Sampler UQ

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Sampler Team and Contributors

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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**

[1] ÚJV Řež, a.s., Czech Republic

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

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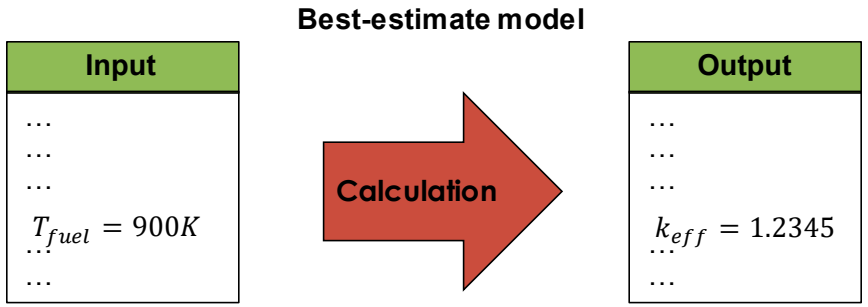
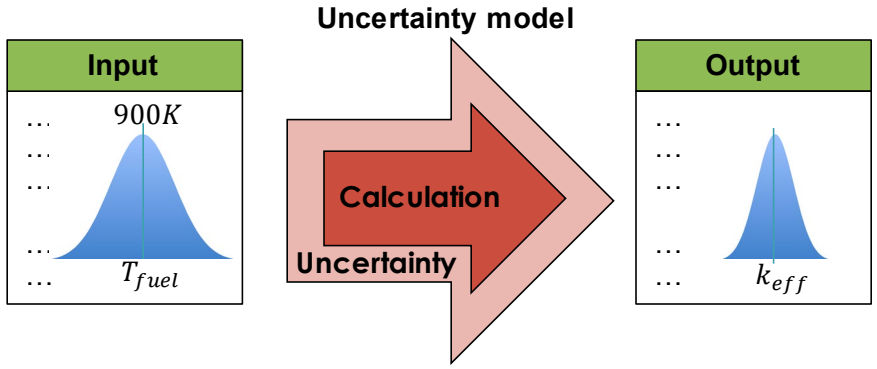
How confident are you in your results?

"A simulation result without some type of uncertainty quantification (UQ) has no value"

- Conventional UQ for simulations includes:
  A. Sensitivity/parametric studies lead to understanding of possible output variation due to due to input data
     "k_{eff} stays 0.1 % of the nominal value for ± 100 K change (uncertainty) in fuel temp"

  B. Comparison of a similar calculation to measurement (validation) leads to understanding of bias
     "SCALE predicts less 2% error in actinides measured from Westinghouse 17x17 UO_2 assemblies, we should expect similar bias in our 17x17 UO_2 actinide predictions."





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Sampler : Complete Uncertainty Quantification in SCALE Simulations

- Leading edge sampling-based uncertainty propagation
  - Every number in the model can have uncertainty which is propagated to uncertainty in outputs
  - Rigorous the best-estimate plus uncertainty (BEPU) methodology
    - Order of 10^5 data variables compared to a few variables in a parametric study)
  - Applicable to
    - Every input (cross section, clad thickness, fuel temperature, decay constant, composition, etc.)
    - Every SCALE sequence (TRITON, Polaris, ORIGEN, MAVRIC, etc.)
  - Capable of handling non-linear problems
    - 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
  - Automated processes for parametric studies

