Sampler Sensitivity Indices

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Uncertainty and sensitivity analysis methods

Uncertainty analysis	What is the uncertainty of our output quantity due to uncertainties in the input?
Sensitivity analysis	Which input parameter is significant for the observed output uncertainty?

Perturbation theory

Random sampling approach

Uncertainty and sensitivity analysis methods

- **Perturbation theory**:
  - Determine sensitivity coefficients of output with respect to the input cross sections
  - Application of "sandwich formula": multiply coefficient vector with covariance matrix
  - **Sensitivity analysis is byproduct**

→ **SCALE/TSUNAMI**

- **Random sampling approach**:
  - Sampling of input cross sections based on covariance matrices
  - Run calculation with perturbed input cross sections
  - Statistical analysis of output: mean value, standard deviation, etc.

→ **SCALE/SAMPLER**

How do we determine which nuclide reactions are important for the observed output uncertainty in case of random sampling?

Squared multiple correlation coefficient R²

$$R_A^2 = \overline{\boldsymbol{\rho}}_{Y,A}^T \cdot \overline{\overline{\boldsymbol{C}}}_{AA}^{-1} \cdot \overline{\boldsymbol{\rho}}_{Y,A}.$$

with

$$\overline{\boldsymbol{\rho}}_{Y,A} = \begin{pmatrix} \rho(Y, \Sigma_{\mathrm{A},1}) \\ \dots \\ \rho(Y, \Sigma_{A,k}) \end{pmatrix}$$

Y: Output quantity,
A: Nuclide reaction, e.g. U-235 fission
$\Sigma_{A,i}$: Sampled cross section of A, energy group i,
ρ: Pearson sample correlation coefficient,
$\boldsymbol{C}_{A,A}^{-1}$: Inverse sample correlation matrix of A.

Requirement:
Sample size **>>** number of sampled cross sections for A (often number of energy groups)

- R^2 is determined for all reactions of all requested nuclides
- Ranking according to size reveals top contributors

Squared multiple correlation coefficient R^2

Characteristics

- $0 \leq R^2_A \leq 1$
- $R^2_A = 0$, if Y is not correlated to any of the cross sections of A
- $R^2_A = 1$, if Y is a linear function of only the cross sections of A
- R^2_A only captures linear effects

Interpretation

- R_A^2: expected amount by which the total output variance would be reduced in case the true values of the cross sections of nuclide reaction A would become known
- R_A^2 captures the contribution to the output variance caused by the uncertainties of nuclide reaction A including the fraction of uncertainties that it has in common with other nuclide reactions due to dependencies

Semi-partial squared multiple correlation coefficient SPC²

Squared semi-partial multiple correlation coefficient SPC²

$$SPC_A^2 = R_{tot}^2 - R_B^2$$

- R^2_{tot} is the total squared multiple correlation coefficient between the output Y and all input cross sections
- R^2_B is the squared multiple correlation coefficient between the output Y and the complementary group of cross sections B
- **Requirement: sample size larger than <u>total</u> number of sampled input parameters**

Interpretation

- SPC_A^2 describes the variance of the output quantity which is expected to remain when the true values of the complementary parameter group Σ_B became known
- SPC_A^2 is the fraction of the variance of Y that is caused by all parameters, Σ_A and Σ_B, less the fraction that is only caused by the complementary group Σ_B

Application in Sampler

- Sampler calculation:
  - E.g. based on perturbations using 56g covariance library
  - Choose sample size >> 56

```
=sampler

read parameters
n_samples = 1000
library="xn252v7.1"
run_cases= yes
perturb_xs = yes
perturb_geometry = no
mg_factors_library="/path/to/samples-dir"

end parameters

read response[keff]
[…]
end response









read case[pin]
sequence=t-newt
[…]
end sequence
end case
end
```

Application in Sampler

- Sampler calculation:
  - E.g. based on perturbations using 56g covariance library
  - Choose sample size >> 56
- Sensitivity analysis:
  - Request R^2 and or SPC^2 analysis for all relevant nuclides
  - Add path to coverx library
  - Identify important nuclide reactions by analyzing ranking
- Note:
  - Check confidence interval and significance bound
  - Values cannot be compared to TSUNAMI top contributors, but there is a qualitative overlap of top contributing nuclide reactions

```
=sampler

read parameters
n_samples = 1000
library="xn252v7.1"
run_cases= yes
perturb_xs = yes
perturb_geometry = no
mg_factors_library="/path/to/samples-dir"
coverx_library = "/path/to/covlib"
end parameters

read response[keff]
[…]
end response

read sensitivity
type = r2
nuclides = uo2 zirc4 h2o helium end
responseids = keff end
end sensitivity

read sensitivity
type = spc2
nuclides = u-235 u-238 h-1 end
responseids = keff end
end sensitivity

read case[pin]
sequence=t-newt
[…]
end sequence
end case
end
```

Response of interest

New sensitivity block

Application in Sampler

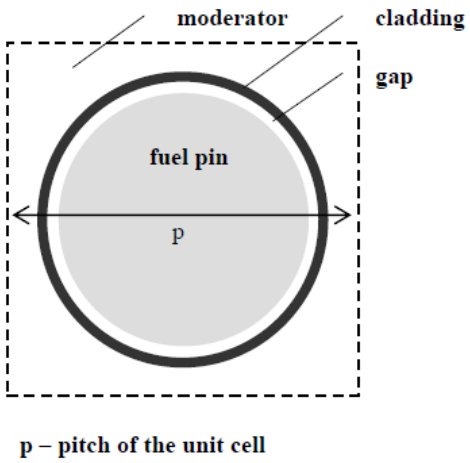
Squared multiple correlation coefficient R^2

```
  pin:keff
   Nuclide        Reaction            R^2       95% conf.       95% sign.
     u-235   prompt.fiss.n   4.024177e-01   4.086680e-02   3.129315e-02
     u-238         n,gamma   2.995198e-01   3.182379e-02   7.392106e-02
     u-238         elastic   2.348276e-01   2.628225e-02   5.776727e-02
...
```

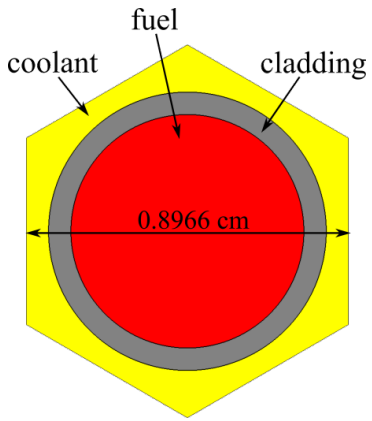
Semi-partial squared multiple correlation coefficient SPC^2

```
  pin:keff
 Total R^2     9.956444e-01
 95% conf.     5.880898e-04
   Nuclide        Reaction           SPC^2       95% conf.
     u-235   prompt.fiss.n   2.217445e-01   2.461164e-02
     u-238         n,gamma   5.174938e-02   6.722998e-03
     u-235             chi   4.845597e-02   6.338892e-03
...
```

