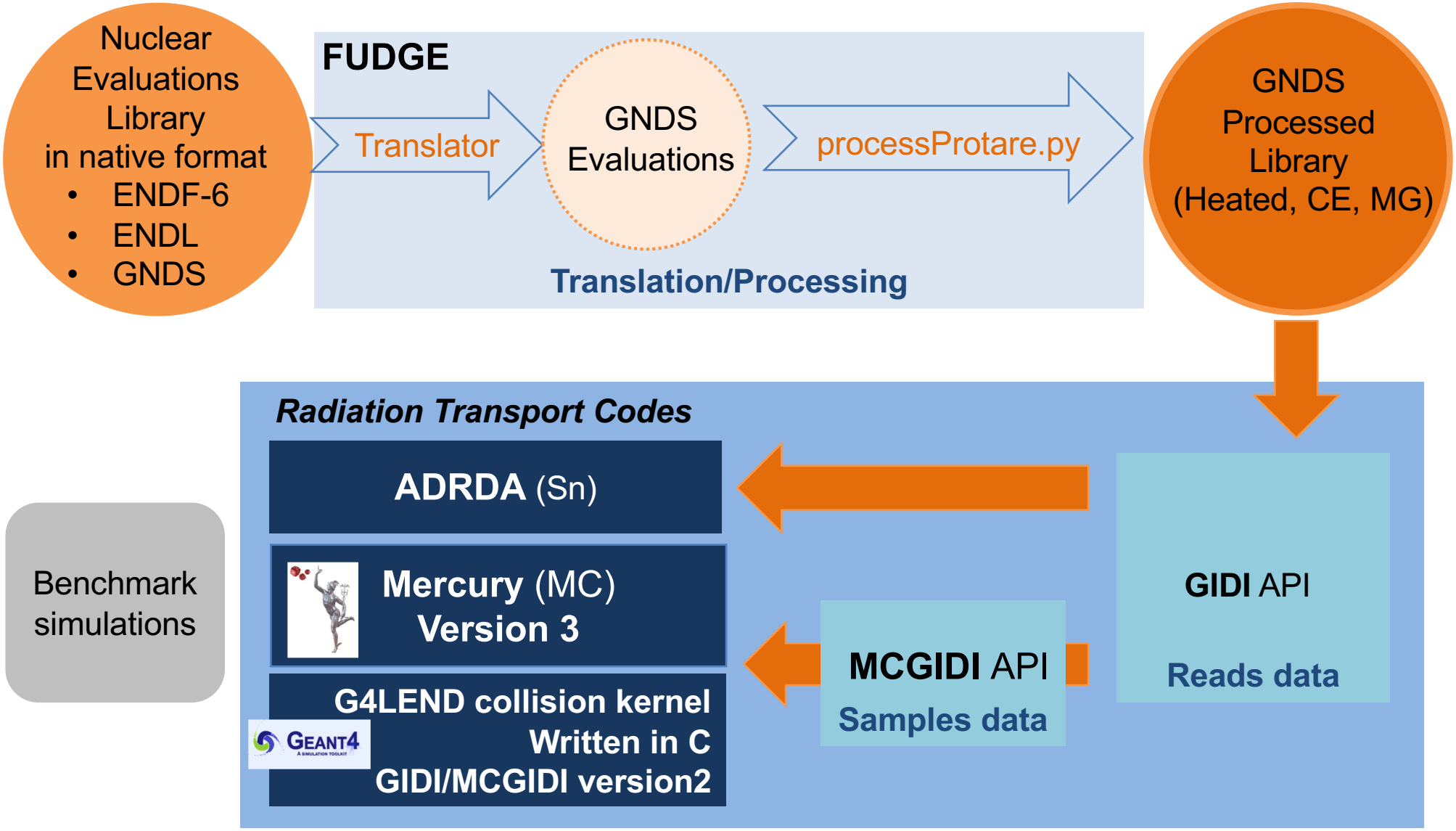
- GNDS: Generalized Nuclear Data Structure
  - New international “format” for storing nuclear evaluated and processed data.
  - Replacement for ENDF-6, ACE, etc. formats

- FUDGE: For Updating Data and Generating Evaluations
  - LLNL’s nuclear data management package.

- GIDI: General Interaction Data Interface
  - LLNL’s low-level C++ API for accessing GNDS data.

- MCGIDI: Monte Carlo General Interaction Data Interface
  - LLNL’s low-level C++ API for Monte Carlo sampling of “nuclear” reaction data.

GNDS: from evaluated data to transport simulations



Why GNDS?