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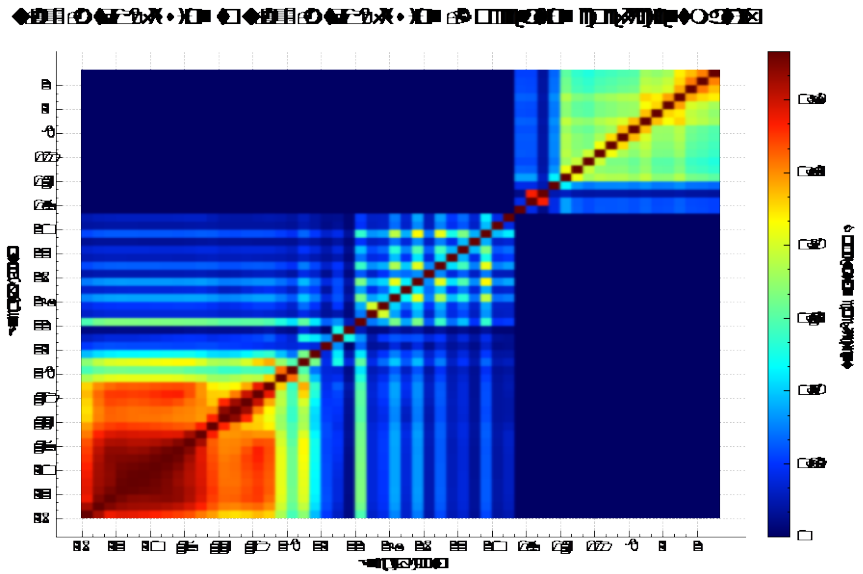
Sampler: Complete Uncertainty Quantification in SCALE Simulations

- Coupled with highly recognized, the most complete, nuclear data covariance libraries, Sampler can propagate uncertainties in depletion calculations using
  - Neutron cross section libraries (ENDF/B VII.1, ENDF/B VIII*)
  - Fission yield libraries
  - Decay libraries (branching rations, decay constants)
  - Kinetics parameters*



- Propagate uncertainties in any model parameter
  - Assign distributions to variables
  - Use variables in place holders #{myvariable}
  - Use SIREN to avoid any modification to input

- Considered a as reference solution for OECD/NEA benchmark for **U**ncertainty **A**nalysis in **M**odeling (UAM) of LWR core calculations

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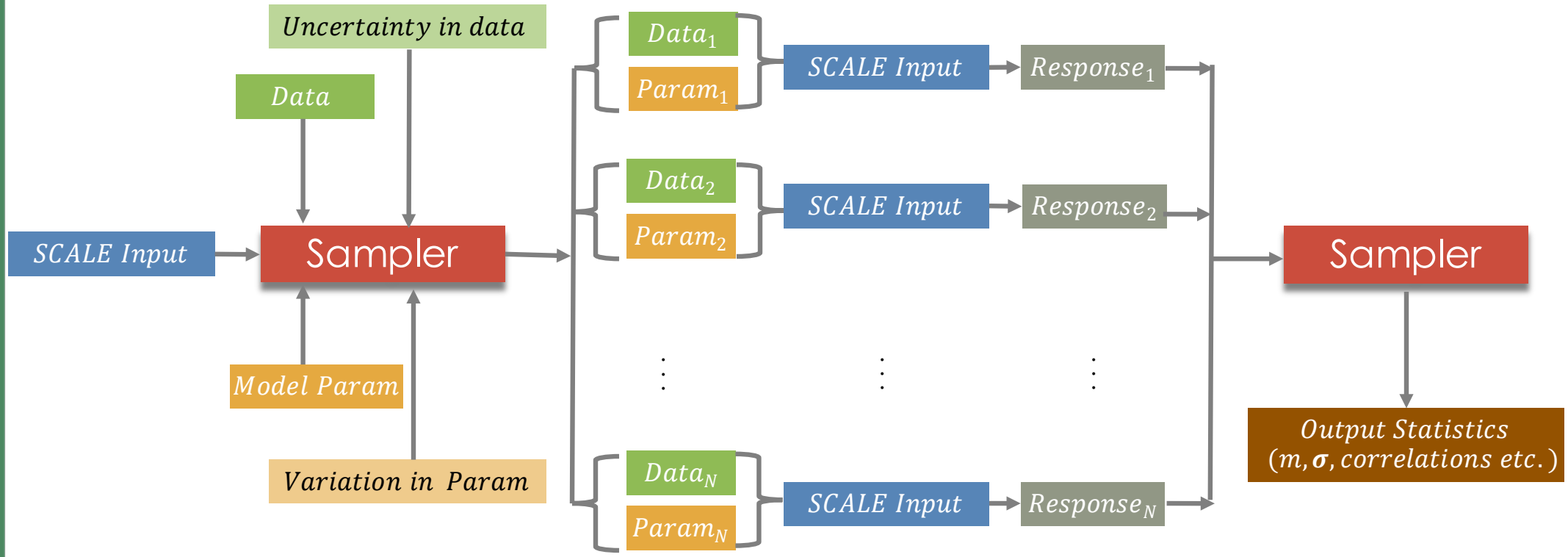
SCALE/SAMPLER Analysis Flow



