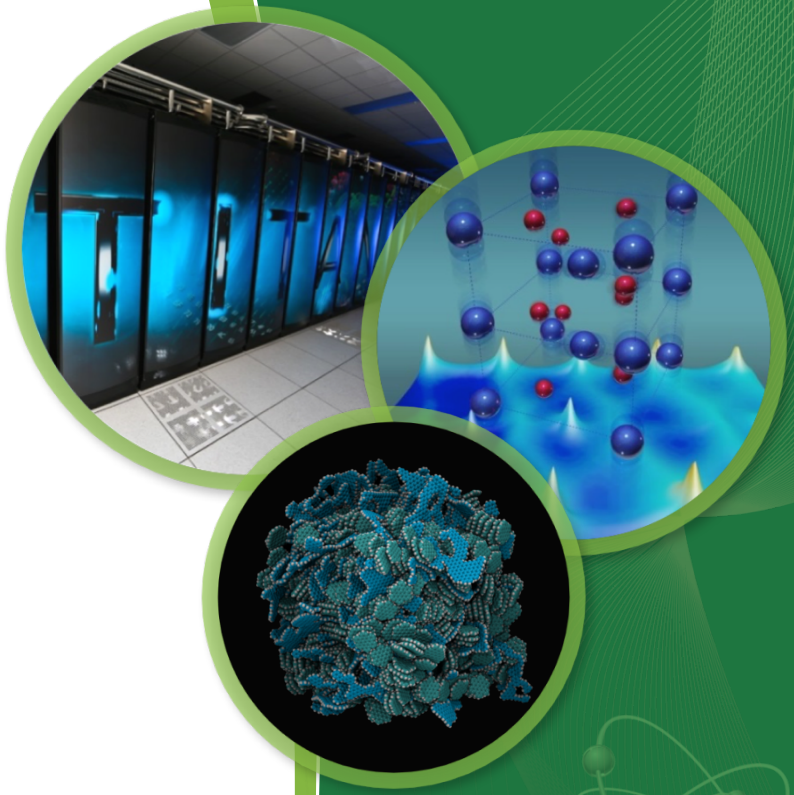
Uncertainty in Anything:
The Future with SCALE/Sampler

