SCALE Uncertainty Quantification Methodology for Criticality Safety Analysis of Used Nuclear Fuel

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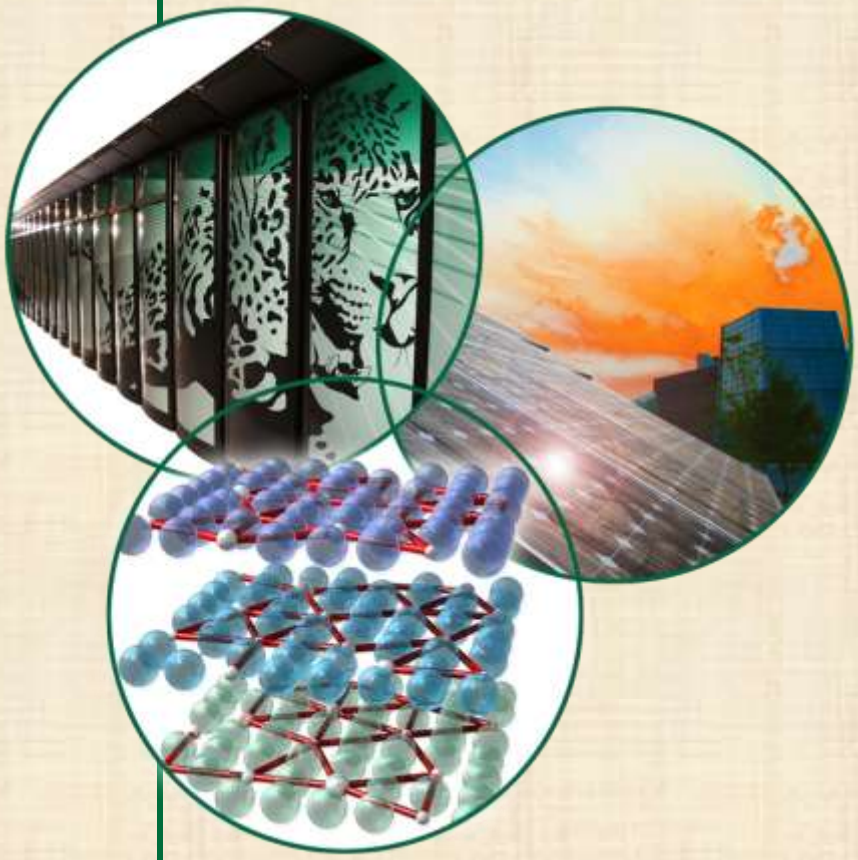

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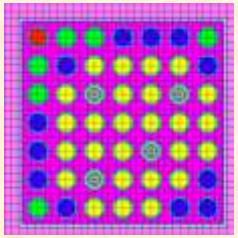
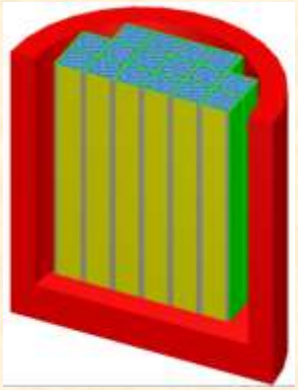
Criticality Analysis of Used Nuclear Fuel (UNF) is Required in Several Areas

- Spent fuel storage pools
- UNF cask design and evaluation
- UNF transportation accident scenarios
- Burnup credit

- ***Uncertainties and biases in computed k_{eff} impact safety margins and economics***

Flowchart of UNF Criticality Analysis





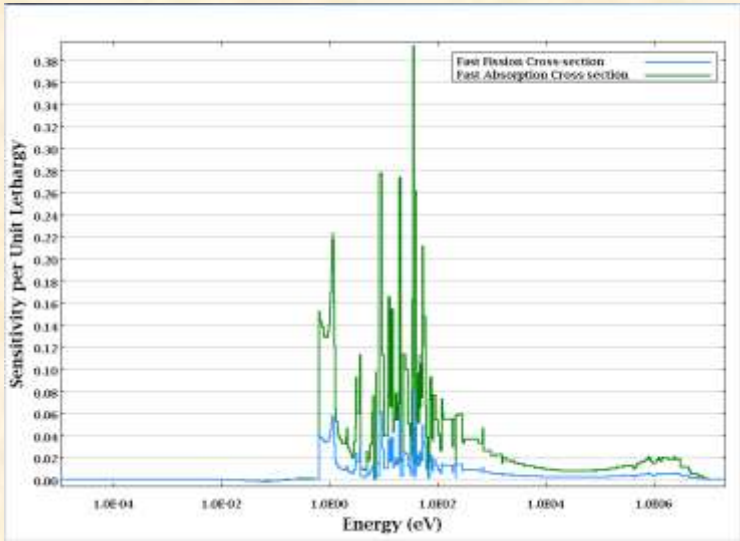
Uncertainty in k_{eff} for UNF Systems Depends on …