Uncertainty in Data

- cross sections
- fission yields
- decay
- kinetics*

Variation in Parameters

- uniform
- beta
- normal
- truncated normal

- arithmetic expressions
  mU238=1-mU235
  radius=diameter/2

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Using A SCALE Sequence Input in Sampler

```
=%sampler
read parametric
 variables= radius end
 n_samples= 11 end
end parametric
'
read case[PuH2O]
  import="/myhome/Pu239-h2o_sphere.inp"
end case

read variable[radius]
  distribution=uniform
  minimum=5 maximum=15 value=10
  siren="/csas5/geometry/global_unit/sphere/dimensions/r"
  cases= PuH2O end
end variable

end
```

your original input

```
=%sampler
read parameters
  n_samples=100
  library="broad_n"
  perturb_xs=yes
end parameters

read case[pin]
sequence=polaris
lib "borad_n"
system PWR
geom W17 : ASSM 1 1.26
com c_f3 :UOX=3.0
mat FUEL.1 : c_f3 10.26
pin F :0.41 0.418 0.475
      :FUEL.1 GAP CLAD
state ALL : temp=560
mesh FUEL : nr=3
end sequence
end case

read response [keff]
  type=grep
  regexp="Transport: k-eff = *:scale.number:"
  regexp=":scale.number:"
end response

end
```


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Sampler Perturbation/Propagation of Uncertain Data

Nuclear Data Perturbations

burst.inp | burst.out | burst_sampler.inp | burst

document | SCALE 6.2.1 | Run | View... | Edit...

```
=shell
    cp ${INPDIR}/burst.inp burst.inp
end

=%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
```

Input Parameter Perturbations

```
comp cuox  : UOX 3.5
comp cfuel : WT
             cuox=95.0 GD2O3=5.0
```

```
comp cuox  : UOX #{enr}
comp cfuel : WT
             cuox=100-#{gd} GD2O3=#{gd}
```

place holders

require input modification

```
read variable[enr]
   distribution=normal
   value=3.5
   stdev=0.01
   min=3.45
   max=3.55
end variable
```

siren

no input change

```
read variable[enr]
   distribution=normal
   value=3.5
   stdev=0.01
   min=3.45
   max=3.55
   siren =
"/polaris/composition/uox/enr/value"
end variable
```


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Input Parameter Perturbations

Expression

```
read variable[a]
…
end variable
read variable[b]
…
end variable

read variable[ID]
  distribution=expression
  expression="53-cos(a)+exp(b)/2"
  cases= c1 end
end variable
```

Operator	Operator
+	floor(x)
+	ceil(x)
-	round(x)
-	roundn(x,n)
*	cos(x)
/	sin(x)
%	tan(x)
^	sec(x)
==	csc(x)
!=	cot(x)
<	sinh(x)
>	cosh(x)
<=	tanh(x)
>=	log(x)
and	log10(x)
or	exp(x)
nand	clamp(l,x,u)
xor	inrange(l,x,u)
nor	sgn(x)
abs(x)	sqrt(x)
min(x,…n)	root(x,y)
max(x,…n)	true
avg(x,…n)	false
Sum(x,…n)	if(cond,true,false)
mul(x,…n)	floor(x)
floor(x)	ceil(x)

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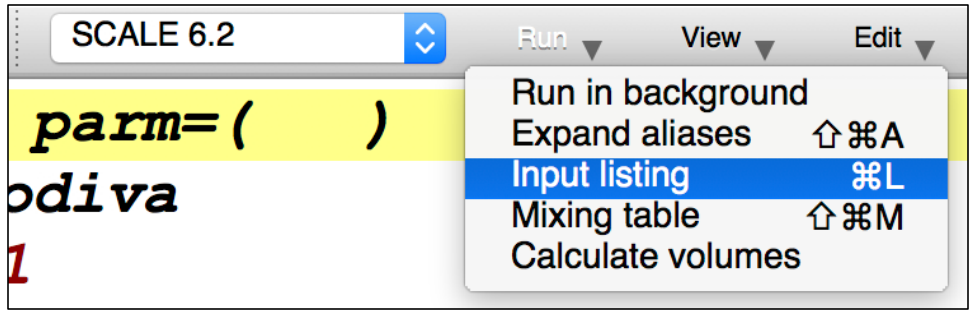
Scale Input Retrieval Engine (SIREN) Overview