W. A. Wieselquist

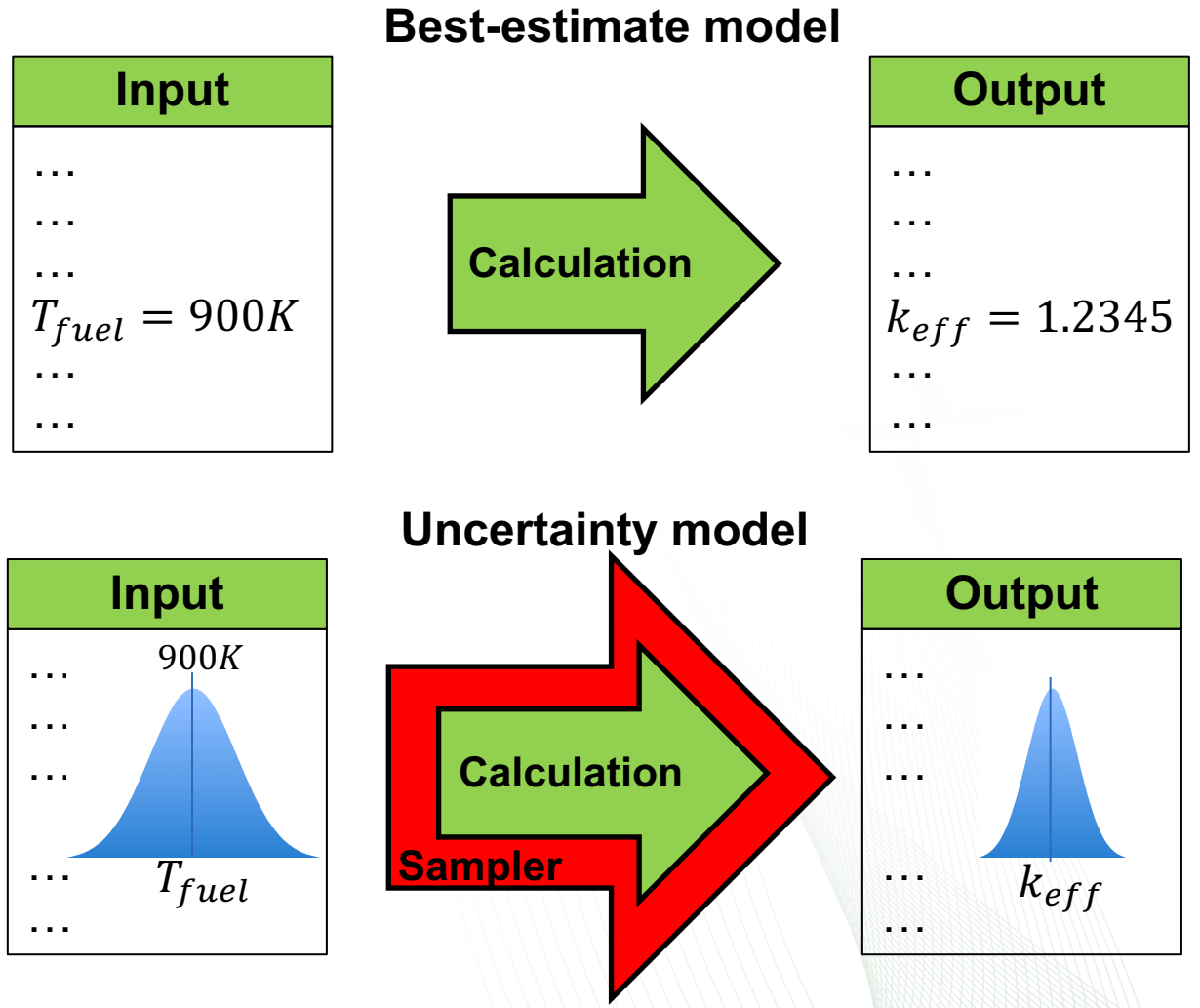


ORNL is managed by UT-Battelle
for the US Department of Energy

OAK RIDGE
National Laboratory

Goal is Complete Uncertainty Quantification in SCALE Simulations

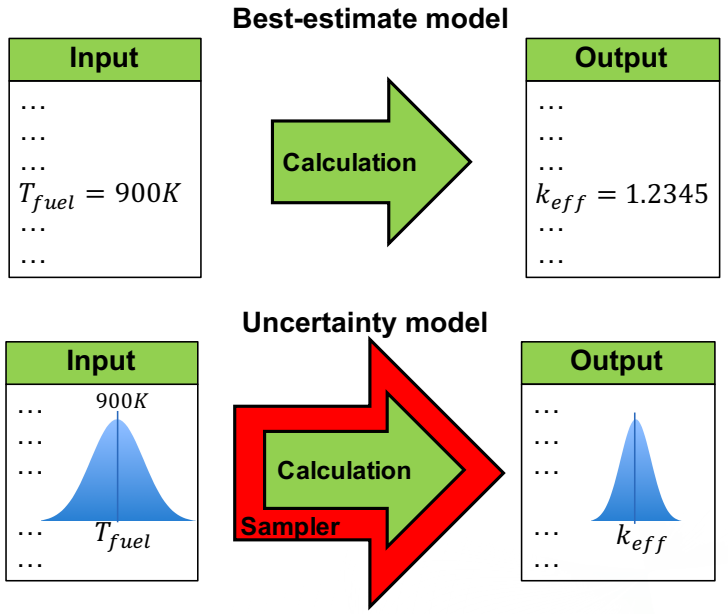
- **Complete** means every **number** in the model can have **uncertainty** which is propagated to uncertainty in outputs
  - Known as the best-estimate plus uncertainty (BEPU) methodology
  - Must be applicable to
    - ***every input***
      cross section, clad thickness, fuel temperature, decay constant, composition, etc.
    - ***every SCALE sequence***
      TRITON, Polaris, ORIGEN, MAVRIC, etc.
  - Time-dependent problems may introduce non-linearity, $\Delta f \not\approx \frac{\partial f}{\partial x}\Delta x$, which first-order perturbation theory methods (TSUNAMI) cannot resolve
- Requirements lead to **sampling-based** uncertainty propagation approach:
  SCALE/**Sampler**



Why do we need Sampler?

Simulation without some type of uncertainty quantification (UQ) has low value

- Conventional UQ for simulations includes
  - A. Sensitivity/parametric studies lead to understanding of possible output variation
    "Let me make sure that Y stays within ~5% of nominal for fuel temperatures ±100 K."
  - B. Comparison of a similar calculation to measurement (validation) leads to understanding of bias
    "We typically have 3% error in actinides and 10% in fission products (except for Gd and Eu) for Westinghouse 17x17 UO_2 assemblies."
- Sampler UQ provides
  - automated processes for parametric studies (A)
  - rigorous BEPU capability (more rigorous than A)



Big UQ Question
What do we do when BEPU and B disagree?

"Sampler predicts 10% uncertainty in the Sm-147 content of a spent fuel sample but a comparison to measurement says we only under-predict by 3%?"

SCALE 6.2 Sampler Team

W. A. Wieselquist*
M. L. Williams*
F. Havluj[1]
R. A. Lefebvre*
W. Zwermann[2]
M. Klein[2]
D. Wiarda*
M. T. Pigni*
I. C. Gauld*
M. A. Jessee*
U. Mertyurek*
J. P. Lefebvre*
K. J. Dugan[3]
B. T. Rearden*

* ORNL

[1] ÚJV Řež, a. s., Czech Republic

[2] Gesellschaft für Anlagen- und Reaktorsicherheit (GRS)

[3] Texas A&M University

HISTORY

2010 **Initiation**

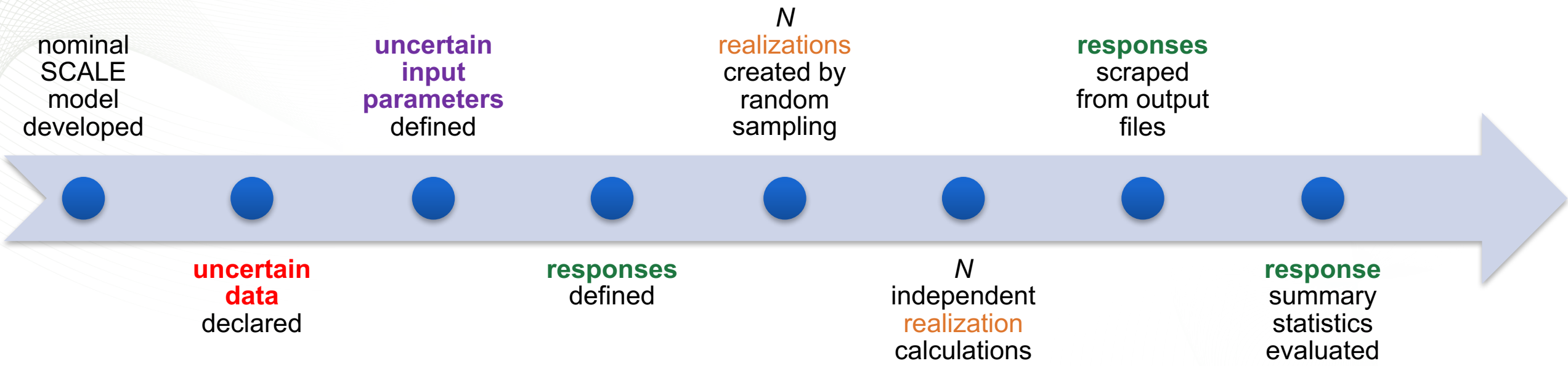
Several RNSD staff & students working toward a sampling-based UQ methodology as part of UQ R&D

