OAK RIDGE National Laboratory

Sampler Applied to Source Term Uncertainty

2018 SCALE Users' Group Tutorial

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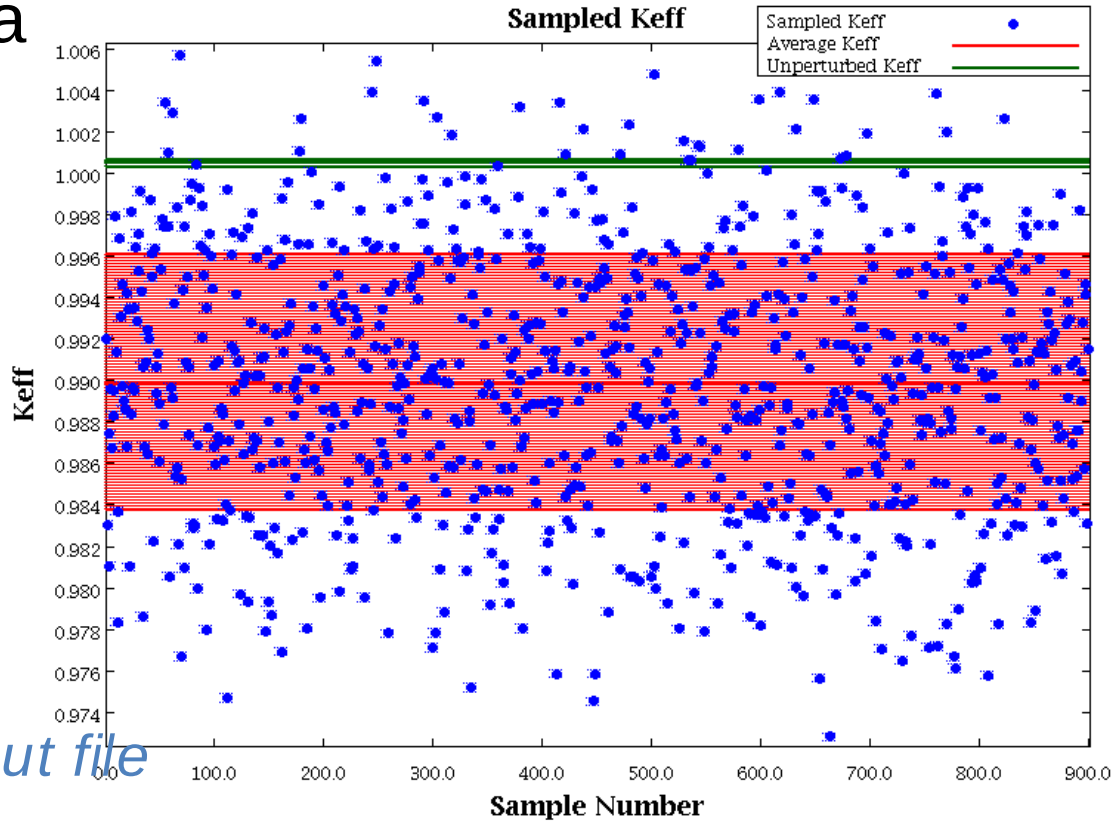
U.S. DEPARTMENT OF ENERGY

Sampler: A Module for Statistical Uncertainty Analysis with SCALE Sequences

Calculates uncertainty in *any* result of a SCALE computation* due to two basic types of uncertainty

- nuclear data uncertainty
  - cross sections
  - fission yield data
  - decay data
- input parameter uncertainty
  - geometry
  - composition
  - *and anything else that appears in an input file*



**multi-group only in SCALE 6.2*

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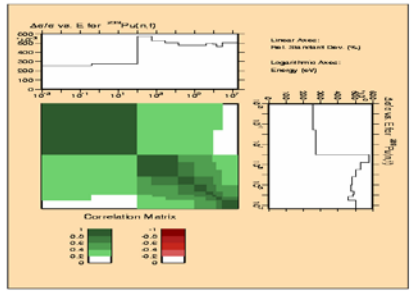
Sampler Overview
Nuclear Data Uncertainty

Sources of Sampler Nuclear Data Uncertainty

- Cross section covariances:

ENDF-VII.1 supplemented by other sources (SCALE cov. library)

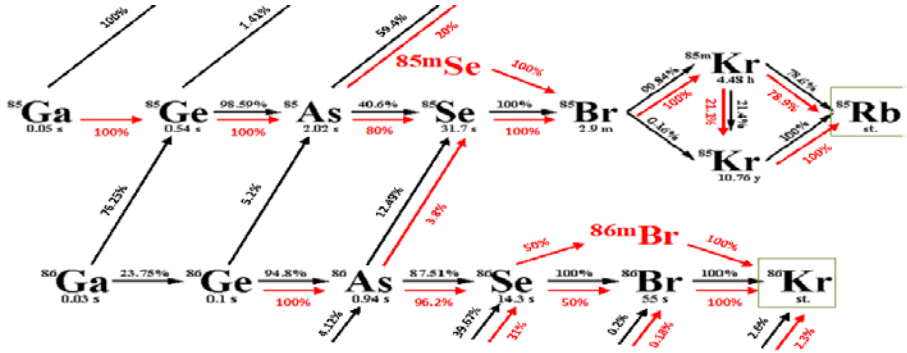


Pu-239 fission covariance

- Fission product yield:

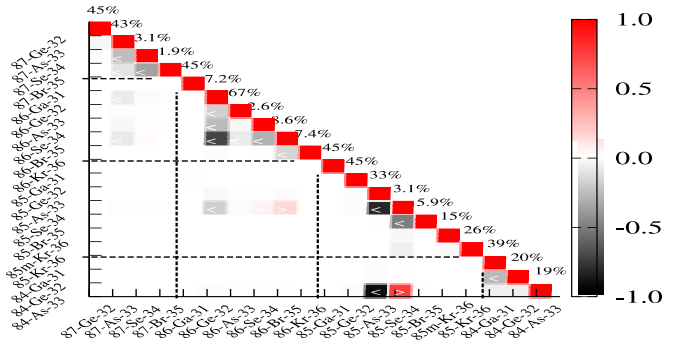
Standard deviations from ENDF/B-VII; correlations generated by combining independent and cumulative yields

Mass A=85-87 yields



- Decay data:

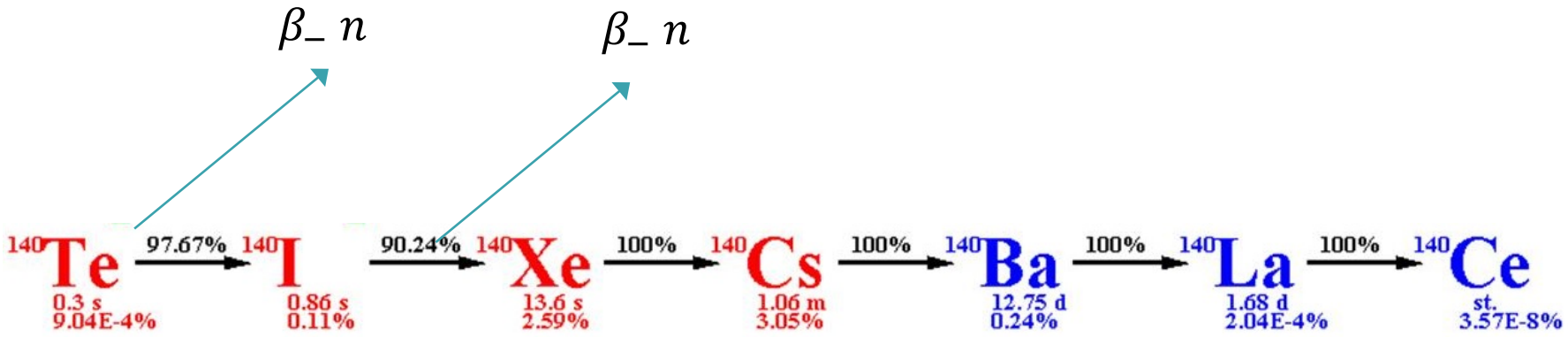
ENDF-VII.1 modified to include branching correlations due to constraint that branch sum=1.0



Yield covariance

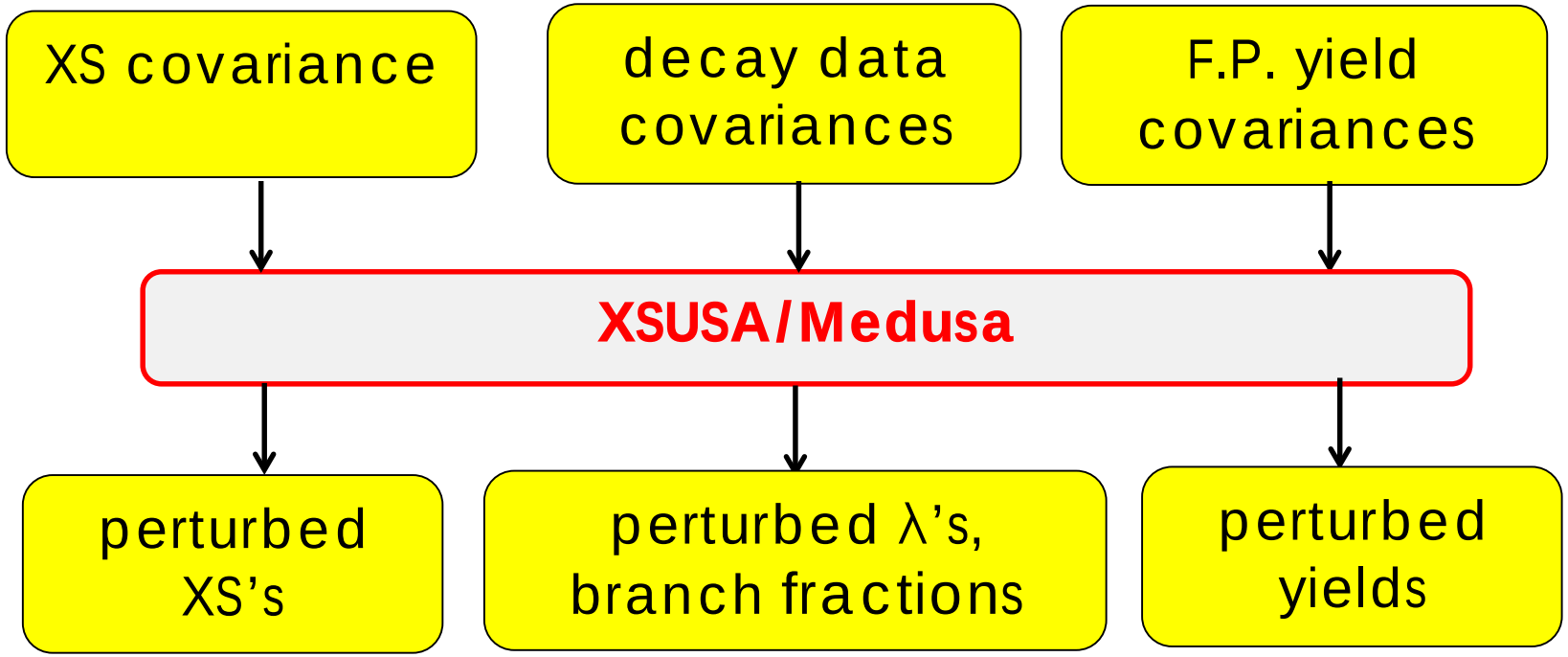
More Detail on Uncertainties In Fission Product Yields

- Independent FP yields are mainly from model calculations…
  →have large uncertainties
- Cumulative FP yields based largely on measurements…
  →have smaller uncertainties
- Beta-delayed neutron branching ratios
  →usually have large uncertainties



half-life
integral fission yield

Generation of Perturbed Nuclear Data Samples



ANS MC2015 - Joint International Conference on Mathematics and Computation (M&C), Supercomputing in Nuclear Applications (SNA) and the Monte Carlo (MC) Method • Nashville, TN • April 19-23, 2015, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2015)

UNCERTAINTY AND SENSITIVITY ANALYSIS IN CRITICALITY CALCULATIONS WITH PERTURBATION THEORY AND SAMPLING

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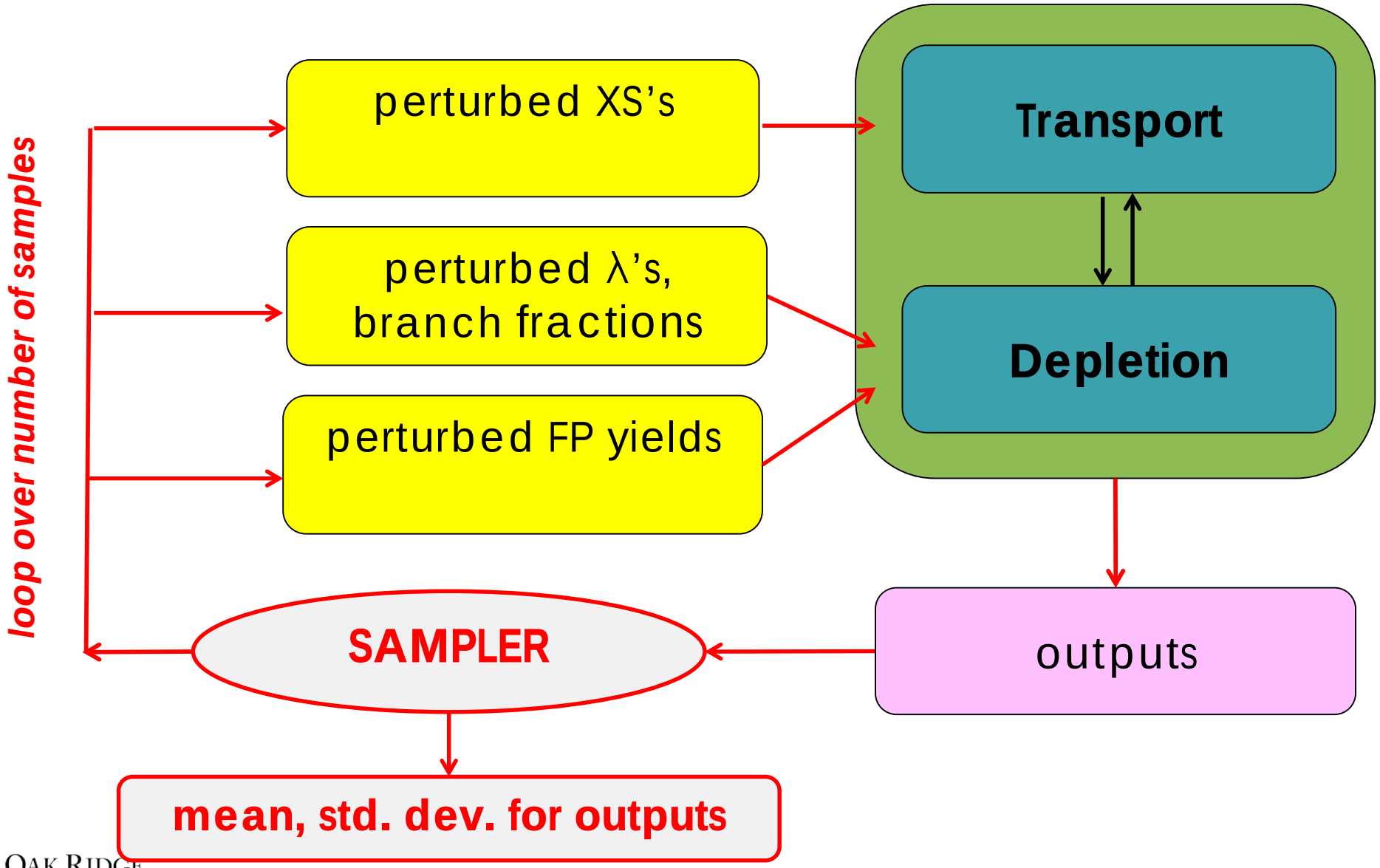
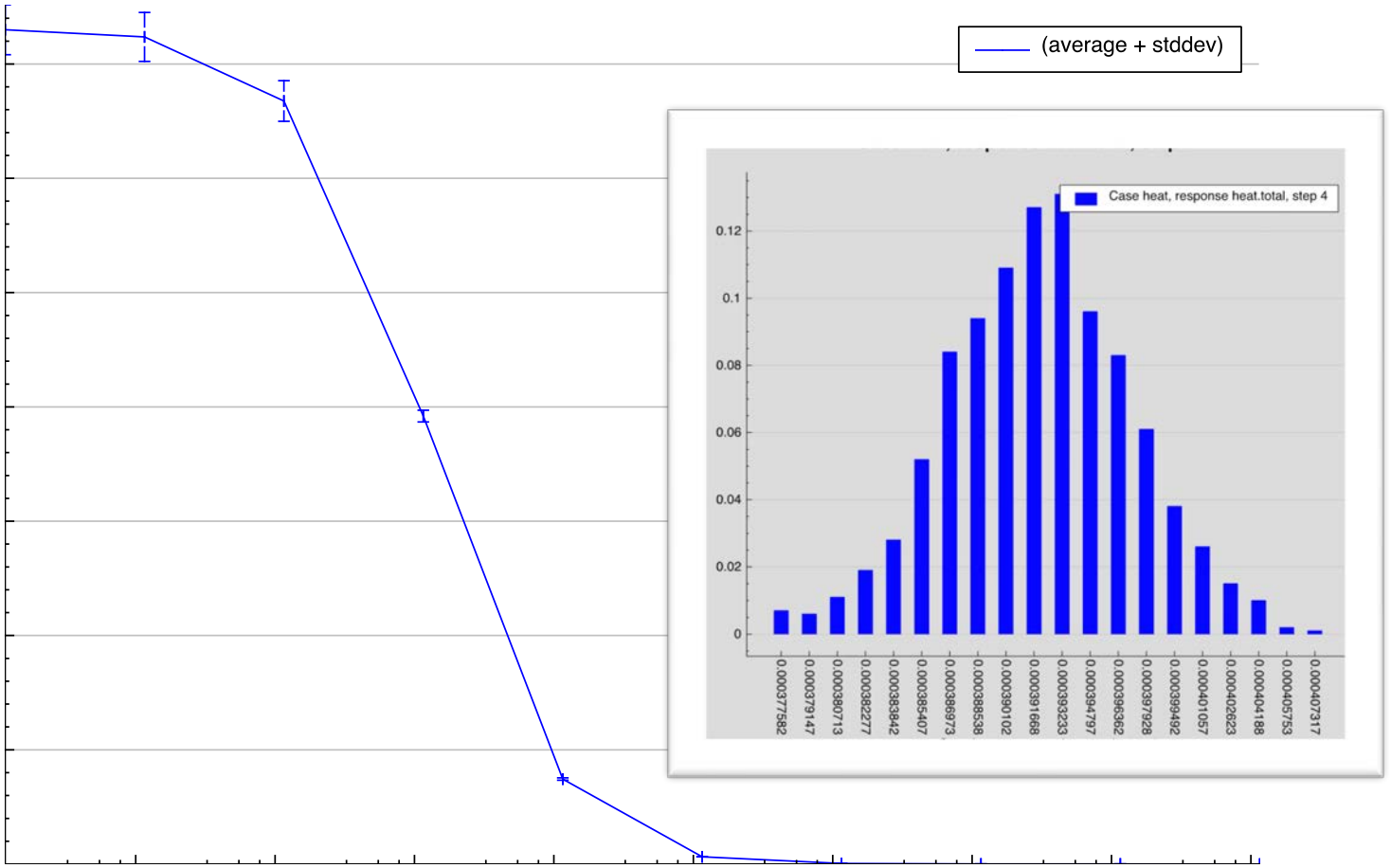
UQ Calculations with Coupled Transport/Depletion

