



Implementing history based GPT capabilities to the official Serpent 2 Monte Carlo code

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Outline

- ▶ Background.
- ▶ Porting the implementation to Serpent 2.1.29.
- ▶ Verification against original implementation.
- ▶ Initial runtime and memory consumption comparisons.
- ▶ Some words about XGPT.
- ▶ Applications and future work.

Background

Background

The collision-history based sensitivity/perturbation calculation methodology is a nice Monte Carlo way for GPT equivalent sensitivity/perturbation calculations (and more).

Methodology is described in¹.

Requires only two real changes to the Monte Carlo simulation:

- ▶ Keeping track of events that neutrons experience.
- ▶ Increasing the track-length sampling cross section to obtain more tentative interactions and rejecting some of the tentative interactions².

By following the number of accepted and rejected events of different sorts, the effects of various perturbations can be estimated on various responses.

The derivation of the methodology for different responses relies on the idea of neutron weight-perturbation as a "post-tracking" step using the collision history collected during the tracking.

¹ M. Aufiero et al. "A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT.". *Annals of Nuclear Energy* **85** (2015), 245–258.

² Every cross section is doubled but 50 % of the interactions are rejected.

Background

Sensitivity of procreating to going to the gym

Start with a group of people:

Gen 1: 

People only go to gym based on an every morning throw of a d4:

$$P(\text{go to gym today}) = 0.25$$



If $P(\text{go to the gym})$ would be higher, would people have more children?

Sensitivity of procreating to going to the gym

If $P(\text{go to the gym})$ would be higher, would people have more children?

Let's double the probability, but reject 50 % of the gym: $P(\text{go to the gym}) = 0.5$



no gym



gym, maybe...



Gym rejected













Gym accepted



Everyone keeps a tally of their "Tally = Accepted - Rejected".

Sensitivity of procreating to going to the gym

On population level the expected lifetime tally value is 0:

Person:										
Tally:	+5	-3	+1	0	+9	-3	-7	-3	+2	-1

What's more, the expected lifetime tally value of anyone is 0 regardless of the length of their life.

To analyze the sensitivity of procreation to the probability of going to the gym we'll look at, say, the 10th generation of descendants of our original population:

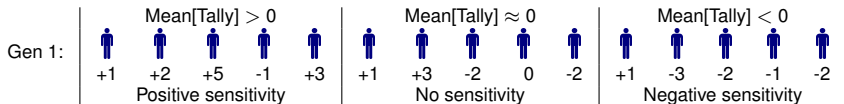
Gen 10: 

or more accurately their 10th grandparents who are a subset of the original population:

Gen 1: 

Sensitivity of procreating to going to the gym

When looking at the tally values for these grandparents there are three possibilities:



Same can be done for neutrons:

Instead of P(go to the gym) we have, e.g. P(get captured by ^{238}U at 1 keV).

Collision history

During neutron tracking, store information about sampled events such as:

- ▶ Interactions (elastic scattering, capture, fission, etc.).
- ▶ Sampled energies, e.g. fission neutron energy for χ -sensitivities.
- ▶ Sampled angles, e.g. sampled scattering cosine.

For each event store:

- ▶ Event type.
- ▶ Event energy.
- ▶ Event nuclide.
- ▶ Event material.
- ▶ Event weight.
- ▶ Accepted or rejected.

Calculated sensitivities

Sensitivities can be scored separately for different nuclides and materials.

Sensitivities are scored on an energy-grid and/or angular-grid, but sensitivities to perturbations that are continuous in energy and/or angle can be calculated with a small amount of additional work using the so-called xGPT approach³.

