

Serpent and nuclear & atomic data

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VTT – beyond the obvious

Outline

- Serpent in a nutshell in 2022.
- Radiation transport and depletion capabilities of Serpent.
- Serpent and nuclear data uncertainties
- Nuclear data related plans for the next 3+3 years.

Serpent overview

Serpent is a continuous-energy Monte Carlo neutron and photon transport code:

- Developed at VTT since 2004
- Physics models for neutron, photon and coupled neutron/photon transport simulations
- Originally developed for reactor physics calculations
- OpenMP/MPI parallelization
- Support for various geometry types (CSG, mesh, CAD, etc...)
- Built-in routines for group constant generation, burnup calculation and variance reduction
- Multi-physics interface for external coupling
- User-friendly, adaptable, no external dependencies, no wrappers

Serpent started out as a reactor physics code, but is currently used for a wide range of fission, fusion and other radiation and particle transport applications.

- Website: <https://serpent.vtt.fi/serpent/>
- Current base version Serpent 2.2 (May 2022).
- Over 1000 users in 250 organizations in 43 countries.

Neutron transport

- Based on a combination of surface tracking and delta tracking.
 - Complemented with additional rejection sampling to model density and temperature distributions separately from the geometry model.
- Multiple intercompatible geometry models:
 - Constructive Solid Geometry (surfaces, cells, universes)
 - CAD-geometry model based on STL solids (triangulated closed surfaces).
 - Unstructured mesh based geometry with support for OpenFOAM mesh format.
- Interaction physics modelled with ENDF laws and standard collision kinematics.
 - ACE libraries currently produced with NJOY to a fixed set of temperatures.
 - Additional temperature treatment of cross sections either as a preprocessing step (Doppler preprocessor) or on-the-fly (Target Motion Sampling).
 - Doppler Broadening Resonance Correction for elastic scattering target velocity sampling.
 - Probability table based unresolved resonance treatment.

Depletion

- Transmutation cross sections evaluated based on ACE format interaction cross sections.
 - Direct 1 group evaluation or spectrum collapse.
- Combined with ENDF NFY and decay data to construct the burnup matrix.
 - Branching ratios for reactions can have a major effect on results.
- Matrix exponential solved with CRAM.
 - Higher order predictor corrector methods with substeps to describe evolution of reaction rates during burnup step.
- Collision based domain decomposition for very large burnup problems.

Photon transport

- Uses ACE format interaction cross sections.
- Includes models for:
 - The photoelectric effect.
 - Rayleigh scattering.
 - Compton scattering.
 - Electron-positron pair production.
 - Atomic relaxation.
 - Thick target bremsstrahlung.
- Photon physics modelling between Monte Carlo codes differs much more than neutron physics modelling.
- Input data for models from multiple sources.

