SERPENT workshop
Cambridge,
17-19 September 2014

Perturbation/sensitivity calculations with Serpent

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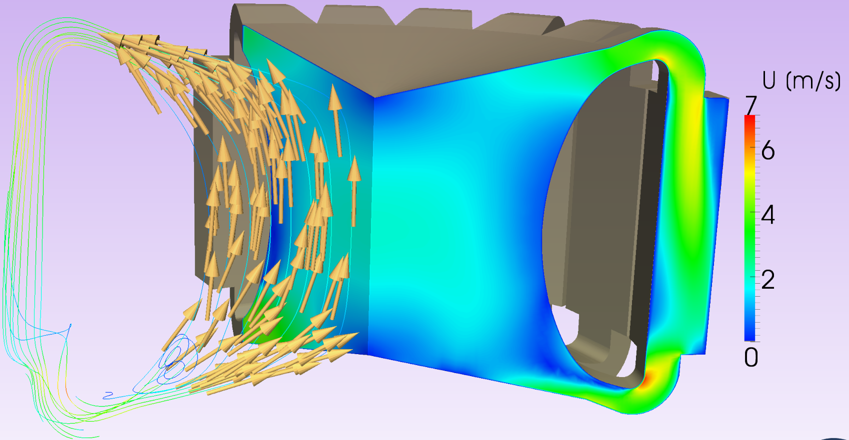
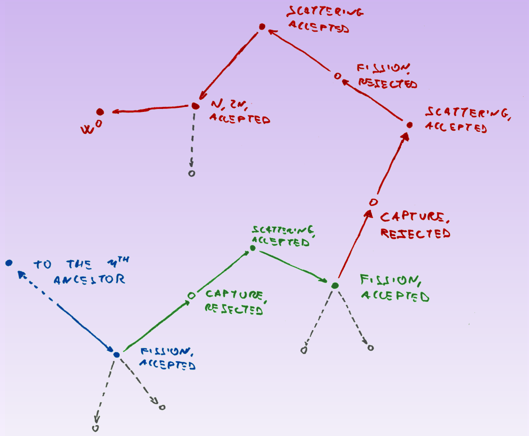
Calculating the "complete" β_{eff} uncertainty in MSRs

...coupling CFD and neutron transport in the MSFR



Nuclear data + DNP decay constants + fluid flow

A collision history-based approach to GPT calculations



Considered response functions

Effect of a perturbation of the parameter x on the response R :

$$S_x^R \equiv \frac{dR/R}{dx/x}$$

Considered response functions:

$R = k_{\text{eff}}$ Effective multiplication factor

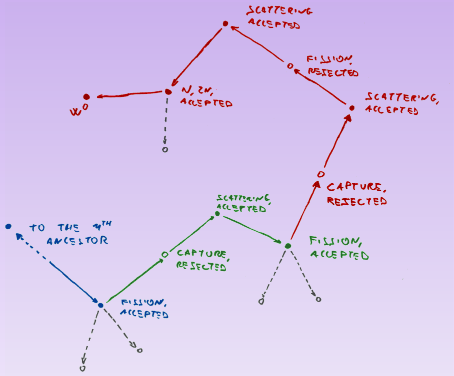
(Simple extension of IFP method, briefly presented last year @Berkeley)

$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle}$ Reaction rate ratios

$R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}$ Bilinear ratios (Adjoint-weighted quantities)

$R = ?$ Something else

Particle's weight perturbation



All the cross sections (and probability distributions) are artificially increased by a factor f .

Events are rejected with a probability of $(1 - 1/f)$.

$f = 0.5$

$$w^* \simeq w^0 \cdot \left(1 + \frac{d\Sigma_{n,2n}}{\Sigma_{n,2n}}\right) \cdot \left(1 + \frac{d\Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{d\Sigma_f}{\Sigma_f}\right) \cdot \left(1 + \frac{d\Sigma_s}{\Sigma_s}\right) \cdot \left(1 - \frac{d\Sigma_c}{\Sigma_c}\right) \cdot$$
$$\cdot \left(1 + \frac{d\Sigma_f}{\Sigma_f}\right) \cdot \left(1 + \frac{d\Sigma_s}{\Sigma_s}\right) \cdot \left(1 + \frac{d\Sigma_f}{\Sigma_f}\right) \ldots$$

The general idea...

Adopting the distribution of the corrected particles weight in the reference system as unbiased estimator of the "exact" neutron flux distribution in the perturbed system.

Re-normalization of the total population weight.

Convergence of the propagation (latent?) generations.

Particle's weight perturbation

x = **nuclear data** for reaction r, on the isotope i, in the material m, in the incident neutron energy bin e, in the volume s (outgoing neutron energy bin e' and scattering cosine bin l)

$$\frac{\partial w_n}{\partial x / x} \simeq w_n \cdot \sum_{g=(\alpha-\lambda)}^{\alpha} \left({}^{(n,g)}ACC_x - {}^{(n,g)}REJ_x \right)$$

α = present generation
λ = number of propagation generations

ACC_x = accepted events x in the history of the particle n
REJ_x = rejected events x

Reaction rate ratios (method)

$$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle}$$

$$R\,' = \frac{\langle \Sigma_1 + \Delta\Sigma_1, \phi + \Delta\phi \rangle}{\langle \Sigma_2 + \Delta\Sigma_2, \phi + \Delta\phi \rangle}$$

Neglecting cross terms...