- Uncertainties in the criticality calculation, due to
  - Reaction cross sections
- Uncertainties in the depletion calculation for computed burned fuel composition, due to
  - Reaction cross sections
  - Fission product yield data
  - Half-lives
  - Decay branching ratios

SCALE-TSUNAMI Sequences Provide Uncertainty in Criticality Calculations--

- Uses perturbation theory to compute sensitivity coefficients of k_{eff} to nuclear data
- Sensitivity coefficients are folded with nuclear data covariances to obtain k_{eff} uncertainty

sensitivity profile



-- *BUT*, TSUNAMI Can Not Determine Uncertainty in Depletion Calculation of UNF Composition

SCALE-6.2 Includes Two Approaches for Sensitivity/Uncertainty Analysis

- **Perturbation Approach with TSUNAMI Modules**
  - Current capability based on multigroup transport codes: TSUNAMI-3D, TSUNAMI-2D, TSUNAMI-1D
  - Also, new methodology based on continuous energy Monte Carlo is being developed for SCALE-6.2
- ***NEW!* Statistical Sampling with Sampler Module**
  - SCALE-6.2 includes new module ***Sampler*** for statistical uncertainty analysis of any SCALE sequence
  - Makes random perturbations in input data; response uncertainty computed by statistical analysis of output response distribution

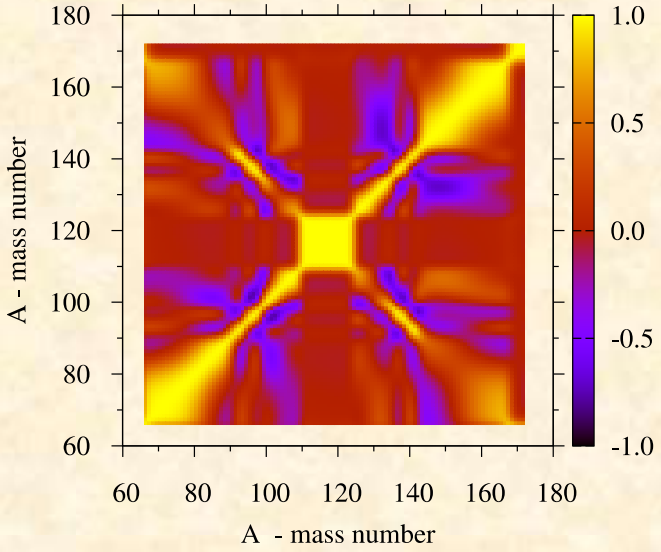
Features of Sampler Module

- A “super-sequence” that executes any Scale sequence using perturbed data parameters
- Performs perturbations in
  - multigroup XS’s, self-shielding data (Bondarenko factors, pointwise XS’s)
  - Fission yields, decay data
  - Model parameters: initial concentrations, dimensions, temperatures, etc.
- Automated statistical analysis for selected responses
- Parallel computations using MPI or OpenMP

Features of Sampler Module, *continued*

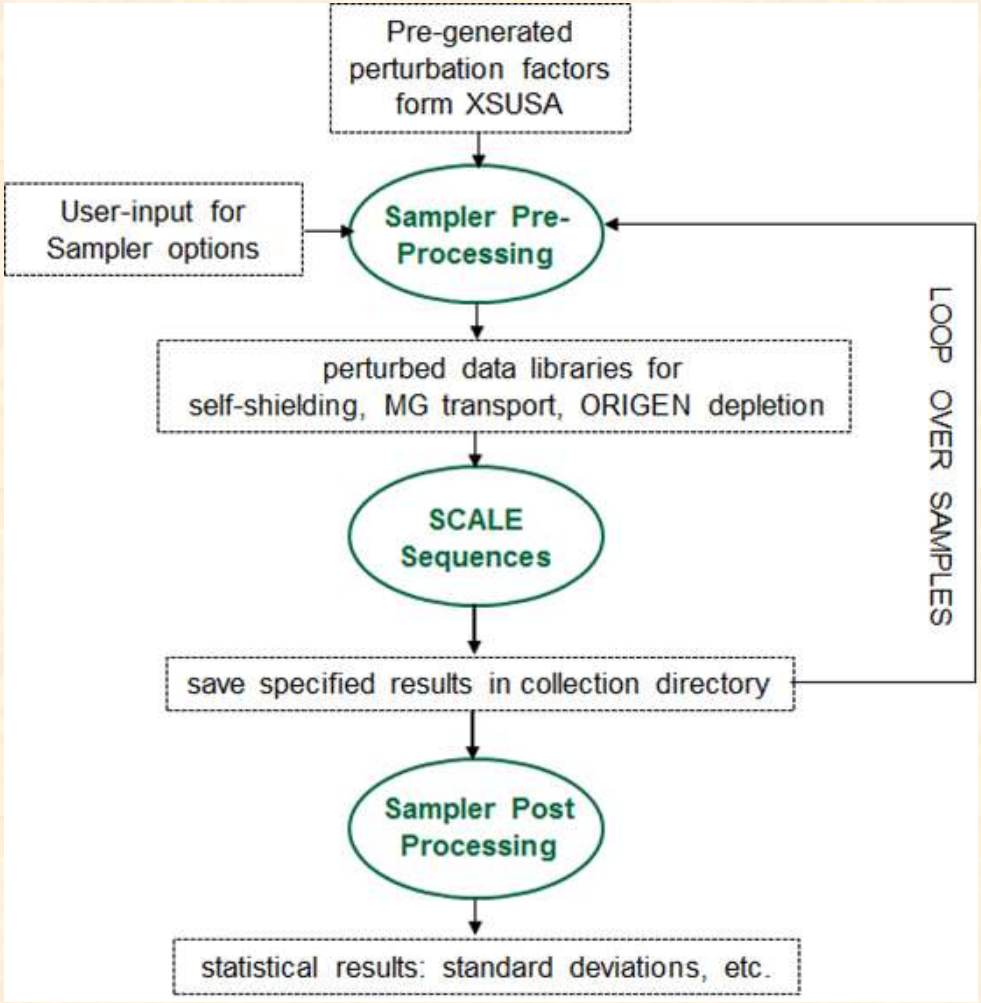
- Uses pre-generated libraries of perturbation factors computed by code such as XSUSA
  - XS perturbations sampled from SCALE Cov library
  - Decay perturbations from ENDF/B-VII uncertainties
  - Yield perturbations sampled from yield covariances developed by ORNL