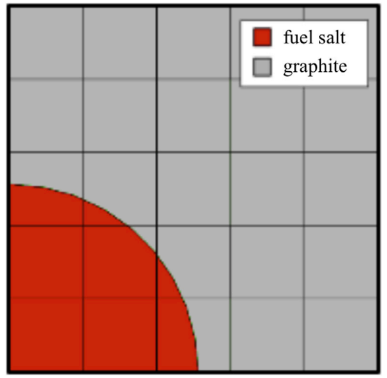
Examples of application



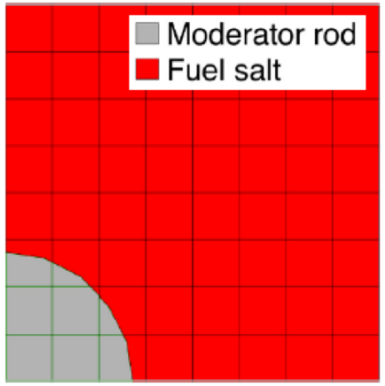
LWR pin



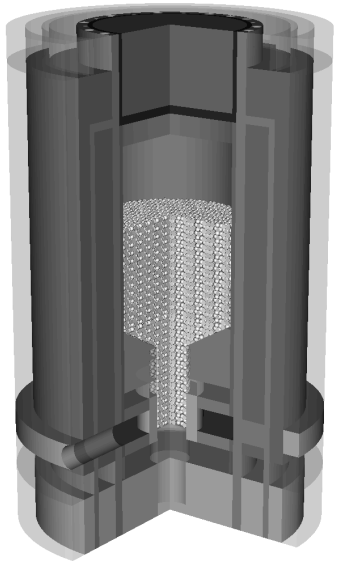
SFR pin



MSR cell:
graphite moderated*



MSR cell:
ZrH moderated*

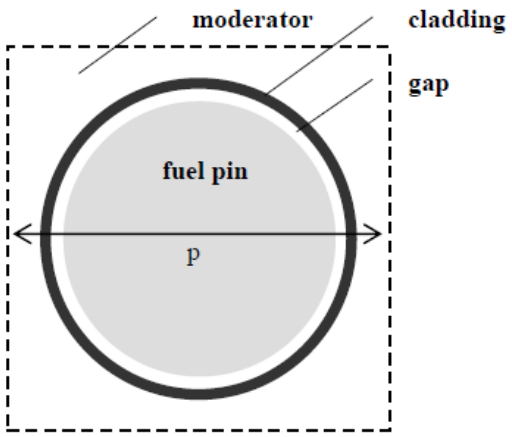


HTR-10

*courtesy of B. Betzler

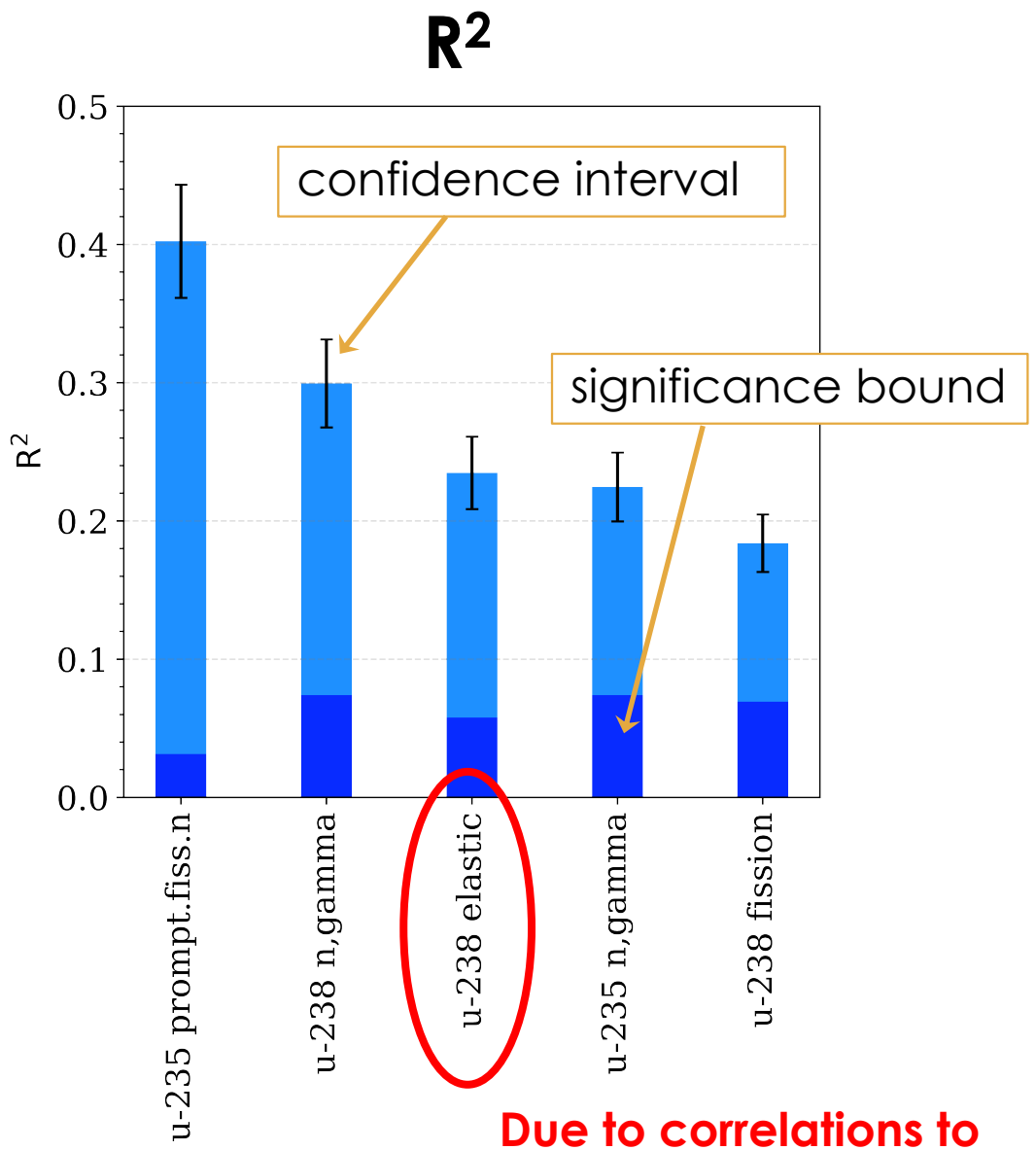
LWR pin cell

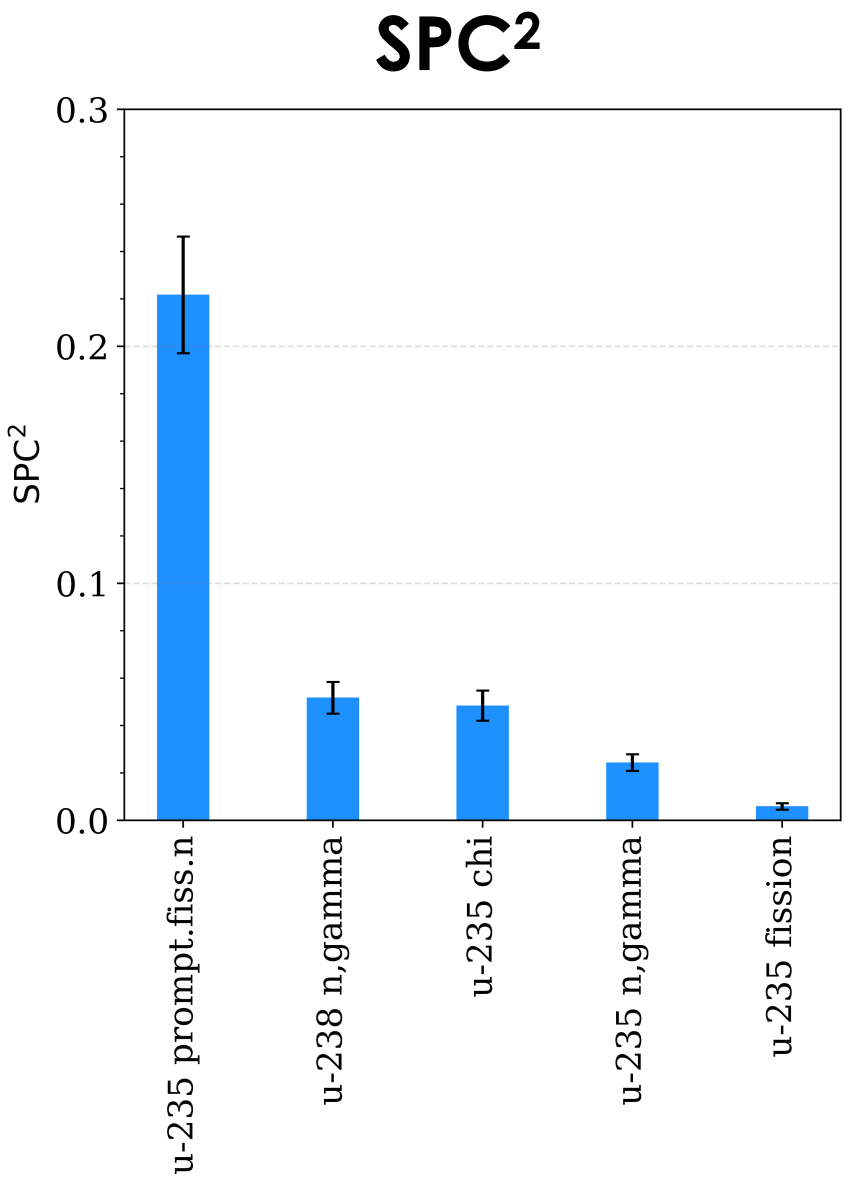
- Neutron transport: NEWT
