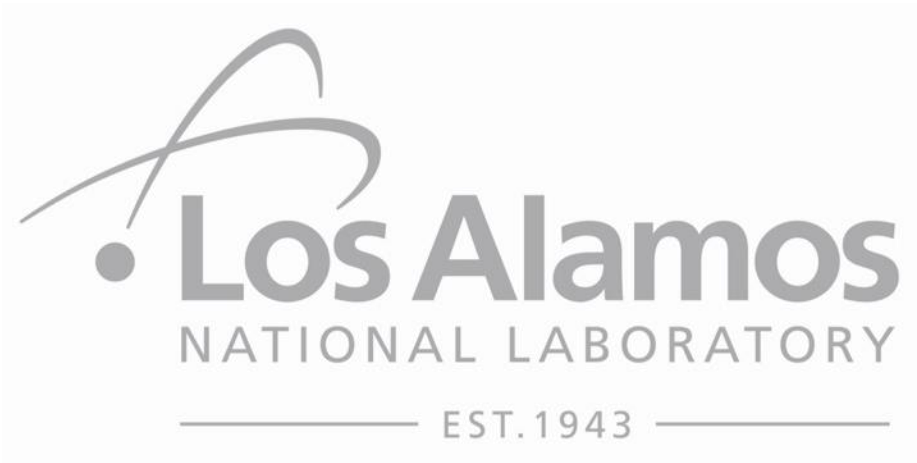
Proposing a JSON structure for calculation results

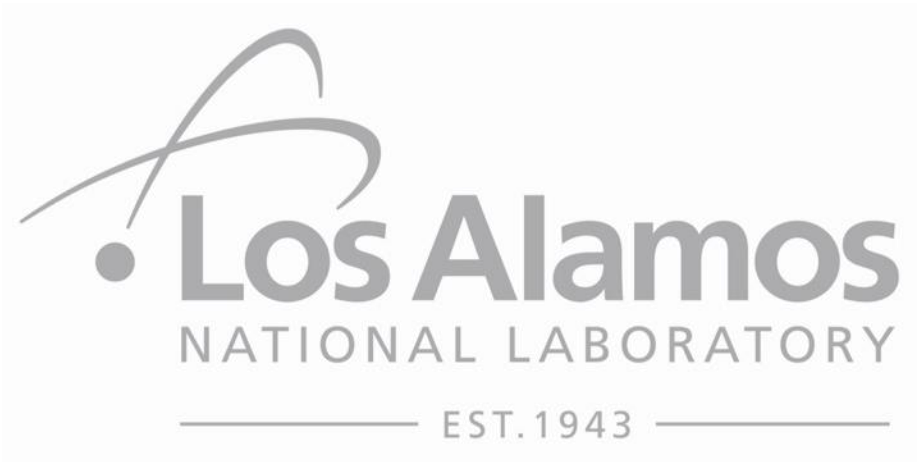


W. Haeck

WPEC SG45, June 24-28, 2019

June 24-28, 2019

WPEC SG45, Paris, France



- **Introduction**
- **Overview**
- **Python coding and examples**

Introduction

Every calculation code gives its result in its own format

- MCNP (LANL): the output file, the mctal file, the ptrac file, etc.
- PARTISN (LANL): the output file, etc.
- MORET (IRSN): the output file, an XML file, etc.

The results we’re interested in are however the same

- Single values: keff, βeff, etc.
- Histogram data: particle spectra, reaction rates, sensitivity profiles, etc.
- Pointwise data: nuclide composition as a function of time, etc.

General calculation results

A calculation result consists of two distinct components

- Attributes (or metadata) that give information about the result
  - What type of result is it?
  - What nuclide and reaction is it for (if it is a reaction rate)?
  - What volume is it for (if it is a particle spectrum)?
  - Which code and version produced the result?
  - Which nuclear data library was used to produce the result?
  - This is what we will want to search and filter on
- The actual calculation result
  - Values for the result: a single value, an array of values, an array of arrays of values, etc.
  - Optional uncertainties: in the same form as the values for the result
  - The structure of the result: a histogram of flux values as a function of incident energy, etc.
  - Optional units for the values and uncertainties
  - This is what we will want to compare, store, exchange, plot, etc.