- Allow reference of any input field
- Does not require changes to existing input. I.e., no placeholders
- Can replace many inputs with a single statement
- Testing with **InputViewer** and **InputSelector** improves usability
- InputViewer conveniently available via **Fulcrum's Run > Input listing** and cursor context



- Functionality is based on the SCALE input parse tree/directory
  - Analogous to file directory listing

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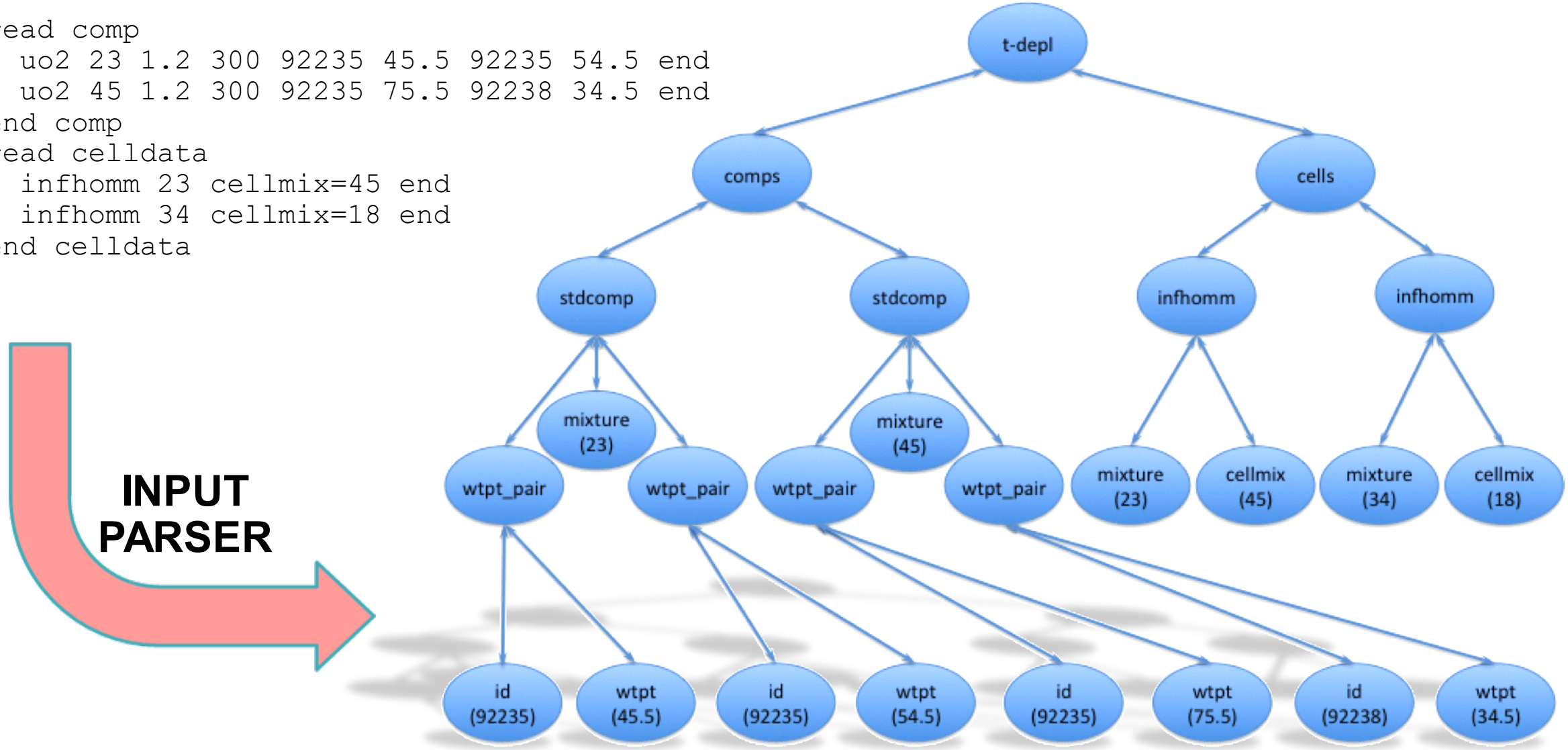
Input Parse Tree Structure Example

```
read comp
  uo2 23 1.2 300 92235 45.5 92235 54.5 end
  uo2 45 1.2 300 92235 75.5 92238 34.5 end
end comp
read celldata
  infhomm 23 cellmix=45 end
  infhomm 34 cellmix=18 end
end celldata
```