- Cross section library: **252g** ENDF/B-VII.1
- Covariance library: **56g** SCALE 6.2
- Sample size: 1,000
- Eigenvalue uncertainty: **0.54%**



p – pitch of the unit cell

LWR pin cell



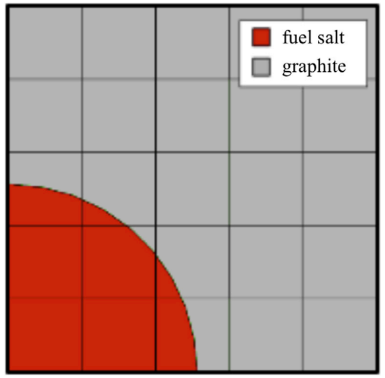


Due to correlations to U-238 n,g and inel.

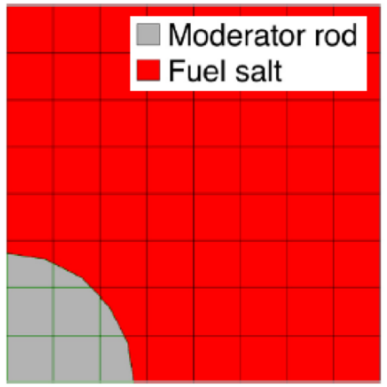
MSR pin cells

- Neutron transport: NEWT
- Cross section library: **252g** ENDF/B-VII.1
- Covariance library: **56g** SCALE 6.2