2010-2016 **Development**

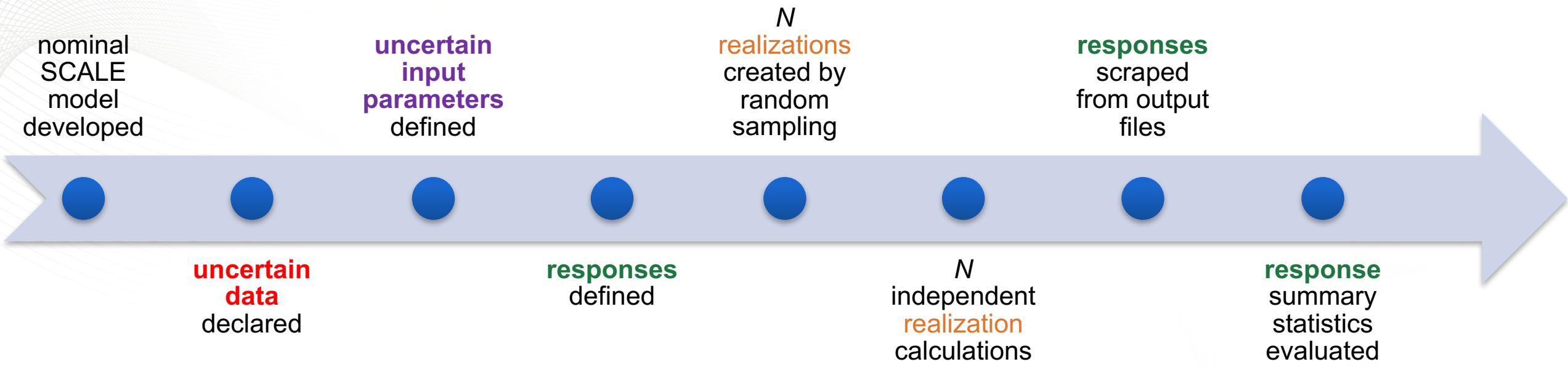
Contributions from students, international collaborators, ORNL applications

2016 **First Release in SCALE 6.2**

SCALE/Sampler Analysis Flow



SCALE/Sampler Analysis Flow



Uncertain Data

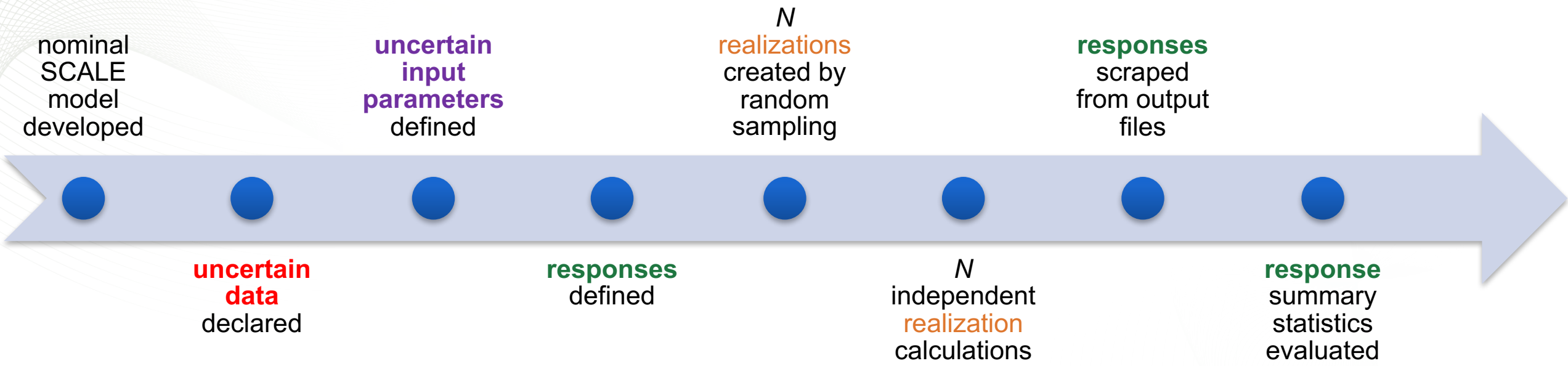
- cross sections
- fission yields
- decay

on the order of 10^5 data variables!

Uncertain Input Parameters

- Distribution Variables
  - uniform
  - beta
  - normal
  - truncated normal
- Expression Variables
  - create new variables (e.g. c=a+b)
  - convert variables to expected input form (e.g. radius=diameter/2)