$$\frac{\Delta R}{R} = \frac{\langle \Delta\Sigma_1, \phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Delta\Sigma_2, \phi \rangle}{\langle \Sigma_2, \phi \rangle} + \frac{\langle \Sigma_1, \Delta\phi \rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\langle \Sigma_2, \Delta\phi \rangle}{\langle \Sigma_2, \phi \rangle}$$

$$S_x^R = \underbrace{\frac{\left\langle \dfrac{\partial\Sigma_1}{\partial x/x}, \phi \right\rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\left\langle \dfrac{\partial\Sigma_2}{\partial x/x}, \phi \right\rangle}{\langle \Sigma_2, \phi \rangle}}_{\textit{direct terms}} + \underbrace{\frac{\left\langle \Sigma_1, \dfrac{\partial\phi}{\partial x/x} \right\rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\left\langle \Sigma_2, \dfrac{\partial\phi}{\partial x/x} \right\rangle}{\langle \Sigma_2, \phi \rangle}}_{\textit{indirect terms}}$$

Reaction rate ratios (method)

Considering track-length estimators (for simplicity)...

$$\langle \Sigma_1, \phi \rangle = \mathrm{q} \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \ell_t \Sigma_1$$

$$\left\langle \Sigma_1, \frac{\partial \phi}{\partial x / x} \right\rangle = \mathrm{q} \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \frac{\partial w_n / w_n}{\partial x / x} \cdot \ell_t \Sigma_1$$

$$\left\langle \Sigma_1, \frac{\partial \phi}{\partial x / x} \right\rangle = \mathrm{q} \cdot \sum_{n \in \alpha} \sum_{t \in n} w_n \left[\sum_{g=(\alpha-\lambda)}^{\alpha} \left(ACC_x^{(n,g)} - REJ_x^{(n,g)} \right) \right] \ell_t \Sigma_1$$

Reaction rate ratios (method)

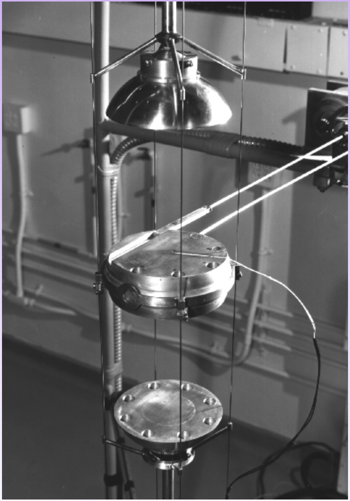
Indirect terms:

$$\frac{\left\langle \Sigma_1, \dfrac{\partial \phi}{\partial x/x} \right\rangle}{\langle \Sigma_1, \phi \rangle} = \frac{q \cdot \sum\limits_{n\,\in\,\alpha} \sum\limits_{t\,\in\,n} w_n \left[\sum\limits_{g=(\alpha-\lambda)}^{\alpha} \left(ACC_x^{(n,g)} - REJ_x^{(n,g)} \right) \right] \ell_t \Sigma_1}{q \cdot \sum\limits_{n\,\in\,\alpha} \sum\limits_{t\,\in\,n} w_n \cdot \ell_t \Sigma_1}$$

Average net number of x events (i.e., real - virtual) in the last λ generations, weighted on the contributions to the track length estimator of $\langle \Sigma_1, \phi \rangle$

Indirect part of S_x^R is obtained as the difference between the average number of net x events in the last λ generations, weighted on the tally contributions for two generic detectors $\langle \Sigma_1, \phi \rangle$ and $\langle \Sigma_2, \phi \rangle$

Reaction rate ratios (results)



$$R = \frac{\iiint \phi(\mathbf{r}, E) \cdot \sigma_f^{^{238}U}(E)\, dE\, d\mathbf{r}}{\iiint \phi(\mathbf{r}, E) \cdot \sigma_f^{^{235}U}(E)\, dE\, d\mathbf{r}}$$

Jezebel (Pu sphere)

PU-MET-FAST-001

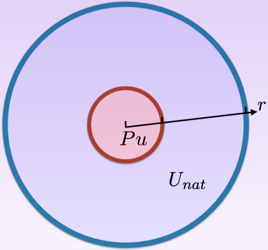
^{238}U/^{235}U fission rate ratio
(measured in the center of the system)

Reaction rate ratios (results)

Flattop-Pu (Popsy)

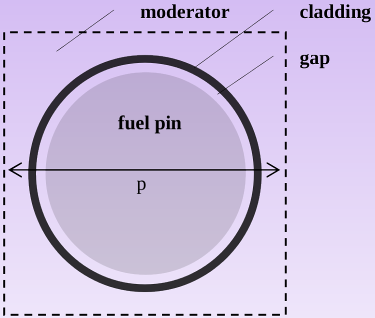
PU-MET-FAST-006

^{238}U/^{235}U fission rate ratio
(measured in the center of the system)



(not in scale)

Reaction rate ratios (results)



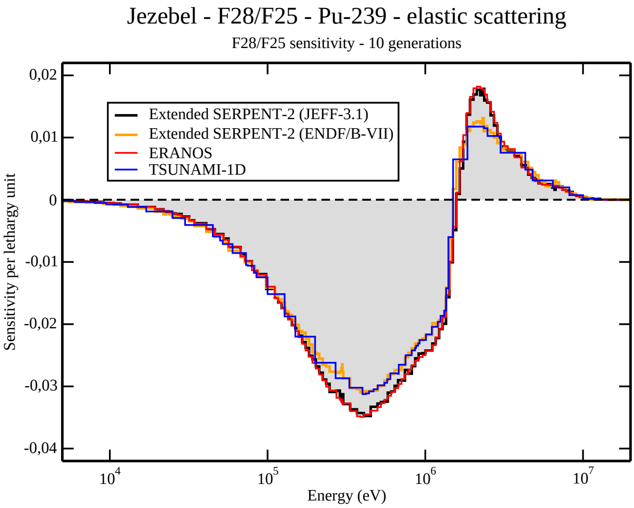
$$R = \frac{\iiint \phi(\mathbf{r}, E) \cdot \sigma_f^{^{238}U}(E)\, dE\, d\mathbf{r}}{\iiint \phi(\mathbf{r}, E) \cdot \sigma_f^{^{235}U}(E)\, dE\, d\mathbf{r}}$$