U238 yield correlation matrix with chain-yield constraints(*)

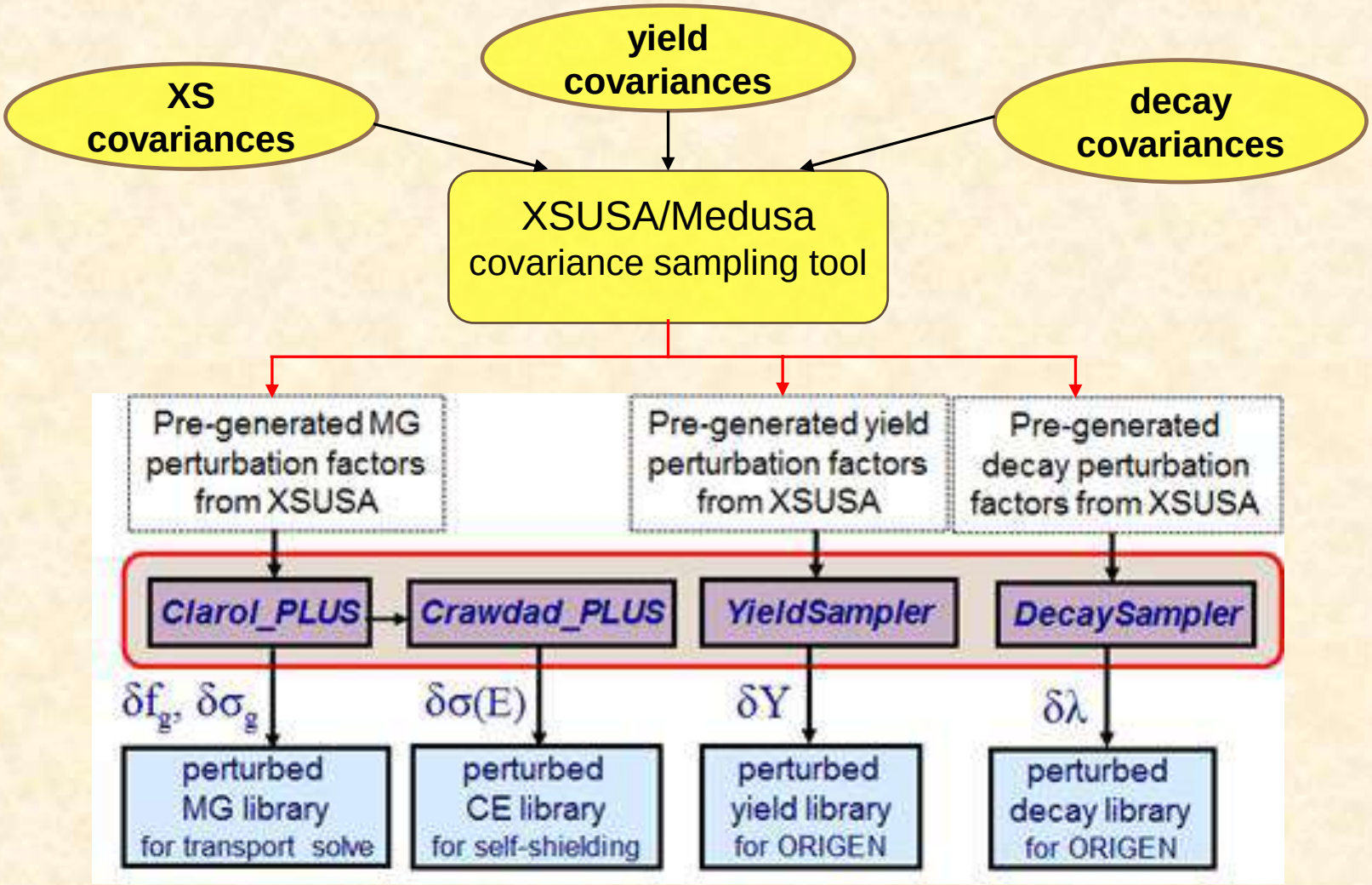


(*) from Pigni et al

Overview of Sampler Calculations



Generation of Perturbed Data Libraries



Typical Sampler Input for Assembly Burnup:

```
=sampler
read parameters
    n_samples=200    perturb_XS=yes
    perturb_yield=yes
    library="v7-252"
end parameters
read case
 sequence=t-depl
     (SCALE input for  t-depl sequence)
 end sequence
end case
read responses[nucs]
     type=origen_nuclides
     nuclides = u-235 pu-239 sm-149  end
end responses
read responses[homxs]
     type=triton
     data= kinf  sigma_fission
     sigma_absorption end
end responses
end
```

Sampler Output

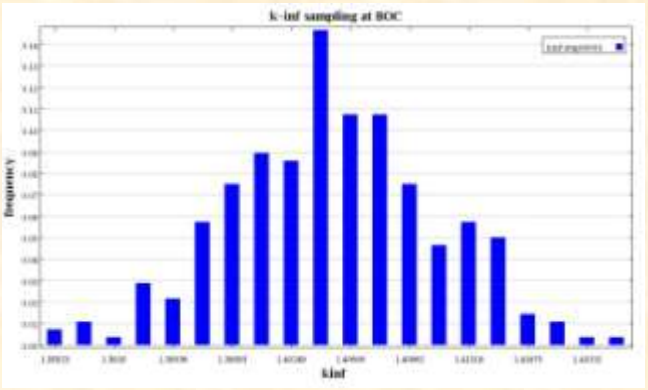
- Sampling results for following types of responses
  - K eigenvalue; (XSDRN, NEWT, KENO)
  - Microscopic reaction rates by nuclide (Newt/Opus)
  - Homogenized/collapsed macro cross sections (Newt)
  - Nuclide concentrations, activities (ORIGEN)