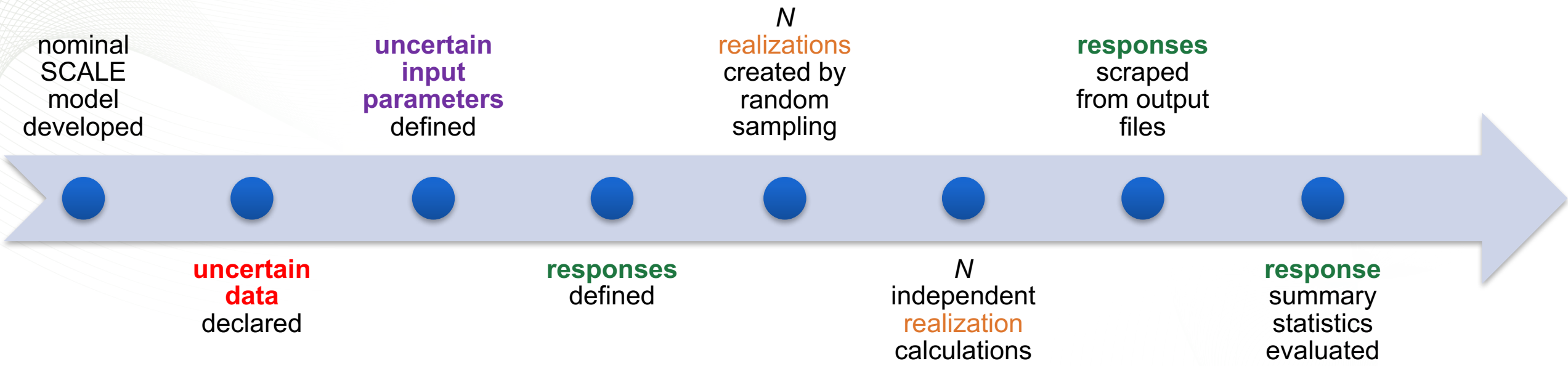
SCALE/Sampler Analysis Flow



Realizations

- Each realization represents a reality, drawn randomly from each variable's distribution
- Sampling error in uncertainty prediction goes as $\frac{1}{\sqrt{N}}$
  - *N=10 → order of magnitude*
  - *N=50 → one significant digit*
  - *N=500 → two significant digits*

SCALE/Sampler Analysis Flow



Responses

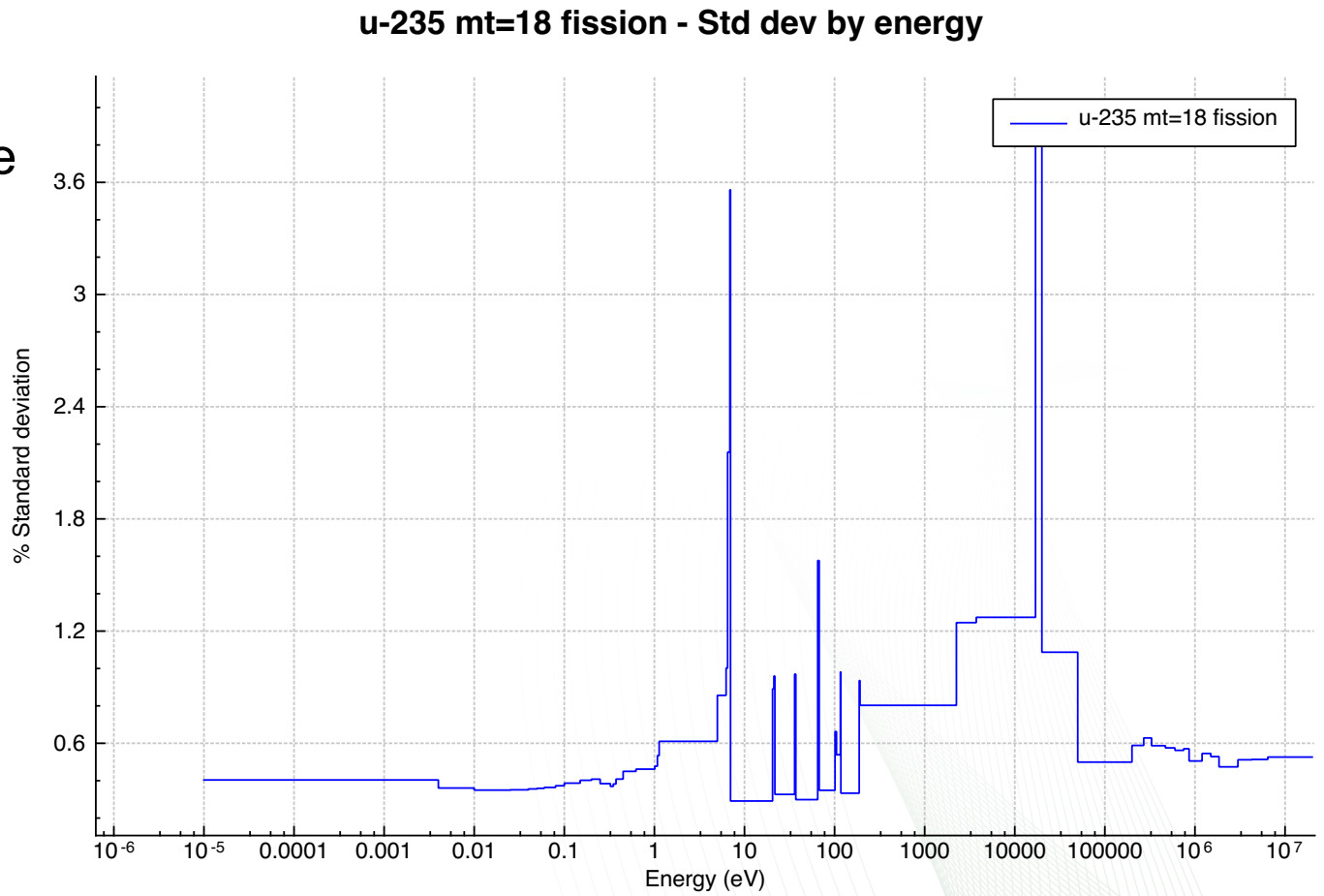
- Any quantity in the main SCALE output file can be treated as an uncertain response
- A few special output files can be processed as well (e.g. ORIGEN isotopics)

Uncertain Nuclear Data

- Cross sections
  - ENDF-VII.1-based covariance matrices
  - Supplemented by other sources to have uncertainty for all isotopes
- Fission product yields
  - Standard deviations from ENDF/B-VII.1
  - Correlations generated using Bayesian procedure considering independent/cumulative yields and decay pathways
- Decay data
  - ENDF-VII.1-based uncertainty
  - Correlations introduced by simple constraints on branching ratios