UAM TMI-1 PWR pin-cell

$^{238}U/^{235}U$ fission rate ratio in the fuel pellet

Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @PSI



Reaction rate ratios (results)

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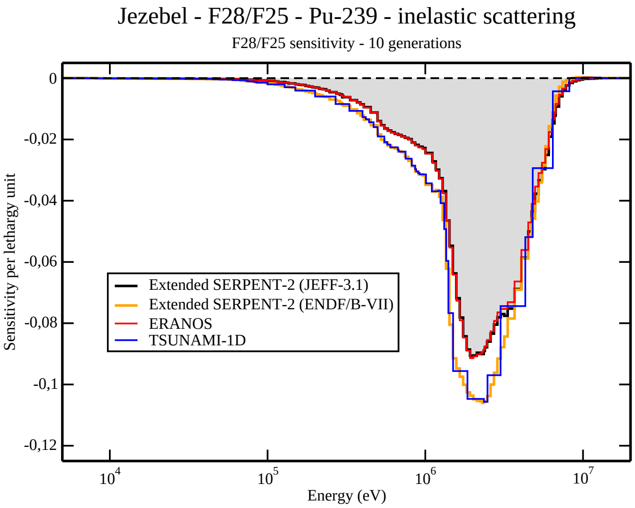

Reaction rate ratios (results)

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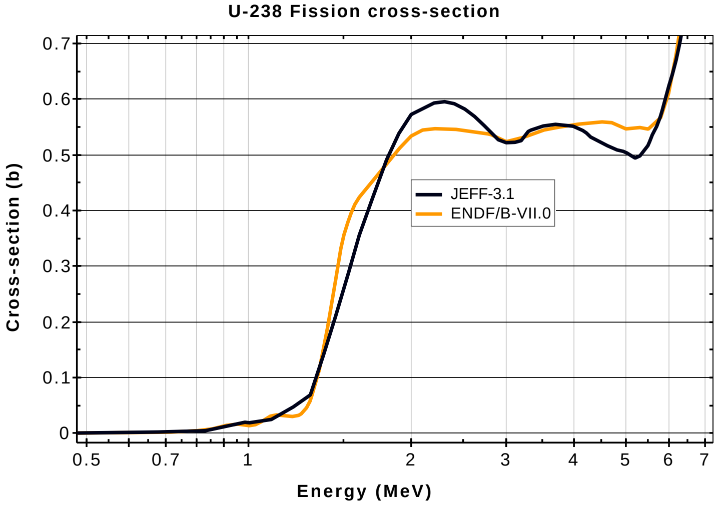
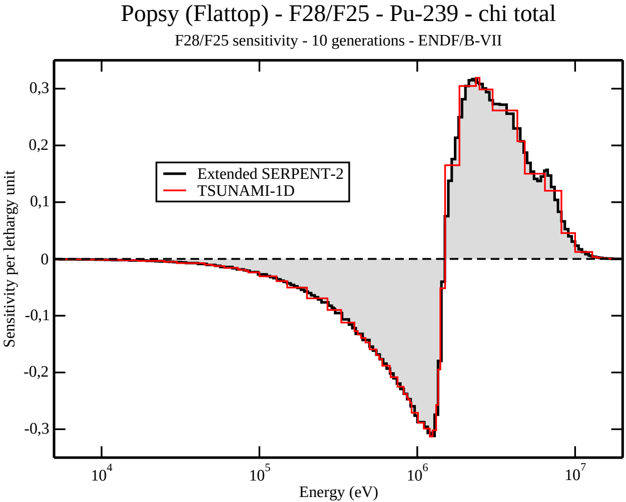


Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @PSI



Reaction rate ratios (results)

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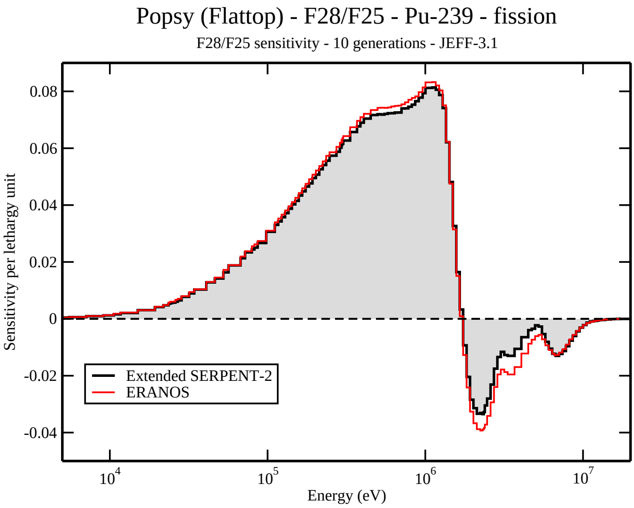

Reaction rate ratios (results)