General calculation results

There are some requirements to a structure to store these

- A result should stand by itself
  - I don’t need to look in multiple places to be able to understand it
  - For example: for a particle spectrum, I should have the group structure at the same time, etc.
- It should be calculation code agnostic
  - I don’t need to know where it came from to understand it
- It should be result type agnostic
  - I can use it for any result, even the ones I have not thought of yet
- It should be relatively easy to interact with through different scripting or programming languages
  - I can use it in python or C++, etc.
- It should be relatively light weight, as in not impose a heavy infrastructure

- It should not be Microsoft excel – that should be obvious …

General calculation results

```
[ { 'type' : 'effectiveMultiplicationFactor',
    'data' : { 'values' : [ 1.0000 ],
               'uncertainties' : [ 0.0001 ] } },
  { 'type' : 'sensitivityProfile',
    'response' : 'keff',
    'parameter' : 'xs',
    'particleId' : 'neutron',
    'nuclide' : '92235',
    'reaction' : 'fission',
    'material' : 'total',
    'data' : { 'values' : [ -1.7129e-17, 1.4106e-09 ],
               'uncertainties' : [ 0.0034, 0.0033 ],
               'structure' : [ { 'name' : 'energy-in',
                                 'type' : 'histogram',
                                 'limits' : [ 1e-11, 10.0, 20.0 ],
                                 'unit' : 'MeV'} ],
               'units' : { 'value' : '%/%', 'uncertainty' : 'relative' } } } ]
```

Attributes

`type` is an essential attribute and should be always be present

- Indicate the type of result we're storing
- Possible values that are currently identified: `effectiveMultiplicationFactor`, `effectiveDelayedNeutronFraction`, `effectiveNeutronGenerationTime`, `thermalFissionFraction`, `aboveThermalFissionFraction`, `averageEnergyCausingFission`, `energyAverageLethargyFission`, `particleSpectrum`, `particleFlux`, `particleCurrent`, `reactionRate`, `sensitivityProfile`

Some attributes will appear based on the value of `type`

- For example, for `sensitivityProfile` :
  - `response` : for which "response function" we have a sensitivity $\partial r/\partial p$, e.g. `keff`
  - `parameter` : the sensitivity of the response is given with respect to a parameter
  - `nuclide` : the nuclide for which a sensitivity profile is given
  - `reaction` : the reaction for which the sensitivity profile is given, e.g. `fission`, `n,gamma`
  - `material` : the material in the model for which the sensitivity is given

Attributes

Some attributes could appear based on the application but should be independent of the value of `type`

For example (we do not use these yet):

- `code` : which calculation code generated the result, e.g. `mcnp`, `cog`, `partisan`, `ardra`
- `date` : the calculation date
- `library` : the nuclear data library, e.g. `endf/b-viii.0`
- `temperature` : the temperature of the material for which the result is given

The way attributes are stored and defined makes it flexible enough for extension

- Retrieving a non-existent attribute is NOT an error, it is simply undefined
- This allows for filters to function properly

Data

As indicated earlier, a calculation result consists of the following:

- A one dimensional array of `values`, this is always present
- An optional one dimensional array of `uncertainties`
- The `structure` of the `values` and `uncertainties`
  - This is a list of dimensions that defines how to interpret the the `values` and `uncertainties`
  - This is not required if the `values` array contains a single value
- An optional set of units, one for a `value` and another one for an `uncertainty`

`values` and `uncertainties` are always an array

- This even applies to a single value (every result needs to look like another one)

Dimensions and the structure of the result

The structure of a result is made up of dimensions, defined by:

- `name` : the name for the dimension, e.g. `energy-in`
- `type` : the type of the dimension, either `histogram` or `points`
- `limits` : the bins or points for which we have data in the current dimension
- `unit` : an optional unit for the dimension

A one dimensional result will have only one dimension, and so on

- A particle spectrum integrated over a given number of energy bins has one dimension
- A sensitivity profile for the fission spectrum can have an incident energy dimension and an outgoing energy dimension
- The order of the dimensions determines the order of the values (obviously)