³M. Aufiero, M. Martin, and M. Fratoni. "XGPT: Extending Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions." *Annals of Nuclear Energy* **96** (2016), 295–306.

k-eff sensitivities

$$S_x^{k_{\text{eff}}} = \frac{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \frac{\partial \mathbf{F}}{\partial x/x} \phi \right\rangle - \left\langle \phi^\dagger, \frac{\partial \mathbf{L}}{\partial x/x} \phi \right\rangle + \left\langle \phi^\dagger, \frac{\partial \mathbf{S}}{\partial x/x} \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \mathbf{F} \phi \right\rangle} \quad (2)$$

Each time a fission occurs, calculate net number of events x in γ :th ancestor generation. Divide by total weight of the generation to obtain estimate for the expected net number of events x per particle.

Bilinear ratios

Sensitivities of responses such as

$$\beta_{\text{eff}} = \frac{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_d \bar{\nu}_d \Sigma_f \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle} \quad (3)$$

$$\ell_{\text{eff}} = \frac{\left\langle \phi^\dagger, \frac{1}{v} \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle} \quad (4)$$

$$\alpha_{\text{cool}} = \frac{\left\langle \phi^\dagger, \Sigma_{t,\text{cool}} \phi \right\rangle}{\left\langle \phi^\dagger, \frac{1}{k_{\text{eff}}} \chi_t \bar{\nu}_t \Sigma_f \phi \right\rangle} \quad (5)$$

Each time a fission occurs, calculate net number of events x from γ :th ancestor generation to the current generation. Weight the net number with the value of the response obtained from ancestor generation γ . Divide with the expected value of the response obtained from ancestor generation γ and subtract the unweighted net number of events x in the summed generations.

Reaction rate ratios

$$R = \frac{\langle \Sigma_1, \phi \rangle}{\langle \Sigma_2, \phi \rangle} \quad (6)$$

First order estimate **direct** and **indirect** terms:

$$S_x^R = \frac{\left\langle \frac{\partial \Sigma_1}{\partial x/x}, \phi \right\rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\left\langle \frac{\partial \Sigma_2}{\partial x/x}, \phi \right\rangle}{\langle \Sigma_2, \phi \rangle} + \frac{\left\langle \Sigma_1, \frac{\partial \phi}{\partial x/x} \right\rangle}{\langle \Sigma_1, \phi \rangle} - \frac{\left\langle \Sigma_2, \frac{\partial \phi}{\partial x/x} \right\rangle}{\langle \Sigma_2, \phi \rangle} \quad (7)$$

Estimation of the indirect term: Each time a detector is scored, calculate net number of events x from γ :th ancestor generation to the current generation. Weight the net number with the detector score value to obtain estimate for

$$\left\langle \Sigma_i, \frac{\partial \phi}{\partial x/x} \right\rangle. \quad (8)$$

The normal detector response provides an estimate for $\langle \Sigma_i, \phi \rangle$.

The divisions and subtraction are conducted for each neutron batch to obtain a statistical estimate for the indirect term.

New implementation

Porting the implementation

- ▶ From Manuele's extension of 2.1.19 to the official version 2.1.29.
- ▶ From static (source-code based) definition to dynamic (input-based) addition of perturbations, responses and options.
- ▶ Standardizing the used data-structures, input- and output-format, adding debugging checks and generally smoothing things out.
- ▶ Learning about the methodology on a source code level.

Internal structure for collision-history style events was included in 2.1.22 for Iterated Fission Probability calculations. Can also be used for tracking other events.

Saves memory as each event is stored only once, even if it is in the collision history of multiple particles.

A small tradeoff in parallel efficiency⁴.

⁴New implementation is still faster at least in tested cases.

Saving memory

Input

Standard input-cards for setting up:

- ▶ Perturbations (`sens pert`).
- ▶ Responses (`sens resp`).
- ▶ General options (`sens opt`).

See up-to-date description in the Serpent-wiki:

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

Setting up perturbations

`sens pert xs all` for perturbing sum reaction cross sections.

`sens pert xs allmt` for perturbing partial reaction cross sections.

`sens pert nubar`

`sens pert chi`

`sens pert eleg 3` for perturbing elastic scattering angular distribution's Legendre moments up to third moment.

