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Title: FAUST - Benchmark and Validation Framework

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FAUST

Benchmark and Validation Framework

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Introduction

Python packages for nuclear data applications and benchmarking

Goals and objectives for FAUST

- Provide input and output processing for different calculation codes
- Allow for exchanging results between different applications and codes
- Running benchmarks and processing the results
- Automate and simplify plot and report generation
- Provide a basis for developing applications useful for nuclear data evaluators

To be used both inside and outside LANL

- All packages are currently hosted internally at LANL
- For example: the LANL ML project and the OECD/NEA WPEC VaNDaL project

Sponsored by ASC-PEM-NP, ASC-ADTM-ML, ASC-V&V-QM, NCSP

Overview of current features

Available packages:

- `result` : storing, serializing, deserialising calculation results
- `sensitivity` : filtering, analysing and using sensitivity data
- `benchmarks` : the material balance table for comparing benchmark inputs
- `mcnp` : extracting data from the mctal and the output file
- `sensmg` : extracting keff and leakage sensitivity profiles (sens_k_x and sens_l_x file)
- `scale` : extracting sensitivity profiles from sdf files (N. Thompson, NEN-2)
- `elementary` : utility package to convert nuclide and reaction identifiers

Work in progress:

- `sensitivity.crater` : evaluate observable changes due to nuclear data changes
- `mcnp.input` : parsing, creating and modifying MCNP input files
- `partisn` : reading and writing binary data files (A. Clark, XCP-3/XCP-5)
- `lmx` : detector events in subcritical multiplication experiments (H. Kistle, NEN-2)

`mcnp` : input and output processing for MCNP

The `mcnp` package is dedicated to MCNP input and output

Extracting results from the MCNP output and mctal file

- Effective multiplication factor, point kinetic values and related information
- Sensitivity profiles (from the output file only)
- Print tables 40, 50 and 60 (material, surfaces and volume information)
- Tally results (from the mctal file only)

Extracting derived data from the print tables

- Balance tables for input comparison (OECD/NEA WPEC VaNDaL project)

Creating, reading and modifying MCNP input file

- Extract information from the input file (dimensions, materials, etc.)
- Modify and regenerate the input file at the request of the user
  - For example: uncertainty analysis in benchmark evaluation

mcnp : input and output processing for MCNP

Processing data from the output file

```
# extract results for multiple output objects in a single go
mcnp = McnpOutput( [ McnpEffectiveMultiplicationFactor(), McnpPointKinetics() ] )
mcnp.extract( 'HEU-MET-FAST-001-001.mcnp.o' )

# retrieve information from the output object
keff = mcnp.data[0]  # mcnp.data is the list of output objects
atff = keff.aboveThermalFissionFraction
aecf = keff.averageEnergyCausingFission
```

Reading and modifying the input file

```
# parse an existing input file
mcnp = McnpInput( 'HEU-MET-FAST-001-001.mcnp' )

# retrieve and modify material related data
heu = mcnp.materials()[0]
u5 = heu.composition[ '92235' ]
heu.composition[ '92235' ] = 1.01
heu.composition.update( { '92235' : 1.0 } )
```

`sensitivity` : tools for sensitivity analysis

Filtering and analysis of the maximum sensitivity

```
# create a filter
select = SensitivityFilter( lowerSensitivity = 10., nuclides = [ 'U235', 'U238' ] )

# select godiva profiles
godiva = profiles[ 'HEU-MET-FAST-001-001-s' ]
godiva = [ profile for profile in godiva if select( profile ) ]

# retrieve maximum sensitivity and sort
table = MaximumSensitivityTable( profiles )
print( table )
```

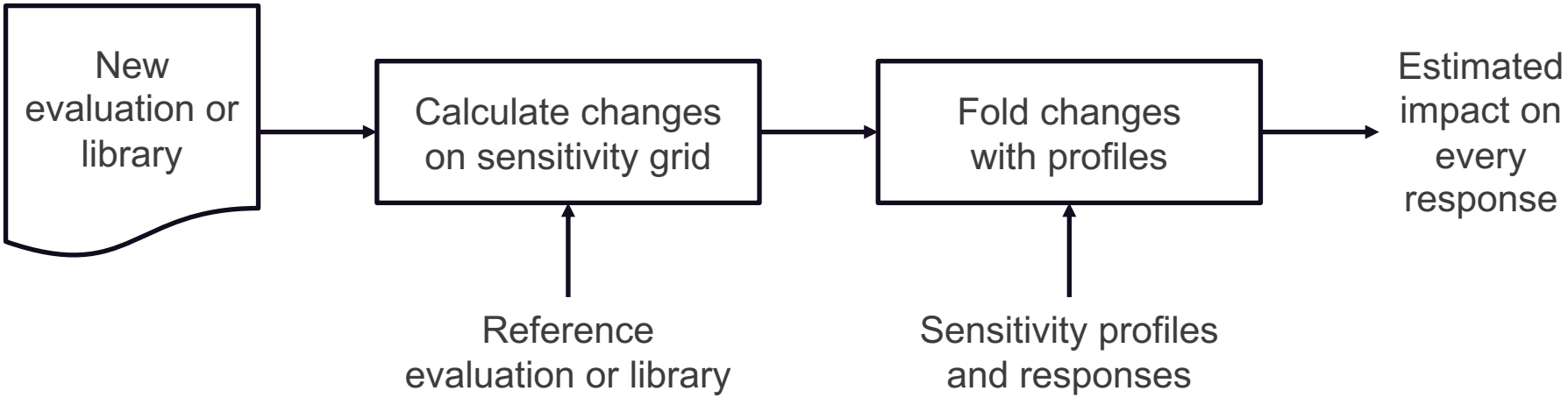
Case	Nuclide	Reaction	Max sensitivity at energy bin [MeV]	Maximum sensitivity [pcm/%]	Integrated sensitivity [pcm/%]
HEU-MET-FAST-001-001-s	U235	total nu	0.4 - 0.9	209.90	982.42
HEU-MET-FAST-001-001-s	U235	prompt nu	0.4 - 0.9	208.48	976.13
HEU-MET-FAST-001-001-s	U235	total	0.4 - 0.9	186.03	804.28
HEU-MET-FAST-001-001-s	U235	fission	0.4 - 0.9	142.86	654.11
HEU-MET-FAST-001-001-s	U235	elastic	0.1 - 0.4	37.78	108.06
HEU-MET-FAST-001-001-s	U235	inelastic	0.4 - 0.9	22.50	79.20