  Sample size: 1,000



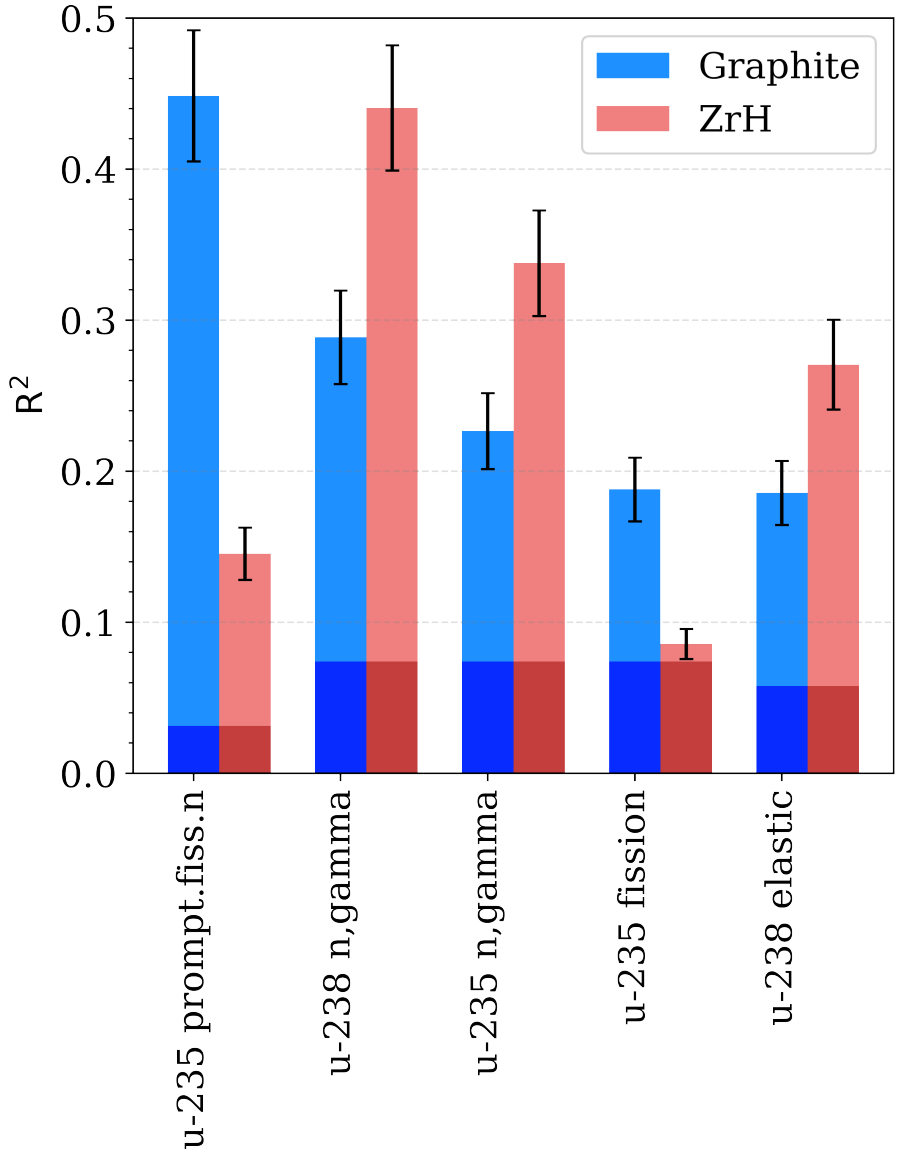
Graphite-moderated MSR unit cell*



MSR unit cell with fuel salt moderated by ZrH rods*

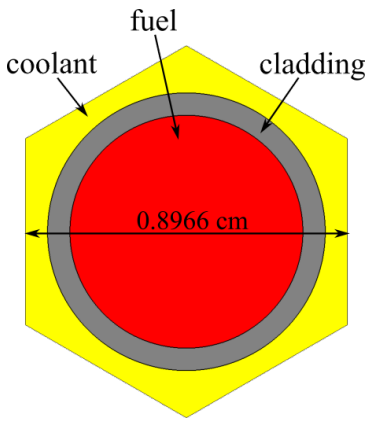
$\Delta k_{inf}/k_{inf}$ Graphite	$\Delta k_{inf}/k_{inf}$ ZrH
0.55%	0.74%

R^2



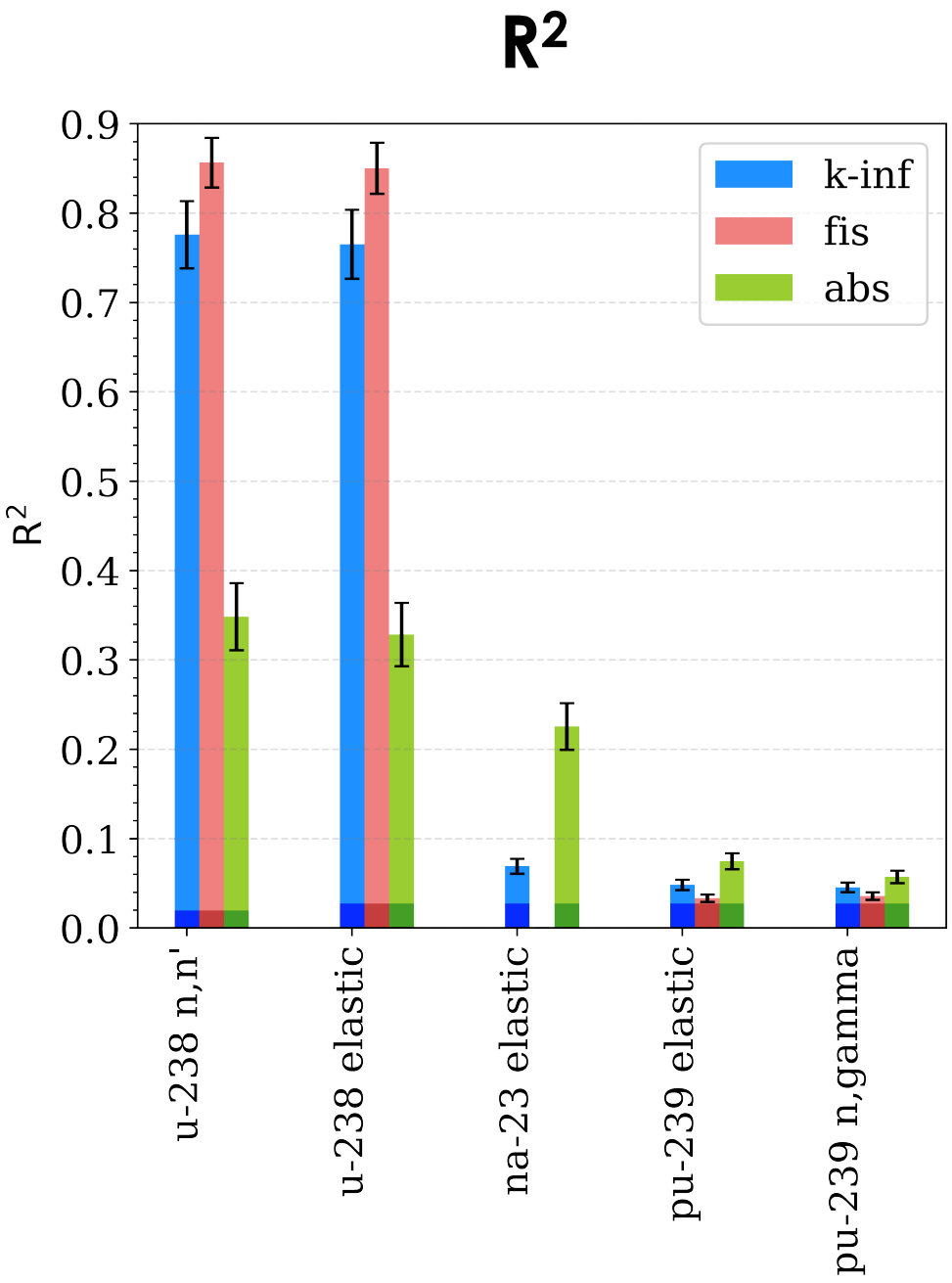
*courtesy of B. Betzler

SFR pin cell



- Neutron transport: NEWT
- Cross section library: **302g** ENDF/B-VII.1
- Covariance library: **17g** SCALE 6.2
- Sample size: 1,000
- Quantities of interest: eigenvalue, collapsed macroscopic fission and absorption cross section