  - Decay heat, radiotoxicity, photon sources (ORIGEN)
  - Shield responses: doses, radiation damage, etc. (Mavric)
- Each response at every time-step includes:
  - Frequency distributions as histogram plot file
  - Mean values and standard deviations in CSV file
  - Results of chi-squared normality test for each response
  - Covariance and correlation coefficients between responses

TMI-1 PWR Assembly Depletion for UAM Benchmark

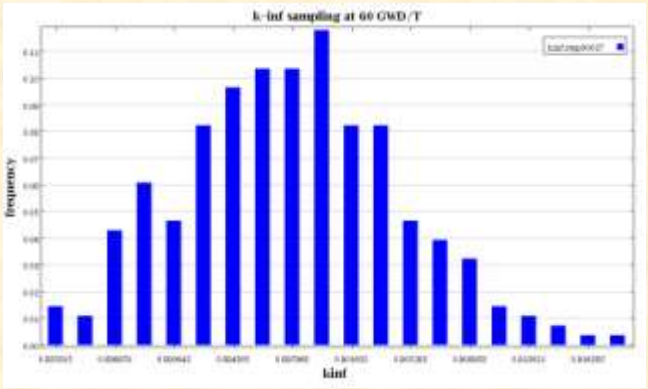
- TMI PWR Assembly, 0-60 GWD/T burnup; 0-100 years cooling
  - Mean values, standard deviations, correlation coefficients computed for 10-GWD/T time steps; and decay times of 1, 3, 5, 10, 50, 100 years after shut down
- Responses considered
  - Time-dependent K_{inf}
  - U235, U238, Pu239, Pu40, Pu241 fission and capture rates
  - Collapsed/homogenized 2-group macro cross sections (XS), for Σ_a, Σ_f, $\nu\Sigma_f$, $\Sigma_{1\rightarrow2}$, D
  - Time-dependent concentrations for 15 actinides and 36 fission products