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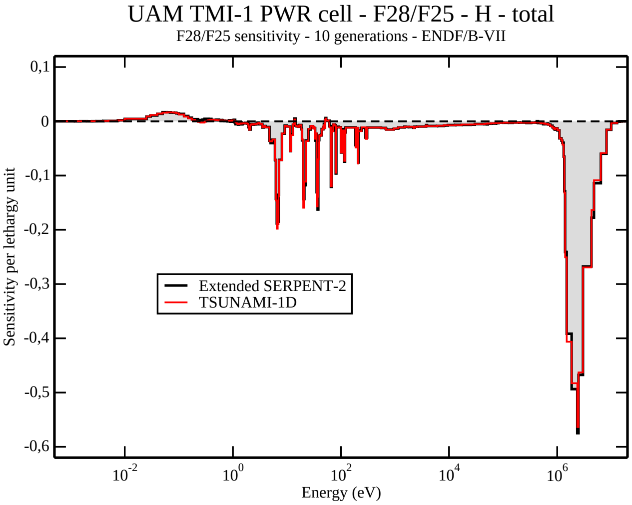

Reaction rate ratios (results)

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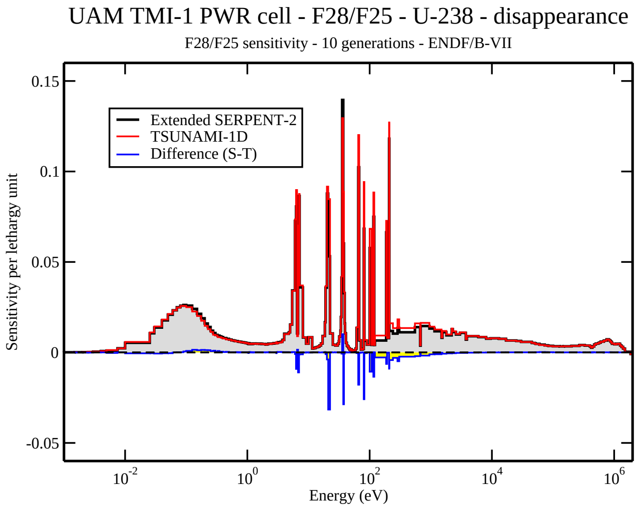


Reaction rate ratios (results)

ERANOS results from Sandro Pelloni @PSI

Energy integrated sensitivity coefficients for Jezebel for the response function R = F28/F25.

x	S_x^R					
	JEFF-3.1			ENDF/B-VII		
	Serpent	Eranos	Rel. diff	Serpent	TSUNAMI-1D	Rel. diff
^{239}Pu σ_{tot}	-0.14856 ± 0.1%	-0.14923	-0.5%	-0.16404 ± 0.1%	-0.16477	-0.4%
^{239}Pu σ_{inl}	-0.13475 ± 0.0%	-0.13308	1.2 %	-0.15996 ± 0.0%	-0.15898	0.6 %
^{239}Pu σ_{ela}	-0.06844 ± 0.2%	-0.06854	-0.1%	-0.06386 ± 0.2%	-0.06396	-0.2%
^{239}Pu σ_{fis}	+0.04750 ± 0.1%	+0.04607	3.0 %	+0.05173 ± 0.1%	+0.05002	3.3 %
^{240}Pu σ_{tot}	-0.01255 ± 0.3%	-0.01243	1.0 %	-0.01407 ± 0.3%	-0.01405	0.1 %
^{239}Pu σ_{dis}	+0.00995 ± 0.1%	+0.01005	-1.0%	+0.01006 ± 0.1%	+0.01008	-0.2%
^{240}Pu σ_{inl}	-0.00822 ± 0.2%	-0.00820	0.2 %	-0.00803 ± 0.2%	-0.00798	0.6 %
^{240}Pu σ_{ela}	-0.00387 ± 0.7%	-0.00384	0.8 %	-0.00403 ± 0.7%	-0.00409	-1.5%
^{239}Pu $\sigma_{n,xn}$	-0.00278 ± 0.2%	-0.00251	9.7 %	-0.00201 ± 0.2%	-0.00193	4.0 %
^{240}Pu σ_{fis}	-0.00103 ± 1.9%	-0.00097	5.8 %	-0.00256 ± 0.7%	-0.00253	1.2 %
^{240}Pu σ_{dis}	+0.00066 ± 0.4%	+0.00066	0.0 %	+0.00062 ± 0.5%	+0.00062	0.0 %
^{241}Pu σ_{tot}	-0.00061 ± 1.6%	-0.00045	26.2% ??	-0.00069 ± 1.5%	-0.00068	1.4 %
^{241}Pu σ_{inl}	-0.00046 ± 0.9%	-0.00047	-2.2%	-0.00061 ± 0.8%	-0.00060	1.6 %

Bilinear ratios (method)

$$R = \frac{\langle \phi^\dagger, \Sigma_1 \phi \rangle}{\langle \phi^\dagger, \Sigma_2 \phi \rangle}$$

Examples:

$$\beta_{\mathrm{eff}} = \frac{\left\langle \phi^\dagger, \dfrac{1}{k_{\mathrm{eff}}} \chi_d \bar{\nu}_d \Sigma_f \phi \right\rangle}{\left\langle \phi^\dagger, \dfrac{1}{k_{\mathrm{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle} \qquad \ell_{\mathrm{eff}} = \frac{\left\langle \phi^\dagger, \dfrac{1}{v} \phi \right\rangle}{\left\langle \phi^\dagger, \dfrac{1}{k_{\mathrm{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle}$$

$$\alpha_{\mathrm{coolant}} = -\frac{\langle \phi^\dagger, \Sigma_{\mathrm{t,coolant}} \phi \rangle}{\left\langle \phi^\dagger, \dfrac{1}{k_{\mathrm{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle}$$