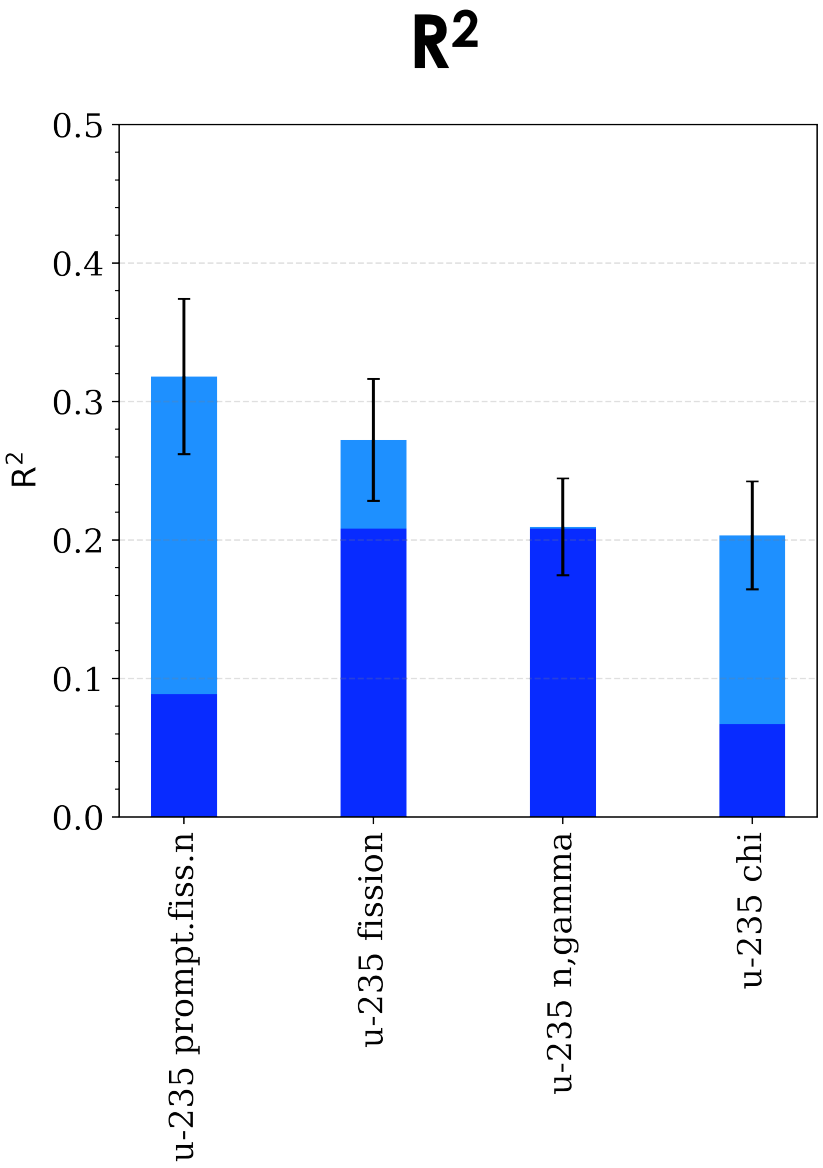
$\Delta k_{inf}/k_{inf}$	$\Delta\Sigma_{fis}/\Sigma_{fis}$	$\Delta\Sigma_{abs}/\Sigma_{abs}$
1.50%	1.54%	0.98%

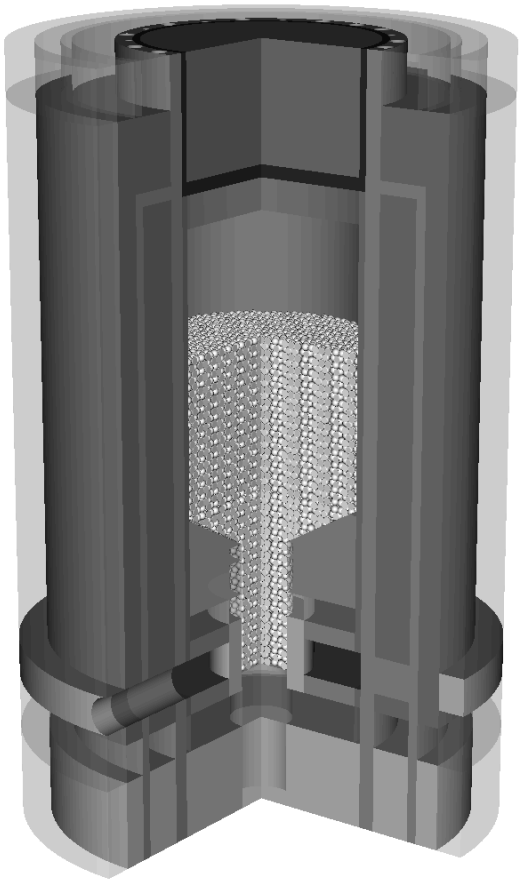


HTR-10

- Model: Full experiment
- Neutron transport: KENO
- Cross section library: **252g** ENDF/B-VII.1
- Covariance library: **56g** SCALE 6.2
- Sample size: **350**
- Eigenvalue uncertainty: **0.68%**

Only four statistically significant R^2 values obtained
→ Increase sample size to lower significance bound and to decrease confidence interval





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Summary and Outlook

- Important nuclides for the output uncertainty with Sampler can be determined in terms of two sensitivity indices
- Sample size plays a major role for confidence and significance of these values
- Indices cannot directly be compared to TSUNAMI output
- Sensitivity analysis will be available in SCALE 6.3

- Extension of sensitivity analysis to time-dependent quantities is planned
- Enabling direct comparison with TSUNAMI is planned
- Feedback from SCALE beta users is very welcome!