Frequency Distributions of Representative Output Responses

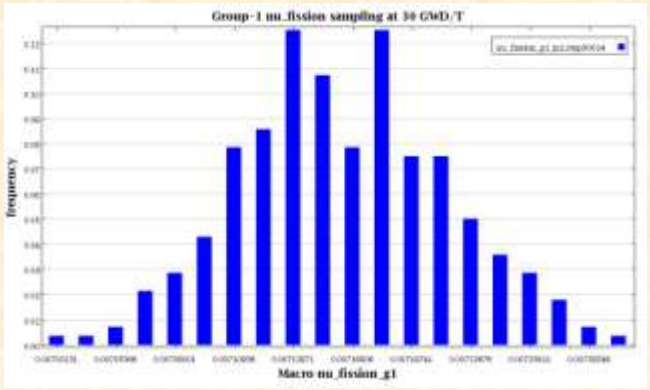
K_{inf} ; 0 GWD/T



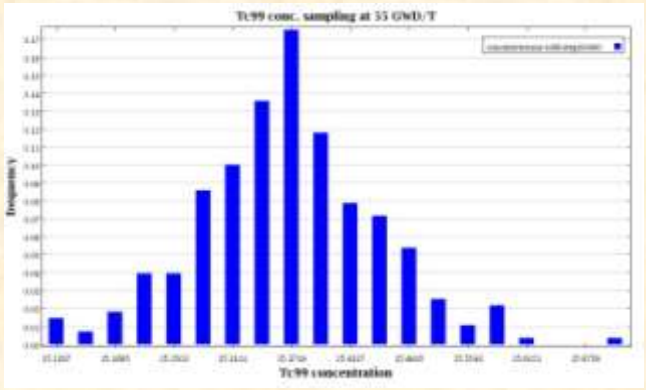
K_{inf} ; 60 GWD/T



Group 1 nu-fission ; 30 GWD/T



Tc-99 concentration; 50 GWD/T



Chi Squared Normality Tests Are Done For Every Response

Example for time-dependent Cs-135 concentration

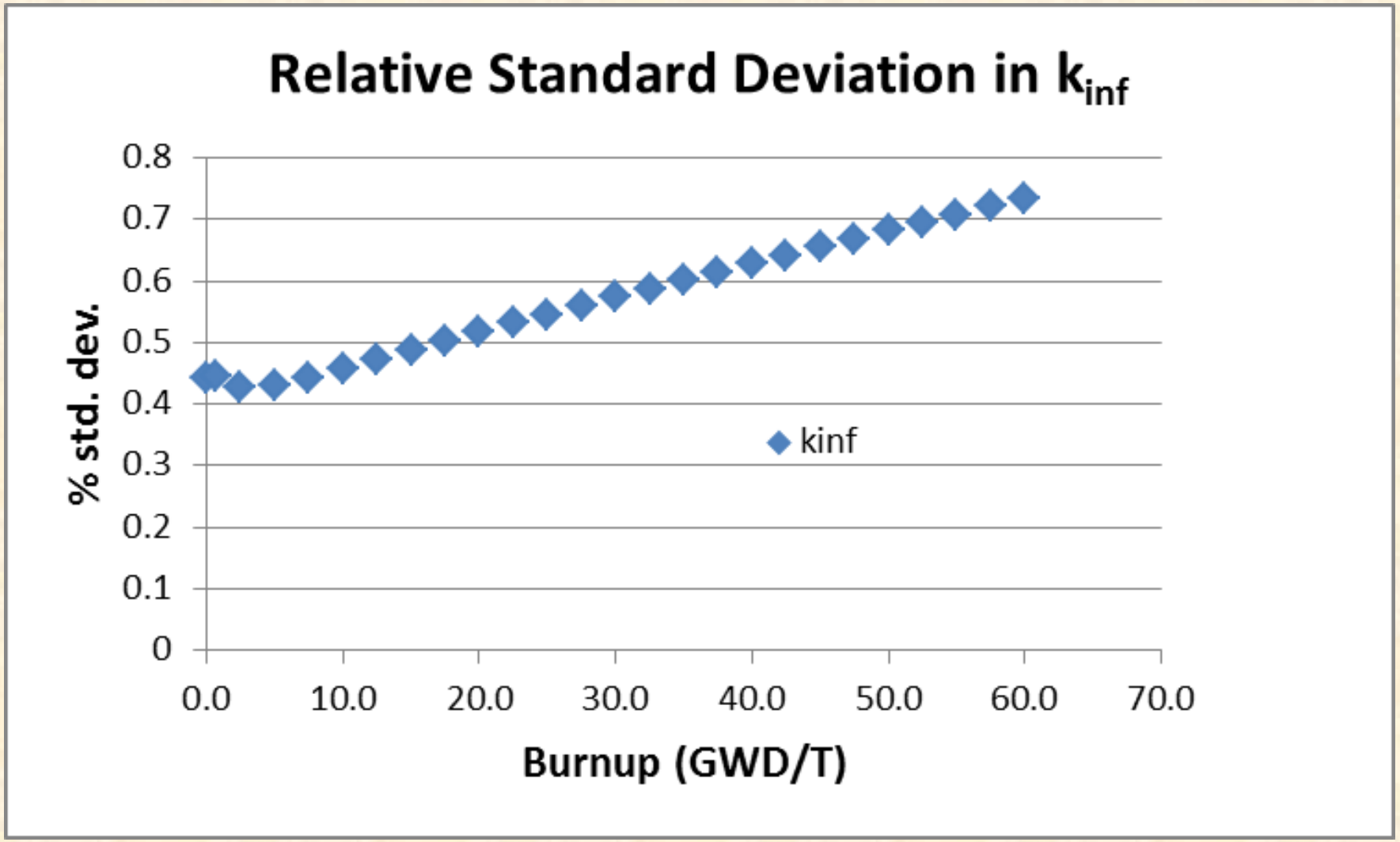
time step	Normal?
27	passed
28	passed
29	failed
30	failed
31	passed
32	passed