Bilinear ratios (method)

$$R' = \frac{\left\langle \phi^\dagger + \Delta\phi^\dagger, (\Sigma_1 + \Delta\Sigma_1)(\phi + \Delta\phi) \right\rangle}{\left\langle \phi^\dagger + \Delta\phi^\dagger, (\Sigma_2 + \Delta\Sigma_2)(\phi + \Delta\phi) \right\rangle}$$

$$\frac{\Delta R}{R} = \frac{\left\langle \phi^\dagger, \Delta\Sigma_1\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \phi^\dagger, \Delta\Sigma_2\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle} + \frac{\left\langle \phi^\dagger, \Sigma_1\Delta\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \phi^\dagger, \Sigma_2\Delta\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle} + \frac{\left\langle \Delta\phi^\dagger, \Sigma_1\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \Delta\phi^\dagger, \Sigma_2\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle}$$

$$S_x^R = \frac{\left\langle \phi^\dagger, \frac{\partial\Sigma_1}{\partial x/x}\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \phi^\dagger, \frac{\partial\Sigma_2}{\partial x/x}\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle} + \frac{\left\langle \phi^\dagger, \Sigma_1\frac{\partial\phi}{\partial x/x} \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \phi^\dagger, \Sigma_2\frac{\partial\phi}{\partial x/x} \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle} +$$

$$+ \frac{\left\langle \frac{\partial\phi^\dagger}{\partial x/x}, \Sigma_1\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_1\phi \right\rangle} - \frac{\left\langle \frac{\partial\phi^\dagger}{\partial x/x}, \Sigma_2\phi \right\rangle}{\left\langle \phi^\dagger, \Sigma_2\phi \right\rangle}$$

Bilinear ratios (method)

Adopting Iterated Fission Probability importance estimators:

$$\mathrm{I}_n^{(\gamma)} = \frac{1}{q'} \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} w_k$$

Importance of neutrons in generation α is calculated as function of the neutron descendants in generation $\alpha + \gamma$

Effect of perturbation on neutron importance:

$$\frac{\partial I_n^{(\gamma)}}{\partial x/x} = \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} \frac{\partial w_k}{\partial x/x} - \frac{1}{{w_n}^2} \frac{\partial w_n}{\partial x/x} \sum_{k \in d_n^{(\gamma)}} w_k$$

Bilinear ratios (method)

Indirect terms...

Effect of perturbation on the forward flux:

$$\left\langle \phi^{\dagger}, \Sigma_1 \frac{\partial \phi}{\partial x/x} \right\rangle = \sum_{n \in \alpha} \sum_{t \in n} \frac{\partial w_n}{\partial x/x} \cdot \ell_t \Sigma_1 \cdot \frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} w_k$$

Effect of perturbation on the adjoint flux:

$$\left\langle \frac{\partial \phi^{\dagger}}{\partial x/x}, \Sigma_1 \phi \right\rangle = \sum_{n \in \alpha} \sum_{t \in n} w_n \cdot \ell_t \Sigma_1 \left(\frac{1}{w_n} \sum_{k \in d_n^{(\gamma)}} \frac{\partial w_k}{\partial x/x} - \frac{1}{{w_n}^2} \frac{\partial w_n}{\partial x/x} \sum_{k \in d_n^{(\gamma)}} w_k \right)$$

Sum of indirect terms (rewritten as function of neutrons in generation $\alpha + \gamma$):

$$\left\langle \phi^{\dagger}, \Sigma_1 \frac{\partial \phi}{\partial x/x} \right\rangle + \left\langle \frac{\partial \phi^{\dagger}}{\partial x/x}, \Sigma_1 \phi \right\rangle = \sum_{k \in (\alpha+\gamma)} \left[w_k \left(\sum_{t \in (-\gamma)_k} \ell_t \Sigma_1 \right) \frac{\partial w_k / w_k}{\partial x/x} \right]$$

Bilinear ratios (method)

Example: effective prompt lifetime

$$R = \frac{\left\langle \phi^\dagger, \frac{1}{v}\phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}}\chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle}$$

Simple IFP estimator for the numerator:

$$\left\langle \phi^\dagger, \frac{1}{v}\phi \right\rangle = \frac{1}{q'} \sum_{k \in (\alpha+\gamma)} w_k \cdot {}^{(-\gamma)}I_k$$

Numerator terms of the perturbation:

$$\frac{\left\langle \phi^\dagger, \frac{1}{v}\frac{\partial \phi}{\partial x/x} \right\rangle}{\left\langle \phi^\dagger, \frac{1}{v}\phi \right\rangle} + \frac{\left\langle \frac{\partial \phi^\dagger}{\partial x/x}, \frac{1}{v}\phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{v}\phi \right\rangle} = \frac{\sum\limits_{k \in (\alpha+\gamma)} w_k \left[\sum\limits_{g=(\alpha-\lambda)}^{(\alpha+\gamma)} \left({}^{(n,g)}ACC_x - {}^{(n,g)}REJ_x \right) \right] {}^{(-\gamma)}I_k}{\sum\limits_{k \in (\alpha+\gamma)} w_k \cdot {}^{(-\gamma)}I_k}$$

Bilinear ratios (method)