`crater` : estimate impact of nuclear data changes

An analysis tool to estimate the impact of nuclear data changes

- Sensitivity profiles provide impact of changing a parameter *p* on a given response R

$$R' = R\left(1 + \sum_{p}\sum_{g} C_{p,g} S^{R}_{p,g}\right)$$



`crater` : estimate impact of nuclear data changes

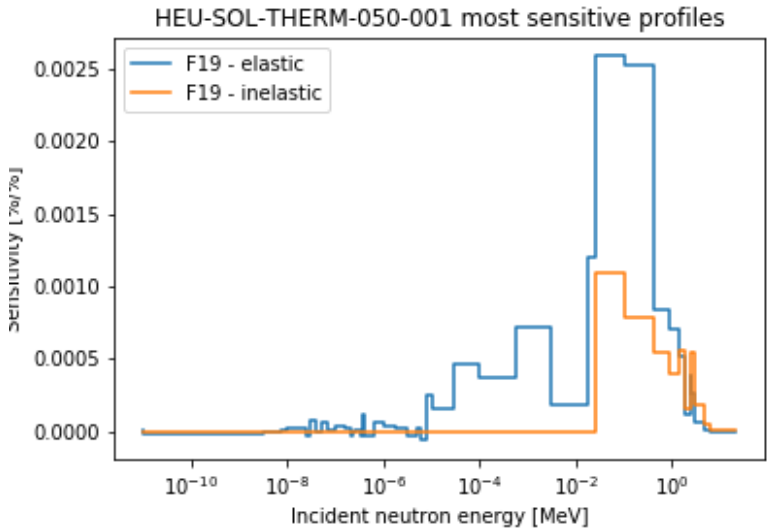
```
# load observables and profiles - both are from MCNP calculations
observables = fromJSON( '/local/json/keff.endf80.20200127.json' )
profiles = fromJSON( '/local/json/sensitivities.crossSection.endf80.20200127.json' )

# create a crater instance using the previously loaded observables and profiles
crater = Crater( observables, profiles )

# create input
changes = CraterInput()
changes.xs.structure = [ 1e-11, ..., 20.0 ] # standard 44 group structure

# change F19 inelastic scattering (can be done by ratio or relative change)
changes.xs.addRatio( 'F19', 'inelastic',
                     [ 1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
                       1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
                       1., 1., 1., 1., 1., 1., 1., 1., 1., 1.,
                       1., 1., 1., 0.937, 1.964, 1.128, 1., 1., 1., 1.,
                       1., 1., 1., 1. ] )

# verify changes - check if the nuclide,reaction pairs actually have sensitivities
crater.verify( changes )

# calculate the impact of these changes - using the same format as the original MCNP observables
newObservables = crater.impact( changes )
```

`crater` : estimate impact of nuclear data changes

For this F19 example, 1029 benchmark cases were considered

- 107 of these lead to changes in the keff value
- 79 of these change by more than 10 pcm
- Mainly for `HEU-SOL-THERM-050`, `U233-SOL-INTER-001`, `U233-SOL-THERM-015`

Case	Before	After	Impact
HEU-SOL-THERM-050-001	1.00587	1.00693	0.00106
HEU-SOL-THERM-050-002	1.00120	1.00200	0.00080
HEU-SOL-THERM-050-003	1.00249	1.00375	0.00126
HEU-SOL-THERM-050-004	1.00257	1.00347	0.00090
HEU-SOL-THERM-050-005	0.99976	1.00024	0.00048
HEU-SOL-THERM-050-006	1.00755	1.00837	0.00082
HEU-SOL-THERM-050-007	0.99622	0.99740	0.00118
HEU-SOL-THERM-050-008	0.99633	0.99719	0.00086
HEU-SOL-THERM-050-009	0.99471	0.99591	0.00120
HEU-SOL-THERM-050-010	0.97854	0.97921	0.00067
HEU-SOL-THERM-050-011	0.99026	0.99077	0.00051



Where we would like to go …

`mephisto` : a benchmark run and result collection system

- Scalable to work on a single PC or a cluster (or maybe a heterogeneous system)