Motivation: *to easily share evaluated and processed data across institutions within a modern framework*

- ENDF celebrates its 50th anniversary +/-2 years
- Format rooted in 80-column punch cards era
- Initially supported neutrons, later expanded to other particles, as projectiles or outgoing particles following reactions
- Stores evaluated data
- Difficult to add new types of data, to expand uncertainties, to allow for higher precision

- Nuclear Data community recognized the need for a more flexible format taking advantage of modern programming languages and computing architectures
- GNDS international effort under OECD/NEA/WPEC
- New ENDF/B-VIII.0 library released in ENDF-6 and GNDS format

GNDS design

- GNDS is very hierarchical
- Defines structure and not format
  - Data can be stored in a file using XML, HDF5, etc.
- Structure follows physics
- Stores data for one PROTARE (PROjectile, TARget, Evaluation)
  - e.g., γ+Fe for ENDF/B-VIII.0
- Supports simultaneous storage of
  - Evaluated, and processed Monte Carlo and multi-group data
  - Multi-temperature data
  - Enabled via styles and component/forms
- More information at **https://www.oecd-nea.org/science/wpec/sg38/**

ENDF-6 and GNDS data organization

ENDF-6

Levels with **numerical identifiers**

Tape: file with 1 or more materials

MAT: material computed from ZA

MF: file ->data type

- Resonance parameters
- Angular distribution
- …

MT: section -> reactions

GNDS

Levels with **string identifiers**

PROjectile TARget Evaluation

Styles

- Evaluated,
- Heated continuous energy,
- Heated multigroup…

Reactions

for each reaction

- Cross sections
- Output channels
- Available energy
- Available momentum

FUDGE: For Updating Data and Generating Evaluation

- FUDGE toolkit
  - Python 2.7 with extension in C and C++ to handle computationally expensive tasks
- Translate LLNL ENDL and ENDF-6 to GNDS and GNDS to ENDF-6
- LLNL principal code for managing and processing Nuclear data
  - Manage, manipulate, view, check and process in ENDL and GNDS data
  - Also handles processed data
  - Generate ACE files
- Download fudge via **http://www.nndc.bnl.gov/endf/codes/FUDGE/index.html**
- **Open Source** released under BSD license

Status of Translation/Processing of ENDF to GNDS

- FUDGE handles all properly formatted ENDF-6 formatted files
  - In ENDF/B-VII.1, VIII.0

- Photon/electron ENDF sub-libraries:

ENDF sub-libraries		Translated ENDF to GNDS	Processed ENDF to GNDS
Photo-at	EPDL	✓	✓
Electron	EEDL	✓	-
Atomic_relax	EADL	✓	-