Uncertain Nuclear Data

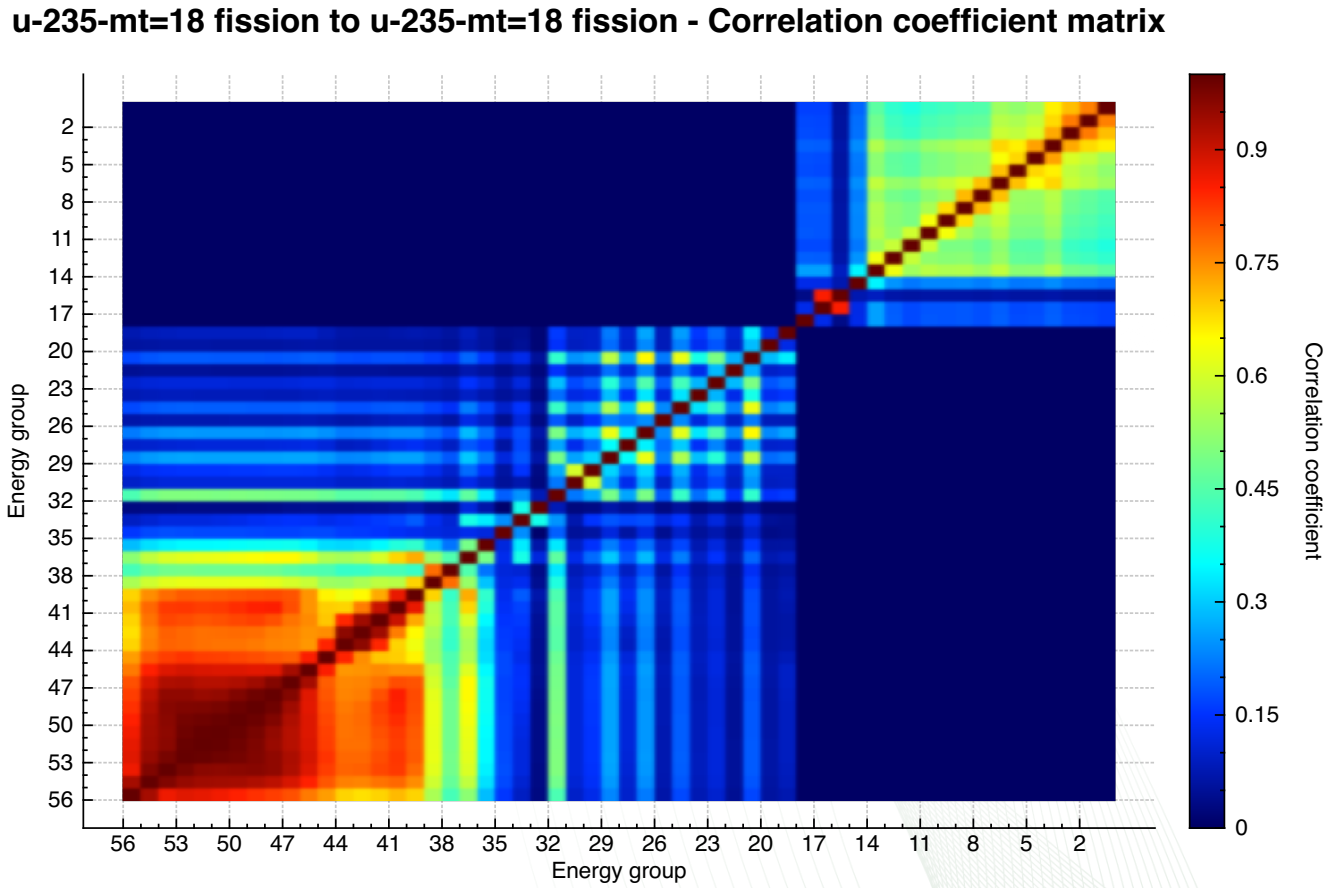
- Cross sections
  - ENDF-VII.1-based covariance matrices
  - Supplemented by other sources to have uncertainty for all isotopes
- Fission product yields
  - Standard deviations from ENDF/B-VII.1
  - Correlations generated using Bayesian procedure considering independent/cumulative yields and decay pathways
- Decay data
  - ENDF-VII.1-based uncertainty
  - Correlations introduced by simple constraints on branching ratios



Output directly from Fulcrum!

Uncertain Nuclear Data

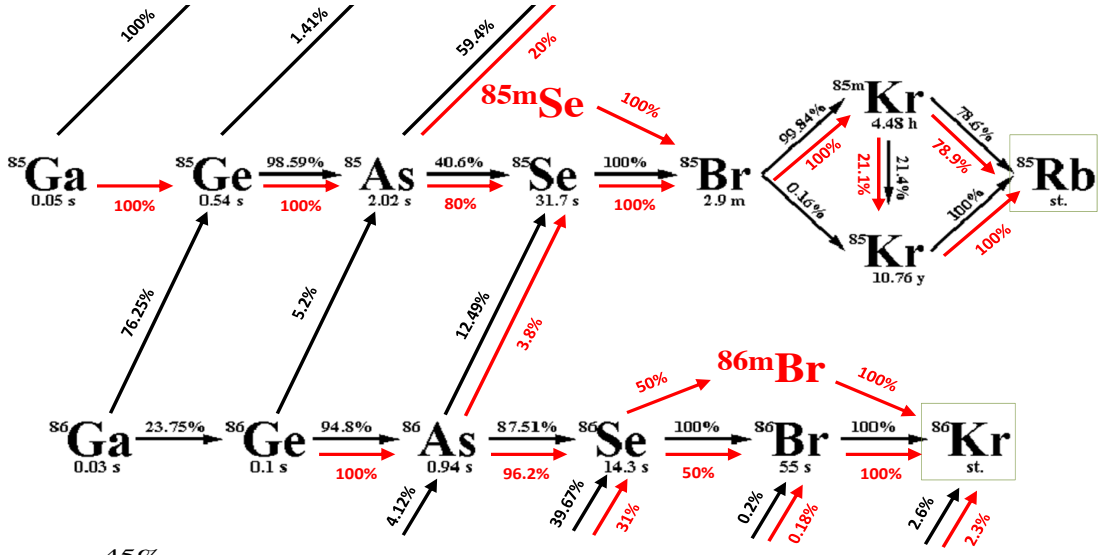
- Cross sections
  - ENDF-VII.1-based covariance matrices
  - Supplemented by other sources to have uncertainty for all isotopes
- Fission product yields
  - Standard deviations from ENDF/B-VII.1
  - Correlations generated using Bayesian procedure considering independent/cumulative yields and decay pathways
- Decay data
  - ENDF-VII.1-based uncertainty
  - Correlations introduced by simple constraints on branching ratios