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InputViewer | List input fields

- **InputViewer** is a utility located in bin processes the input and returns the tree to the screen as a directory listing
  - Can be more usefully redirected to a file for later reference
- Syntax:

  `SCALE/bin/InputViewer path/to/`*`file.inp`*

- This is *not* like running a SCALE job, it's an interactive process
- SCALE input and InputViewer output provided on next two slides

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KENO comp block listing

```
=csas5 parm=()
godiva
ce_v7.1_endf
read composition
 uranium      1 den=18.742 1 300
              92235 93.7112
              92238 5.2686
              92234 1.0202   end
end composition
```

```
/
/csas5
/csas5/decl(=)
/csas5/decl(csas5)
/csas5/parmdata
/csas5/parmdata/decl(parm)
/csas5/parmdata/assign(=)
/csas5/parmdata/lparen(()
/csas5/parmdata/rparen())
/csas5/title
/csas5/title/word(godiva)
/csas5/xslib
/csas5/xslib/word(ce_v7.1_endf)
/csas5/comps
/csas5/comps/decl(read composition)
/csas5/comps/stdcomp
/csas5/comps/stdcomp/decl(uranium)
/csas5/comps/stdcomp/mixture(1)
/csas5/comps/stdcomp/roth
/csas5/comps/stdcomp/roth/decl(den)
/csas5/comps/stdcomp/roth/assign(=)
/csas5/comps/stdcomp/roth/value(18.742)
/csas5/comps/stdcomp/vf(1)
/csas5/comps/stdcomp/temp(300)
/csas5/comps/stdcomp/wtpt_pair
/csas5/comps/stdcomp/wtpt_pair/id(92235)
/csas5/comps/stdcomp/wtpt_pair/wtpt(93.7112)
/csas5/comps/stdcomp/wtpt_pair
/csas5/comps/stdcomp/wtpt_pair/id(92238)
/csas5/comps/stdcomp/wtpt_pair/wtpt(5.2686)
/csas5/comps/stdcomp/wtpt_pair
/csas5/comps/stdcomp/wtpt_pair/id(92234)
/csas5/comps/stdcomp/wtpt_pair/wtpt(1.0202)
/csas5/comps/stdcomp/term(end)
/csas5/comps/term(end composition)
```


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KENO parameter and geometry blocks

```
read param
  htm=no
end param
read geometry
global unit 1
 sphere 1 1   8.741
end geometry
end data
end
```

```
/csas5/parameters
/csas5/parameters/decl(read param)
/csas5/parameters/htm
/csas5/parameters/htm/decl(htm)
/csas5/parameters/htm/assign(=)
/csas5/parameters/htm/value(no)
/csas5/parameters/term(end param)
/csas5/geometry
/csas5/geometry/decl(read geometry)
/csas5/geometry/global_unit
/csas5/geometry/global_unit/decl(global unit)
/csas5/geometry/global_unit/id(1)
/csas5/geometry/global_unit/sphere
/csas5/geometry/global_unit/sphere/decl(sphere)
/csas5/geometry/global_unit/sphere/mixture(1)
/csas5/geometry/global_unit/sphere/biasid(1)
/csas5/geometry/global_unit/sphere/dimensions
/csas5/geometry/global_unit/sphere/dimensions/r(8.741)
/csas5/geometry/term(end geometry)
/csas5/term(end data)
/csas5/term(end)
```