- Verification of translation

GIDI & MCGIDI: General Interaction Data Interface

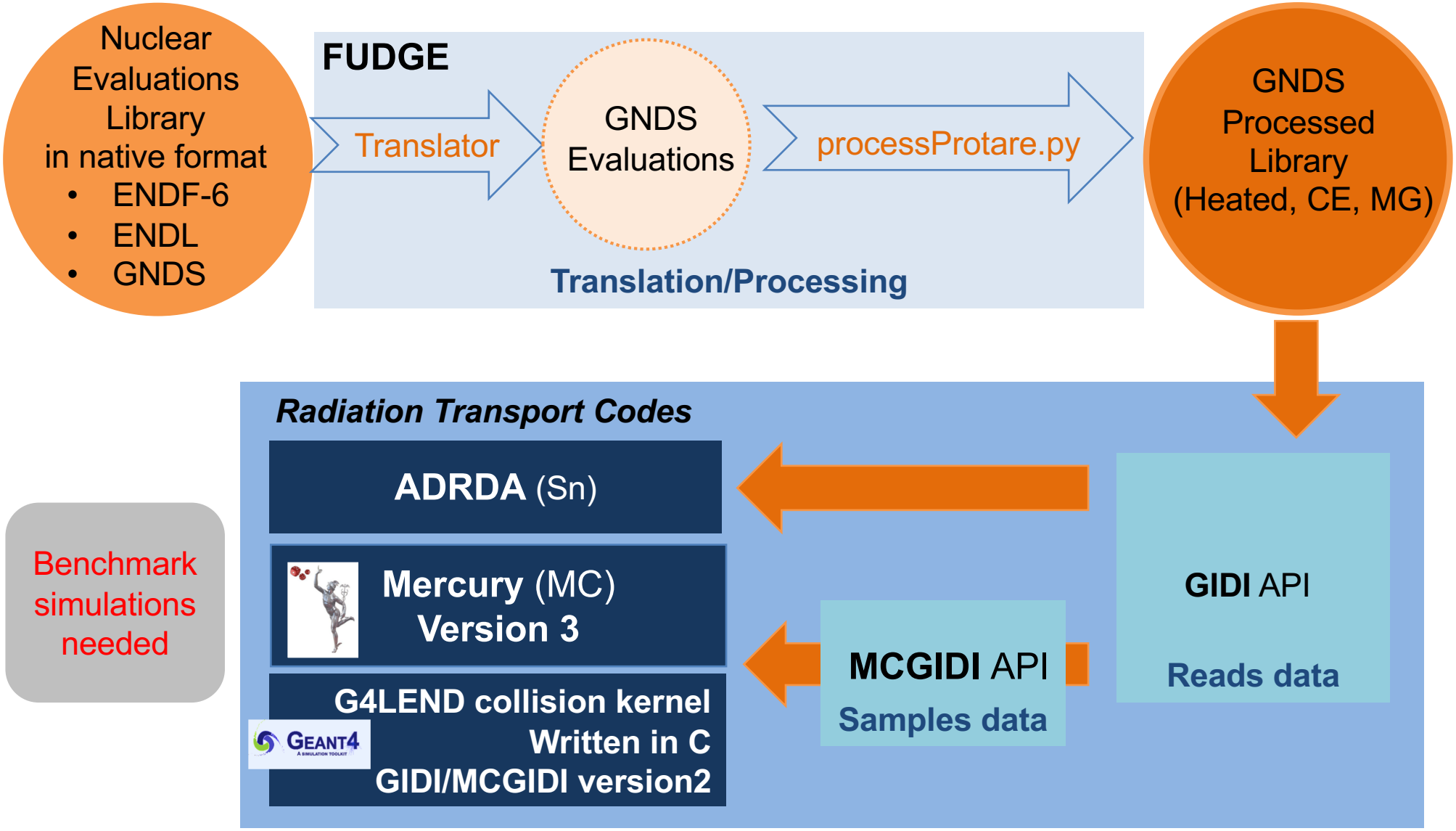
- **GIDI** version 3
  - C++ API to read GNDS files for transport codes
  - Can get data at any level in GNDS structure
  - Multi-group collapsing
    - For vectors and matrices
    - Transport correction
  - Calculates multi-group energy deposition
  - Complete for neutrons, photons and charged particles

- **Open Source** will be released *soon* under BSD license

- **MCGIDI** version 3: Monte Carlo GIDI
  - C++ API to store and sample for Monte Carlo transport codes
  - Uses GIDI to read data, then puts it into better form for optimal MC sampling
  - Handles point-wise cross sections and pdf/cdf distributions
  - Supports GPUs
  - Will sample a reaction for a protare and outgoing distribution
  - Angular biasing
  - multi-group support for cross sections

- Currently working on:
  - point-wise energy deposition
  - fixed-grid support for cross sections, deposition energy, etc.

Need Validation of GNDS photoatomic data/transport codes



Simple formats to share/combine data easily

- Similar to xsdir file for MCNP
- A “library” is defined as a collection of protares
  - at LLNL, we generate a “map” file

```
<map>
<import path="neutrons/all.map"/>
<import path="protons/all.map"/>
<import path="photo-nuclear/all.map"/>
<import path="photo-atomic/all.map"/>
</map>
```

all.map file for photons

```
<map>
<protare projectile="photon" target="O"
evaluation="ENDF/B-8.0"
path="photo_atomic/photo_atomic-008_O_000.xml"/>
<protare projectile="photon" target="H"
evaluation="ENDF/B-8.0"
path="photo_atomic/photo_atomic-001_H_000.xml"/>
<protare projectile="photon" target="Al"
evaluation="ENDF/B-8.0"
path="photo_atomic/photo_atomic-013_Al_000.xml"/>
</map>
```

- Community still needs to define common
  - multi-group boundaries structure or format
  - flux structure or format

Top level of GNDS file

```
– <reactionSuite projectile="photon" target="U" evaluation="ENDF/B-7.1" format="1.10" projectileFrame="lab">
  + <styles></styles>
  + <documentations></documentations>
  + <PoPs name="protare_internal" version="1.0" format="0.1"></PoPs>
  + <reactions></reactions>
  + <sums></sums>
  + <applicationData></applicationData>
</reactionSuite>
```