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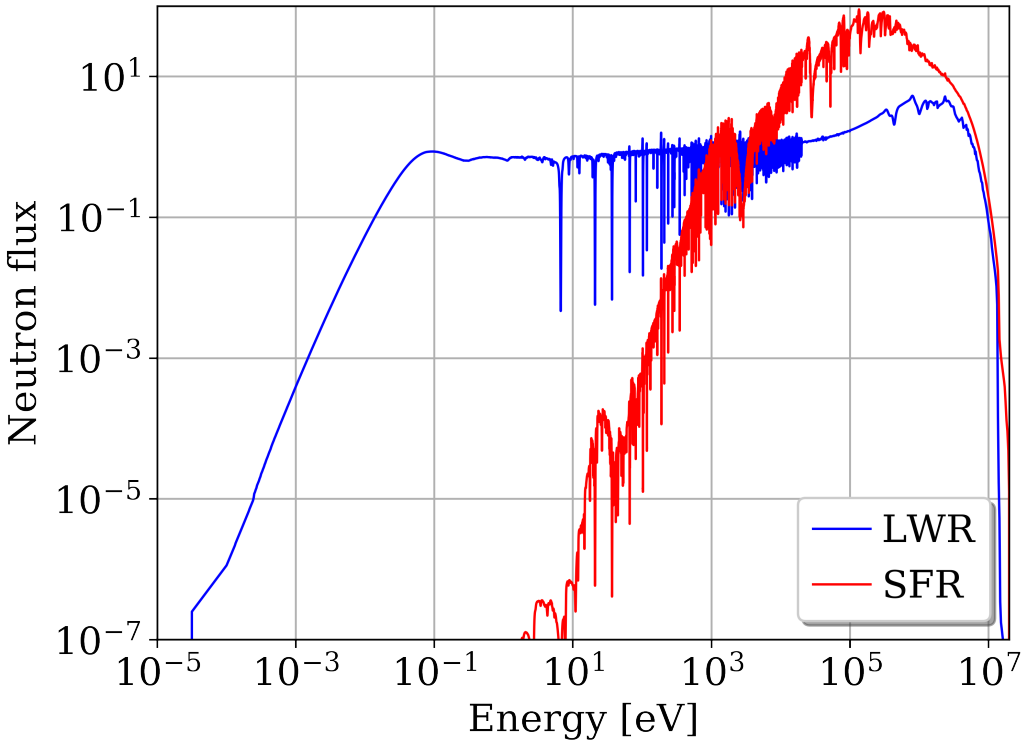
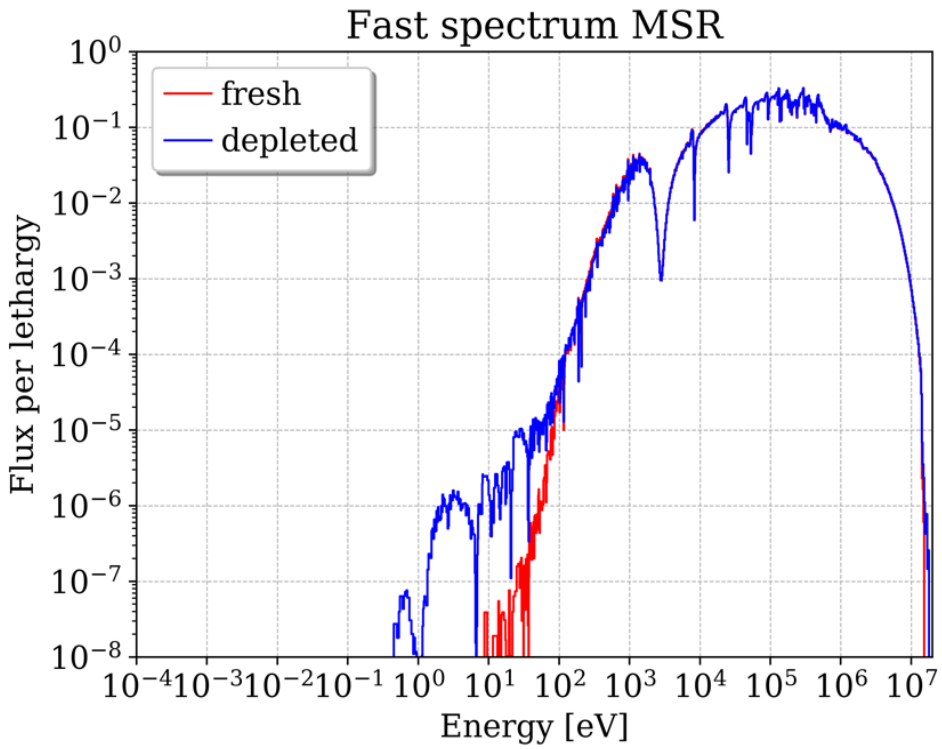
Backup