`sens pert zailist 942390 942400 sum total`

`sens pert matlist innerfuel outerfuel sum total`

See up-to-date description in the Serpent-wiki:

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

Setting up responses

```
sens resp keff
```

```
sens resp leff
```

```
sens resp beff
```

```
sens resp void coolant
```

```
sens resp detratio myDet1 myDet2
```

See up-to-date description in the Serpent-wiki:

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

Setting up options

```
sens opt egrid myScale44
```

```
sens opt latgen 10
```

```
sens opt direct 0.25
```

```
sens opt history
```

See up-to-date description in the Serpent-wiki:

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

Output

Sensitivities in MATLAB-readable format in a separate output file:

- ▶ `input_sens.m`

Energy grid boundaries and bin lethargy widths are also included for ease of plotting and processing.

Indices for different materials, nuclides and perturbations are also included for ease of use.

Possibility to tally and print out the results using a lower number of latent generations (`sens opt history`). Can be useful in determining the required number of latent generations.

See up-to-date description in the Serpent-wiki:

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations

Verification

Verification

Verification of the methodology in the extended 2.1.19 against various computational tools has been executed previously¹³⁴⁵.

Now the verification was conducted for the new implementation against the old implementation in the three cases included in ¹:

- ▶ Jezebel (unreflected plutonium metal alloy sphere).
- ▶ Popsy/Flattop (plutonium metal alloy sphere reflected by natural uranium blanket).
- ▶ HZP pin-cell for TMI1 from the UAM benchmark.

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³ I. A. Kodeli, M. Aufiero, and W. Zwermann. "Comparison of deterministic and Monte Carlo codes SUS3D, Serpent and XSUSA for beta-effective sensitivity calculations." In *proc. M&C 2017. Jeju, Korea, Apr. 2017*.

⁴ I. A. Kodeli et al. "OECD/NEA intercomparison of deterministic and Monte Carlo cross-section sensitivity codes using SNEAK-7 benchmarks." In *proc. M&C 2017. Jeju, Korea, Apr. 2017*.

⁵ G. Baiocco, A. Petruzzi, and M. Aufiero. "Uncertainty quantification using SCALE 6.2 and GPT techniques implemented in Serpent." In *proc. M&C 2017. Jeju, Korea, Apr. 2017*.

Jezebel

The considered responses were

- ▶ Effective multiplication factor.
- ▶ Effective prompt neutron generation time.
- ▶ $^{238}\text{U}/^{235}\text{U}$ fission rate ratio in the center of the plutonium core (spectral index).

The considered perturbations were

- ▶ Reaction cross sections and $\bar{\nu}$ as well as the three first Legendre moments of the elastic scattering angular distribution **of**
- ▶ ^{239}Pu and ^{240}Pu **tallied on**
- ▶ Vitamin-J 175 group structure.

Jezebel – energy-integrated sensitivities

keff sensitivity					
942390 total xs	:	+0.824027	[+0.823467	+0.824587]	(0.068 % 2 sigma)
0.69 sigma	:	+0.824399	[+0.823888	+0.824910]	(0.062 % 2 sigma)
942390 ela scatt xs	:	+0.063917	[+0.063456	+0.064377]	(0.720 % 2 sigma)
0.56 sigma	:	+0.063673	[+0.063259	+0.064087]	(0.650 % 2 sigma)
942390 sab scatt xs	:	+0.000000	[+0.000000	+0.000000]	(0.000 % 2 sigma)
0.00 sigma	:	+0.000000	[+0.000000	+0.000000]	(0.000 % 2 sigma)
942390 inl scatt xs	:	+0.039305	[+0.039038	+0.039572]	(0.680 % 2 sigma)
0.38 sigma	:	+0.039401	[+0.039163	+0.039639]	(0.604 % 2 sigma)
942390 capture xs	:	-0.007455	[-0.007491	-0.007419]	(0.480 % 2 sigma)
0.40 sigma	:	-0.007469	[-0.007501	-0.007436]	(0.438 % 2 sigma)
942390 fission xs	:	+0.728260	[+0.728042	+0.728478]	(0.030 % 2 sigma)
0.06 sigma	:	+0.728273	[+0.728069	+0.728477]	(0.028 % 2 sigma)
942390 nxn xs	:	+0.000516	[+0.000498	+0.000535]	(3.600 % 2 sigma)
0.21 sigma	:	+0.000520	[+0.000504	+0.000536]	(3.092 % 2 sigma)
942390 nubar total	:	+0.965769	[+0.965694	+0.965844]	(0.008 % 2 sigma)
0.80 sigma	:	+0.965826	[+0.965758	+0.965894]	(0.007 % 2 sigma)
942390 nubar prompt	:	+0.964010	[+0.963933	+0.964087]	(0.008 % 2 sigma)
0.66 sigma	:	+0.964058	[+0.963989	+0.964127]	(0.007 % 2 sigma)
942390 nubar delayed	:	+0.001759	[+0.001743	+0.001776]	(0.960 % 2 sigma)