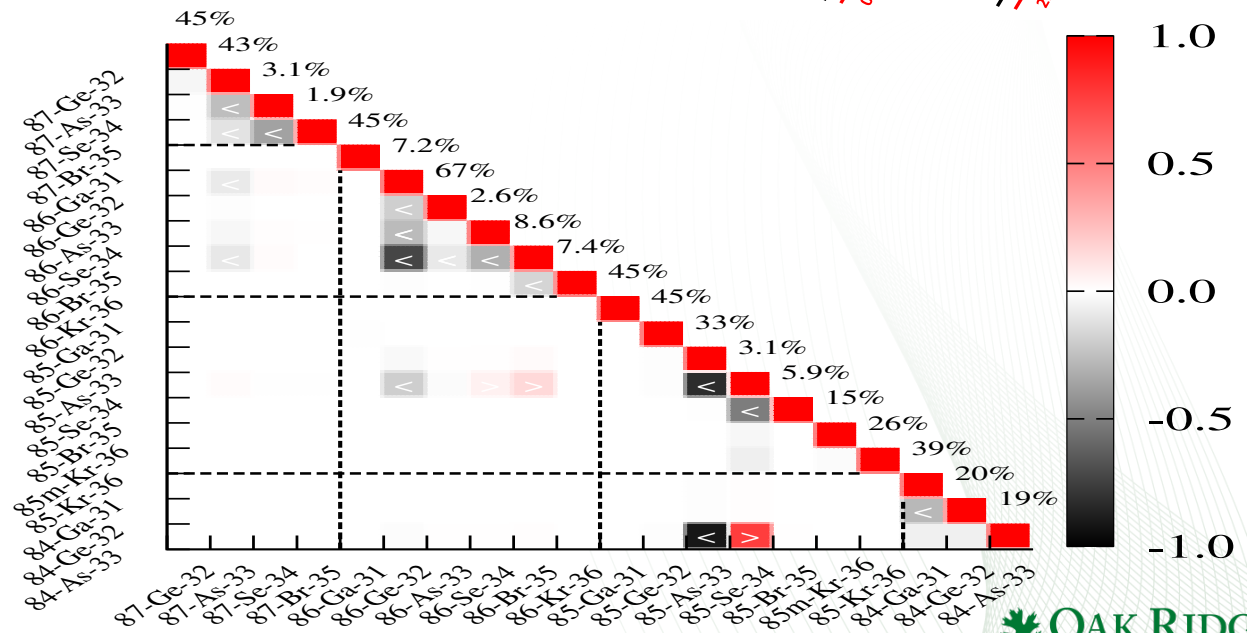


Output directly from Fulcrum!

Uncertain Nuclear Data

- Cross sections
  - ENDF-VII.1-based covariance matrices
  - Supplemented by other sources to have uncertainty for all isotopes
- Fission product yields
  - Standard deviations from ENDF/B-VII.1
  - Correlations generated using Bayesian procedure considering independent/cumulative yields and decay pathways
- Decay data
  - ENDF-VII.1-based uncertainty
  - Correlations introduced by simple constraints on branching ratios