LWR, SFR and fast MSR flux

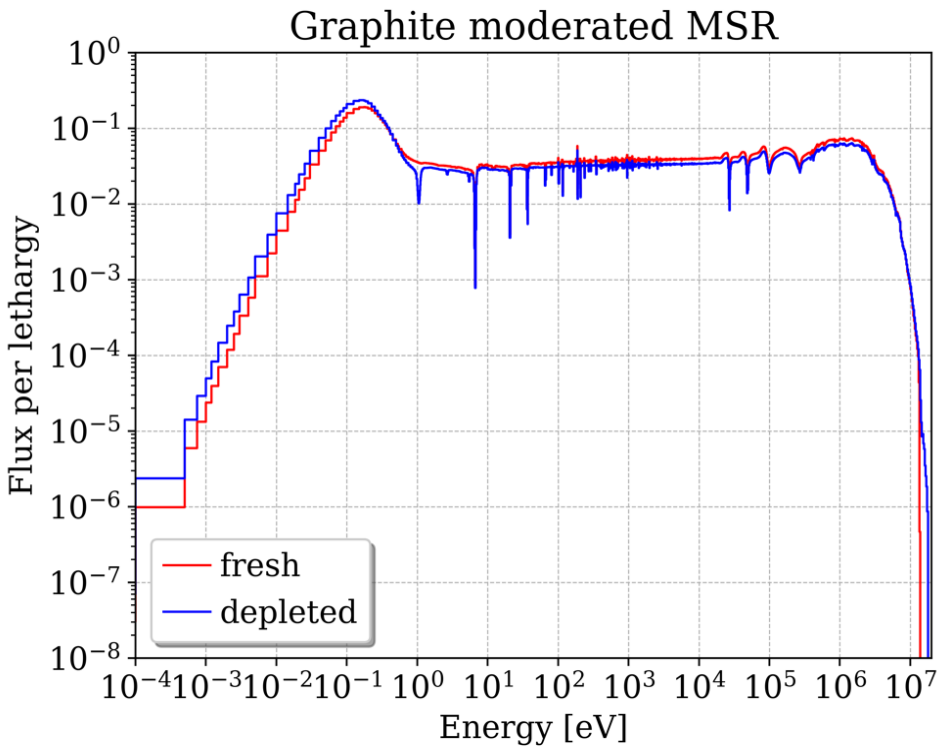
Normalized neutron flux

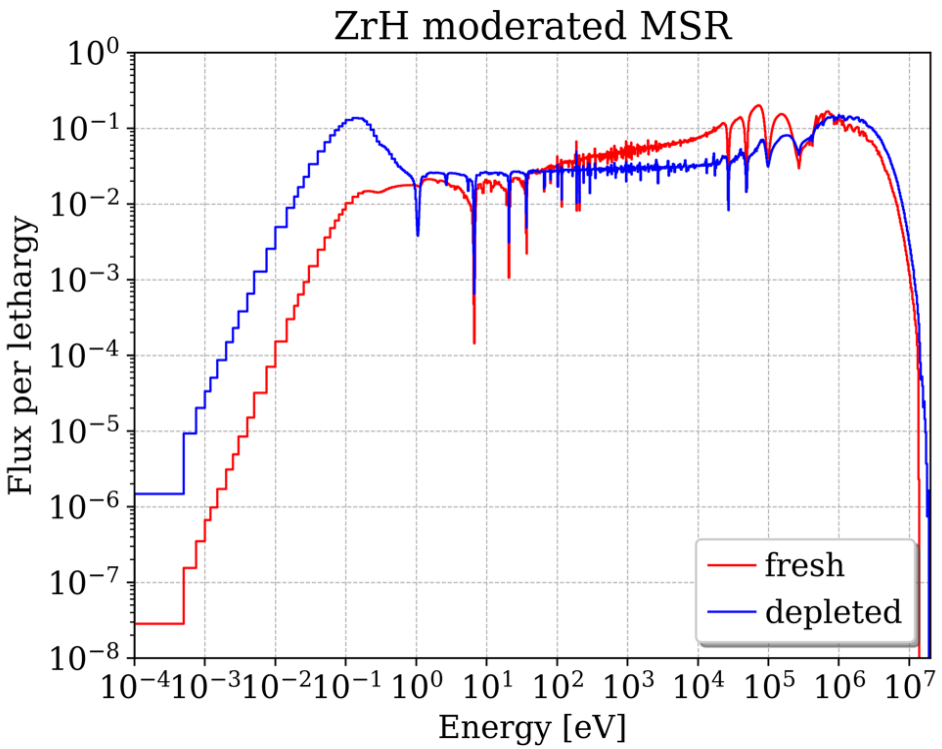




Moderated MSR flux

Normalized neutron flux

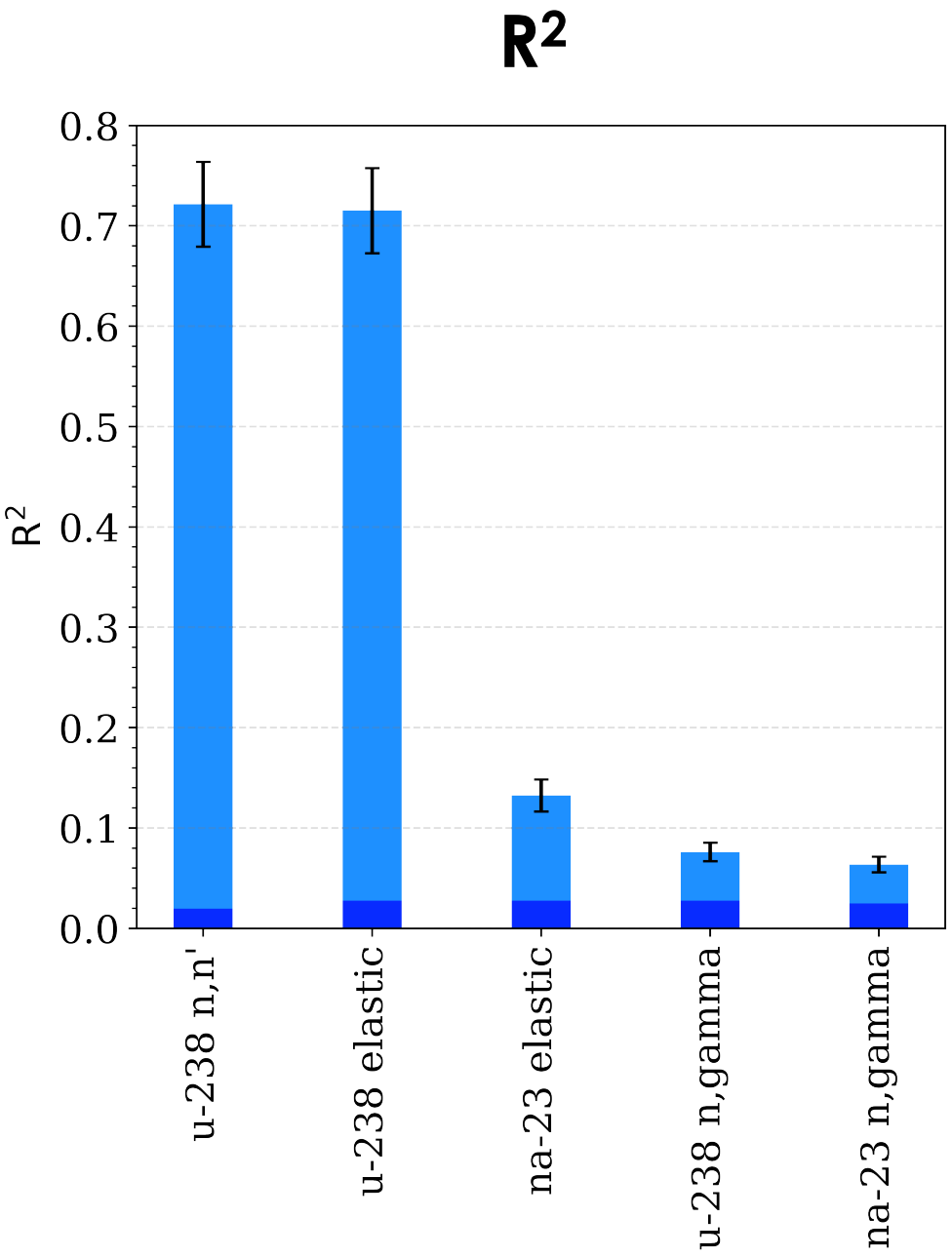




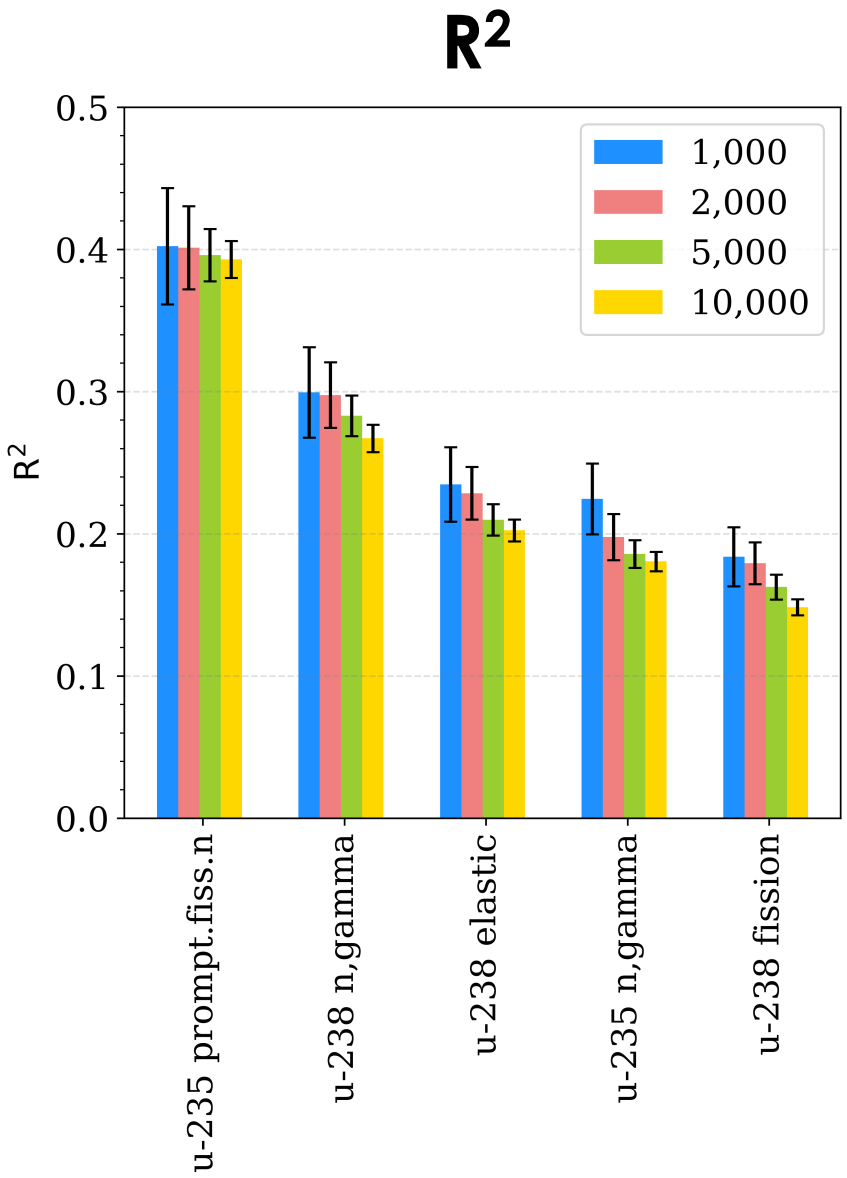
MSR cell – fast spectrum

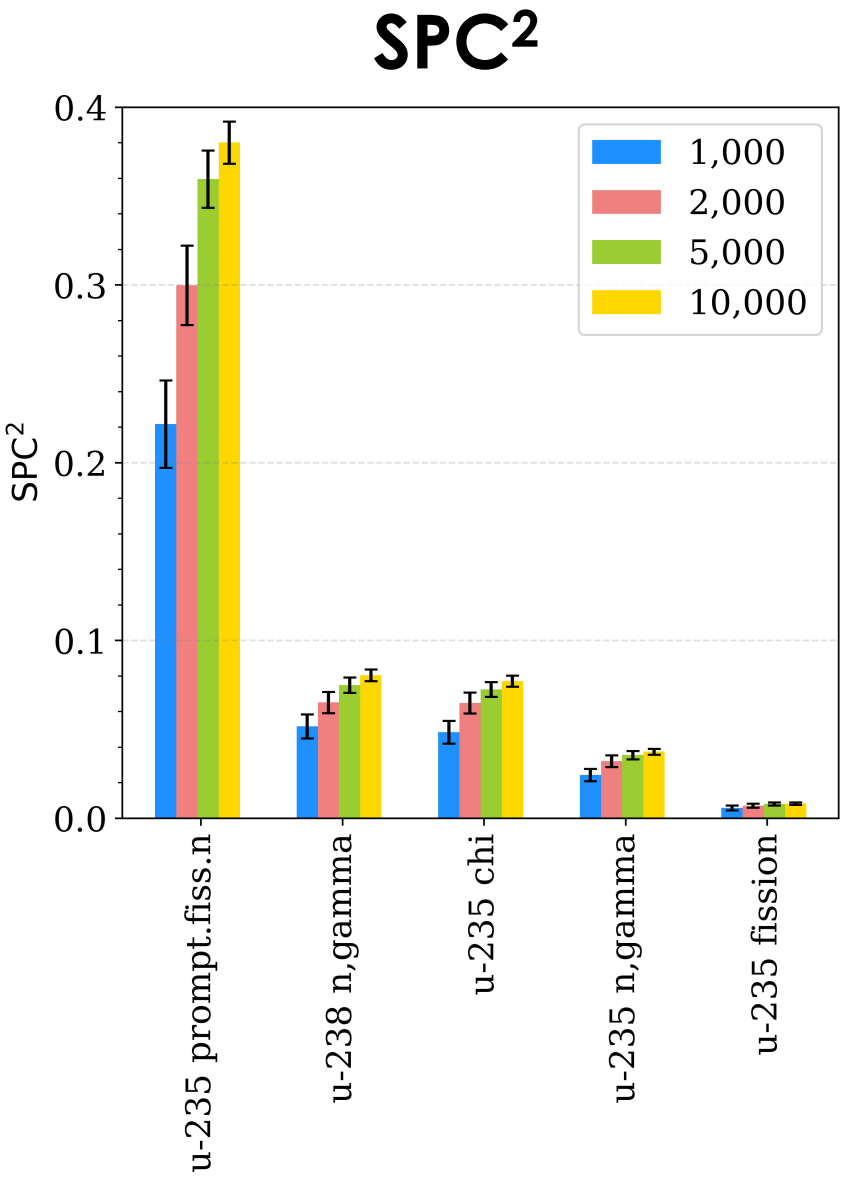
- Model: homogeneous mixture
- Neutron transport: NEWT
- Cross section library: **302g** ENDF/B-VII.1
- Covariance library: **17g** SCALE 6.2

  Sample size: 1,000
- Eigenvalue uncertainty: **1.85%**



LWR pin cell – various sample sizes





SAMPLER and TSUNAMI uncertainties

	LWR pin	SFR pin		
Code	$\Delta k_{inf}/k_{inf}$	$\Delta k_{inf}/k_{inf}$	$\Delta \Sigma_{fis}/\Sigma_{fis}$	$\Delta \Sigma_{abs}/\Sigma_{abs}$
TSUNAMI	0.55%	1.52%	1.54%	0.98%
Sampler, N=1,000	0.54%	1.50%	1.54%	0.98%

	MSR cells		