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Composition examples

Changing isotopic weight percent in a uranium composition:

```
siren="/csas5/comps/stdcomp/wtpt_pair[id='92234']/wtpt"
```

Changing ^{235}U number density in a composition:

```
siren="/csas5/comps/stdcomp[name='u-235']/aden"
```

Changing O-16 number density in two identical compositions:

```
siren="/csas5/comps/stdcomp[name='o-16'][mixture='1',mixture='10']/aden"
```

Changing theoretical density of a UO_2 mixture:

```
siren="/csas5/comps/stdcomp[name='uo2']/roth/value"
```


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InputSelector | Input Field Selection

- InputSelector is an interactive utility, like InputViewer
- Arguments are input file and SIREN statement

```
SCALE/bin/InputSelector ="/csas5/comps/stdcomp[name='u-235']/aden"
```

- InputSelector is invaluable for confirming that SIREN statements will work as intended

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Integration in variable blocks

```
read variable[u234_wo]
   distribution=uniform
   value=1.0202
   min=1
   max=1.0404
   siren="/csas5/comps/stdcomp/wtpt_pair[id='92234']/wtpt"
   cases= godiva end
end variable

read variable[u235_wo]
   distribution=normal
   value=93.7112
   stddev=0.05
   min=93.5
   max=93.9224
   siren="/csas5/comps/stdcomp/wtpt_pair[id='92235']/wtpt"
   cases= godiva end
end variable
```


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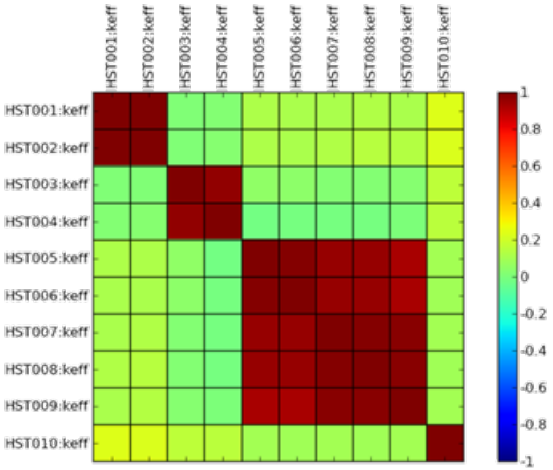
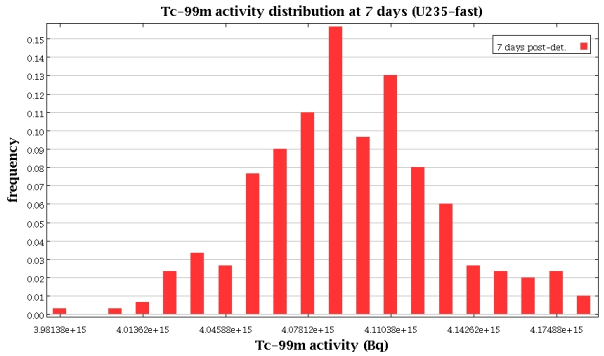
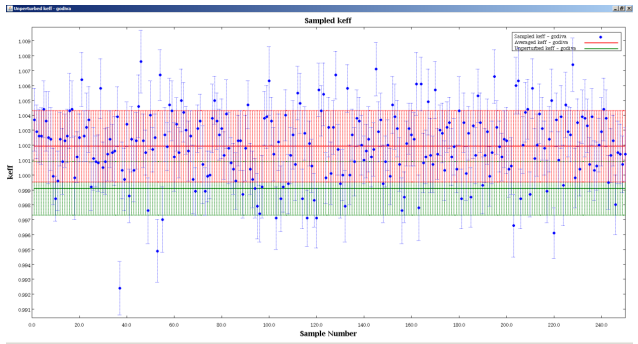
Post Processing

- Creates response tables as requested
  - Average values, correlations and covariances between responses