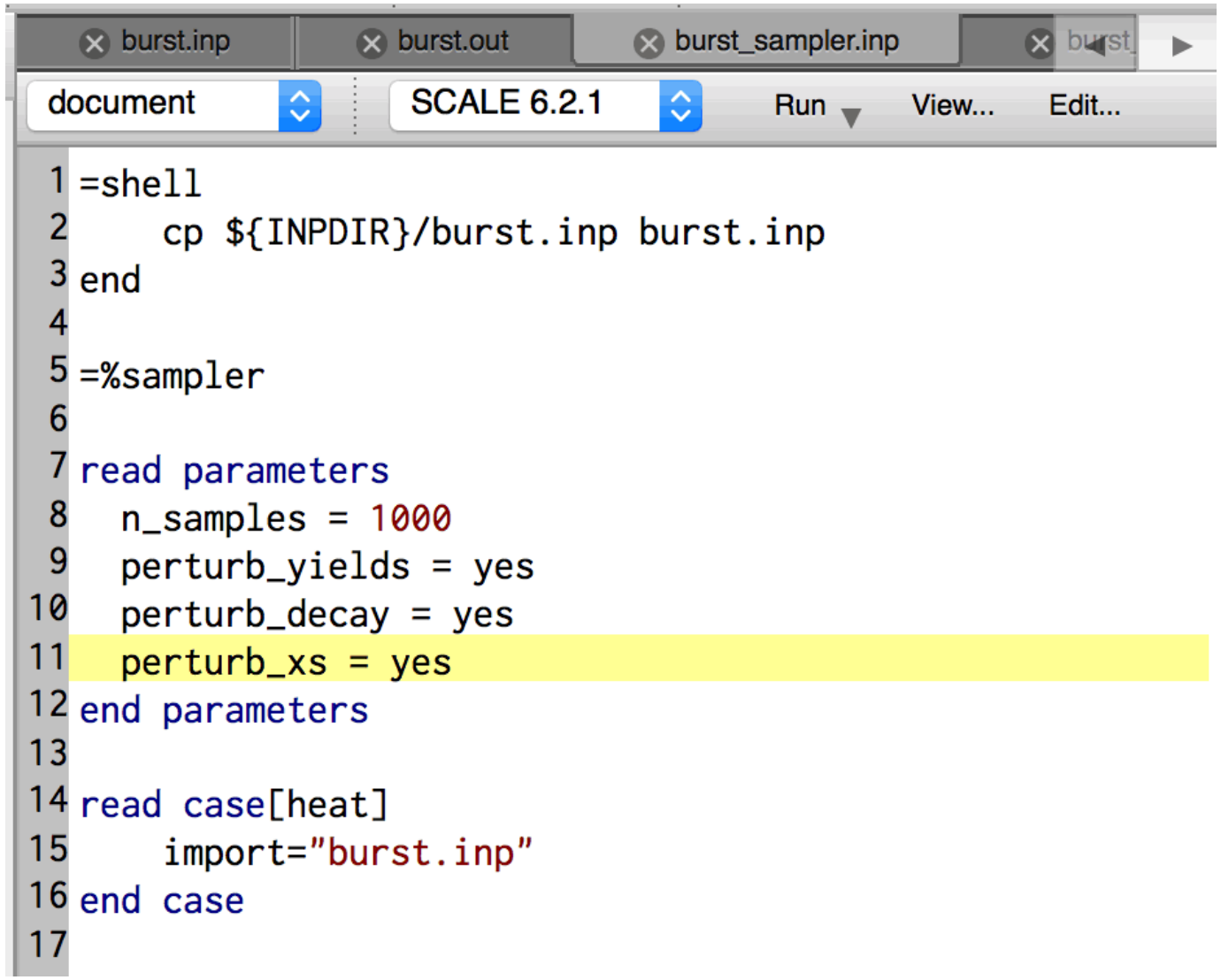


U-235 Fission Burst
with FP Yield and Decay Data Uncertainties




```
'generate ORIGEN f33 library
=couple
Fission Yield Library

0$$ a3 80 21 0 33 e
1$$ a2 1 a4 1 a18 238 e 1t
9**
 13z 1.25 0.3 223z
2t
done
end

'ORIGEN calculation
=origen
case{
    lib{ file="ft33f001" }
    time{
        t=[ 1e-6 1e-5 1e-4 1e-3
            1e-2 1e-1 1    1e1
            1e2  1e3  1e4  1e5 1e6]
        units=SECONDS
    }
    flux=[4r 1.0e15 9r0]

    mat{
        iso[ u235=1 ]
        units=GRAMS
    }

    save{
        file="ft71f001"
        steps=ALL
    }
}
end

'post-process Watts
=opus
  time=seconds
  minposition=5
  units=watts
end
```

Nuclear Data Perturbations are Easy




```
read parameters
     n_samples       = 1000
     perturb_xs      = yes
     perturb_decay   = yes
     perturb_yields  = yes
end parameters
```

Notes

- only 1000 pre-calculated nuclear data perturbations available
- with nuclear data-only import="x.inp" makes sampler "case" trivial

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Sampler Overview
Input Parameter Uncertainty

Perturbation of Compositions and Geometry

- Can be used to quantify uncertainties, or to calculate correlation coefficients
- User selects appropriate distribution and parameters for sampling composition and geometry inputs
  - Available distributions: uniform, normal *(can be truncated)*, and beta
- Simple mathematical expressions can also be used to calculate perturbed inputs
- Perturbations applied to specified cases allowing identical realizations for shared characteristics
- Case input can be included in Sampler input or modified via the SCALE Input Retrieval Engine (SIREN)

Two Options for Declaring Input Parameters are Uncertain

- **Easy way → PLACEHOLDERS**
  Substitute number in input with #{variable_name} and define variable

Polaris Composition

```
comp c_u    : ENRU 3.5
comp c_uox  : FORM
              c_u=1.0 o=2.0
comp c_fuel : WT
              c_uox=95.0 GD2O3=5.0
```

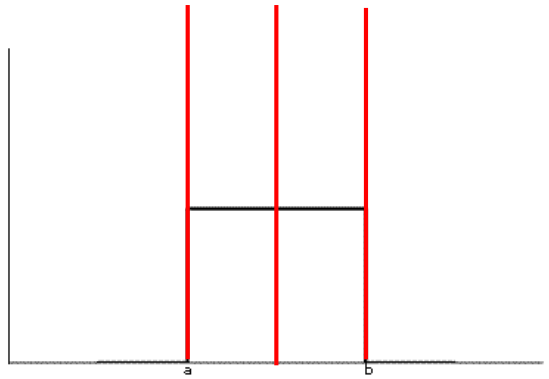
With Placeholder Variables

```
comp c_u    : ENRU #{enr}
comp c_uox  : FORM
              c_u=1.0 o=#{stoich}
comp c_fuel : WT
              c_uox=#{uox} GD2O3=#{gd}
```

- **Hard way → SIREN**
  Declare an uncertain variable with a special "XPATH" like /path/to/variable *(will cover later)*

Variable Blocks – Uniform Distribution

```
read variable[enr]
   distribution=uniform
   value=3.5
   min=3.45
   max=3.55
end variable
```



required
optional

```
read variable[ID]
  distribution=uniform
  minimum=a
  maximum=b
  value=c
  cases=c1 end
end variable
```

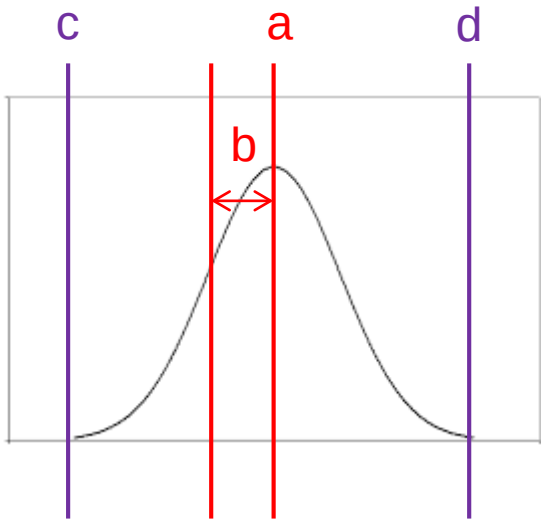
NOTE: value c will be unperturbed value

Polaris Example

```
comp c_u     : UO2 #{enr}
comp c_uox   : FORM
               c_u=1.0 o=#{stoich}
comp c_fuel  : WT
               c_uox=#{uox} GD2O3=#{gd}
```

Variable Blocks – Normal Distribution

```
read variable[stoich]
   distribution=normal
   value=2.00
   stddev=0.01
   min=1.98
   max=2.02
end variable
```



Polaris Example

```
comp c_u     : ENRU #{enr}
comp c_uox   : FORM
               c_u=1.0 o=#{stoich}
comp c_fuel  : WT
               c_uox=#{uox} GD2O3=#{gd}
```

required
optional

```
read variable[ID]
  distribution=normal
  value=a
  stddev=b
  minimum=c
  maximum=d
  cases=c1 end
end variable
```

NOTE: value c, d are used to truncate

Variable Blocks – Expression

```
read variable[uox]
   distribution=expression
   expression="100.0 - gd"
end variable
```

```
read variable[gd]
   distribution=normal
   value=5.0
   stddev=0.1
end variable
```

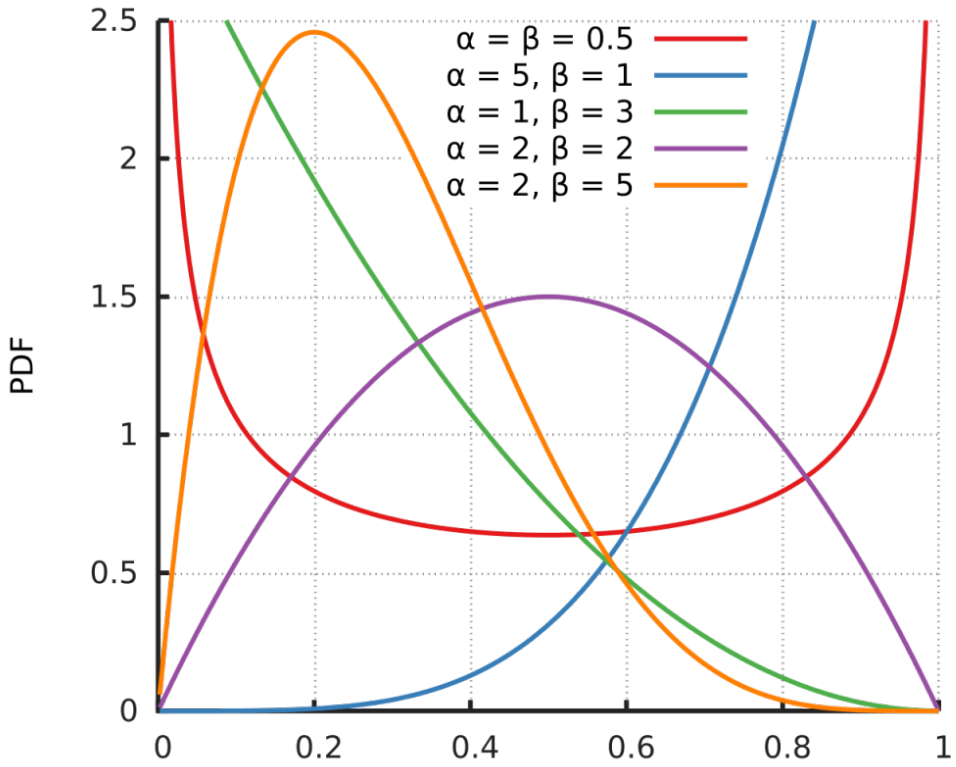
Polaris Example

```
comp c_u    : ENRU #{enr}
comp c_uox  : FORM
              c_u=1.0 o=#{stoich}
comp c_fuel : WT
              c_uox=#{uox} GD2O3=#{gd}
```

Variable Blocks – Beta Distribution

```
read variable[r_f]
    distribution=beta
    value=0.4096
    minimum=0.4090
    maximum=0.4100
    beta_a=2
    beta_b=1
end variable
```

```
pin 1 : #{r_f} 0.418 0.475
      : FUEL   GAP   CLAD
```

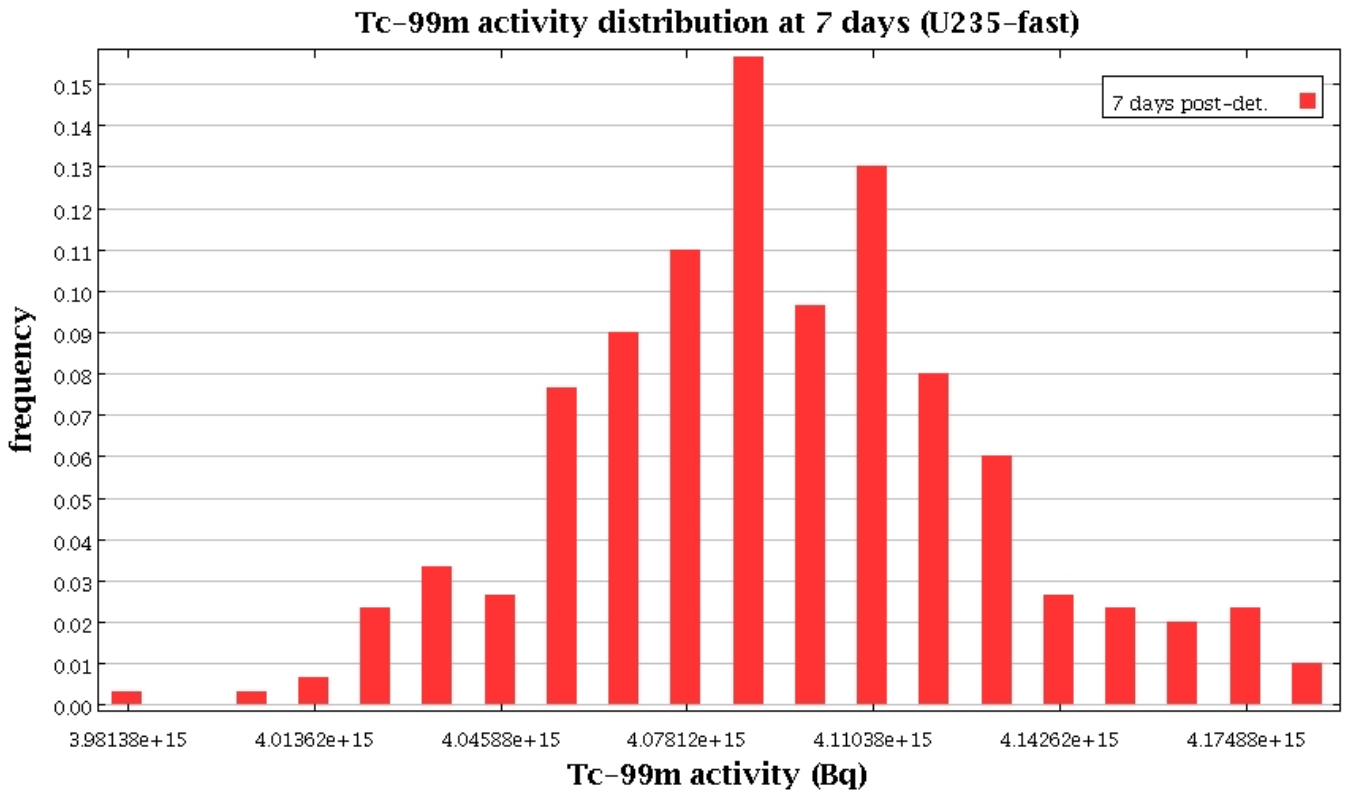



```
read variable[ID]
  distribution=beta
  beta_a=α
  beta_b=β
  minimum=c
  maximum=d
  value=e
  cases= c1 end
end variable
```

NOTE: α, β, c, d define distribution and value e will be used as unperturbed value