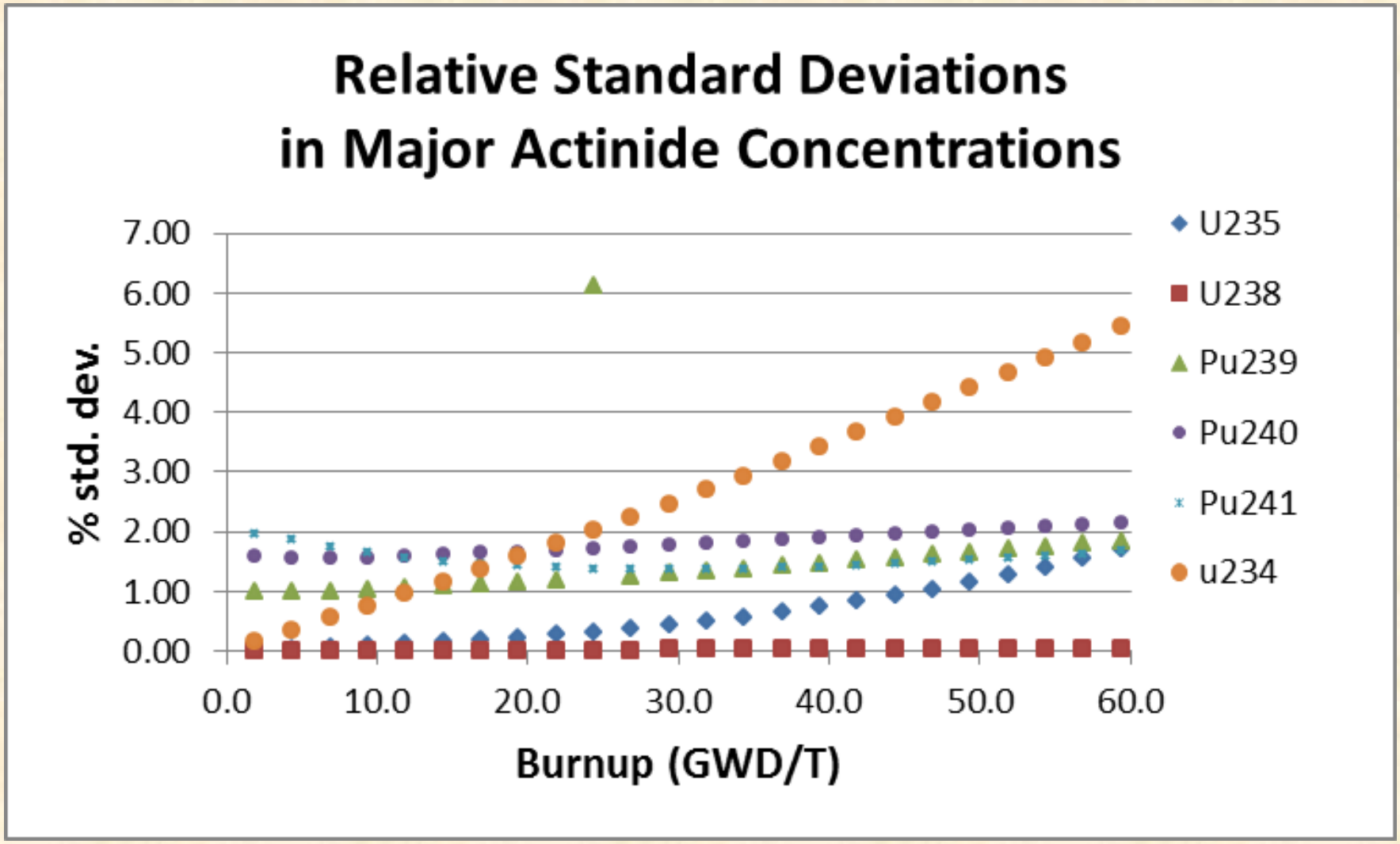
SUMMARY

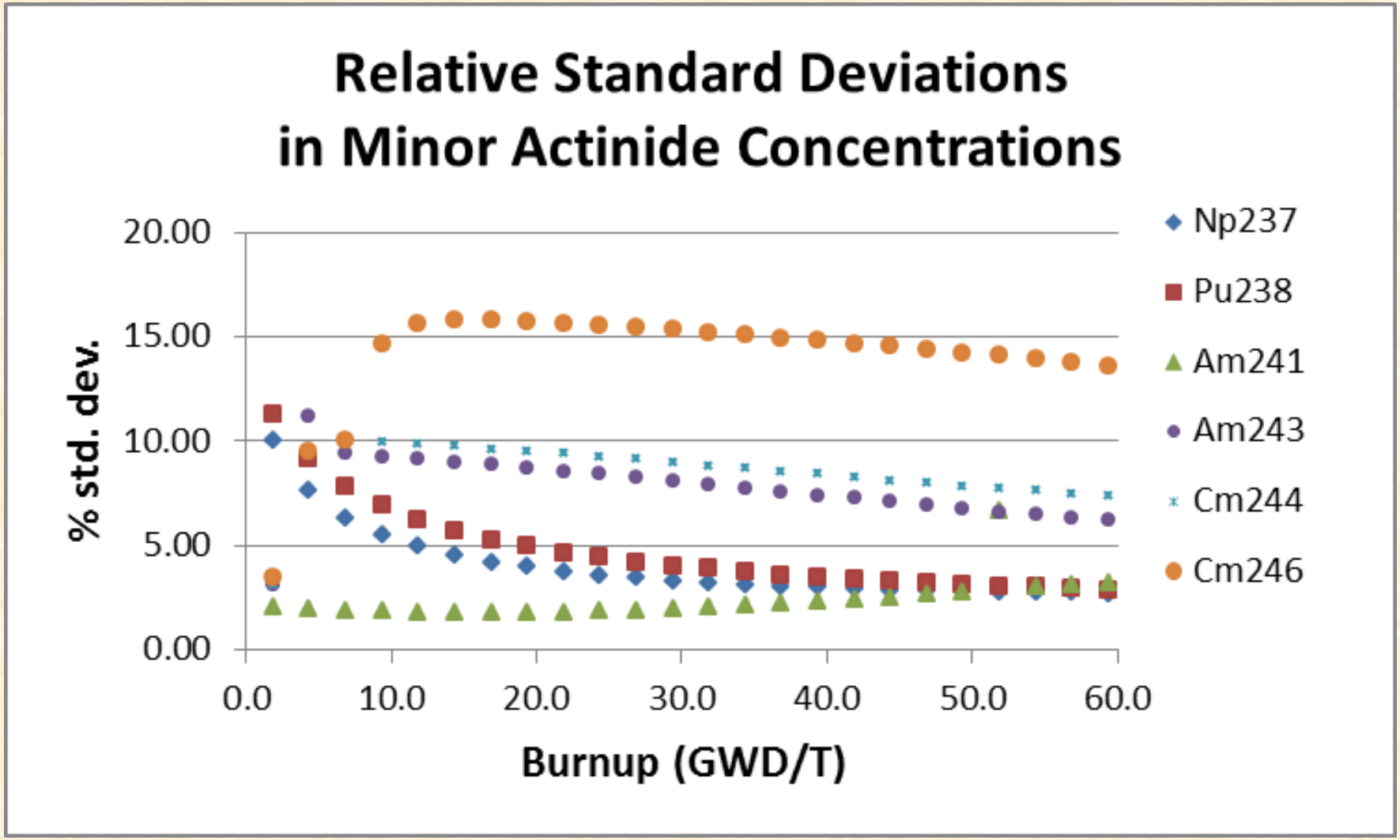
- SCALE-6.2 will include new capabilities and data for uncertainty analysis
  - ENDF/B-VII.1 covariances for many nuclides
  - Fission yields and decay data covariances
  - Sampler statistical uncertainty analysis module
- Sampler is comprehensive super-sequence that greatly extends SCALE uncertainty analysis