Denominator terms:

$$\frac{\left\langle \phi^{\dagger}, \mathbf{F}\frac{\partial\phi}{\partial x/x} \right\rangle}{\left\langle \phi^{\dagger}, \mathbf{F}\phi \right\rangle} + \frac{\left\langle \phi^{\dagger}, \frac{\partial \mathbf{F}}{\partial x/x}\phi \right\rangle}{\left\langle \phi^{\dagger}, \mathbf{F}\phi \right\rangle} + \frac{\left\langle \frac{\partial\phi^{\dagger}}{\partial x/x}, \mathbf{F}\phi \right\rangle}{\left\langle \phi^{\dagger}, \mathbf{F}\phi \right\rangle} = \frac{\sum\limits_{k\,\in\,(\alpha+\gamma)} w_k \left[\sum\limits_{g=(\alpha-\lambda)}^{(\alpha+\gamma)} \left({}^{(n,g)}ACC_x - {}^{(n,g)}REJ_x \right)\right]}{\sum\limits_{k\,\in\,(\alpha+\gamma)} w_k}$$

We finally obtain the sensitivity coefficient for ℓ_{eff} :

$$S_x^{\ell_{\text{eff}}} = \frac{E\left[{}^{(-\gamma)}I \cdot \sum\limits^{history} (ACC_x - REJ_x) \right]}{E\left[{}^{(-\gamma)}I \right]} - E\left[\sum\limits^{history} (ACC_x - REJ_x) \right] =$$

$$= \frac{COV\left[{}^{(-\gamma)}I \,,\, \sum\limits^{history} (ACC_x - REJ_x) \right]}{E\left[{}^{(-\gamma)}I \right]}$$

Bilinear ratios (method)

Everything is much more simple...

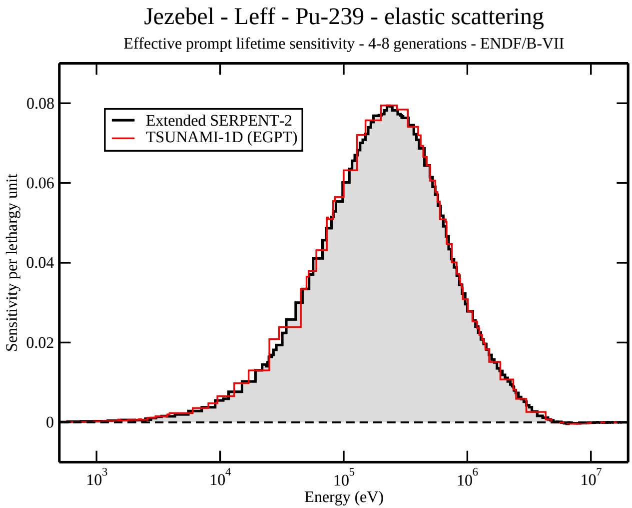
If the quantity R can be estimated as the ratio of two generic Monte Carlo responses

$$\mathrm{R} = \frac{E\left[e_1\right]}{E\left[e_2\right]}$$

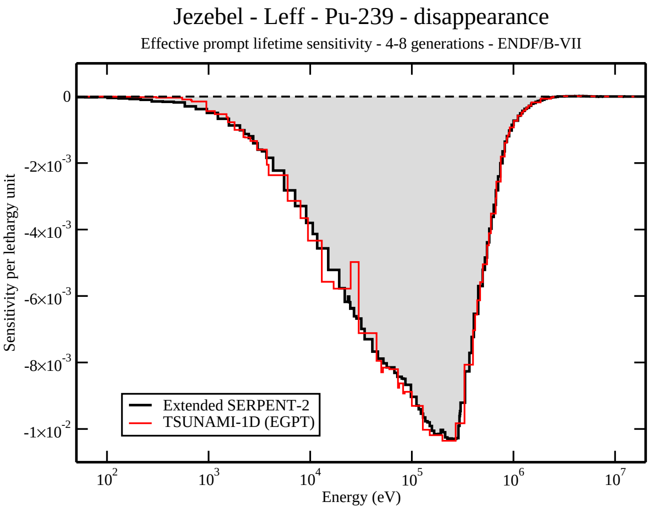
the sensitivity coefficient of R with respect to x can be obtained as:

$$S_x^R = \frac{COV\left[e_1 \, , \sum^{history} \left(ACC_x - REJ_x\right)\right]}{E\left[e_1\right]} - \frac{COV\left[e_2 \, , \sum^{history} \left(ACC_x - REJ_x\right)\right]}{E\left[e_2\right]}$$

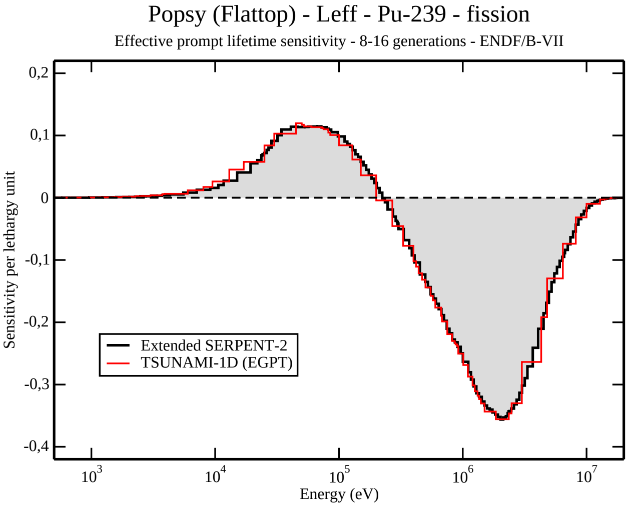
Bilinear ratios (results)



