Calculating the impact of nuclear data changes with Crater

W. Haeck, A. R. Clark, M. W. Herman

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Introduction: accelerating the nuclear data pipeline

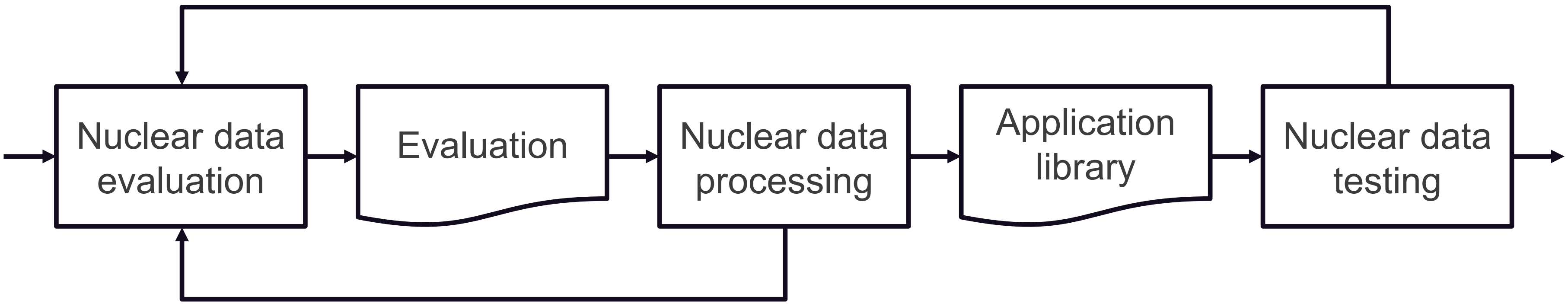
Accelerating the nuclear data pipeline

- Getting good nuclear data to applications faster
- An objective of the nuclear data community

Nuclear data testing: just one of the feedback loops

- This process takes time: hundreds to thousands of calculations
- A solution: using sensitivity profiles to assess impact

$$S = \frac{p}{r}\frac{\partial r}{\partial p}$$



Using sensitivities to assess changes to a response

Sensitivity: change in a response due to change of a parameter

$$S = \frac{p}{r}\frac{\partial r}{\partial p} \approx \frac{p}{r}\frac{\Delta r}{\Delta p}$$

Assuming the change is small enough so that linear perturbation theory applies

$$\Delta r = S\frac{\Delta p}{p}r \qquad r' = r\left(1 + S\frac{\Delta p}{p}\right) \qquad r' = r\left(1 + \sum_g S_g \frac{\Delta p_g}{p_g}\right)$$

When applying multiple changes in independent parameters

$$r' = r\left(1 + \sum_i \sum_g S_{i,g}\frac{\Delta p_{i,g}}{p_{i,g}}\right)$$

NDAST (OECD/NEA): an existing tool that allows us to do this

- Only for effective multiplication factors, not other responses
- Using a graphical user interface, not in command line

Faust & Crater

Faust: python packages for nuclear data applications and validation

Goals and objectives

- 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
  - Benchmark selection for testing purposes using sensitivity and similarity
  - Sensitivity analysis and folding to assess the impact of nuclear data changes
  - Nuclear data format and physics testing