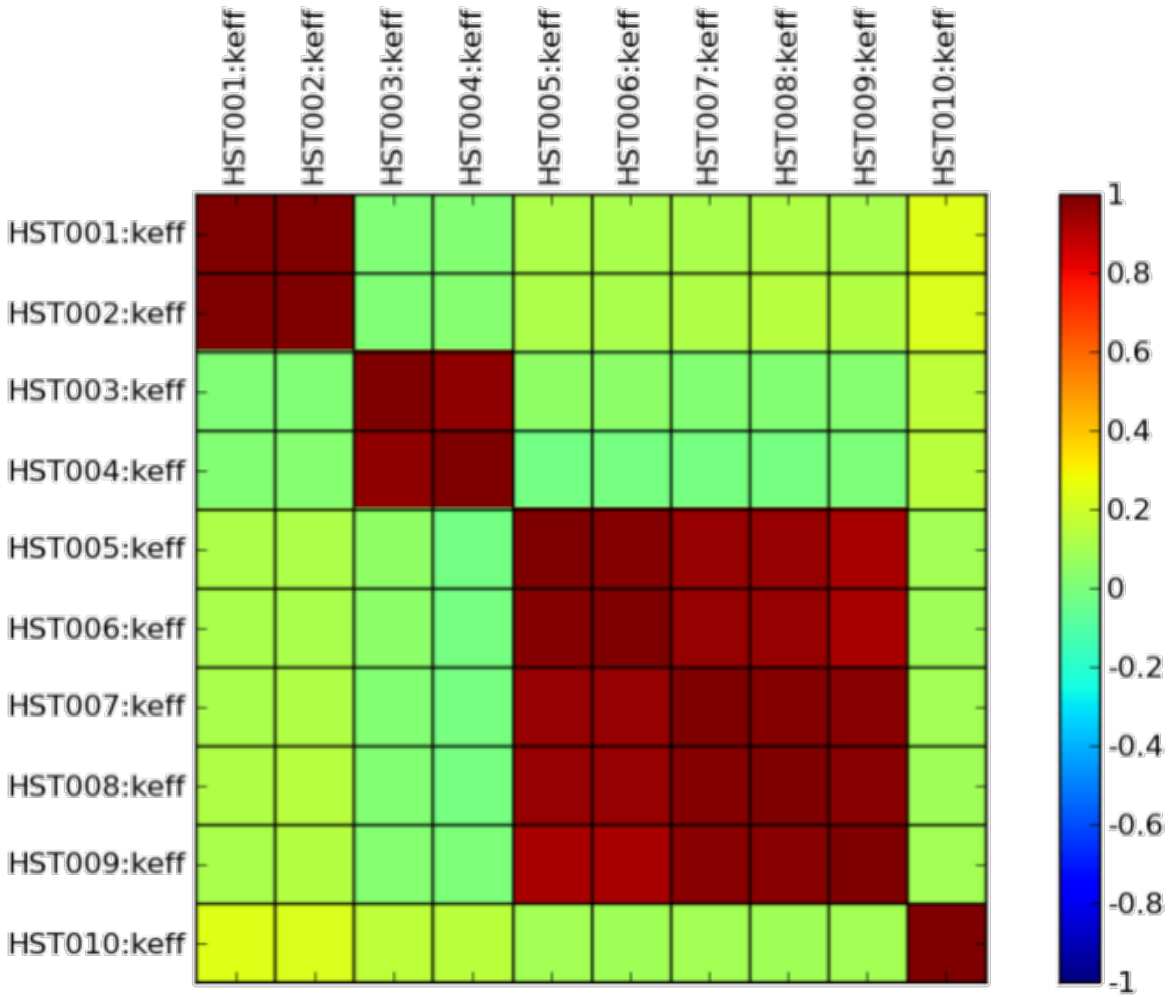
Post-processing

- **Creates response tables as requested**
  - Average values, correlations, covariances, etc.
- **Correlations created for multiple cases** (e.g. critical experimental correlations)
- **PTP plot files**
  - Running averages, histograms, scatter plots



Critical Experiment Correlations

- Correlations of responses are automatically computed
- For example, can calculate correlations between k-eff of various critical benchmark configurations, e.g.
  - two experiments use the same fuel rods or same reflector and this should be taken into account
- For validation calculations, should preferentially choose one case from each ***correlated*** block

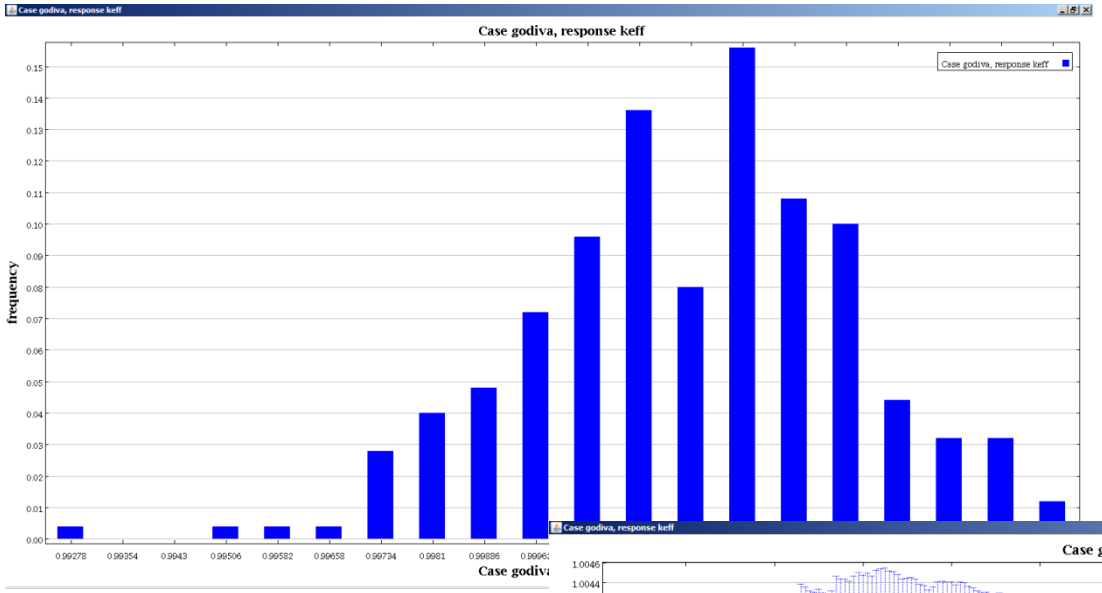


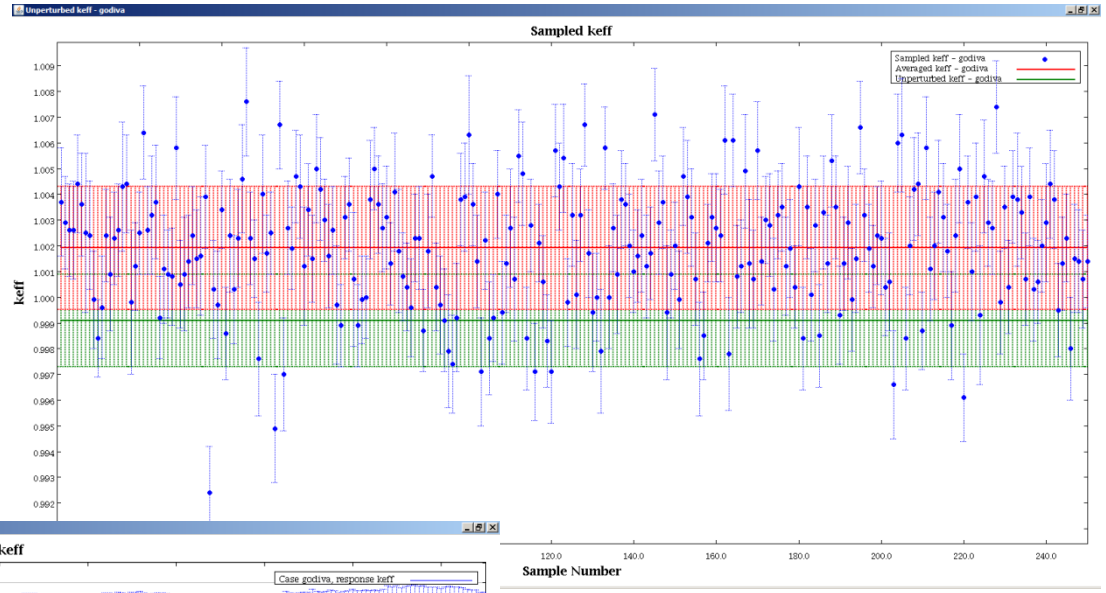
Critical Experimental Correlations

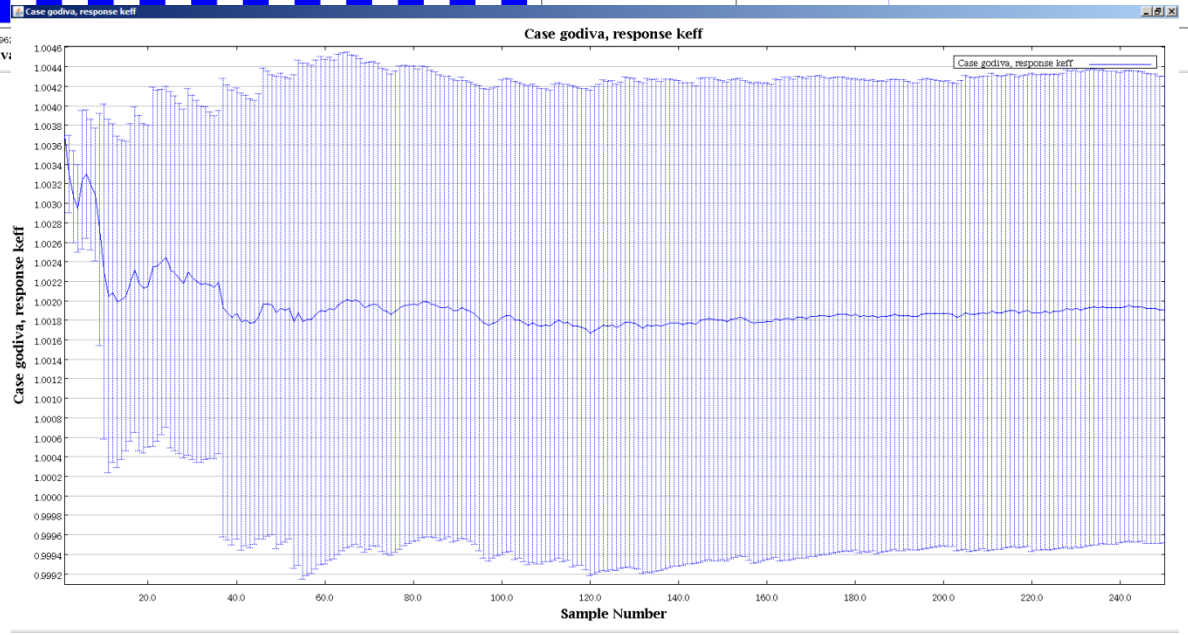
UAM LWR Benchmark

- OECD/NEA benchmark for **U**ncertainty **A**nalysis in **M**odeling (UAM) of LWR core calculations
- Propagation of nuclear data and manufacturing uncertainties, through core calculations, to quantify uncertainties in core responses (e.g. nodal power and burnup distributions)
- Phase I – BOC pin, lattice, core neutronics
- Phase II – lattice physics depletion
- Phase III – coupled TH/neutronics full-core steady-state and transient analysis
- Each phase contains specifications for
  - TMI
  - Peach Bottom
  - VVER
  - PWR LEU/MOX core (aka Gen III)

Plot Examples







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Summary

- Sampler is a wrapper for uncertainty quantification
  - In any (multi-group) SCALE calculation
- Leading-edge nuclear data uncertainty
  - Fission product yield uncertainty
  - Decay data uncertainty
  - Multi-group cross section uncertainty
- Input parameter perturbations
  - Assign distributions to variables
  - Use variables in placeholders #{myvariable}
  - Or use SIREN to avoid copy/paste input

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Sampler Example
Decay Uncertainty Propagation

Uncertainty in Rn-222 Activity

Problem

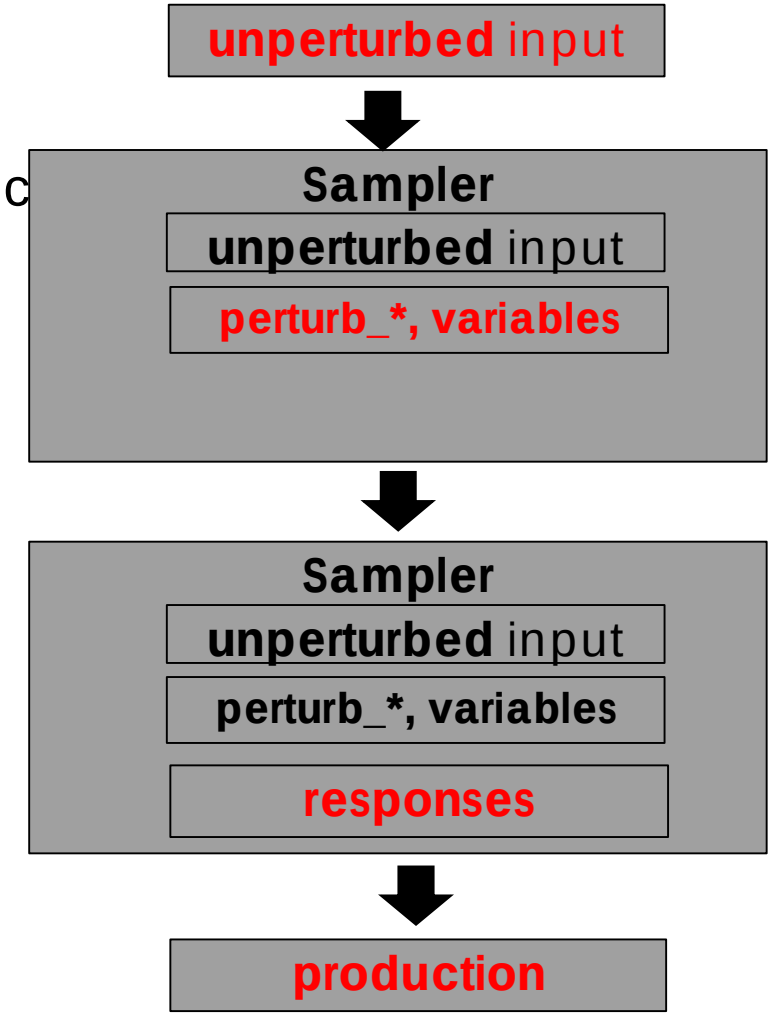
Decay 1 mol of U-238 for 1 billion years

Goals

- Determine uncertainty in Radon-222 (^{222}Rn) activity
- Gain familiarity with
  - the Sampler process
  - Sampler directories and results files
- Discuss limits of decay uncertainty calculation

The Sampler Process

1. Create the "unperturbed" SCALE input
   - be certain that it **works**!
   - make sure it produces the outputs you want (f71, plt, etc
2. Wrap it in Sampler
   - use `n_samples=2`, `force_run=yes`, `run_cases=no`
   - verify you have the desired `perturb_*=yes`
   - verify variables are sampled correctly
3. Verify responses
   - use `n_samples=2`, `force_run=no`, `run_cases=yes`
   - NOTE: **greps** almost always take a few iterations
4. Start "production" run
   - `n_samples=100` (or more)!

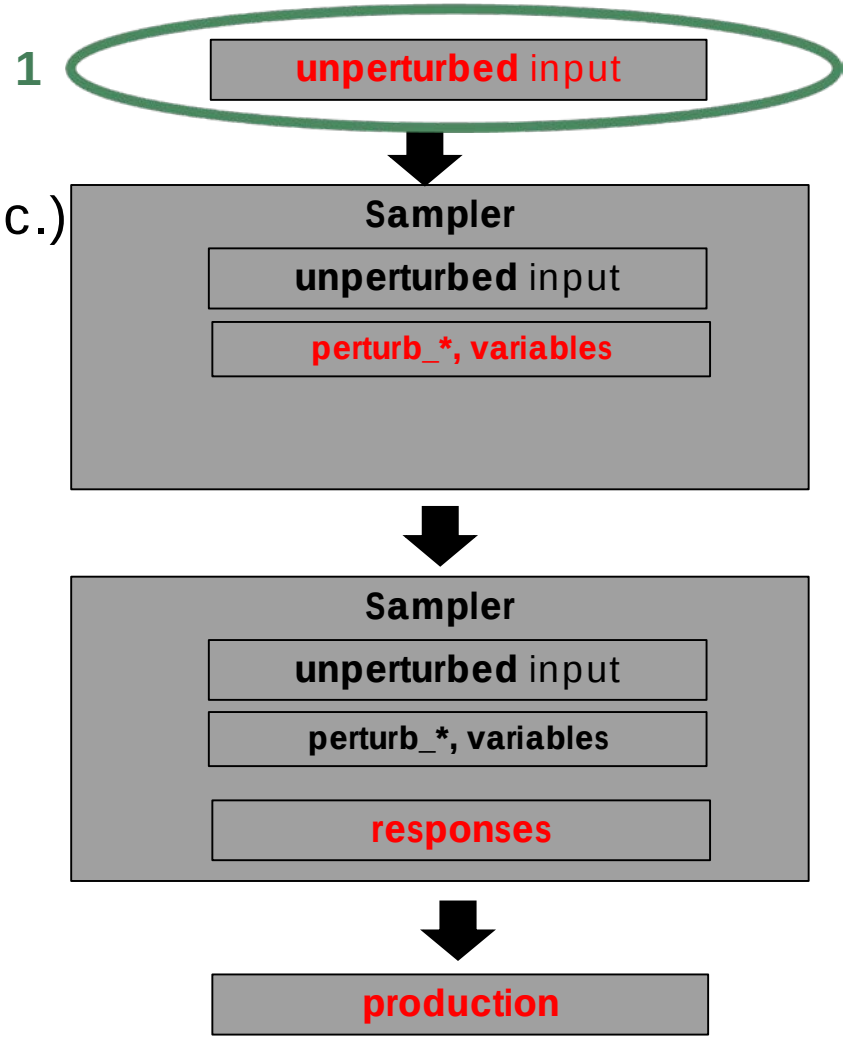


The Sampler Process: Step 1

Create the "unperturbed" SCALE input

- **be certain that it works!**
- make sure it produces the outputs you want (f71, plt, etc.)

```
'rn222.inp decays 1 mol u238 for 1e9 years
'  produces output: f71 (moles) and plt (curies)
=origen
case{
    title="U238 decay chain"
    lib{ file="end7dec" }
    time{ units=years t=[3L 1e1 1e9] }
    mat{ iso=[u238=1.0] }
    print{ nuc{ units=[moles curies] } }
    save=yes
}
end
=opus
library="end7dec"
units=curies
end
```