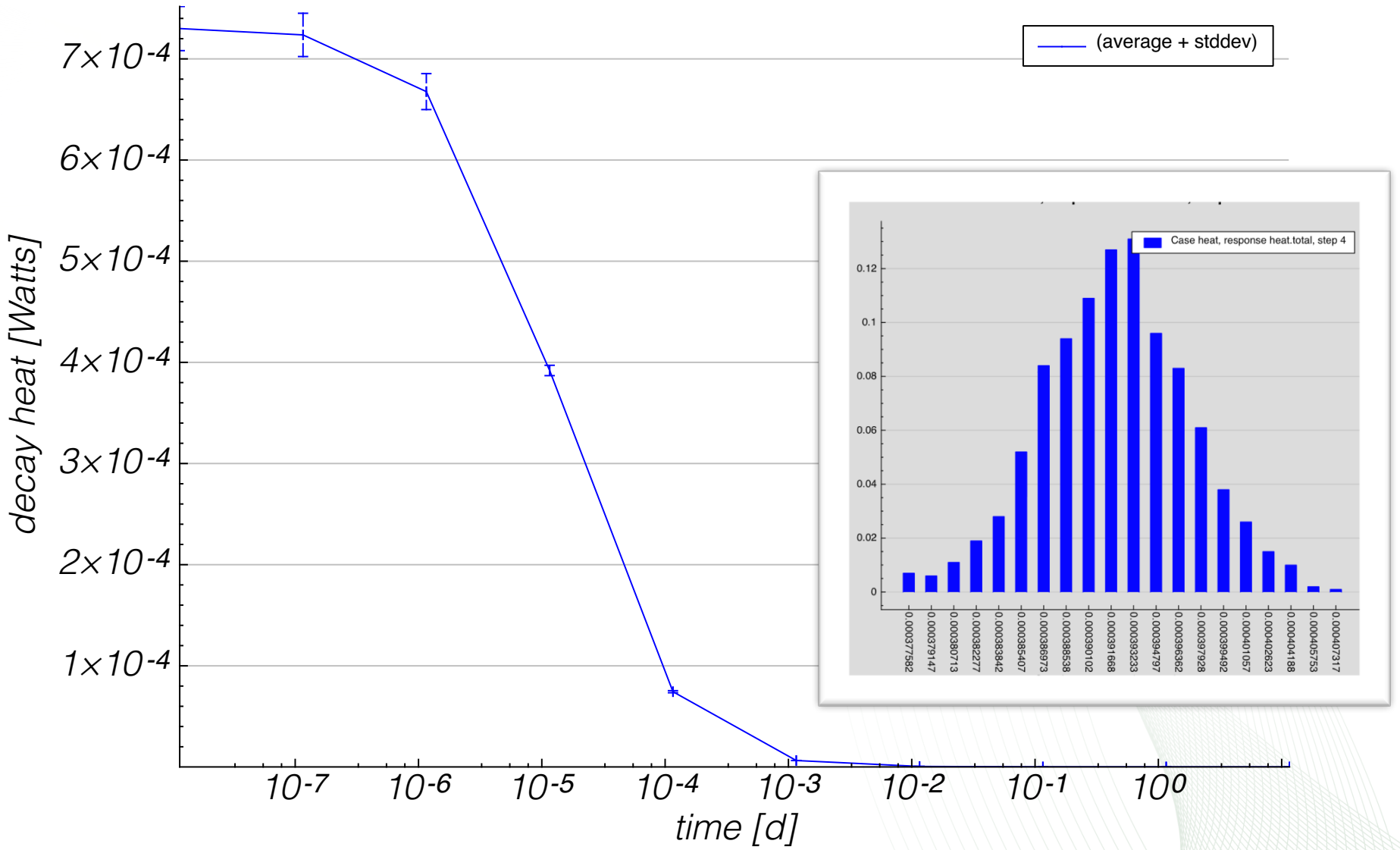


OAK RIDGE National Laboratory

Example Impact of FP Yield and Decay Data Uncertainties For U235 Fission Burst

Nominal Input

```
'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
```

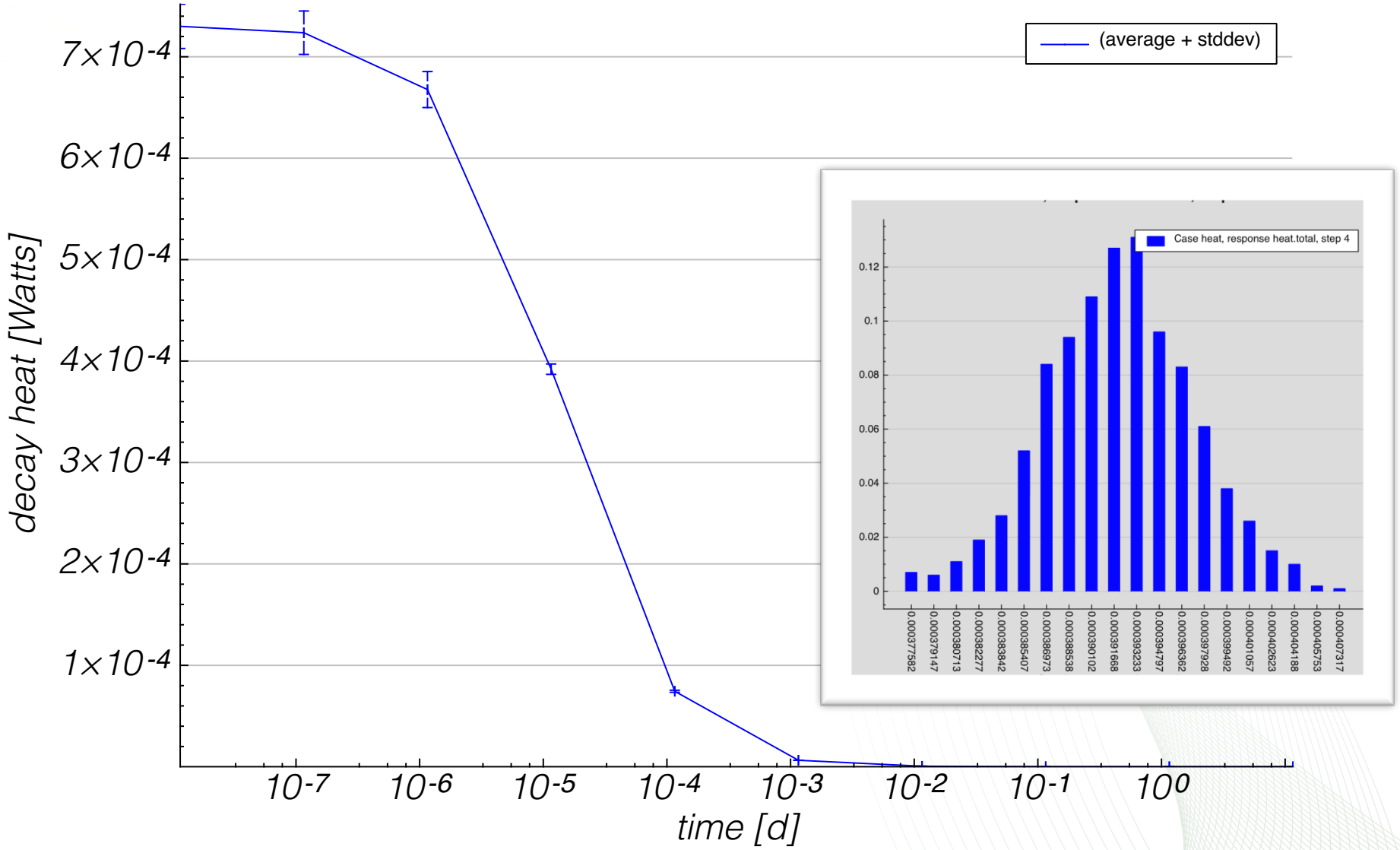


OAK RIDGE National Laboratory

Example Impact of FP Yield and Decay Data Uncertainties For U235 Fission Burst

Sampler Input

```
=%sampler

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

read case[heat]
    import="burst.inp"
end case

read response[heat]
  type=opus_plt
  ndataset=0
  nuclides=total end
end response

end
```



OAK RIDGE National Laboratory

Uncertain Input Parameters

- **Method 1: Placeholders**
  - Substitute any number in input with #{variable_name}
  - Define variable

- **Method 2: SIREN**
  - SCALE Input Retrieval Engine
  - Define variable
  - Link variable to an input “XPATH”