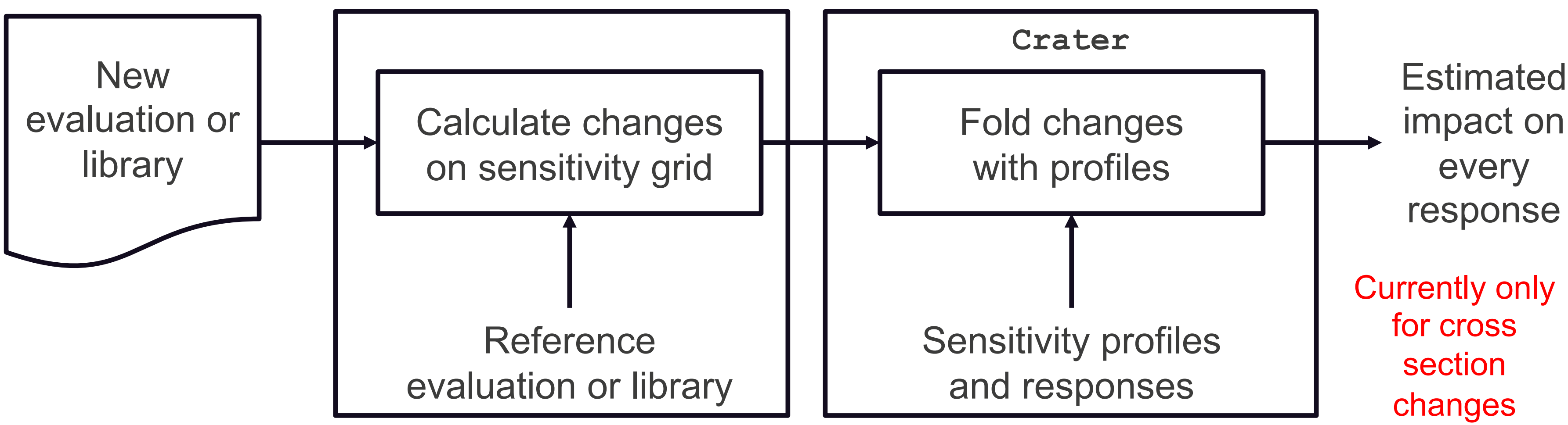
Crater: estimate impact of nuclear data changes

`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

$$r' = r\left(1 + \sum_{p}\sum_{g} c_{p,g} S_{p,g}^{r}\right)$$



Response values and sensitivity profiles

```
[ { "type" : "effectiveMultiplicationFactor",
    "data" : { "values" : [ 1.0000 ],
               "uncertainties" : [ 0.0001 ] } },
  { "type" : "sensitivityProfile",
    "response" : "effectiveMultiplicationFactor",
    "parameter" : "crossSection",
    "particleId" : "neutron",
    "nuclide" : "U235",
    "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" } } } ]
```

We'll need a database for this data

ENDF/B-VIII.0 MCNP results for ~1100 ICSBEP benchmarks

- Values for k_{eff}, β_{eff} and Λ_{eff}
- Three group spectra
- Fission fractions
- Average energy causing fission
- Energy of the average lethargy causing fission
- Sensitivity profiles

A lot of data: 1.3 GB json file for the cross section sensitivities alone

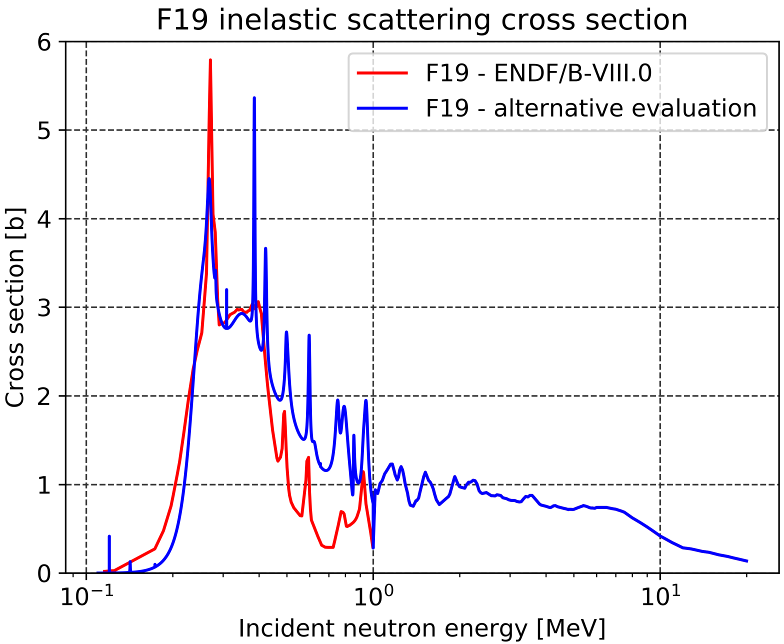
Example code

```
# load observables and cross section sensitivity 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 cross section (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 )
```