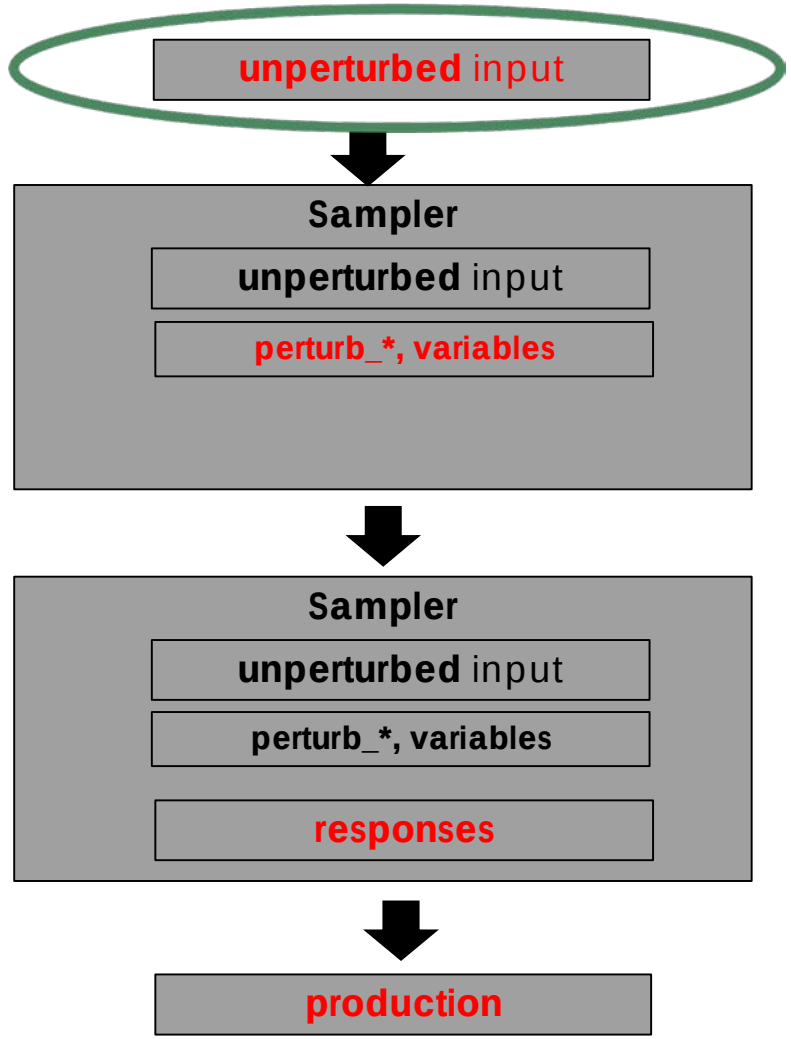
The Sampler Process: Step 1

Create the "unperturbed" SCALE input

- be certain that it **works**!
- **make sure it produces the outputs you want (f71, plt, etc.)**

.out file

```
=================================================================================================================================
=   Nuclide concentrations in curies for case '1' (#1/1)                                                                        =
=   U238 decay chain                                                                                                            =
---------------------------------------------------------------------------------------------------------------------------------
  (relative cutoff; integral of concentrations over time >   1.00E-06 % of integral of all concentrations over time)
.
               0.0E+00y    1.0E+01y    1.0E+03y    1.0E+05y    1.0E+07y    1.0E+09y
  tl-206       0.0000E+00  1.4583E-23  1.8040E-16  9.4921E-12  1.0702E-10  9.1781E-11
  tl-210       0.0000E+00  3.1186E-20  2.8293E-14  1.4887E-09  1.6784E-08  1.4394E-08
  pb-210       0.0000E+00  1.0891E-17  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  pb-214       0.0000E+00  1.4848E-16  1.3470E-10  7.0875E-06  7.9908E-05  6.8531E-05
  bi-210       0.0000E+00  1.0891E-17  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  bi-214       0.0000E+00  1.4850E-16  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  po-210       0.0000E+00  1.0891E-17  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  po-214       0.0000E+00  1.4847E-16  1.3470E-10  7.0875E-06  7.9907E-05  6.8530E-05
  po-218       0.0000E+00  1.4851E-16  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  at-218       0.0000E+00  2.9701E-20  2.6945E-14  1.4178E-09  1.5985E-08  1.3709E-08
  rn-218       0.0000E+00  2.9701E-23  2.6945E-17  1.4178E-12  1.5985E-11  1.3709E-11
  rn-222       0.0000E+00  1.4851E-16  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  ra-226       0.0000E+00  1.4851E-16  1.3473E-10  7.0890E-06  7.9924E-05  6.8544E-05
  th-230       0.0000E+00  1.0294E-13  1.0351E-09  7.0889E-06  7.9924E-05  6.8544E-05
  th-234       0.0000E+00  8.0048E-05  8.0048E-05  8.0047E-05  7.9924E-05  6.8544E-05
  pa-234m      0.0000E+00  8.0048E-05  8.0048E-05  8.0047E-05  7.9924E-05  6.8544E-05
  pa-234       0.0000E+00  1.2808E-07  1.2808E-07  1.2808E-07  1.2788E-07  1.0967E-07
  u-234        0.0000E+00  2.2388E-09  2.2569E-07  1.9692E-05  7.9924E-05  6.8544E-05
  u-238        8.0048E-05  8.0048E-05  8.0048E-05  8.0047E-05  7.9924E-05  6.8544E-05
------------
  totals      8.0048E-05  2.4028E-04  2.4050E-04  3.3085E-04  1.1191E-03  9.5973E-04
=================================================================================================================================
```

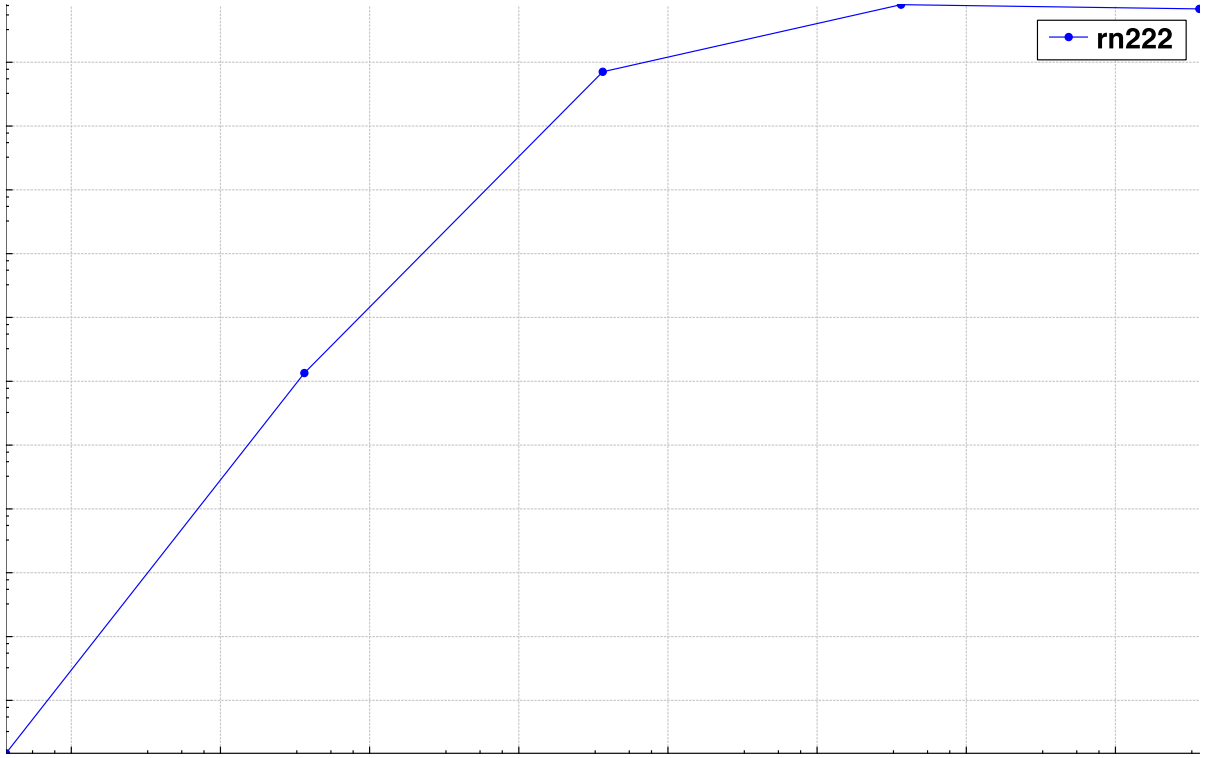


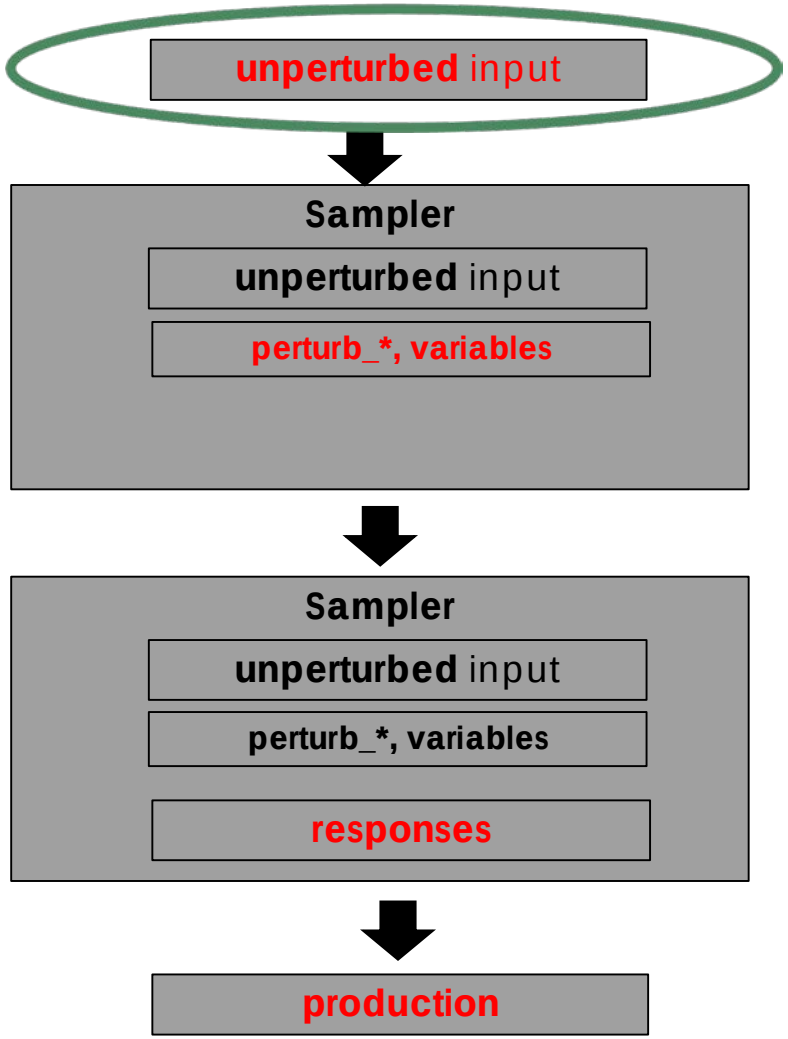
The Sampler Process: Step 1

Create the "unperturbed" SCALE input

- be certain that it **works**!
- **make sure it produces the outputs you want (f71, plt, etc.)**

.plt file viewed in Fulcrum





The Sampler Process: Step 2

Wrap it in Sampler

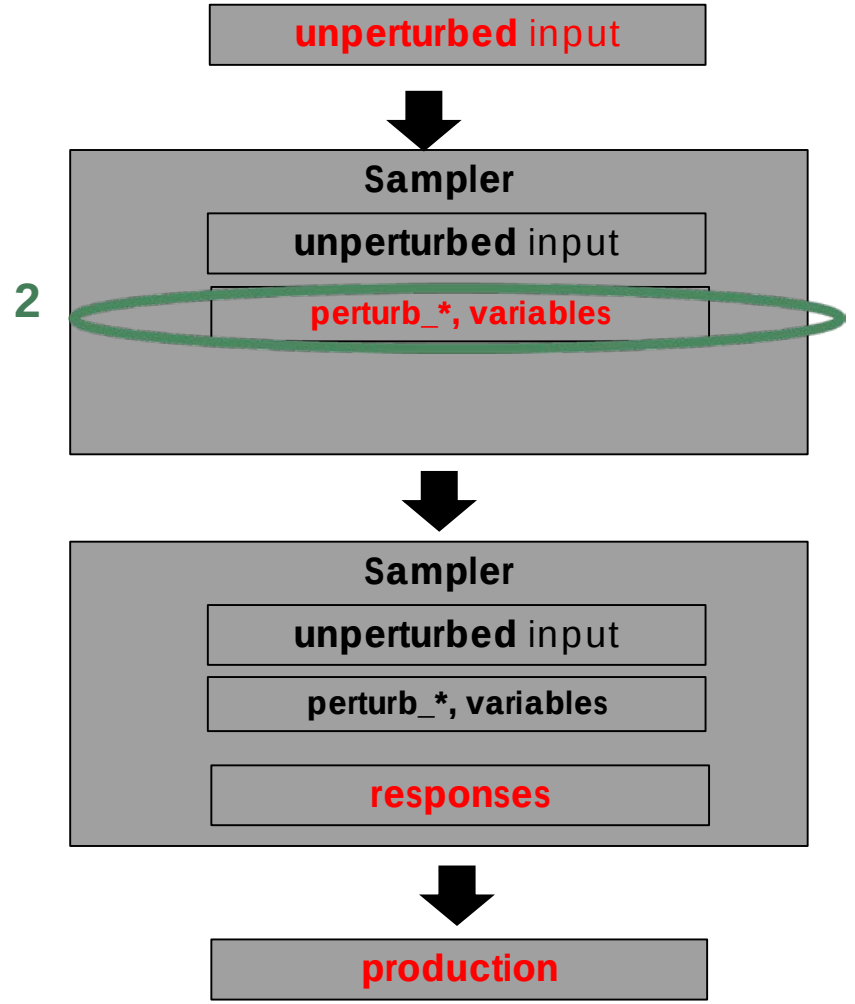
- use `n_samples=2`, `force_run=yes`, `run_cases=no`
- verify you have the desired `perturb_*=yes`
- verify variables are sampled correctly

```
'rn222_uq.starter.inp is a basic sampler template for
'an ORIGEN followed by an OPUS
=sampler

read parameters
'n_samples=100
'force_run=no
'run_cases=yes
'perturb_decay=yes
'perturb_yields=yes
'perturb_xs=yes
'perturb_geometry=yes
end parameters

read case[c1]
sequence{PASTE_ORIGEN}sequence
sequence{PASTE_OPUS}sequence
end case

end
```



The Sampler Process: Step 2

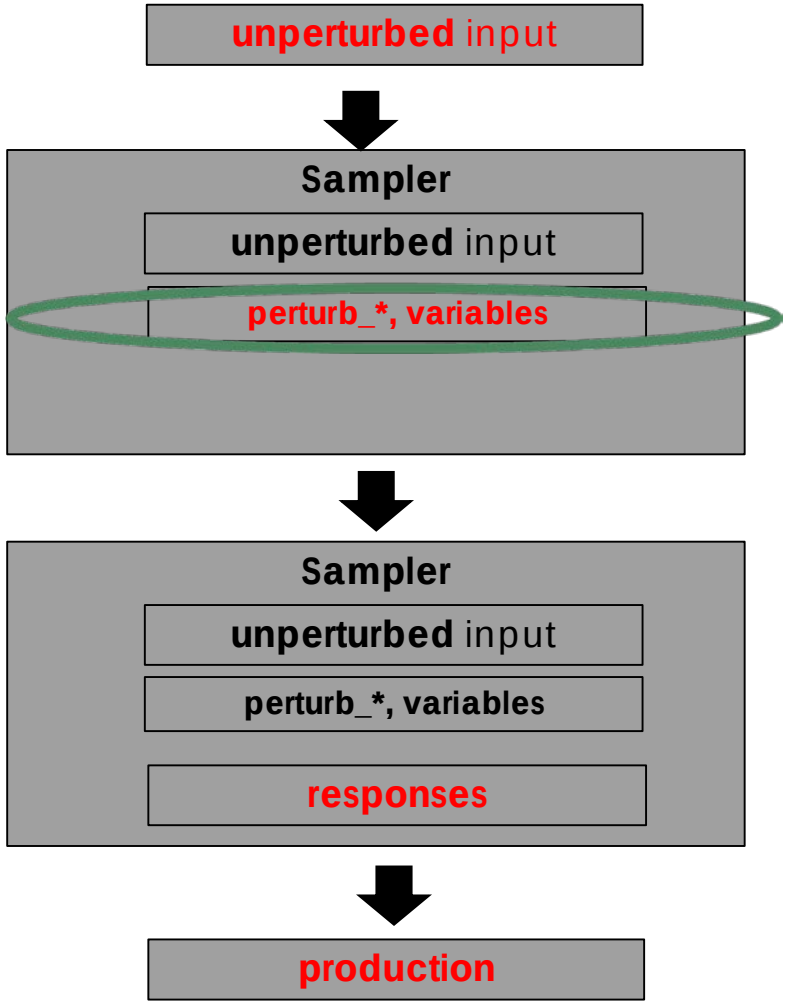
Wrap it in Sampler

- use `n_samples=2`, `force_run=yes`, `run_cases=no`
- verify you have the desired `perturb_*=yes`
- verify variables are sampled correctly

```
'rn222_uq.1.inp shows how to paste sequences in to a single case
=sampler
…
read case[c1]
sequence=origen
case{
    title="U238 decay chain"
    lib{ file="end7dec" }
    time{ units=years t=[3L 1e1 1e9] }
    mat{ iso=[u238=1.0] }
    print{ nuc{ units=[moles curies] } }
    save=yes
}
end sequence
sequence=opus
library="end7dec"
units=curies
end sequence
end case

end
```