Jezebel

72 non-zero energy-integrated sensitivities were calculated (unique nuclide, perturbation mode and response)

- ▶ 73.6 % were within combined 1σ interval.
- ▶ 99.2 % were within combined 2σ interval.
- ▶ 100 % were within combined 3σ interval.

Jezebel

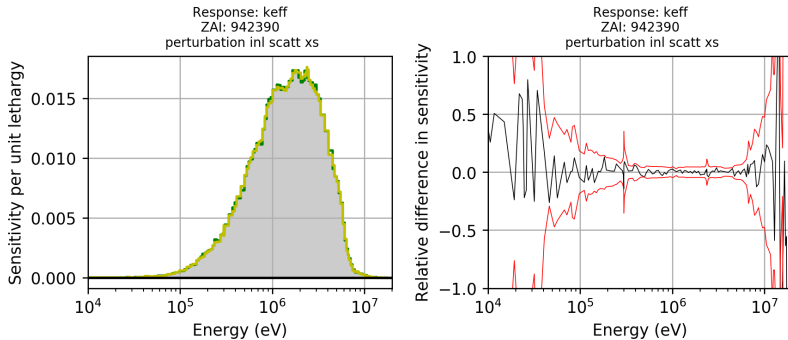


Figure 2: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Jezebel

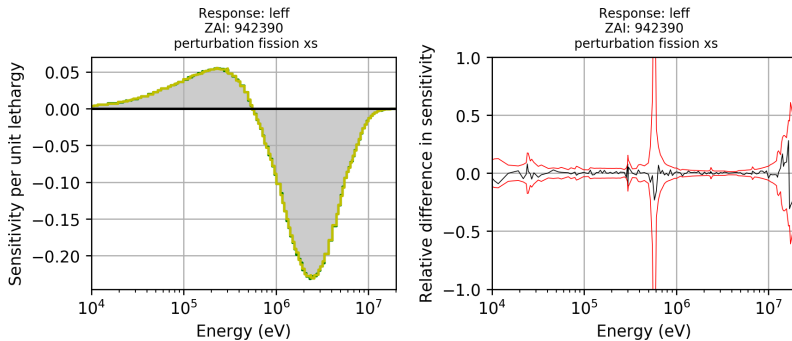


Figure 3: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Flattop

The considered responses were

- ▶ Effective multiplication factor.
- ▶ Effective prompt neutron generation time.
- ▶ Effective delayed neutron fraction.
- ▶ $^{238}\text{U}/^{235}\text{U}$ fission rate ratio in the center of the plutonium core (spectral index).

The considered perturbations were

- ▶ Reaction cross sections, nubar and fission spectrum as well as the three first Legendre moments of the elastic scattering angular distribution **of**
- ▶ ^{239}Pu and ^{240}Pu **tallied on**
- ▶ Vitamin-J 175 group structure.