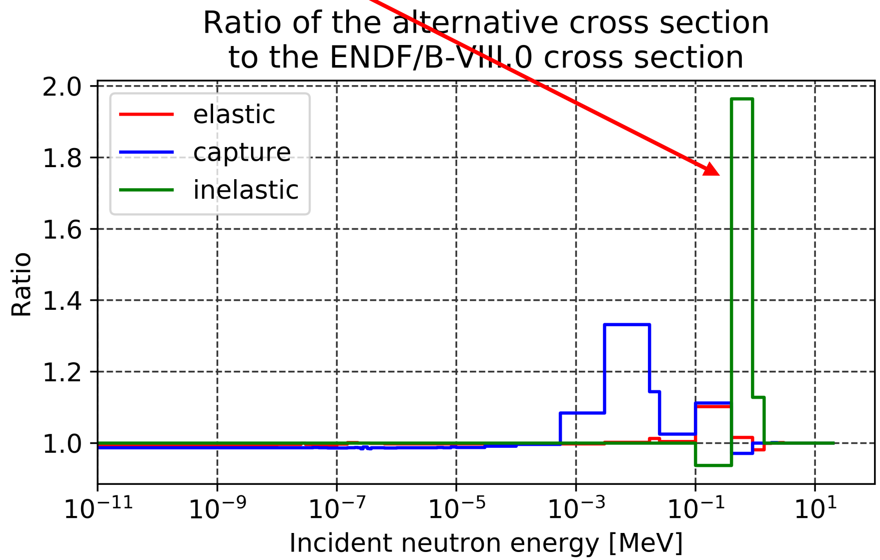
An example: an alternative evaluation for F19

ML work at LANL indicated a potential issue in ENDF/B-VIII.0 F19

- It was found that inelastic scattering was too low between 0.5 and 1 MeV
- An alternative evaluation was proposed for ENDF/B-VIII.0 but ultimately not adopted



One could argue that this is not a small change



An example: an alternative evaluation for F19

For this F19 example, 1029 benchmark cases were considered

- Only 107 of these contain F19
- 79 of these change by more than 10 pcm
- The largest change is smaller than 150 pcm
- Mainly for `HEU-SOL-THERM`, `U233-SOL-INTER`, `U233-SOL-THERM`

This represents a change of ~0.15%

For this example, we have verified these values against MCNP6.2

Before we get to the results, some fun facts:

- Crater: just a few seconds of calculation time for 1000 benchmarks
- MCNP6.2: from hours to days to weeks
  - Depending on the number benchmarks
  - Depending on precision

OK, so this isn't entirely true since GB sized json files take a few minutes to read

An example: an alternative evaluation for F19

Compared to MCNP6.2, Crater gives “statistically equivalent” results

- 60% of the Crater Δkeff are within one standard deviation of the MCNP6.2 Δkeff
- Only 1 value is outside of three standard deviations

Case	Original MCNP6.2	Crater estimate	MCNP6.2 estimate	Crater Δkeff	MCNP6.2 Δkeff	MCNP6.2 σ(Δkeff)	Impact
HST-009-001	1.00094	1.00154	1.00198	60	104	18	< 3
HST-009-002	1.00192	1.00237	1.00231	45	39	20	< 1
HST-009-003	1.00204	1.00240	1.00246	36	42	18	< 1
HST-009-004	0.99695	0.99710	0.99728	15	33	18	< 1
HST-050-001	1.00587	1.00693	1.00654	106	67	21	< 2
HST-050-002	1.00120	1.00200	1.00204	80	84	21	< 1
HST-050-003	1.00249	1.00375	1.00360	126	111	21	< 1
HST-050-004	1.00257	1.00347	1.00344	90	87	23	< 1
HST-050-005	0.99976	1.00024	1.00093	48	117	23	> 3
HST-050-006	1.00755	1.00837	1.00844	82	89	20	< 1
HST-050-007	0.99622	0.99740	0.99748	118	126	20	< 1
HST-050-008	0.99633	0.99719	0.99752	86	119	21	< 2
HST-050-009	0.99471	0.99591	0.99620	120	149	20	< 2
HST-050-010	0.97854	0.97921	0.97941	67	87	20	< 2
HST-050-011	0.99026	0.99077	0.99069	51	43	20	< 1

What's next?

Extend this capability to other higher dimensional responses

- keff is essentially a single response r with a corresponding profile S_g
  - The response is 0D, the sensitivity profile is 1D in incident neutron energy
- In a time of flight spectrum, every time bin i is a single response r_i with profile $S_{g,i}$
  - The response is 1D in time, the sensitivity profile is 2D in time and incident neutron energy

The question is how do we get these higher dimensional profiles?