2



The Sampler Process: Step 2

Wrap it in Sampler

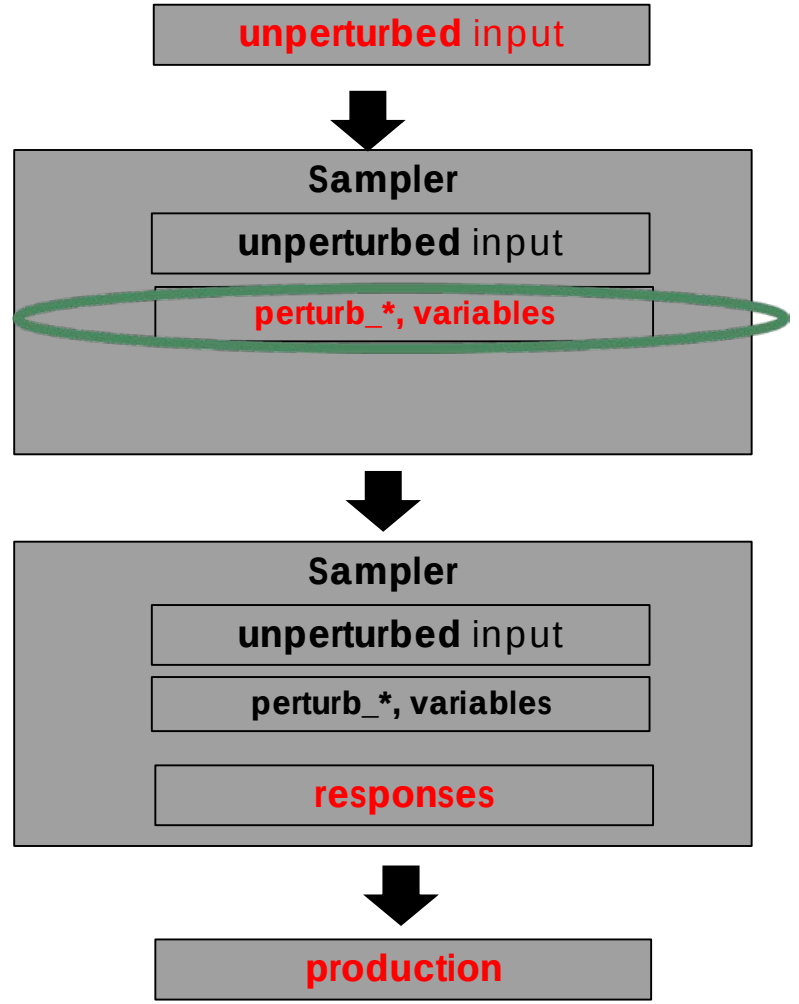
- **use n_samples=2, force_run=yes, run_cases=no**
- **verify you have the desired perturb_*=yes**
- verify variables are sampled correctly

```
'rn222_uq.2.inp shows options for variable testing
=sampler
read parameters
n_samples=2
force_run=yes
run_cases=no
perturb_decay=yes
'perturb_yields=yes
'perturb_xs=yes
'perturb_geometry=yes
end parameters

read case[c1]
…
end case

end
```

2



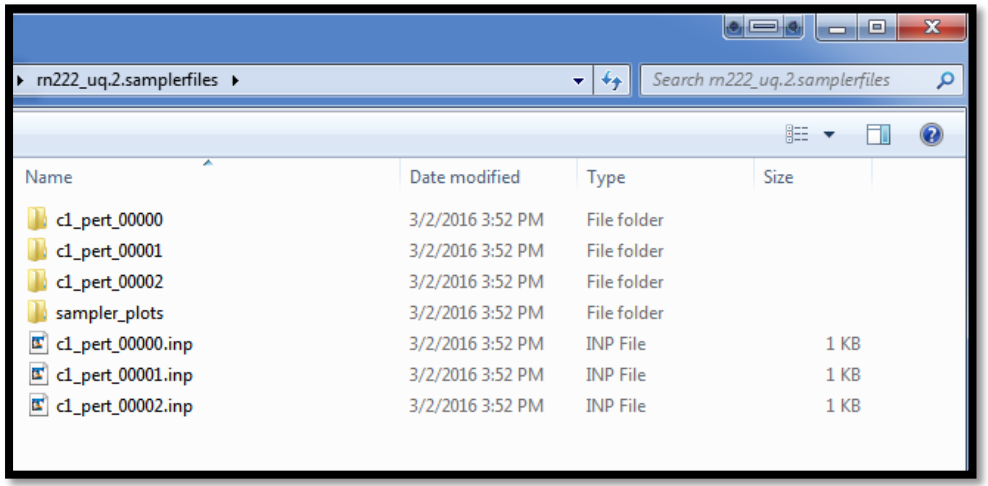
The Sampler Process: Step 2

Wrap it in Sampler

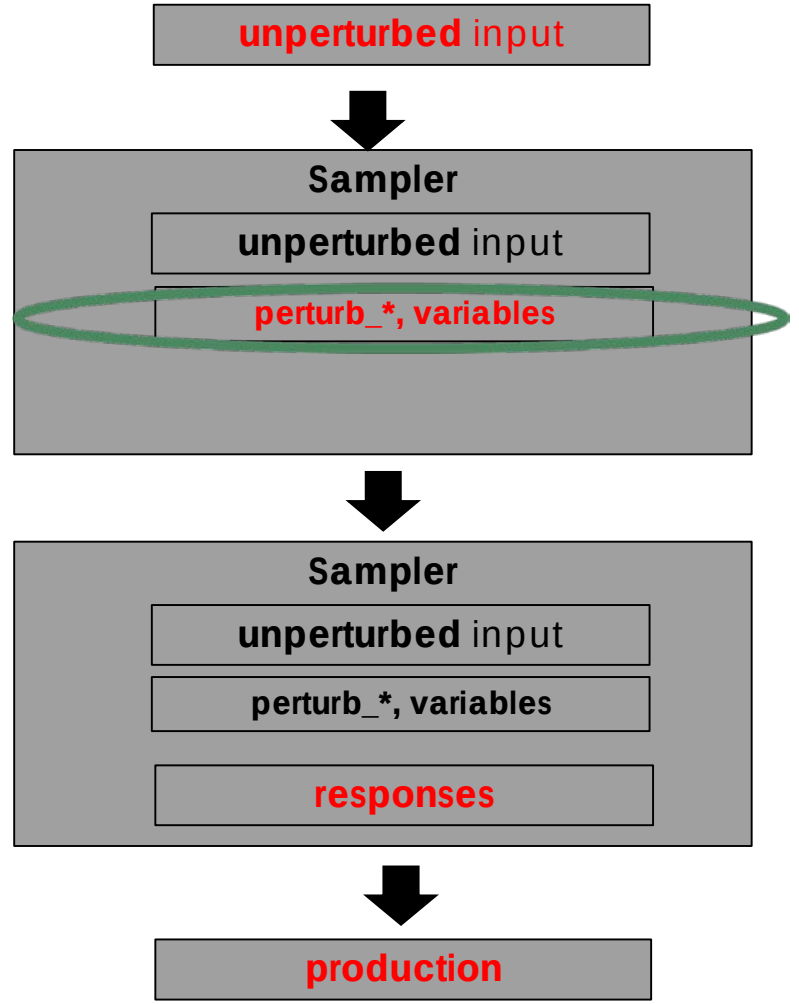
- use `n_samples=2`, `force_run=yes`, `run_cases=no`
- verify you have the desired `perturb_*=yes`
- verify variables are sampled correctly (don't need)

rn222_uq.2.out file

```
…
*********************************************************************************************************
*                                                Sampling                                               *
*********************************************************************************************************
      case |            run#           type          index           new?                  sample directory
-----------+-----------------------------------------------------------------------------------------------
        c1 |               1    unperturbed         #00000            yes rn222_uq.2.samplerfiles/c1_pert_00000
        c1 |               2         random         #00001            yes rn222_uq.2.samplerfiles/c1_pert_00001
        c1 |               3         random         #00002            yes rn222_uq.2.samplerfiles/c1_pert_00002
…
```



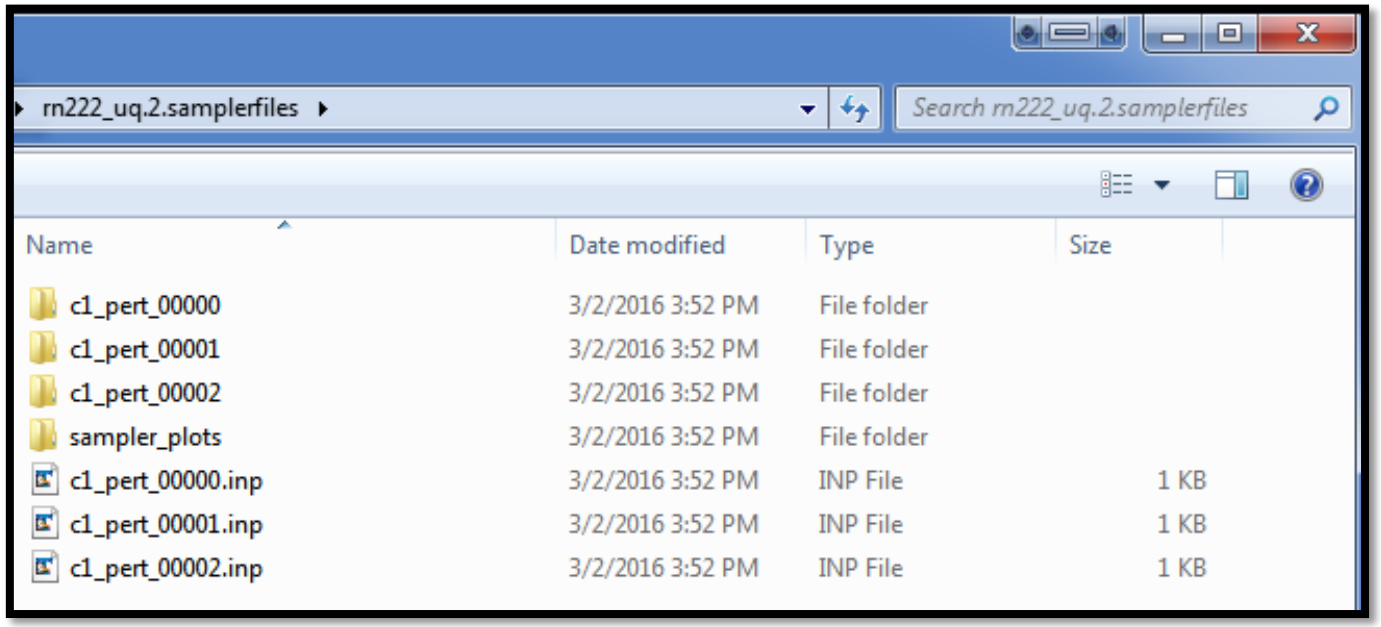
2



Sample Inputs

sample input naming scheme: <case_id>_pert_JJJJJ.inp

- c1 was <case_id>
- 5-digit perturbation index JJJJJ
  - 00000 for unperturbed
  - 00001 for first sample
  - 00002 for second
  - etc.



Sample Inputs Created by Sampler

compare c1_pert_00000.inp and c1_pert_00001.inp

```
=origen
case{
    title="U238 decay chain"
    lib{ file="end7dec" }
    time{ units=years t=[3L 1e1 1e9] }
    mat{ iso=[u238=1.0] }
    print{ nuc{ units=[moles curies] } }
    save=yes
}
end
=opus
library="end7dec"
units=curies
end
```

```
=shell
  ln -sf C:\SCALE-6.2\data\perturb\end7dec_0000  end7dec
end

=origen
case{
    title="U238 decay chain"
    lib{ file="end7dec" }
    time{ units=years t=[3L 1e1 1e9] }
    mat{ iso=[u238=1.0] }
    print{ nuc{ units=[moles curies] } }
    save=yes
}
end
=opus
library="end7dec"
units=curies
end
```

links in perturbed decay data

The Sampler Process: Step 3

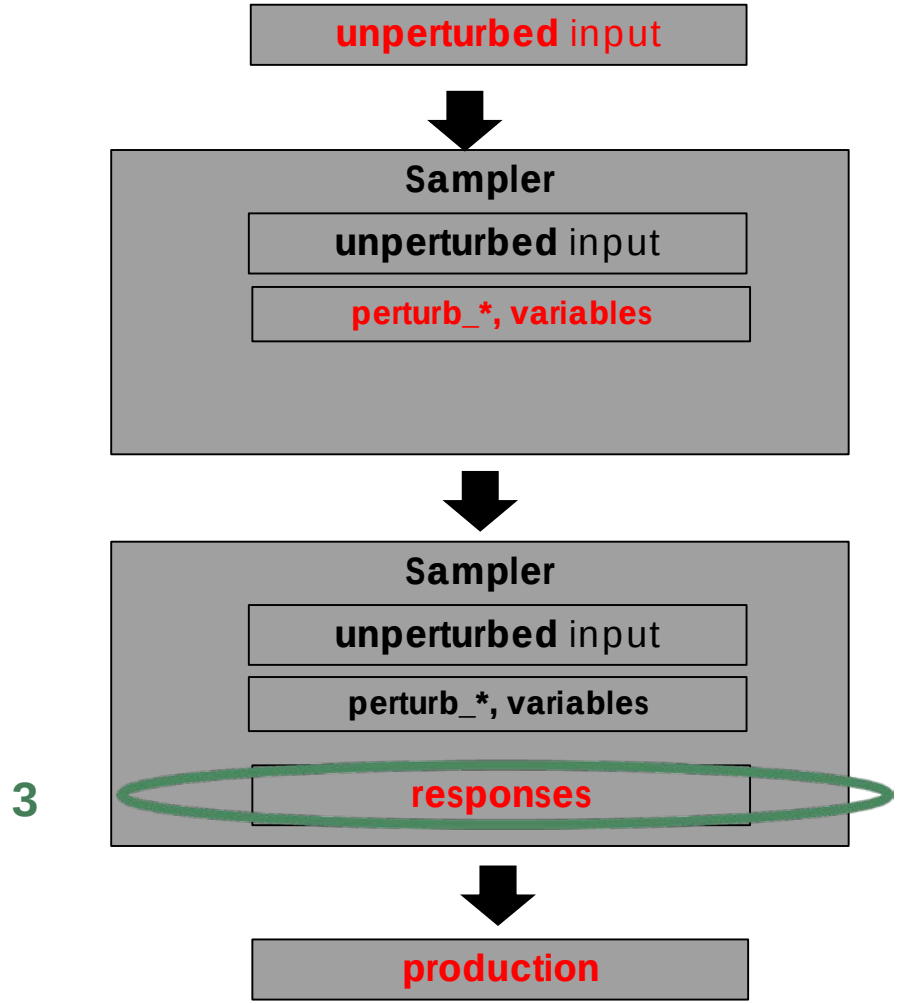
Verify responses

- use `n_samples=2`, `force_run=no`, `run_cases=yes`
- NOTE: **greps** almost always take a few iterations

```
'rn222_uq.3.inp shows options for response testing
=sampler
read parameters
n_samples=2
force_run=no
run_cases=yes
perturb_decay=yes
'perturb_yields=yes
'perturb_xs=yes
'perturb_geometry=yes
end parameters

read case[c1]
…
end case

end
```

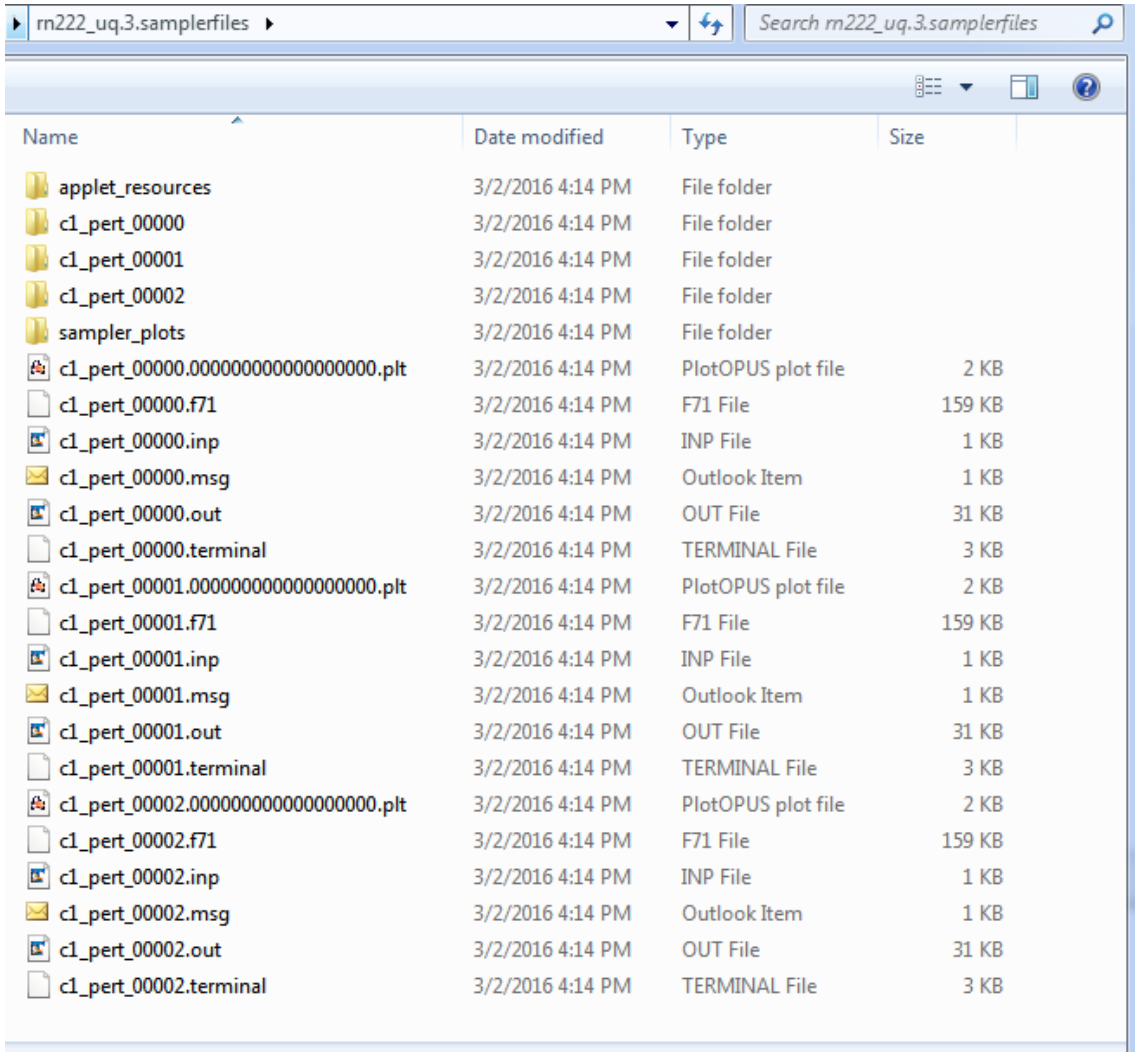


3

Sample Outputs Created by Sampler

now, when we run with **run_cases=yes**,
we get all the output files
we got for original case,
but now for all samples