Flattop

192 non-zero energy-integrated sensitivities were calculated (unique nuclide, perturbation mode and response)

- ▶ 75.5 % were within combined 1σ interval.
- ▶ 100.0 % were within combined 2σ interval.
- ▶ 100.0 % were within combined 3σ interval.

Flattop

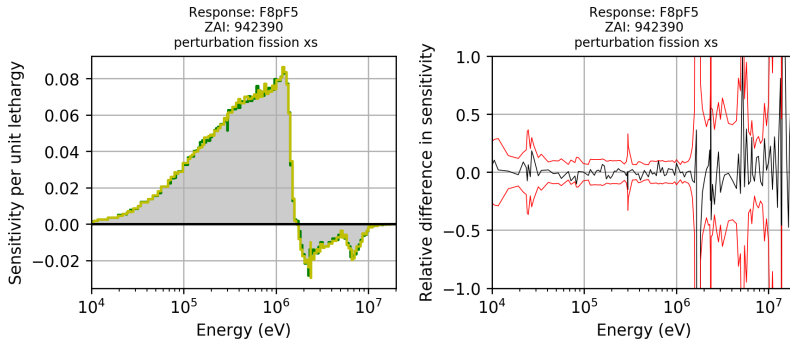


Figure 4: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Flattop

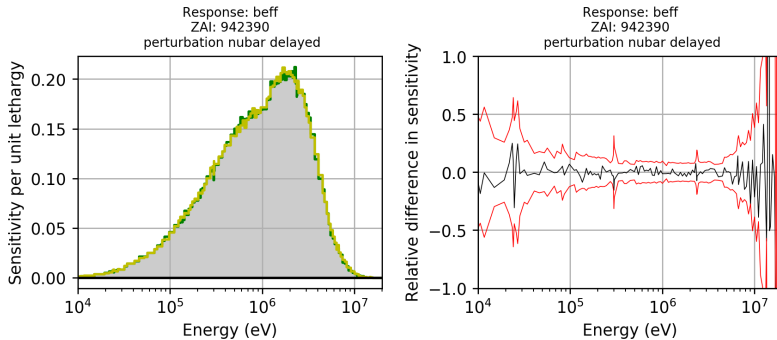


Figure 5: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Flattop

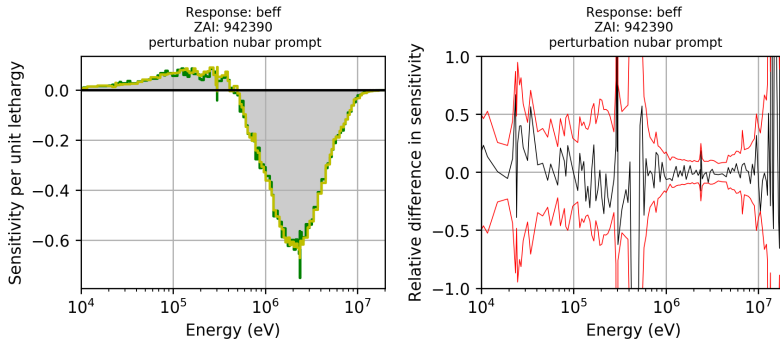


Figure 6: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Flattop

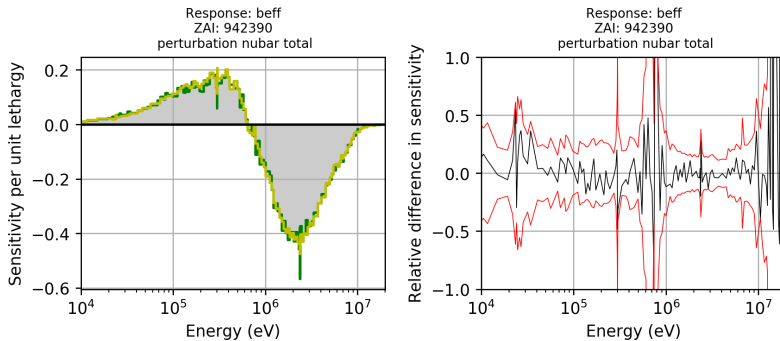


Figure 7: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

TMI1 HZP pin-cell

The considered responses were

- ▶ Effective multiplication factor.
- ▶ Void reactivity coefficient.
- ▶ $^{238}\text{U}/^{235}\text{U}$ fission rate ratio in the fuel pellet (spectral index).