Dimensions and the structure of the result

The dimension `type` can be mixed over multiple dimensions

- I can use a first dimension that gives me points in time followed by a second dimension that gives me histograms for each point in time (e.g. changes in particle spectrum as a function of time)

```
[ { 'name' : 'time', 'type' : 'points',
    'limits' : [ 0, 1, 2 ], 'unit' : 'days' },
  { 'name' : 'energy', 'type' : 'histogram',
    'limits' : [ 1e-5, 1.0, 2e+7 ], 'unit' : 'eV' } ]
```

The number of values and uncertainties is directly linked to the dimension

- Dimensions must be present as soon as there is more than 1 value in the arrays

Python interface

```
# retrieve attribute information with the 'attributes' property on Result
type = result.attributes.type          # 'sensitivityProfile'
nuclide = result.attributes.nuclide    # '92235'
reaction = result.attributes.reaction # 'fission'
date = result.attributes.date          # None, 'date' attribute is not present

# retrieve the data
values = result.values                 # result.data.values also works here
groups = result.structure[0].limits
valueUnit = result.units.value

# data can also be retrieved through its own property
data = result.data
values = data.values
groups = data.structure[0].limits
valueUnit = data.units.value
```

Python interface

```
# factory functions to create new results from data

# overloaded functions to allow for flexibility
myResult = makeKeffResult( 1.0001 )
myResult = makeKeffResult( 1.0001, 0.0005 ) # the uncertainty is optional
myResult = makeEffectiveNeutronGenerationTimeResult( 5.62578, 'ns' )
myResult = makeEffectiveNeutronGenerationTimeResult( 5.62578, 0.00713, 'ns' )

# can be provided for every result type to make it easier for the user
myResult = makeKeffResult( ... )
myResult = makeEffectiveDelayedNeutronFractionResult( ... )
myResult = makeEffectiveNeutronGenerationTimeResult( ... )
myResult = makeAverageNeutronEnergyCausingFissionResult( ... )
myResult = makeAboveThermalFissionFractionResult( ... )
myResult = makeSensitivityResult( ... )

# note: we may change this for a fluent builder interface
```

Python interface

```
# we have an interface over MCNP and SENSMG outputs to use this structure
mcnp = McnpOutput( [ McnpEffectiveMultiplicationFactor(),
                     McnpPointKinetics(),
                     McnpSensitivityProfiles() ] )
mcnp.extract( 'HEU-MET-FAST-001-001.mcnp.o' )

# retrieve the results
results = {}
results[ 'HEU-MET-FAST-001-001' ] = mcnp.toResults()

# we have json serialisation and deserialization in place
toJSON( results, 'mcnp.results.json', indent = 2 )
resultsFromJSON = fromJSON( 'mcnp.results.json' )

# results and resultsFromJSON are the same
print( results == resultsFromJSON ) # should be true
```

Python interface

```
# getting keff and above thermal fission fraction for a set of benchmarks
benchmarks = []
keffValues = []
atffValues = []

# go over the results for each benchmark
for name, list in results :
    keff = [ result.values[0] for result in results
                if result.attributes.type == 'effectiveMultiplicationFactor' ]
    atff = [ result.values[0] for result in results
                if result.attributes.type == 'aboveThermalFissionFraction' ]
    if keff and atff :
        benchmarks.append( name )
        keffValues.append( keff[0] )
        atff.append( atff[0] )

# now we can go plot this data ...
```

Python interface

```
# another filter example: get all sensitivity profiles for U235 xs
nuclide = '92235'
search = [ result for result in results
            if result.attributes.type == 'sensitivityProfile' and
               result.attributes.nuclide == nuclide ]

# retrieve and print all reactions of U235 for which we have profiles
reactions = [ result.attributes.reaction for result in search ]
print( reactions )   # [ 'fission' ]
```

Considerations for the future

Use a NoSQL document database for storing results

- MongoDB, CoachDB, etc.
- Would allow easier searching instead of having to loop all the time

Open source the python coding and release it for VaNDaL