but we need to define "responses" for Sampler to process the output



The Sampler Process: Step 3

Verify responses

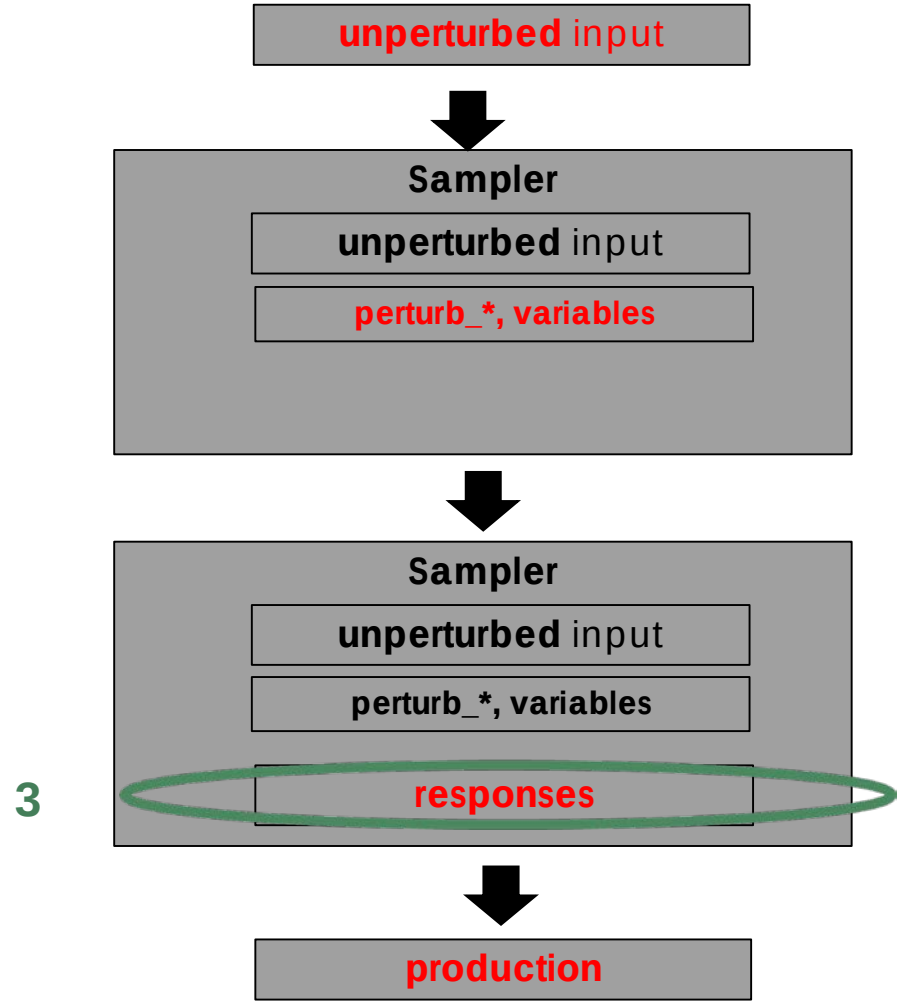
- use `n_samples=2`, `force_run=no`, `run_cases=yes`
- NOTE: **greps** almost always take a few iterations

```
'rn222_uq.3.inp shows options for response testing
=sampler
…

'process case/mixture 1 in ft71f001 file
read response[moles]
    type=origen_nuclides
    mixture=1
    nuclides=rn-222 end
end response


'process *0.plt file
read response[curies]
    type=opus_plt
    ndataset=0
    nuclides=rn-222 total end
end response
end
```

just a name



3

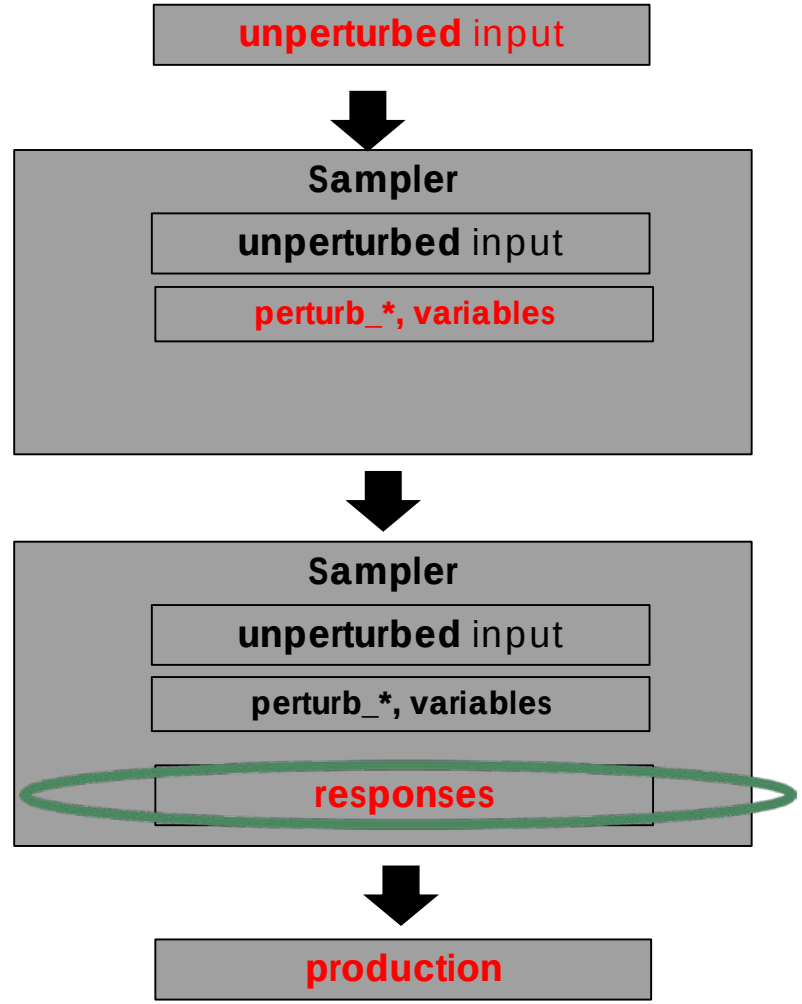
The Sampler Process: Step 3

Verify responses

- use `n_samples=2`, `force_run=no`, `run_cases=yes`
- NOTE: **greps** almost always take a few iterations

rn222_uq.3.out file

```
Average + std. deviation table 2 (c1:curies.rn222, c1:curies.total)
   time(d) |                          c1:curies.rn222                          c1:curies.total
-----------+-------------------------------------------------------------------------------------
         0 |       0.0000e+00 +/- 0.0000e+00 (0.00 %)      8.0010e-05 +/- 0.0000e+00 (0.00 %)
      3653 |       1.4780e-16 +/- 4.5461e-19 (0.31 %)      2.4077e-04 +/- 5.4365e-07 (0.23 %)
    365300 |       1.3413e-10 +/- 4.1899e-13 (0.31 %)      2.4100e-04 +/- 5.3541e-07 (0.22 %)
 3.653e+07 |       7.0763e-06 +/- 6.9442e-09 (0.10 %)      3.3117e-04 +/- 5.9067e-07 (0.18 %)
 3.653e+09 |       7.9947e-05 +/- 4.9216e-08 (0.06 %)      1.1197e-03 +/- 2.4944e-06 (0.22 %)
 3.653e+11 |       6.8557e-05 +/- 3.2998e-08 (0.05 %)      9.5987e-04 +/- 2.1203e-06 (0.22 %)
```

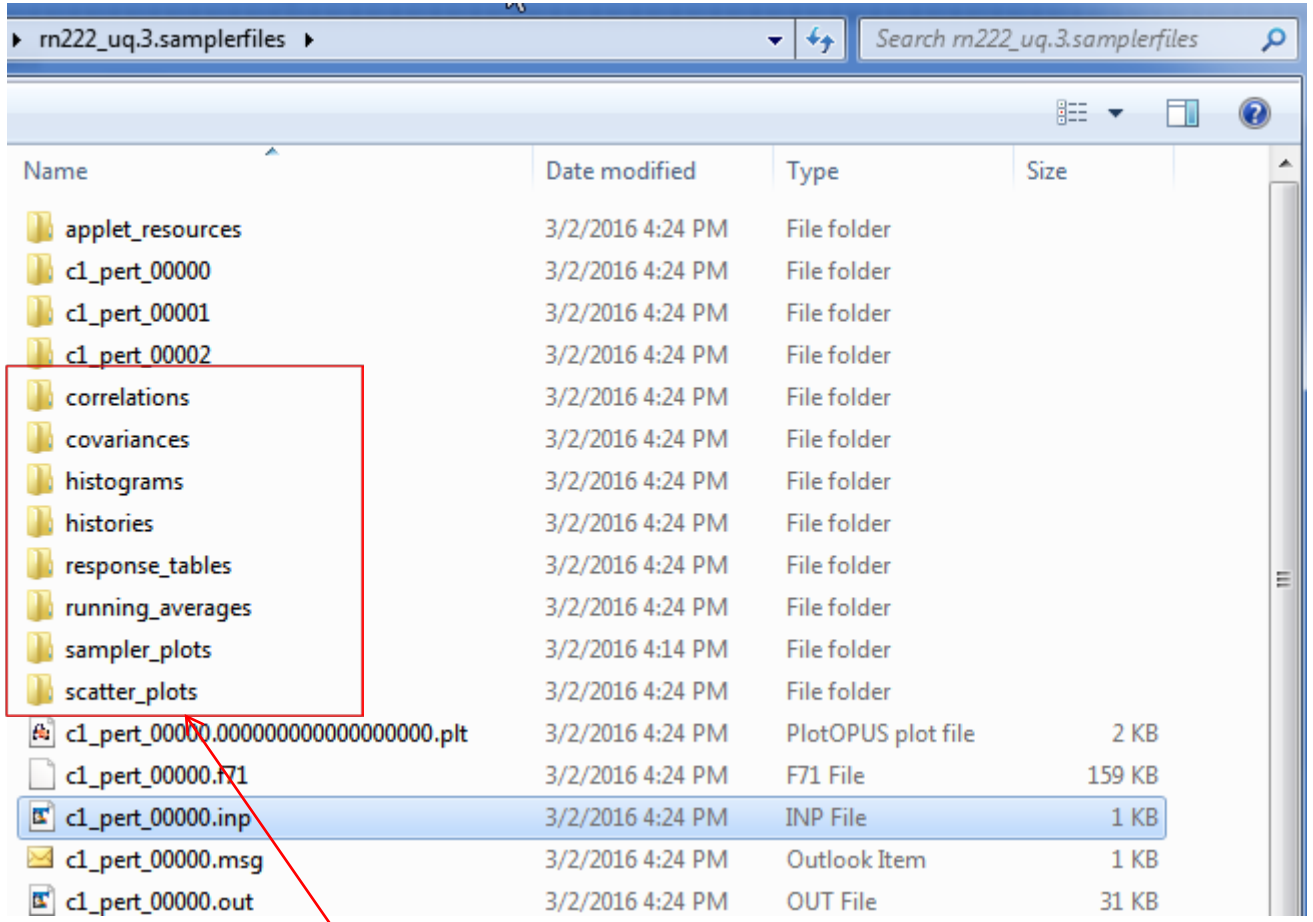


3

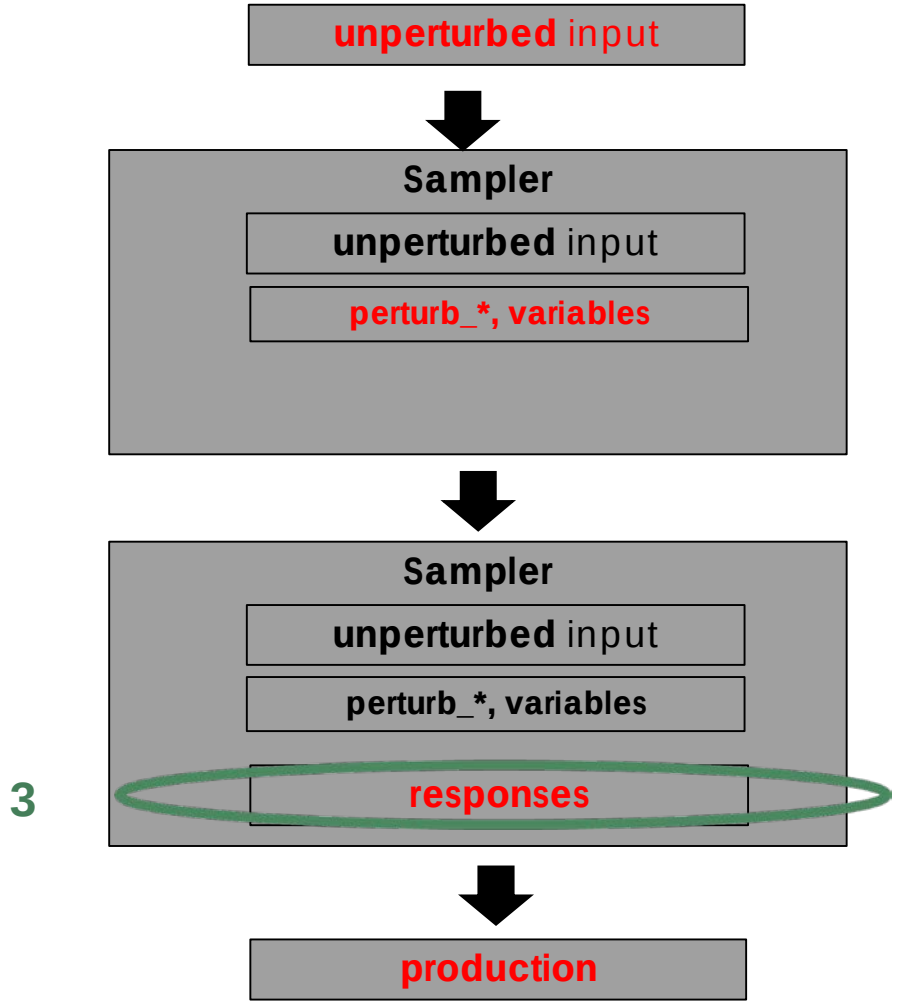
IMPORTANT: Do not attempt to interpret uncertainties, yet! There were only two samples!

The important thing is that we get some result and the process appears to be working as expected.

Sampler response files



new directories with response files!



3

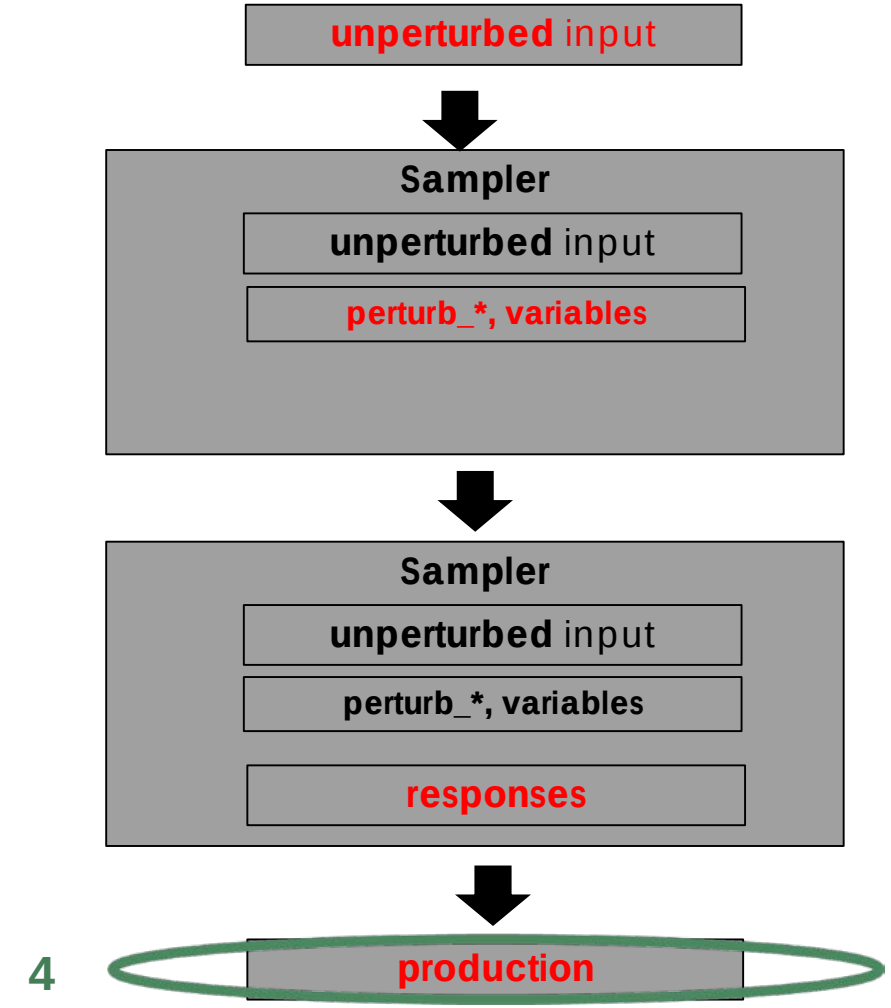
The Sampler Process: Step 4

Start "production" run !!!