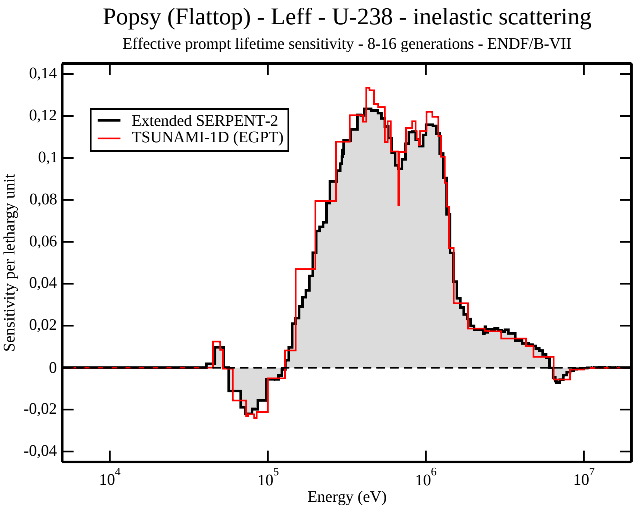
Bilinear ratios (results)



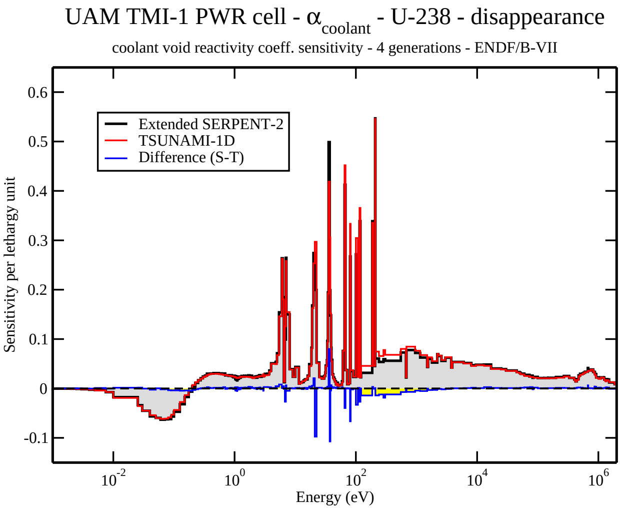
Bilinear ratios (results)



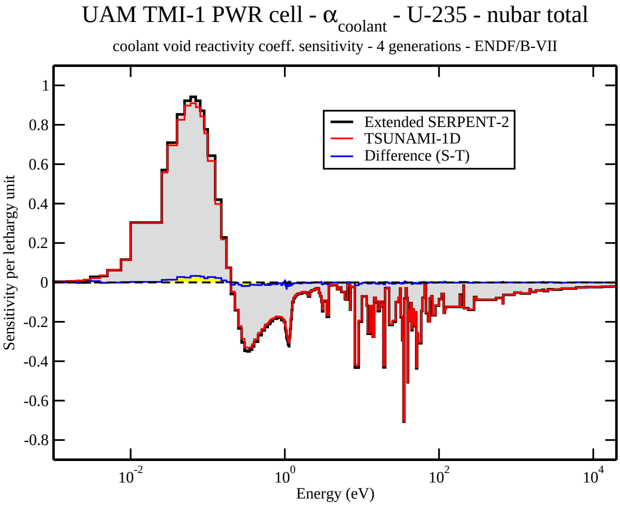
Bilinear ratios (results)



Bilinear ratios (results)



Bilinear ratios (results)



Scattering distributions

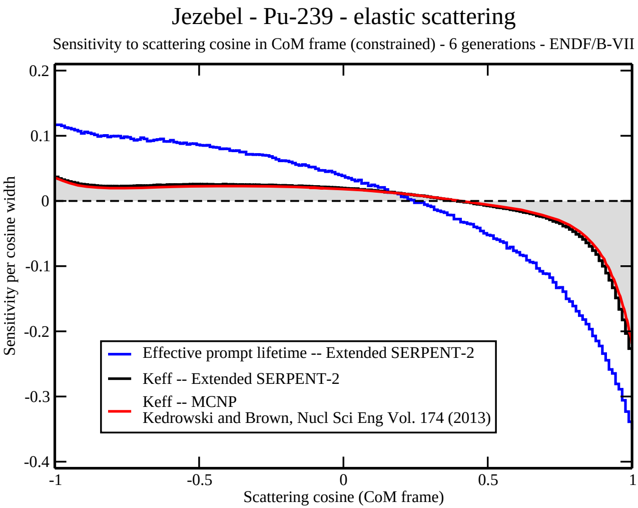
The method can be extended to scattering distribution sensitivities:

At each scattering event, two pairs of outgoing energy/scattering angle are sampled

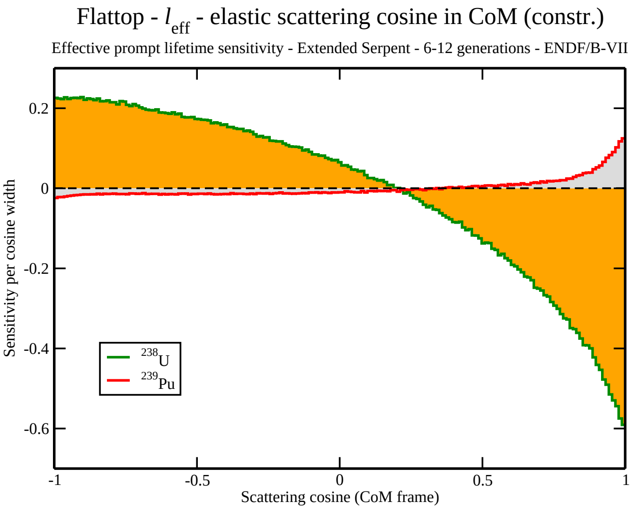
One is accepted as real event, the other is rejected as virtual