The considered perturbations were

- ▶ Reaction cross sections and nubar **of**
- ▶ ^1H , ^{16}O , ^{235}U , ^{238}U **tallied on**
- ▶ SCALE 44 group structure.

TMI1 HZP pin-cell

79 non-zero energy-integrated sensitivities were calculated (unique nuclide, perturbation mode and response)

- ▶ 67.1 % were within combined 1σ interval.
- ▶ 83.5 % were within combined 2σ interval.
- ▶ 86.1 % were within combined 3σ interval.

TMI1 HZP pin-cell

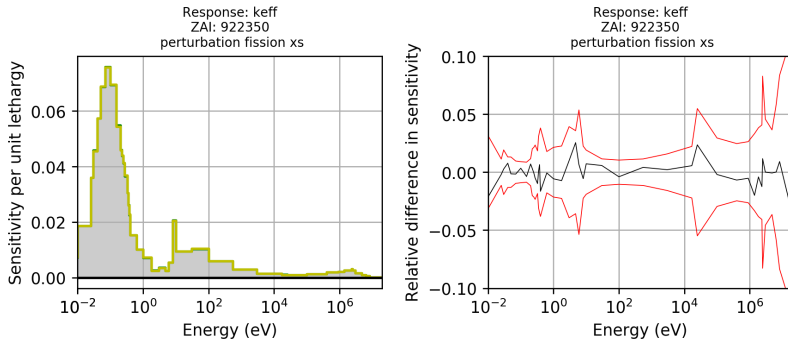


Figure 8: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

TMI1 HZP pin-cell

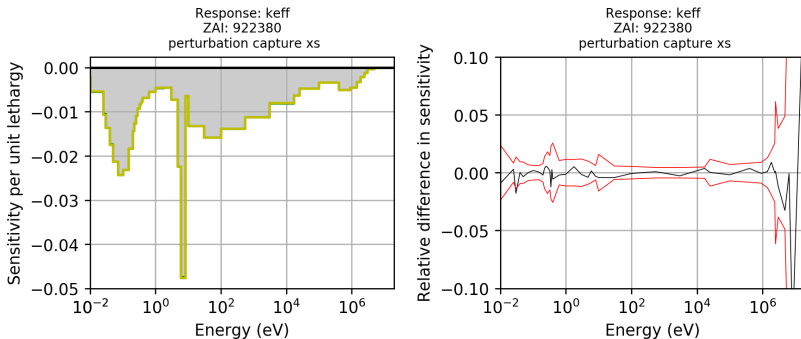


Figure 9: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

TMI1 HZP pin-cell

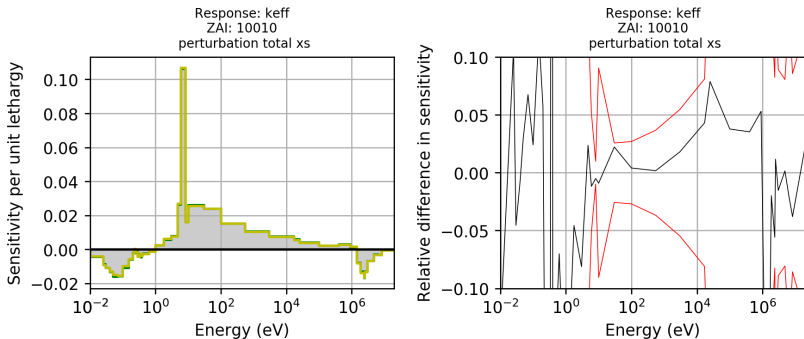


Figure 10: **Left:** Energy dependent sensitivity profile. **Yellow** line indicates old implementation, **green** line indicates new implementation. **Right:** Relative difference in energy dependent sensitivity (New/Old - 1) with 2σ statistical deviations (**red** lines).