- n_samples=100 (or more)!

```
'rn222_uq.final.inp has n_samples=100
=sampler
read parameters
n_samples=100
force_run=no
run_cases=yes
perturb_decay=yes
'perturb_yields=yes
'perturb_xs=yes
'perturb_geometry=yes
end parameters
…
end
```

should take ~3 minutes with 4 threads, i.e. invoke scale with `scalerte -I 4`

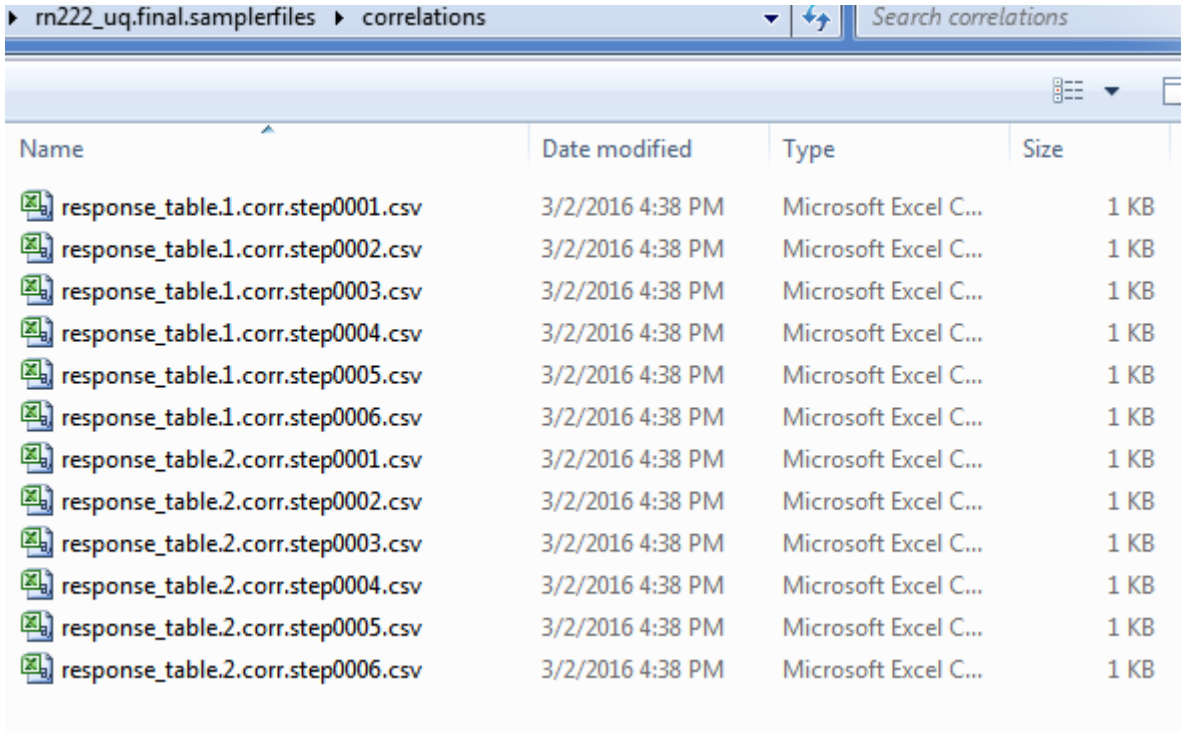


Now Analysis Begins…

a survey of directory contents

- **correlations/ covariances** – csv* sample correlation/sample covariance matrix
  - between each pair of defined responses in a response set
  - do not believe ρ≈0 unless you have many samples (n_samples ≈1000)
  - cannot compute if responses do not vary (e.g. for isotopics at time=0)

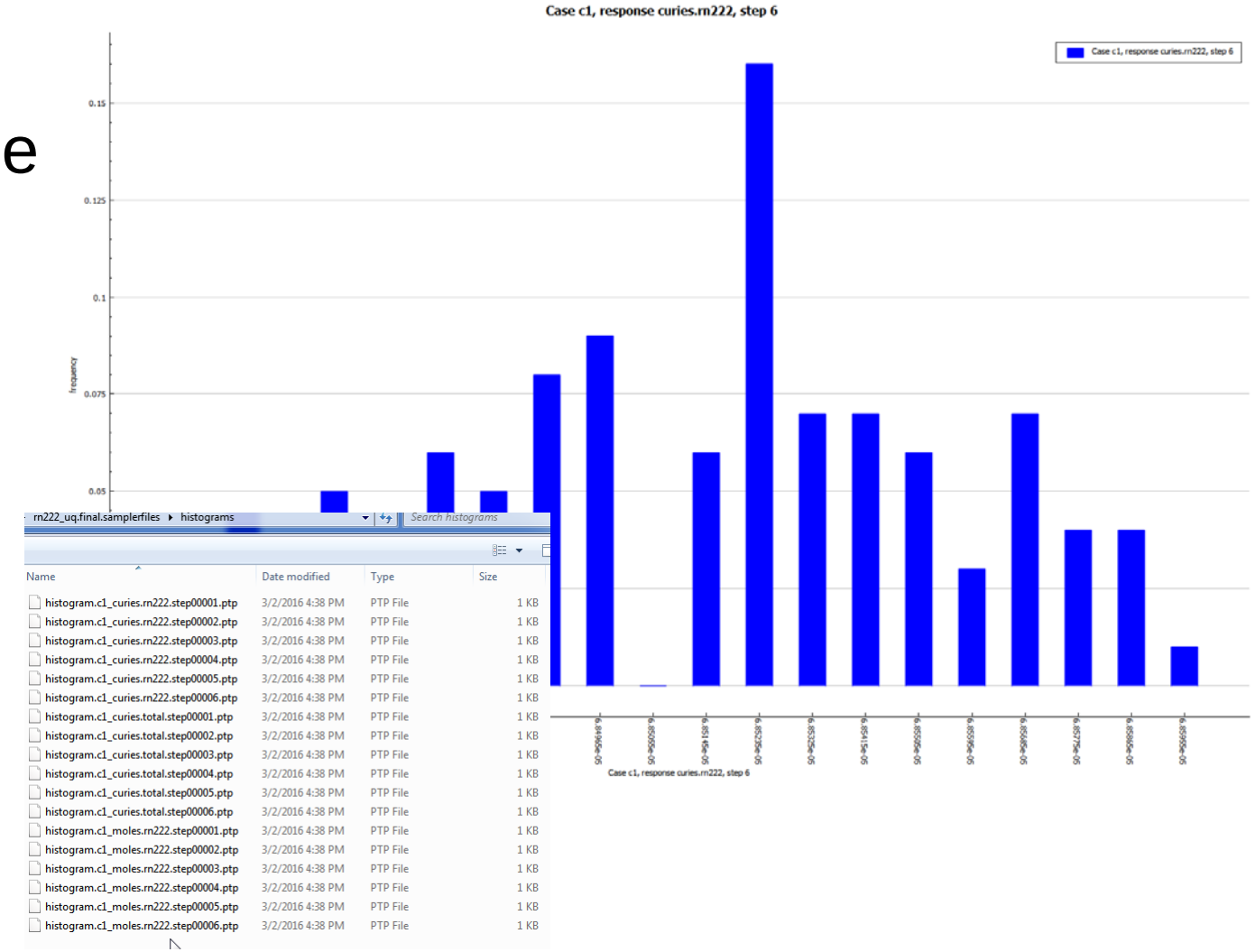
* our csv is **semi-colon (;) separated** not comma (,) separated to avoid international incidents where "," is used as the decimal
e.g. "3,14" instead of "3.14"



Now Analysis Begins…

a survey of directory contents

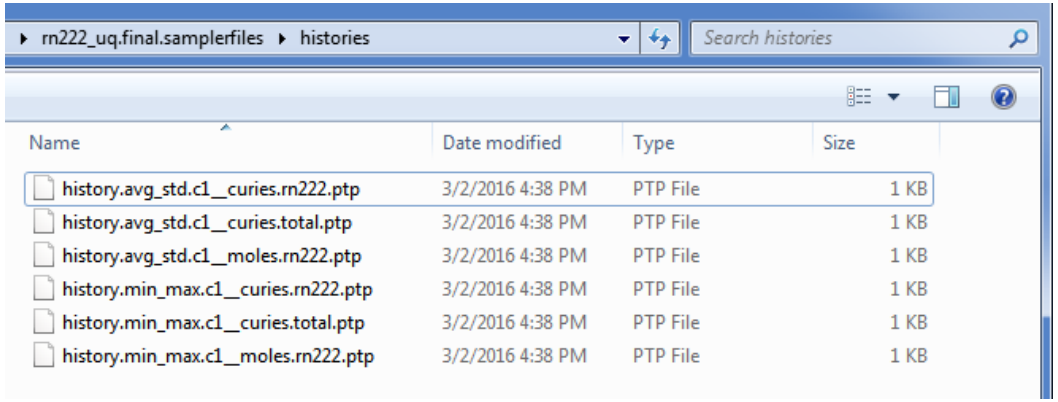
- **histograms** – ptp files with histograms for each response
  - one for each time value of the response
  - 20 bins
  - plottable in Fulcrum (also right-click on plot→save as→image)

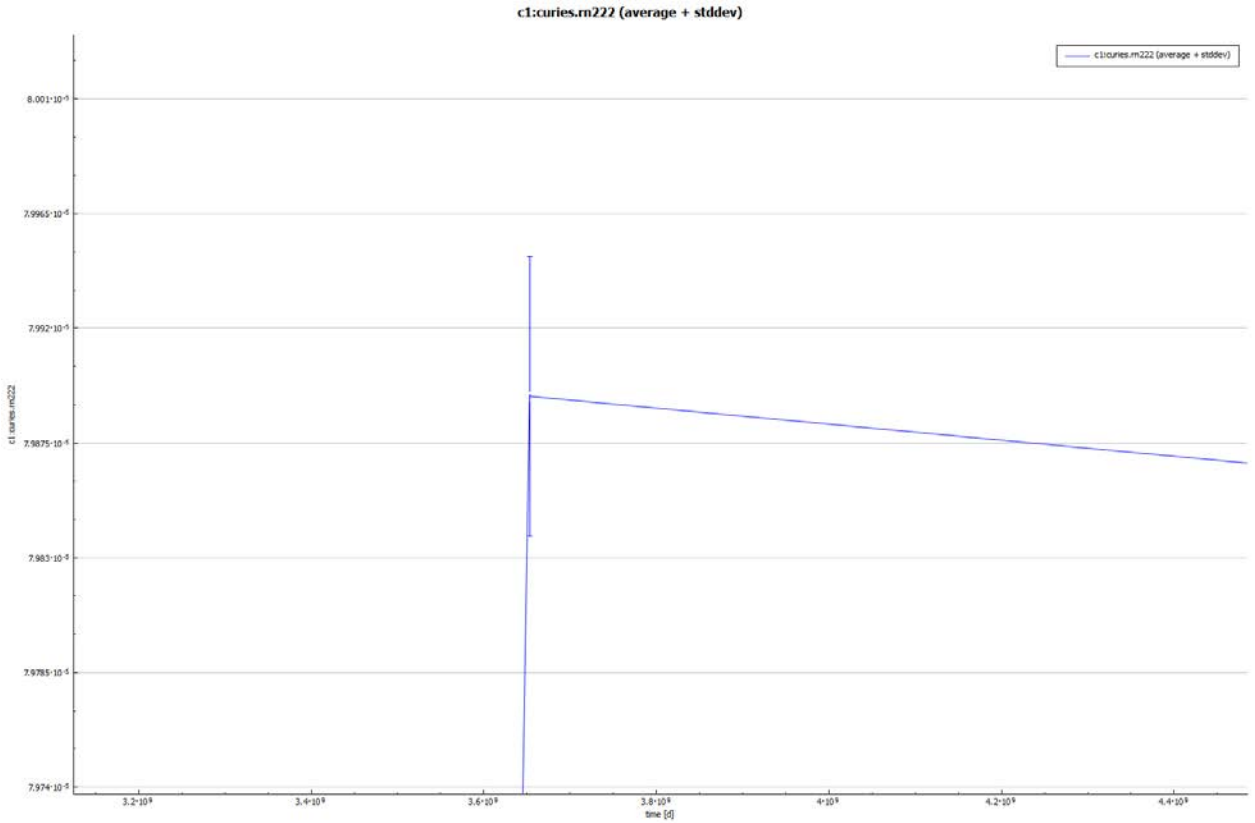


Now Analysis Begins…

a survey of directory contents

- **histories** – ptp files with time-dependent response
  - average with standard deviation
  - also average with min/max

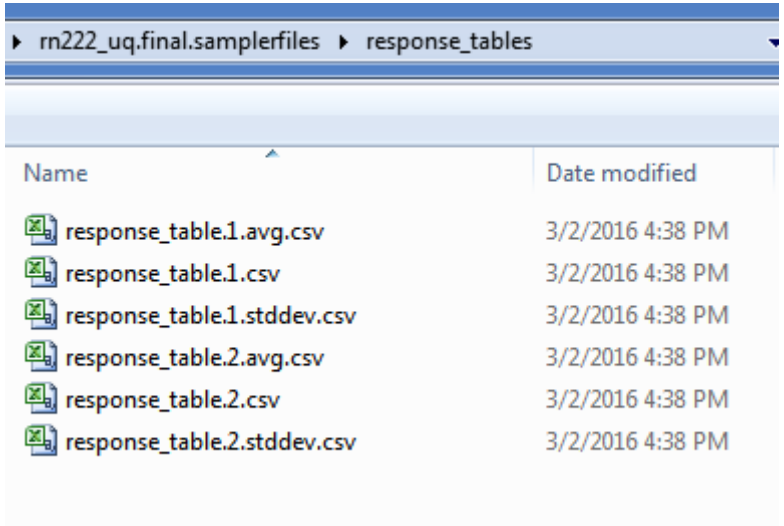




Now Analysis Begins…

a survey of directory contents

- **response_tables** – csv files
  - every response
  - every time point
  - versions for sample/standard deviation/average



A	B	C	D	E
sample	time(d)	c1:moles.rn222		
1	0	0.00E+00	+/-	0.00E+00
1	3652.78	4.35E-24	+/-	0.00E+00
1	365278	3.94E-18	+/-	0.00E+00
1	3.65E+07	2.07E-13	+/-	0.00E+00
1	3.65E+09	2.34E-12	+/-	0.00E+00
1	3.65E+11	2.01E-12	+/-	0.00E+00
2	0	0.00E+00	+/-	0.00E+00
2	3652.78	4.31E-24	+/-	0.00E+00
2	365278	3.92E-18	+/-	0.00E+00
2	3.65E+07	2.07E-13	+/-	0.00E+00
2	3.65E+09	2.34E-12	+/-	0.00E+00
2	3.65E+11	2.01E-12	+/-	0.00E+00
3	0	0.00E+00	+/-	0.00E+00

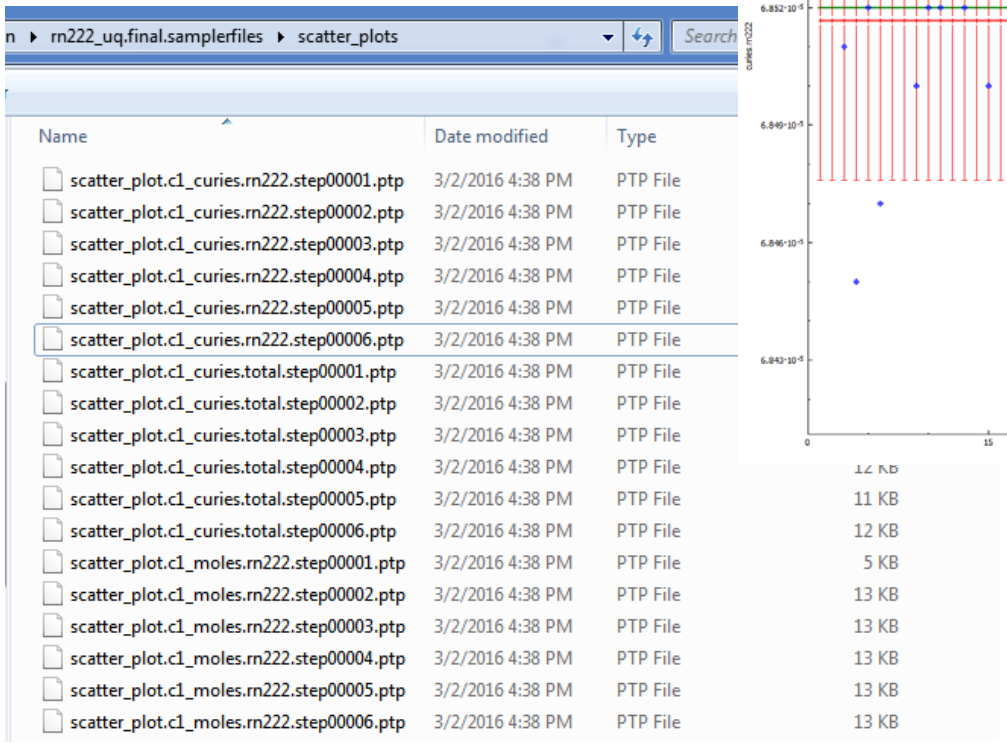
solution uncertainty

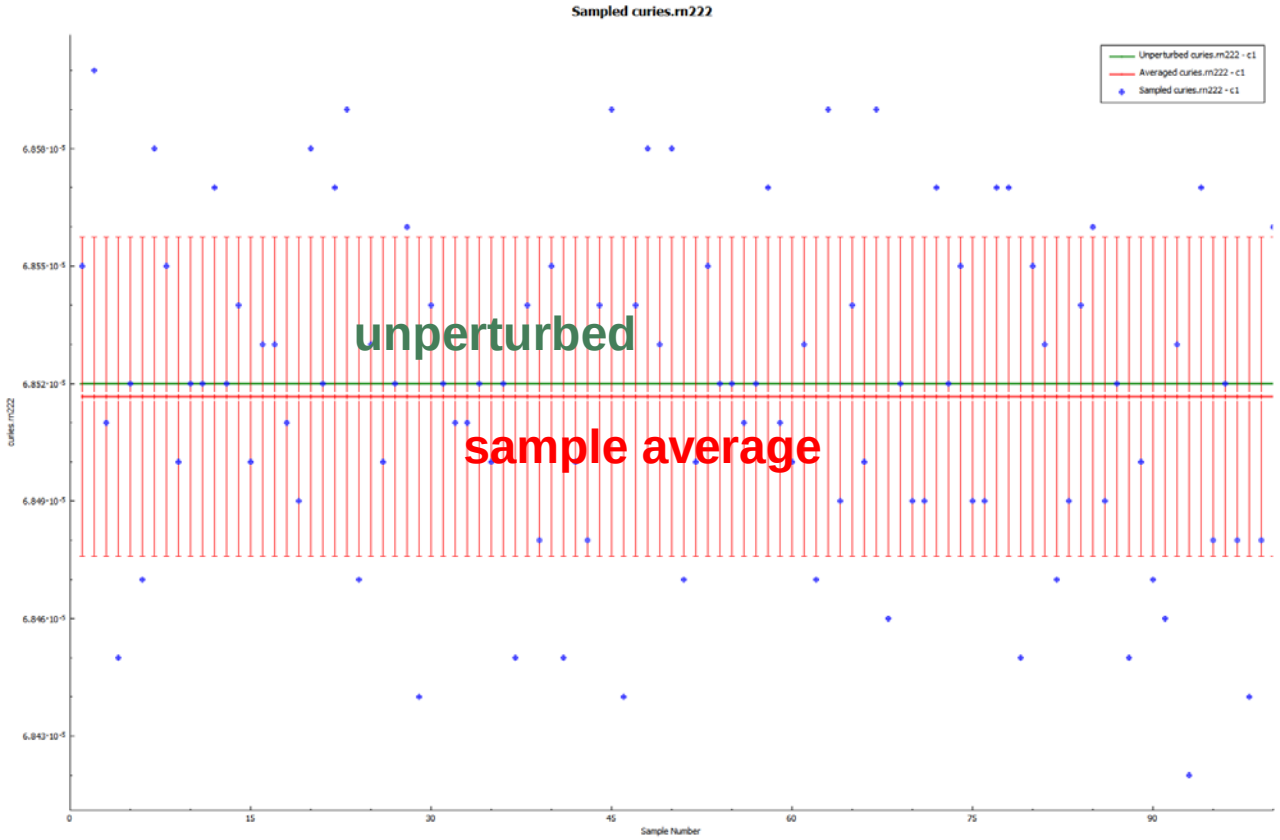
(only populated by Monte Carlo transport methods)

Now Analysis Begins…

a survey of directory contents

- **scatter_plots** – ptp files showing data points
  - average vs. unperturbed!