Uncertain Input Parameters

- **Method 1: Placeholders**
  - Substitute any number in input with #{variable_name}
  - Define variable

- **Method 2: SIREN**
  - SCALE Input Retrieval Engine
  - Define variable
  - Link variable to an input “XPATH”

```
read composition
 uranium     1 den=18.742 1 300
               92235   #{u235_wo}
               92238   #{u238_wo}
               92234   #{u234_wo} end
end composition
…
read variable[u235_wo]
   distribution=normal
   value=93.7112
   stddev=0.05
end variable

read variable[u234_wo]
   distribution=uniform
   value=1.0202
   min=1
   max=1.0404
end variable

read variable[u238_wo]
   distribution=expression
   expression="100.0 - u235_wo - u234_wo"
end variable
```

Uncertain Input Parameters

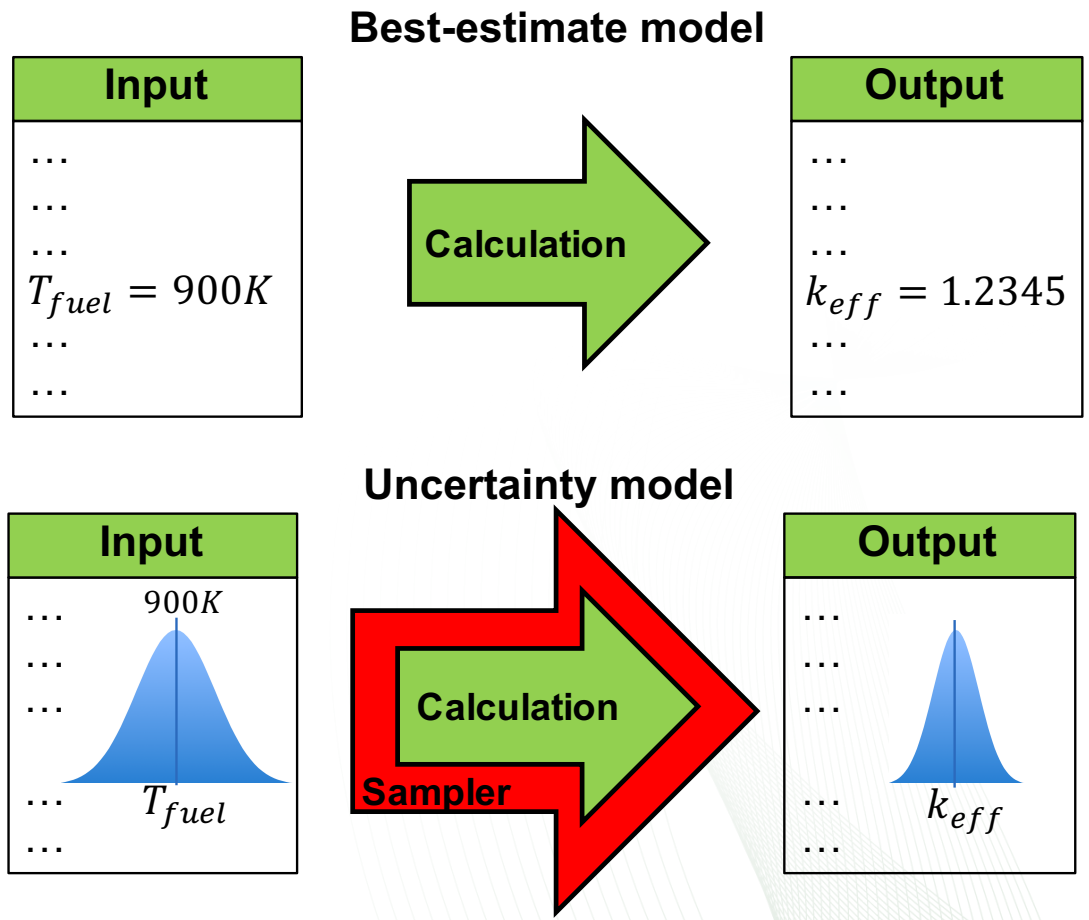
- **Method 1: Placeholders**
  - Substitute any number in input with #{variable_name}
  - Define variable

- **Method 2: SIREN**
  - SCALE Input Retrieval Engine
  - Define variable
  - Link variable to an input “XPATH”

```
read composition
 uranium      1 den=18.742 1 300
                92235    93.7112
                92238     5.2686
                92234     1.0202 end
end composition
…
read variable[u235_wo]
   distribution=normal
   value=93.7112
   stddev=0.05
   siren="/*/comps/stdcomp/wtpt_pair/id[92235]/wtpt"
end variable

read variable[u234_wo]
   distribution=uniform
   value=1.0202
   min=1
   max=1.0404
   siren="/*/comps/stdcomp/wtpt_pair/id[92234]/wtpt"
end variable

read variable[u238_wo]
   distribution=expression
   expression="100.0 - u235_wo - u234_wo”
   siren="/*/comps/stdcomp/wtpt_pair/id[92238]/wtpt"
end variable
```

Summary

- Sampler is a new *Super Sequence* capable of driving a best-estimate plus uncertainty (BEPU) analysis
  - Applicable to any SCALE calculation
  - Easy inclusion of nuclear data uncertainty
  - Association of distributions to any input variable
- Leading-edge nuclear data uncertainty
  - Fission product yield uncertainty
  - Decay data uncertainty
  - Multi-group cross section uncertainty (CE in SCALE 6.3)



The Future

- **SCALE 6.3**
  - CE data perturbations, i.e. can use Sampler with CE-KENO
  - Expanding fission product yield uncertainty
  - Data as a response
  - Rank partial correlation coefficient
- **Beyond**
  - More useful "sensitivity" information out of sampling results
  - **Tackle the Big UQ Question**

    What do we do when BEPU and validation disagree?

    Opportunities!
    - Improve data (data assimilation)
    - Improve model (calibration)