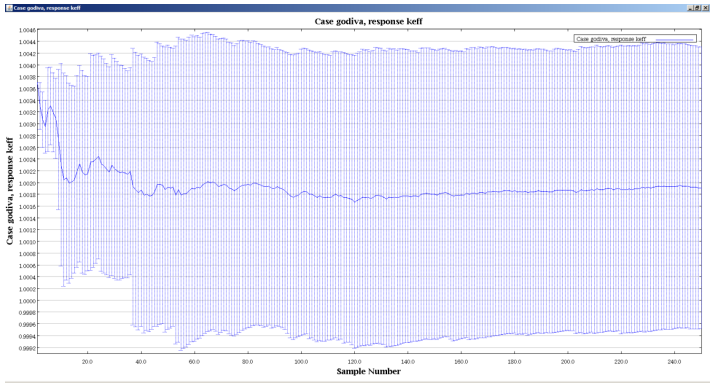




- Correlations created for multiple cases *(e.g. critical experimental correlations)*



- PTP plot files
  - Running averages, histograms, scatter plots



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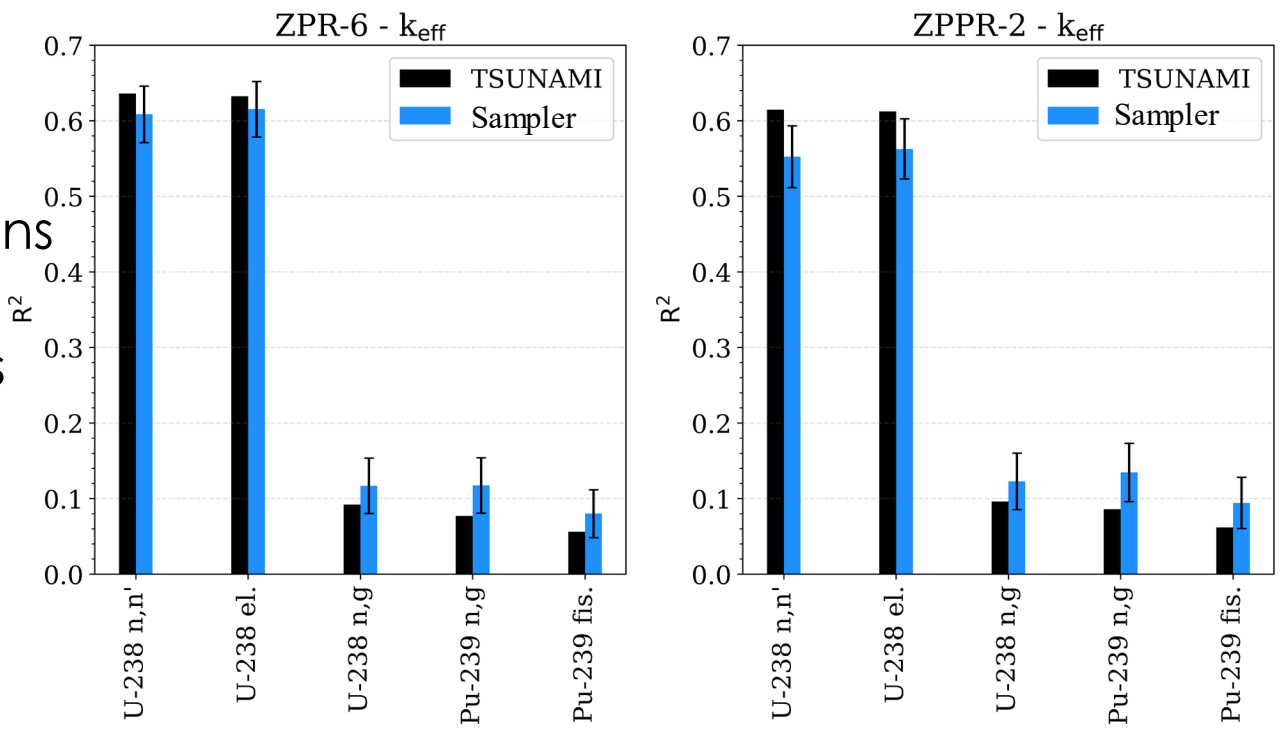
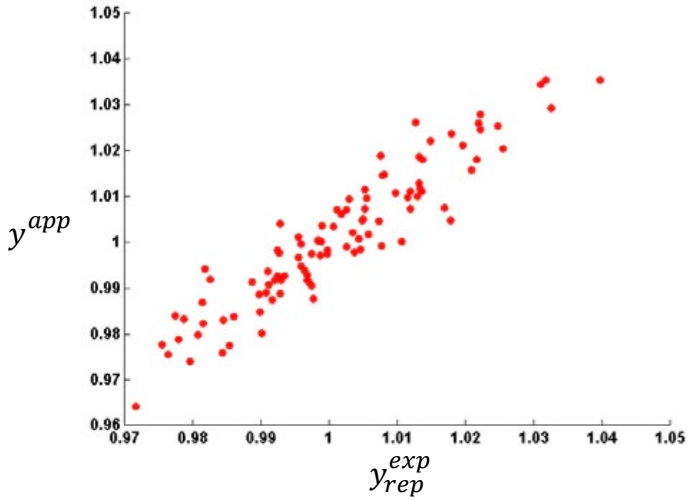
More in SCALE 6.3