Performance comparison

The verification simulations were executed using direct scoring (`sens opt direct <frac>`). Event based scoring would save some memory with a slight cost in running time.

The simulated neutron population was 10k neutrons per cycle, 50 inactive cycles, 100k active cycles for TMI1, 200k for fast systems.

Calculations with 20 cores on a node with two Intel(R) Xeon(R) CPU E5-2690 v2.

	Running time		Memory consumption ¹	
	2.1.19 (ext)	2.1.29	2.1.19 (ext)	2.1.29
Jezebel	14.3 h	11.7 h	6.7 GB	5.7 GB
Flattop	11.7 h	8.2 h	11.9 GB	6.0 GB
TMI1	115.7 h	28.3 h	6.5 GB	5.2 GB

¹ Read from `ALLOC_MEMSIZE` in `<input>_res.m`.

XGPT

eXtended Generalized Perturbation Theory²

Basic GPT approach gives us the sensitivity vector \bar{S} where each element S_g gives the sensitivity of k-eff to XS perturbation in a specific energy group.

If we have a perturbation extending through the whole energy range and, we can multiply the sensitivity vector \bar{S} with the perturbation vector \bar{P} to obtain the total sensitivity for the perturbation.

$$S_{\text{tot}} = \bar{P}^T \bar{S} = \sum_{g=0}^{g=N_g} P_g \times S_g$$

In XGPT we can have a continuous energy perturbation $P(E)$ and we'll calculate

$$S_{\text{tot}} = \int_{E_{\text{min}}}^{E_{\text{max}}} P(E) S(E) dE$$

inside the simulation.

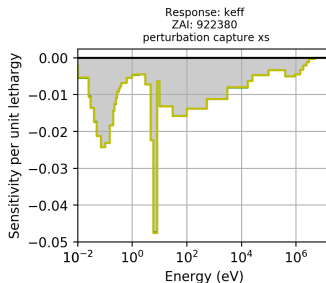


Figure 11: K-eff sensitivity in TM11 pin-cell to U-238 capture cross section.

²M. Aufiero, M. Martin, and M. Fratoni. "XGPT: Extending Monte Carlo Generalized Perturbation Theory capabilities to continuous-energy sensitivity functions." *Annals of Nuclear Energy* **96** (2016), 295–306.

Interesting applications

In addition to the clear applications in uncertainty quantification and propagation, the sensitivity calculation capabilities have other applications such as:

- ▶ Calculation of void reactivity coefficient?
- ▶ Calculation of Doppler reactivity coefficient (XGPT).
- ▶ Advanced depletion schemes⁶.
- ▶ Advanced coupled calculation schemes⁷⁸ (partly XGPT).

Time will tell if the methodology is really feasible for the applications above. Most likely, using GPT is good when the number of perturbations and/or responses is large. Otherwise statistical sampling is probably better.

⁶D. Kotlyar et al. "A perturbation-based susbtep method for coupled depletion Monte-Carlo codes." *Annals of Nuclear Energy* **102** (2017), 236–244.

⁷M. Aufiero and M. Fratoni. "Stabilization and convergence acceleration in coupled Monte Carlo–CFD calculations: the Newton method via Monte Carlo Perturbation Theory." *In proc. M&C 2017. Jeju, Korea, Apr. 2017.*

⁸D. Kotlyar et al. "Iteration-free coupled Monte Carlo with thermal hydraulic method." *In proc. M&C 2017. Jeju, Korea, Apr. 2017.*

Future work

Implementation

These would be nice things:

- ▶ Perturbation of scattering cosine (output).
- ▶ Direct part of reaction rate ratios.
- ▶ Better ways for xGPT.
 - Spatial distributions using multi-physics interface formats.
 - Cross section derivatives calculated inside Serpent.
- ▶ Multi-bin detectors for reaction rate ratios.
- ▶ Variance equalization.
- ▶ Runtime and memory comparisons (what affects resource consumption and how?).