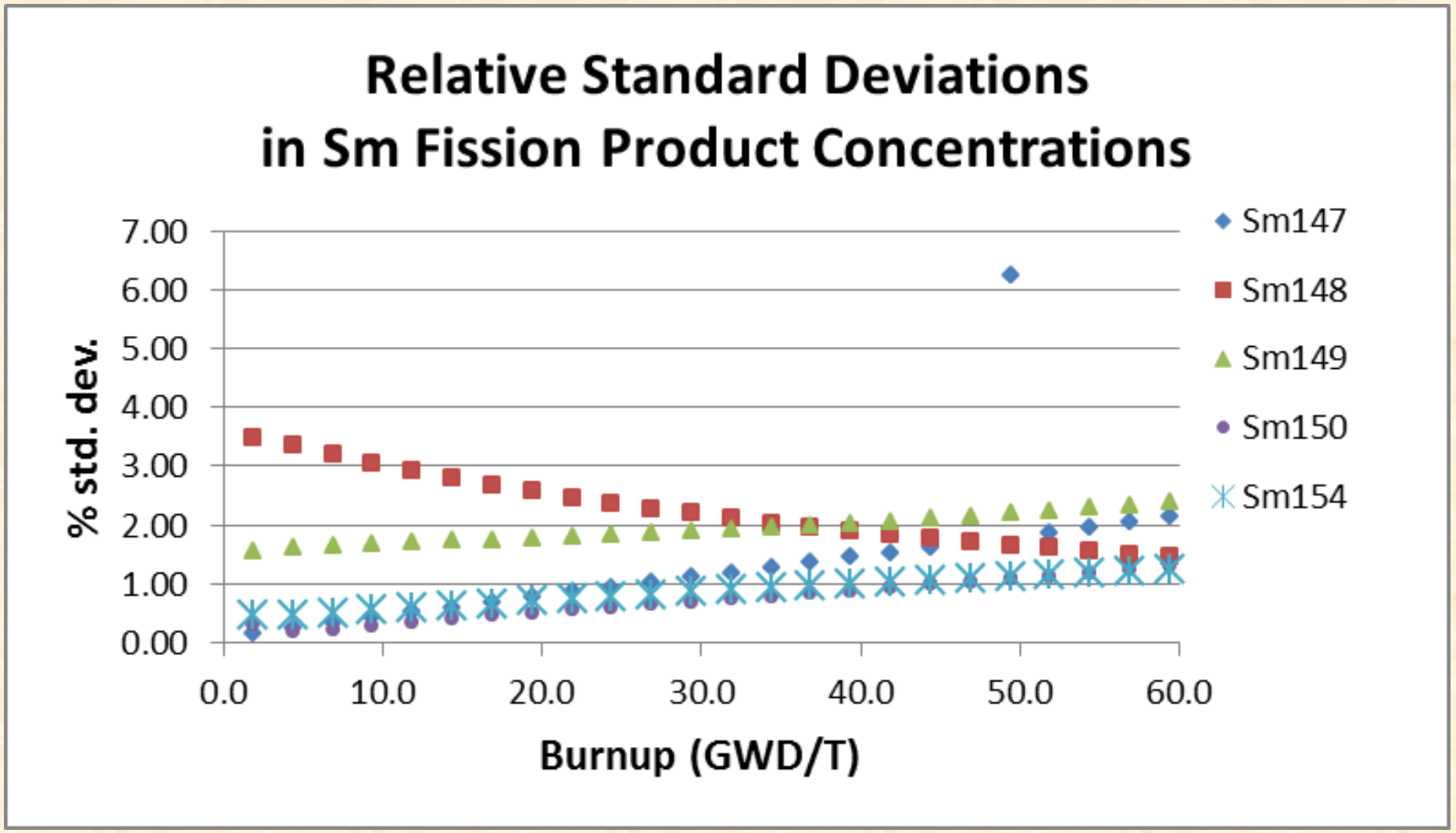
Application of Sampler to Obtain Uncertainty in Burned Fuel Properties

- Sampler used 280 random samples for the "*input data vector*" = { multigroup XS's, Bondarenko factors, pointwise XS's, fission product yields }
  - Perturbations obtained from sampling SCALE covariance libraries
- SCALE TRITON sequence calculation performed for each random sample of the input data vector
  - Newt 2D transport module with 252 group ENDF/B-VII.0
  - Bonami/CENTRM/PMC self-shielding
  - ORIGEN depletion with ~2000 isotopes
- Computations done in parallel with MPI on Linux cluster with 80 CPUs


Relative Standard Deviation in k_{inf}
% std. dev.
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
kinf
0.0
10.0
20.0
30.0
40.0
50.0
60.0
70.0
Burnup (GWD/T)


Relative Standard Deviations
in Major Actinide Concentrations
% std. dev.
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
0.0
10.0
20.0
30.0
40.0
50.0
60.0
Burnup (GWD/T)
U235
U238
Pu239
Pu240
Pu241
u234


Relative Standard Deviations
in Minor Actinide Concentrations
% std. dev.
20.00
15.00
10.00
5.00
0.00
0.0
10.0
20.0
30.0
40.0
50.0
60.0
Burnup (GWD/T)
Np237
Pu238
Am241
Am243
Cm244
Cm246


Relative Standard Deviations
in Sm Fission Product Concentrations
% std. dev.
7.00
6.00
5.00
4.00
3.00
2.00
1.00
0.00
0.0
10.0
20.0
30.0
40.0
50.0
60.0
Burnup (GWD/T)
Sm147
Sm148
Sm149
Sm150
Sm154