Top level of GNDS file

```
– <reactionSuite projectile="photon" target="U" evaluation="ENDF/B-7.1" format="1.10" projectileFrame="lab">
  – <styles>
    – <evaluated label="eval" date="1997-07-01" library="ENDF/B" version="7.1.1">
        <temperature value="0.0" unit="K"/>
        <projectileEnergyDomain min="2044000.0" max="100000000000.0" unit="eV"/>
      </evaluated>
    </styles>
  + <documentations></documentations>
  + <PoPs name="protare_internal" version="1.0" format="0.1"></PoPs>
  – <reactions>
    + <reaction label="U + photon [coherent]" ENDF_MT="502"></reaction>
    + <reaction label="U + photon [incoherent]" ENDF_MT="504"></reaction>
    + <reaction label="e- + e+ + U [pair production: electron field]" ENDF_MT="515"></reaction>
    + <reaction label="e- + e+ + U [pair production: nuclear field]" ENDF_MT="517"></reaction>
    + <reaction label="e- + U{1s1/2}" ENDF_MT="534"></reaction>
    + <reaction label="e- + U{2s1/2}" ENDF_MT="535"></reaction>
    + <reaction label="e- + U{2p1/2}" ENDF_MT="536"></reaction>
    + <reaction label="e- + U{2p3/2}" ENDF_MT="537"></reaction>
    + <reaction label="e- + U{3s1/2}" ENDF_MT="538"></reaction>
    + <reaction label="e- + U{3p1/2}" ENDF_MT="539"></reaction>
    + <reaction label="e- + U{3p3/2}" ENDF_MT="540"></reaction>
    + <reaction label="e- + U{3d3/2}" ENDF_MT="541"></reaction>
    + <reaction label="e- + U{3d5/2}" ENDF_MT="542"></reaction>
    + <reaction label="e- + U{4s1/2}" ENDF_MT="543"></reaction>
    + <reaction label="e- + U{4p1/2}" ENDF_MT="544"></reaction>
    + <reaction label="e- + U{4p3/2}" ENDF_MT="545"></reaction>
    + <reaction label="e- + U{4d3/2}" ENDF_MT="546"></reaction>
    + <reaction label="e- + U{4d5/2}" ENDF_MT="547"></reaction>
    + <reaction label="e- + U{4f5/2}" ENDF_MT="548"></reaction>
    + <reaction label="e- + U{4f7/2}" ENDF_MT="549"></reaction>
    + <reaction label="e- + U{5s1/2}" ENDF_MT="550"></reaction>
    + <reaction label="e- + U{5p1/2}" ENDF_MT="551"></reaction>
    + <reaction label="e- + U{5p3/2}" ENDF_MT="552"></reaction>
    + <reaction label="e- + U{5d3/2}" ENDF_MT="553"></reaction>
    + <reaction label="e- + U{5d5/2}" ENDF_MT="554"></reaction>
    + <reaction label="e- + U{5f5/2}" ENDF_MT="555"></reaction>
    + <reaction label="e- + U{5f7/2}" ENDF_MT="556"></reaction>
    + <reaction label="e- + U{6s1/2}" ENDF_MT="559"></reaction>
    + <reaction label="e- + U{6p1/2}" ENDF_MT="560"></reaction>
    + <reaction label="e- + U{6p3/2}" ENDF_MT="561"></reaction>
    + <reaction label="e- + U{6d3/2}" ENDF_MT="562"></reaction>
    + <reaction label="e- + U{6d5/2}" ENDF_MT="563"></reaction>
    + <reaction label="e- + U{7s1/2}" ENDF_MT="570"></reaction>
    </reactions>
  + <sums></sums>
  + <applicationData></applicationData>
</reactionSuite>
```