- Sensitivity Analysis
  - Identify top contributing nuclide reactions to the output uncertainty.
  - Provide sensitivity indices for parameters other than nuclear data
  - Energy group-wise sensitivity indices



- Similarity Assessment
  - Calculate similarity indices to quantify uncertainty-based similarity between applications and experiments for validation and bias estimate of
    - k_{eff} (c_k)
    - Isotope concentrations (c_{U238}, c_{Pu249})



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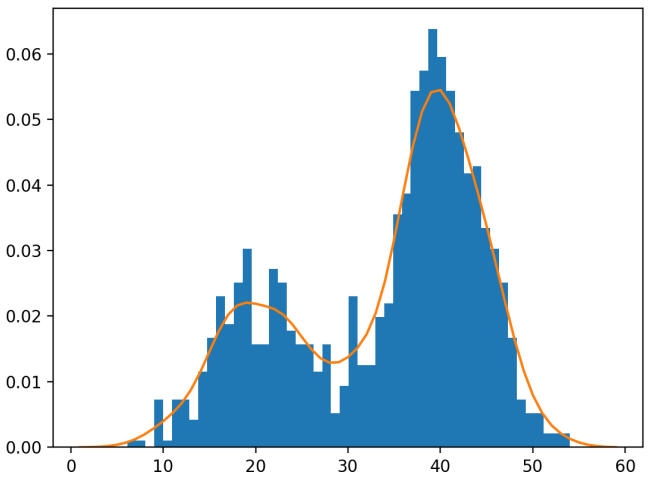
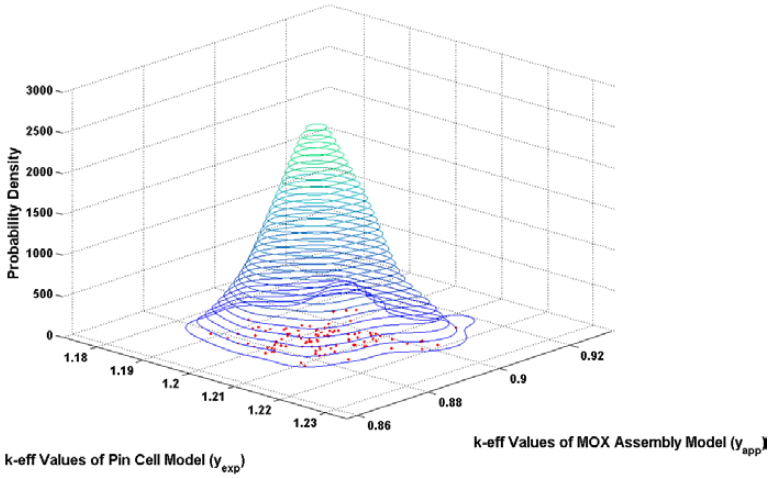
More in SCALE 6.3

- Kernel density estimators:
  - additional analysis of responses with statistical uncertainties (e.g. Mavric or KENO)
  - visualization of response distributions
- User selective and accessible data perturbations:
  - extensive data/response analysis capability for users
  - calculation of user specified correlations (any input to any response)
- CE library perturbation
- Kinetics data perturbation





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