Code	$\Delta k_{inf}/k_{inf}$ Graphite	$\Delta k_{inf}/k_{inf}$ ZrH	$\Delta k_{inf}/k_{inf}$ fast
TSUNAMI	0.56%	0.75%	1.79%
Sampler, N=1,000	0.55%	0.74%	1.85%

	HTR-10
Code	$\Delta k_{inf}/k_{inf}$
TSUNAMI	0.69%
Sampler, N=350	0.68%

TSUNAMI top contributors

LWR pin cell		SFR pin cell		MSR fast spectrum	
Reaction	$\Delta k_{inf}/k_{inf}$	**Reaction**	$\Delta k_{inf}/k_{inf}$	**Reaction**	$\Delta k_{inf}/k_{inf}$
U-235 nubar	0.34%	U-238 inel.	1.35%	U-238 inel.	1.51%
U-238 n,g	0.28%	Na-23 el.	0.28%	Na-23 el.	0.53%
U-235 n,g	0.20%	U-238 n,g	0.23%	U-238 n,g	4.29%

MSR cell: graphite		MSR cell: ZrH		HTR-10	
Reaction	$\Delta k_{inf}/k_{inf}$	**Reaction**	$\Delta k_{inf}/k_{inf}$	**Reaction**	$\Delta k_{inf}/k_{inf}$
U-235 nubar	0.37%	U-238 n,g	0.46%	U-235 nubar	0.38%
U-238 n,g	0.26%	U-235 n,g	0.37%	Graphite el.	0.34%
U-235 n,g	0.20%	U-235 nubar	0.28%	U-235 chi	0.27%