Future work

Applications

- ▶ Uncertainty propagation into Serpent generated group constants.
- ▶ Uncertainty propagation in burnup calculations?
- ▶ Even more advanced depletion schemes?
- ▶ Advanced multi-physics coupling schemes?

Summary and conclusions

- ▶ Basic collision history based sensitivity/perturbation based capabilities have been ported from extended Serpent 2.1.19 to Serpent 2.1.29.
- ▶ Some advanced features will be added in the future updates alongside with quality-of-life improvements for certain specific tasks.
- ▶ The verification calculations show that the implemented routines work as intended.

Summary and conclusions

- ▶ The new implementation has a reduced memory footprint.
- ▶ The new implementation was faster than the old one in all of the tested applications.
- ▶ Some obvious ways to increase the performance are available and will be implemented and tested in the future.
- ▶ In addition to the applications in uncertainty propagation, the capabilities have use in various fields of reactor physics and coupled calculations.

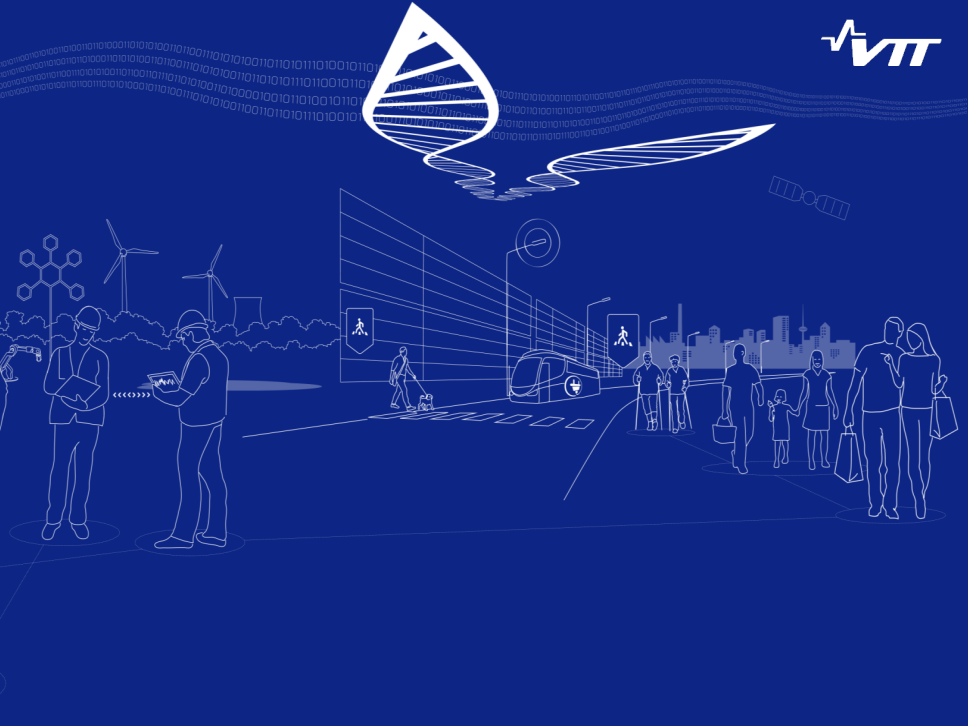
Thank you for your attention!

ville.valtavirta@vtt.fi

Project homepage: montecarlo.vtt.fi

Serpent wiki: serpent.vtt.fi

http://serpent.vtt.fi/mediawiki/index.php/Sensitivity_Calculations





M. Aufiero and M. Fratoni. “Stabilization and convergence acceleration in coupled Monte Carlo–CFD calculations: the Newton method via Monte Carlo Perturbation Theory.” In *proc. M&C 2017*. Jeju, Korea, (Apr. 2017).



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