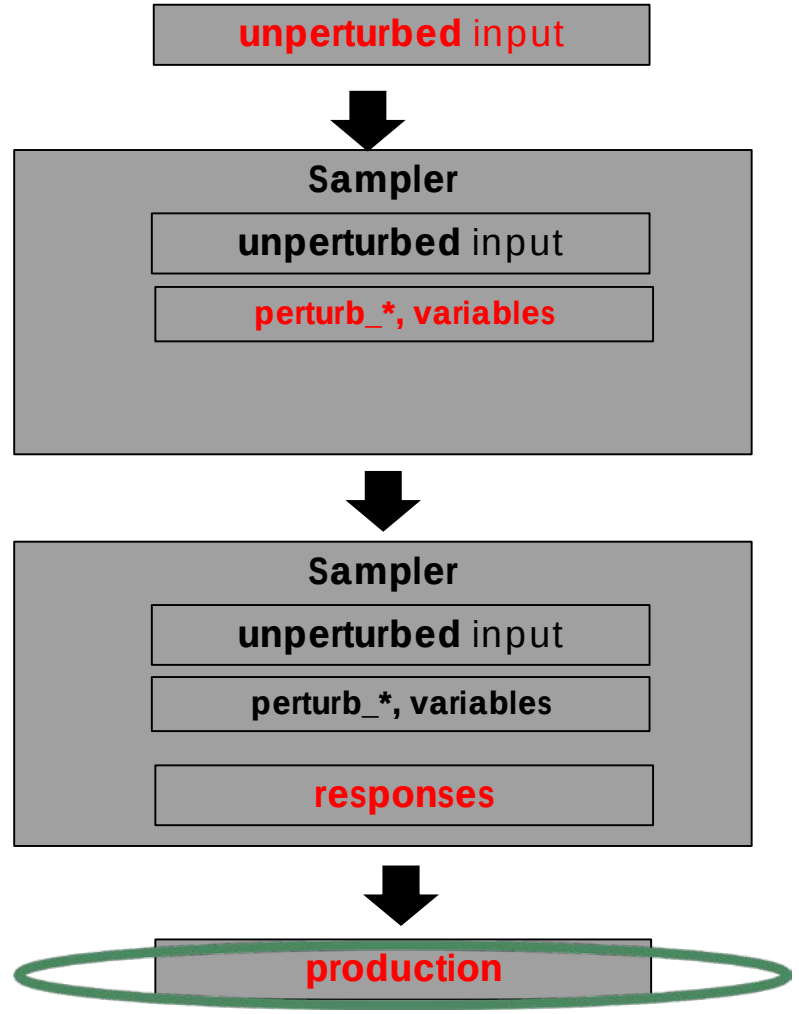


And the Answer is...

Uncertainty peaks at about 0.7% but decreases to 0.07% at long times (~1 billion years)

rn222_uq.final.out file

```
Average + std. deviation table 2 (c1:curies.rn222, c1:curies.total)
   time(d) |                          c1:curies.rn222                          c1:curies.total
-----------+-------------------------------------------------------------------------------
         0 |       0.0000e+00 +/- 0.0000e+00 (0.00 %)      8.0010e-05 +/- 0.0000e+00 (0.00 %)
      3653 |       1.4835e-16 +/- 1.0360e-18 (0.70 %)      2.4042e-04 +/- 1.1034e-06 (0.46 %)
    365300 |       1.3460e-10 +/- 9.0120e-13 (0.67 %)      2.4065e-04 +/- 1.1069e-06 (0.46 %)
 3.653e+07 |       7.0849e-06 +/- 2.7948e-08 (0.39 %)      3.3090e-04 +/- 1.1306e-06 (0.34 %)
 3.653e+09 |       7.9893e-05 +/- 5.4575e-08 (0.07 %)      1.1183e-03 +/- 2.9942e-06 (0.27 %)
 3.653e+11 |       6.8517e-05 +/- 4.0519e-08 (0.06 %)      9.5910e-04 +/- 2.5288e-06 (0.26 %)
```



Some Comments on Decay Uncertainty

- Uncertainty is in general small for decay constants/branching ratios
  - exception is short-lived fission products, e.g. following burst fission
- Including decay uncertainty in a calculation requires direct usage of the "end7dec" ORIGEN decay library
  - COUPLE and ORIGEN **if** they use "end7dec"
    - pre-generated ORIGEN reactor libraries have embedded decay constants
  - **TRITON and Polaris do not use end7dec by default**
- Must explicitly use `library="end7dec"` in OPUS or unperturbed decay constants are used

```
=shell
  ln -sf ${DATA}\perturb\end7dec_0000  end7dec
end

=origen
case{
    title="U238 decay chain"
    lib{ file="end7dec" }
    time{ units=years t=[3L 1e1 1e9] }
    mat{ iso=[u238=1.0] }
    print{ nuc{ units=[moles curies] } }
    save=yes
}
end
=opus
library="end7dec"
units=curies
end
```

OAK RIDGE National Laboratory

Sampler

Time-dependent depletion/decay responses

Overview

Sampler has two types of responses

- **Static responses**
  - grep – search for a specific value in the output (.out) file
  - stdcmp – extract from a standard composition (.stdcmp) file
  - variables – sampled values of non-nuclear data
- **Time-dependent responses**
  - origen_nuclides – extract from an ORIGEN concentration (.f71) file
  - opus_plt – extract from an OPUS plot (.plt) file

Overview

Sampler has two types of responses

- **Static responses**
  - grep – search for a specific value in the output (.out) file
  - stdcmp – extract from a standard composition (.stdcmp) file
  - variables – sampled values of non-nuclear data

Source Terms

- **Time-dependent responses**
  - origen_nuclides – extract from an ORIGEN concentration (.f71) file
  - opus_plt – extract from an OPUS plot (.plt) file

Response type=origen_nuclides

	origen_nuclides
units	fixed (moles)
nuclides	user chooses ***at post-processing time*** *(do not need to rerun sampler to look at different nuclides!)*
filename	*.samplerfiles/ ${SUBDIR}/ ${OUTBASENAME}.f71
format	binary
precision	16 digits

- Multiple names for the file that contains isotopics
  - ORIGEN (binary) concentrations file
  - ft71 file
  - f71 file
- Traditionally has the file name "ft71f001" in the SCALE temporary calculation directory
- There is a SCALE rule to copy it to the user's output directory
  - ft71f001→${OUTBASENAME}.f71
  - e.g.
    my.inp → sequence → ${TMPDIR}/ft71f001 → scalerte finalization → ${OUTDIR}/my.f71

Response type=origen_nuclides

	origen_nuclides
units	fixed (moles)
nuclides	user chooses ***at post-processing time*** *(do not need to rerun sampler to look at different nuclides!)*
filename	*.samplerfiles/ ${SUBDIR}/ ${OUTBASENAME}.f71
format	binary
precision	16 digits

- If you have an **origen_nuclides** response
  - Sampler has it's own rule to copy

    ${TMPDIR}/ft71f001→

    *.samplerfiles/my_pert_c00001.f71→

    ***.samplerfiles/my_pert_c00001/ my_pert_c00001.f71**

  - Sampler must find this file or it redoes the calculation!
  - The extra file copies Sampler sets up must succeed or it will not post-process.

Response type=origen_nuclides

	origen_nuclides
units	fixed (moles)
nuclides	user chooses ***at post-processing time*** *(do not need to rerun sampler to look at different nuclides!)*
filename	*.samplerfiles/ ${SUBDIR}/ ${OUTBASENAME}.f71
format	binary
precision	16 digits

- Once Sampler has saved the ft71f001→ ${SUBDIR}/${OUTBASENAME}.f71, can ask for any of the tracked 2237 nuclides

```
read param
   force_run=no
end param
...
read response[moles]
        type=origen_nuclides
        mixture=1
        nuclides= rn-200 rn-221 rn-222
                rn-223 rn-224 rn-225
                rn-226 end
end response
```

- ft71f001 is just a "stack" of isotopics vectors
  - when read (e.g. by ORIGEN or OPUS), a printout of contents is shown
- Access specific ranges in the ft71f001 using either
  - **step_from=X step_to=Y**
  - **mixture=C** where C is a case number (ORIGEN/Polaris) or mixture id (TRITON)

Response type=opus_plt

	opus_plt
units	**user chooses**
nuclides	user chooses at runtime via powerful ranking or explicit selection
filename	*.samplerfiles/ ${OUTBASENAME}.<n>.plt *(where <n> is a very long integer starting at 0)*
format	text
precision	5 digits

- Each =opus call creates a numbered *.plt file from an ORIGEN concentration file

```
'first opus creates *0.plt file
=opus
data="ft71f001"
library="end7dec"
units=curies
nrank=40
symnuc=rn-222 end
end
```

- The Sampler response accesses the file by the ndataset number (starts at 0)

```
'access *0.plt contents
read response[curies]
    type=opus_plt
    ndataset=0
    nuclides=rn-222 total end
end response
```

Response type=opus_plt

	opus_plt
units	**user chooses**
nuclides	user chooses at runtime via powerful ranking or explicit selection
filename	*.samplerfiles/ ${OUTBASENAME}.<n>.plt *(where <n> is a very long integer starting at 0)*
format	text
precision	5 digits

- By default OPUS gives top 40 nuclides contributing to the units of interest
  - E.g., if units=curies, top 40 curie-producing isotopes
  - In Sampler, only available nuclides can be output—includes powerful total and subtotal, though
  - NOTE: OPUS is a post-processor for ORIGEN, described in the ORIGEN section of the SCALE manual
- OPUS .plt format is simple

```
time (d)
Ci
nuclide
6 24
                0.000e+00 3.653e+03 3.653e+05 3.653e+07 3.653e+09 3.653e+11
            u238 8.001e-05 8.001e-05 8.001e-05 8.001e-05 7.989e-05 6.852e-05
           th234 0.000e+00 8.001e-05 8.001e-05 8.001e-05 7.989e-05 6.852e-05
          pa234m 0.000e+00 8.001e-05 8.001e-05 8.001e-05 7.989e-05 6.852e-05
            u234 0.000e+00 2.238e-09 2.256e-07 1.968e-05 7.989e-05 6.852e-05
           pb210 0.000e+00 1.089e-17 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           bi210 0.000e+00 1.089e-17 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           po210 0.000e+00 1.089e-17 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           po218 0.000e+00 1.484e-16 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           rn222 0.000e+00 1.484e-16 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           ra226 0.000e+00 1.484e-16 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           th230 0.000e+00 1.029e-13 1.035e-09 7.086e-06 7.989e-05 6.852e-05
           bi214 0.000e+00 1.484e-16 1.347e-10 7.086e-06 7.989e-05 6.852e-05
           pb214 0.000e+00 1.484e-16 1.346e-10 7.085e-06 7.987e-05 6.850e-05
           po214 0.000e+00 1.484e-16 1.346e-10 7.084e-06 7.987e-05 6.850e-05
           pa234 0.000e+00 1.280e-07 1.280e-07 1.280e-07 1.278e-07 1.096e-07
           tl210 0.000e+00 3.117e-20 2.828e-14 1.488e-09 1.678e-08 1.439e-08
           at218 0.000e+00 2.969e-20 2.693e-14 1.417e-09 1.598e-08 1.370e-08
           tl206 0.000e+00 1.458e-23 1.803e-16 9.488e-12 1.070e-10 9.174e-11
           rn218 0.000e+00 2.969e-23 2.693e-17 1.417e-12 1.598e-11 1.370e-11
           hg206 0.000e+00 2.068e-25 2.559e-18 1.346e-13 1.518e-12 1.302e-12
           pb209 0.000e+00 2.650e-24 2.404e-18 1.265e-13 1.426e-12 1.223e-12
           bi209 0.000e+00 0.000e+00 5.210e-47 4.726e-41 2.487e-36 3.053e-35
        subtotal 8.001e-05 2.402e-04 2.404e-04 3.307e-04 1.119e-03 9.593e-04
           total 8.001e-05 2.402e-04 2.404e-04 3.307e-04 1.119e-03 9.593e-04
```

Comparison

	opus_plt	origen_nuclides
units	**user chooses**	fixed (moles)
nuclides	user chooses at runtime via powerful ranking or explicit selection	user chooses ***at post-processing time*** *(do not need to rerun sampler to look at different nuclides!)*
filename	*.samplerfiles/ ${OUTBASENAME}.<n>.plt	*.samplerfiles/ ${SUBDIR}/ ${OUTBASENAME}.f71
format	text	binary
precision	5 digits	16 digits

Basic Example 1/2

- Let's return to the simple decay example
  1. Remove all responses
  2. Add a variable **u238** to add uncertainty in the initial isotopics to make things a little more interesting
  3. Make sure to modify so **perturb_geometry=yes**
  4. Let's run 10 samples
  5. Once successful, set **force_run=no**

```
=sampler

read parameters
n_samples=10
force_run=no
run_cases=yes
perturb_decay=yes
perturb_geometry=yes
'perturb_yields=yes
'perturb_xs=yes
end parameters

read case[c1]

sequence=origen
case{
       title="U238 decay chain"
       lib{ file="end7dec" }
       time{ units=years t=[20L 1e0 1e9] }
       mat{ iso=[u238=#{u238}] }
       print{ nuc{ units=[moles curies] } }
       save=yes %produces ft71f001 by default
}
end sequence

sequence=opus
data="ft71f001"
library="end7dec"
units=curies
end sequence

read variable[u238]
distribution=uniform
value=1.0
min=0.9
max=1.1
end variable

end case

end
```

Basic Example 2/2

- Let's return to the simple decay example
  1. Remove all responses
  2. Add a variable **u238** to add uncertainty in the initial isotopics to make things a little more interesting.
  3. Make sure to modify so **perturb_geometry=yes**
  4. Let's run 10 samples
  5. Once successful, set **force_run=no**

Our Sampler case produces one *0.plt file and one .f71 file

6. Verify *0.plt and .f71 exist in your *.samplerfiles directory
7. Add one response for the **type=origen_nuclides** and rerun to see it does not rerun the calculation but adds a response
8. Add one response for **type=opus_plt** and rerun to see it does not rerun the calculation but adds a response
9. Examine the *.samplerfiles/histories files

```
=sampler

read parameters
n_samples=10
force_run=no
run_cases=yes
perturb_decay=yes
perturb_geometry=yes
'perturb_yields=yes
'perturb_xs=yes
end parameters

read case[c1]

...

end case

'access *.f71 contents
read response[moles]
    type=origen_nuclides
    mixture=1
    nuclides= rn-200 rn-221 rn-222
              rn-223 rn-224 rn-225
              rn-226 end
end response

'access *0.plt contents
read response[curies]
    type=opus_plt
    ndataset=0
    nuclides=rn-222 total end
end response

end
```

Advanced Example

- **`origen_nuclides` response**
  1. Create two additional **`origen_nuclides`** responses with different nuclide sets.
  2. Verify the behavior of the **`mixture`**, **`to_step`**, and **`from_step`** ways to isolate the steps.
     - Look in the nominal case output file c1_pert_00000.out for "ORIGEN Concentrations Data Summary" for a list of the available data.
     - Column 1 shows the positions (pos) expected in the `from_step` and `to_step`, e.g. `from_step=1` and `to_step=23` for positions 1 through 23. DO NOT USE THE STEP COLUMN NUMBERS.
     - Column 8 shows the case index (case) which depends on the code producing the f71:
       - TRITON: a mixture identifier
       - ORIGEN: the case index (starting at 1)
       - Polaris: material zone index (look at Polaris output for ordering of zones)

- **`opus_plt` response**
  1. Verify the error produced when adding an **`opus_plt`** response for **`ndataset=1`** without first adding a new **`sequence=opus`**.
  2. Add a new **`sequence=opus`** with units=grams and **rerun** calculation to enable **`ndataset=1`**.
  3. Verify trying to retrieve a nuclide that does not exist in the *.plt file assumes a value of zero.

```
#########################################################################################################################################
#                                                  ORIGEN Concentrations Data Summary                                                   #
#########################################################################################################################################
   pos         time        power         flux       fluence       energy libpos   case   step DCGNAB
   (-)          (s)         (MW)    (n/cm2-s)      (n/cm2)        (MWd)    (-)    (-)    (-)    (-)
     1  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      0 DC----
     2  3.15600e+07  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      1 DC----
     3  8.46659e+07  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      2 DC----
     4  2.27133e+08  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      3 DC----
     5  6.09328e+08  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      4 DC----
     6  1.63464e+09  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      5 DC----
     7  4.38525e+09  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      6 DC----
     8  1.17643e+10  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      7 DC----
     9  3.15600e+10  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      8 DC----
    10  8.46659e+10  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1      9 DC----
    11  2.27133e+11  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     10 DC----
    12  6.09328e+11  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     11 DC----
    13  1.63464e+12  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     12 DC----
    14  4.38525e+12  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     13 DC----
    15  1.17643e+13  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     14 DC----
    16  3.15600e+13  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     15 DC----
    17  8.46659e+13  0.00000e+00  0.00000e+00  0.00000e+00  0.00000e+00      1      1     16 DC----
```

Summary

- Two **time-dependent responses** are especially useful for any SCALE depletion/decay calculation
  - **origen_nuclides** – extract from an ORIGEN concentration (.f71) file
  - **opus_plt** – extract from an OPUS plot (.plt) file (NOTE: OPUS plot files are post-processed .f71 files)
- Each has good/*bad*
  - **origen_nuclides** allows any set of nuclides to be examined without rerunning calculation *but units can only be "moles"*
  - **opus_plt** has flexible units (grams, becquerels) and nuclide selection *but restricts number of nuclides at calculation time*

```
=sampler

read parameters
...
end parameters

read case[c1]
...
end case

'access *.f71 contents
read response[moles]
    type=origen_nuclides
    mixture=1
    nuclides= rn-200 rn-221 rn-222
              rn-223 rn-224 rn-225
              rn-226 end
end response

'access *0.plt contents
read response[curies]
    type=opus_plt
    ndataset=0
    nuclides=rn-222 total end
end response

end
```

More Examples

- origami_operating_history.inp
- polaris_pin.inp