Top level of GNDS file


```
− <reactions>
  + <reaction label="U + photon [coherent]" ENDF_MT="502"></reaction>
  − <reaction label="U + photon [incoherent]" ENDF_MT="504">
    − <doubleDifferentialCrossSection>
      − <incoherentPhotonScattering label="eval" pid="photon" productFrame="lab">
        + <regions1d></regions1d>
        </incoherentPhotonScattering>
      </doubleDifferentialCrossSection>
    − <crossSection>
      − <XYs1d label="eval" interpolation="log-log">
        − <axes>
            <axis index="1" label="energy_in" unit="eV"/>
            <axis index="0" label="crossSection" unit="b"/>
          </axes>
        − <values>
            1.00000000e+00 2.82650000e-06 1.25890000e+00 4.47970000e-06 1.58490000e+00 7.09990000e-06 1.99530000e+00 1.12520000e-05 2.51190000e+00 1.78340000e-05 3.16230000e+00
            2.82650000e-05 3.98110000e+00 4.47960000e-05 5.01190000e+00 7.09970000e-05 6.30960000e+00 1.12520000e-04 7.94330000e+00 1.78330000e-04 1.00000000e+01 2.82640000e-04
            1.25890000e+01 4.47940000e-04 1.58490000e+01 7.09570000e-04 1.99530000e+01 1.12380000e-03 2.51190000e+01 1.78020000e-03 3.16230000e+01 2.82020000e-03 3.98110000e+01
            4.46840000e-03 5.01190000e+01 7.08020000e-03 6.30960000e+01 1.12190000e-02 7.94330000e+01 1.77580000e-02 1.00000000e+02 2.80950000e-02 1.25890000e+02 4.43890000e-02
            1.58490000e+02 7.00070000e-02 1.99530000e+02 1.10090000e-01 2.51190000e+02 1.72400000e-01 3.16230000e+02 2.68220000e-01 3.98110000e+02 4.12580000e-01 5.01190000e+02
            6.21630000e-01 6.30960000e+02 9.13240000e-01 7.94330000e+02 1.30020000e+00 1.00000000e+03 1.79060000e+00 1.25890000e+03 2.39520000e+00 1.58490000e+03 3.14450000e+00
            1.99530000e+03 4.08550000e+00 2.51190000e+03 5.25430000e+00 3.16230000e+03 6.67140000e+00 3.98110000e+03 8.35620000e+00 5.01190000e+03 1.02910000e+01 6.30960000e+03
            1.24380000e+01 7.94330000e+03 1.48290000e+01 1.00000000e+04 1.75140000e+01 1.25890000e+04 2.04260000e+01 1.58490000e+04 2.34800000e+01 1.99530000e+04 2.64240000e+01
            2.51190000e+04 2.92540000e+01 3.16230000e+04 3.19310000e+01 3.98110000e+04 3.41830000e+01 5.01190000e+04 3.60320000e+01 6.30960000e+04 3.74650000e+01 7.94330000e+04
            3.80590000e+01 1.00000000e+05 3.80190000e+01 1.25890000e+05 3.73730000e+01 1.58490000e+05 3.61310000e+01 1.99530000e+05 3.45460000e+01 2.51190000e+05 3.26050000e+01
            3.16230000e+05 3.04610000e+01 3.98110000e+05 2.82050000e+01 5.01190000e+05 2.59050000e+01 6.30960000e+05 2.36220000e+01 7.94330000e+05 2.13870000e+01 1.00000000e+06
            1.92260000e+01 1.25890000e+06 1.71760000e+01 1.58490000e+06 1.52380000e+01 1.99530000e+06 1.34270000e+01 2.51190000e+06 1.17540000e+01 3.16230000e+06 1.02250000e+01
            3.98110000e+06 8.84120000e+00 5.01190000e+06 7.60130000e+00 6.30960000e+06 6.50100000e+00 7.94330000e+06 5.53290000e+00 1.00000000e+07 4.68800000e+00 1.25890000e+07
            3.95600000e+00 1.58490000e+07 3.32610000e+00 1.99530000e+07 2.78720000e+00 2.51190000e+07 2.32850000e+00 3.16230000e+07 1.94010000e+00 3.98110000e+07 1.61250000e+00
            5.01190000e+07 1.33730000e+00 6.30960000e+07 1.10680000e+00 7.94330000e+07 9.14380000e-01 1.00000000e+08 7.54150000e-01 1.25890000e+08 6.21060000e-01 1.58490000e+08
            5.10750000e-01 1.99530000e+08 4.19500000e-01 2.51190000e+08 3.44140000e-01 3.16230000e+08 2.82020000e-01 3.98110000e+08 2.30880000e-01 5.01190000e+08 1.88830000e-01
            6.30960000e+08 1.54310000e-01 7.94330000e+08 1.25990000e-01 1.00000000e+09 1.02800000e-01 1.25890000e+09 8.38090000e-02 1.58490000e+09 6.82820000e-02 1.99530000e+09
            5.55960000e-02 2.51190000e+09 4.52390000e-02 3.16230000e+09 3.67900000e-02 3.98110000e+09 2.99030000e-02 5.01190000e+09 2.42920000e-02 6.30960000e+09 1.97250000e-02
            7.94330000e+09 1.60080000e-02 1.00000000e+10 1.29860000e-02 1.25890000e+10 1.05300000e-02 1.58490000e+10 8.53440000e-03 1.99530000e+10 6.91440000e-03 2.51190000e+10
            5.59980000e-03 3.16230000e+10 4.53350000e-03 3.98110000e+10 3.66880000e-03 5.01190000e+10 2.96810000e-03 6.30960000e+10 2.40040000e-03 7.94330000e+10 1.94070000e-03
            1.00000000e+11 1.56850000e-03
          </values>
        </XYs1d>
      </crossSection>
    + <outputChannel genre="twoBody" process="incoherent"></outputChannel>
    </reaction>
```


- GNDS can accomodate uncertainties and covariances