Implicit, continuous constraining of the sensitivity profiles

Scattering distributions

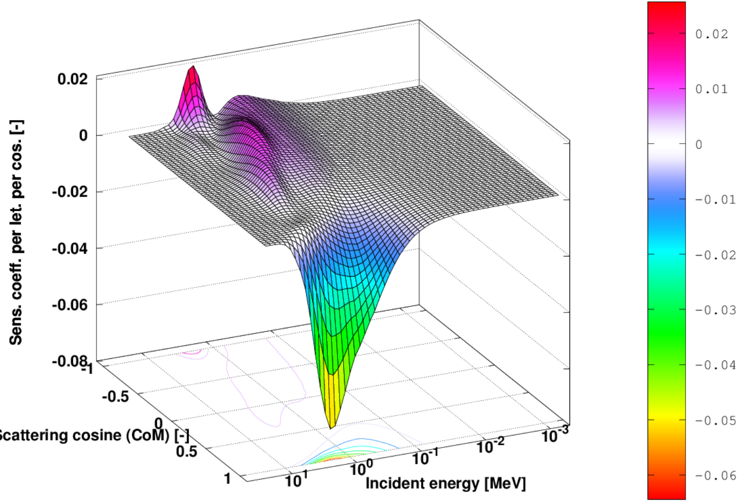


Scattering distributions



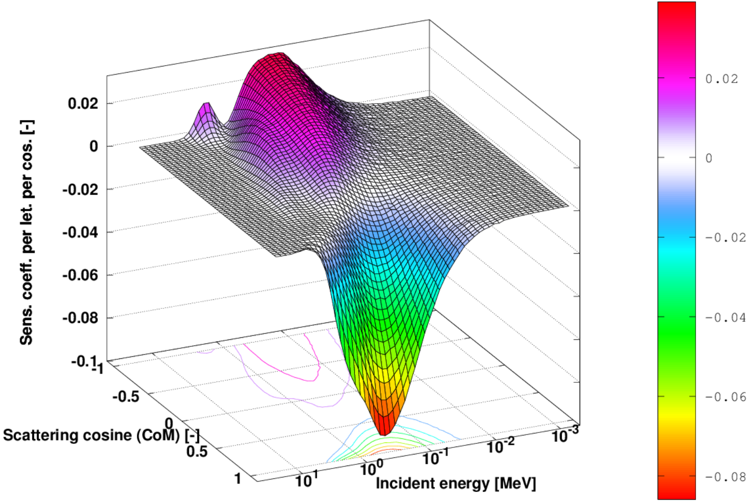
Scattering distributions

Jezebel, k_{eff} sensitivity to elastic scattering distribution



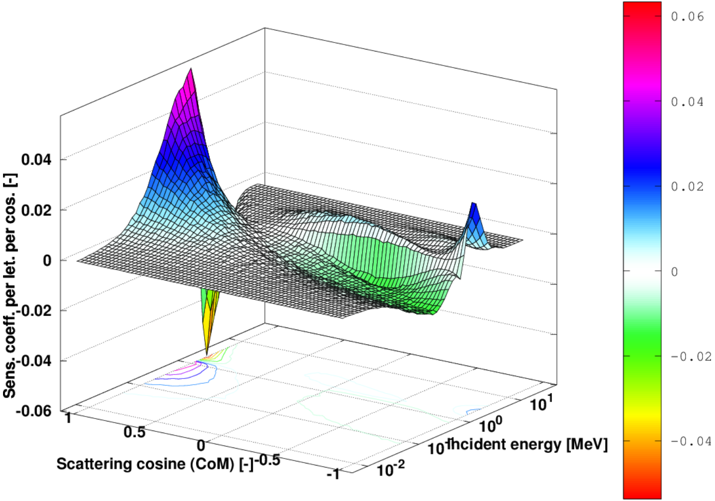
Scattering distributions

Jezebel, ℓ_{eff} sensitivity to elastic scattering distribution



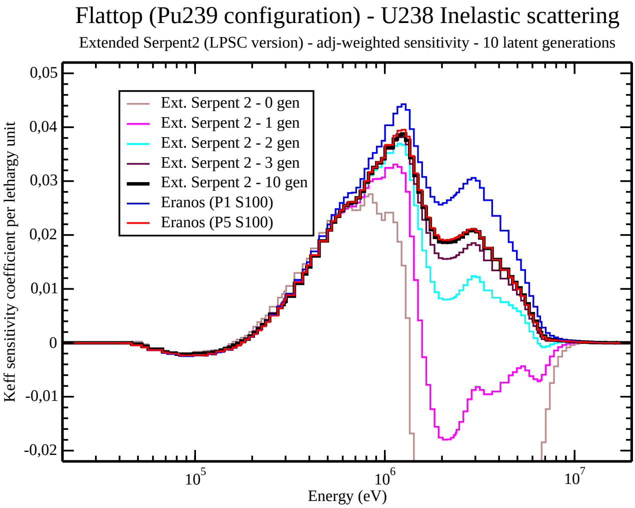
Scattering distributions

Jezebel, $F28/F25$ sensitivity to elastic scattering distribution



Latent generations convergence

ERANOS results from Sandro Pelloni @PSI



Next steps

- **“Complete” β_{eff} uncertainties in MSFR**
- **GPT in Serpent/OpenFOAM for multiphysics application**
- Continuous (E and μ) sensitivity to Legendre moments (from implicitly constrained scattering sensitivities)
- “Exact” perturbations
- Coupled depletion/transport sensitivities...

  ...and comparisons with Total Monte Carlo approach
- Doppler effect

THANK YOU FOR THE ATTENTION

Vue sur l'agglomération Grenobloise depuis le sommet du Moucherotte (Bertrand93)

QUESTIONS? SUGGESTIONS? NEW IDEAS?