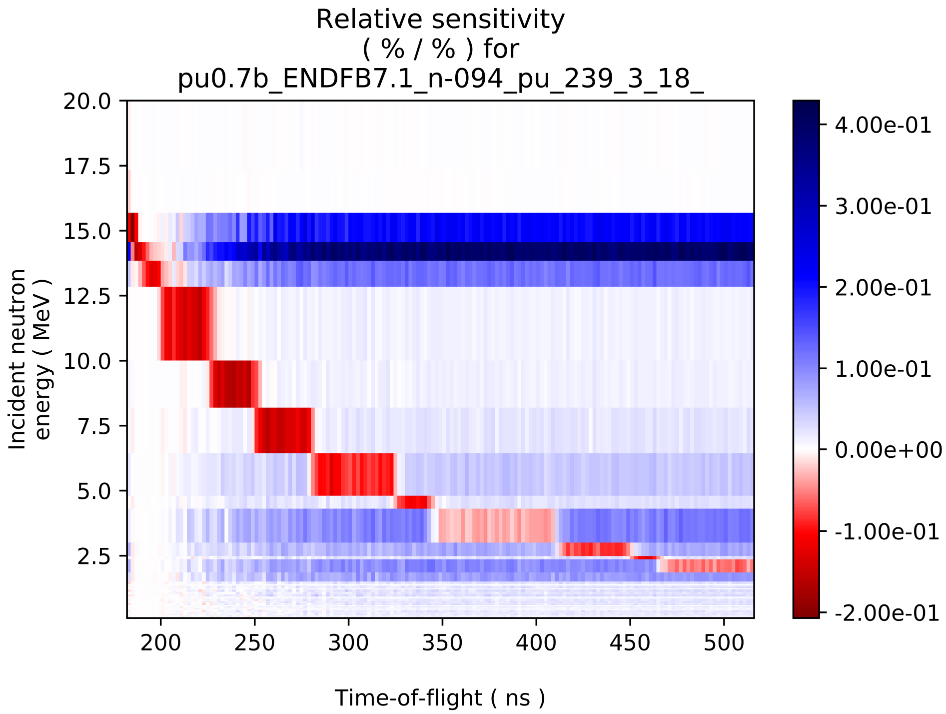
Using central difference calculations is one way

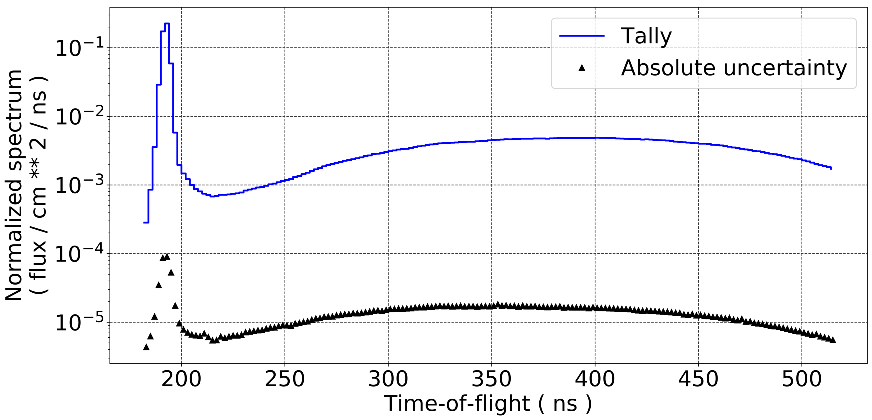
- Perturb one parameter in one group
- Calculate the unperturbed and perturbed responses using MCNP6.2

$$S = \frac{p}{r} \frac{r_{p+\Delta p} - r_{p-\Delta p}}{2\Delta p}$$

What’s next?

An example: Pu239 fission cross section profile for a pulsed sphere





Conclusions

At LANL, work is underway to develop a comprehensive package of python tools for benchmarking, sensitivity analysis, etc.

Crater : calculate the impact of nuclear data changes on responses

- Folds changes in a nuclear data parameter with the corresponding sensitivity profile
- A fast alternative to performing the actual transport calculations
- Currently works only for cross section changes

The future of Crater

- Extend the capability to angular data and particle spectra
- Extend the capability to higher dimensional observables

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