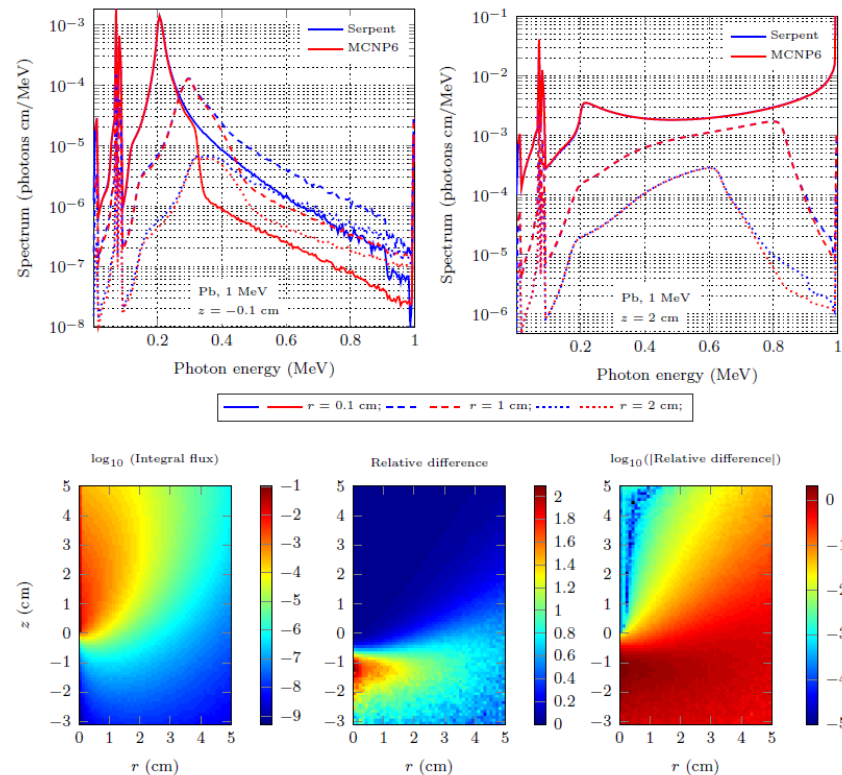


Figure 6.10: At the top row, the volume integrated photon energy spectrum for 1 MeV photon beam in a lead cylinder at six locations of the geometry. At the bottom row, the total integral flux given by Serpent in the cylinder and the relative difference (Eq. (6.1)) compared with MCNP6.

From T. Kaltiaisenaho, "Implementing a photon physics model in Serpent 2", MSc thesis, Aalto University, 2016.
https://aaltodoc.aalto.fi/bitstream/handle/123456789/21004/master_Kaltiaisenaho_Toni_2016.pdf?sequence=1&isAllowed=y

Coupled neutron photon transport

- Photons produced from neutron interactions.
 - Either analog or implicit sampling.
 - Banked in memory to wait for simulation after current neutron transport finishes.
- Utilized for shielding and accurate energy deposition calculations.
- Decay photons not included in the coupled neutron photon calculation.
- Photonuclear interactions included in a separate development branch.
 - Based on ACE-format interaction cross sections.

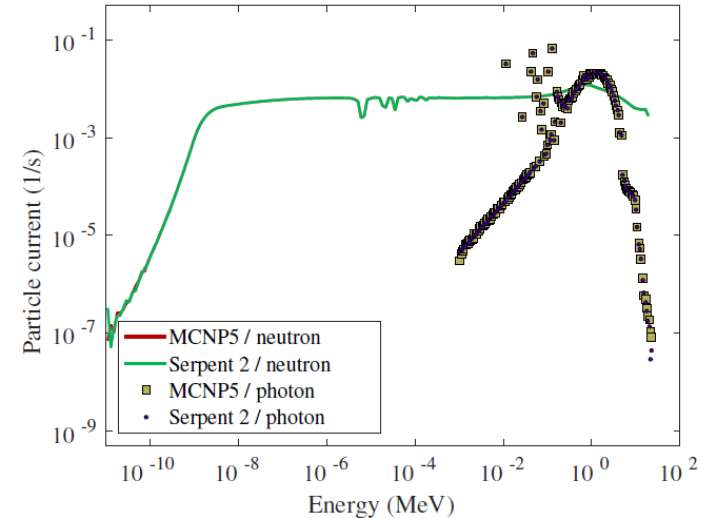


Fig. 1. Example of a “Broomstick” comparison calculation used for validating the photon production routine in Serpent 2 against MCNP5. Out-going neutron and photon current spectra calculated using the two codes. The example case is for ^{238}U from JENDL-4.0.

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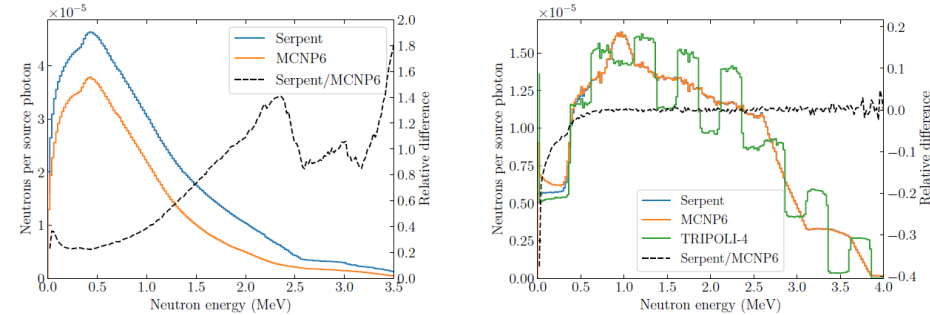


Figure 3: Photoneutron spectra on the surfaces of the tungsten and lead cubes.

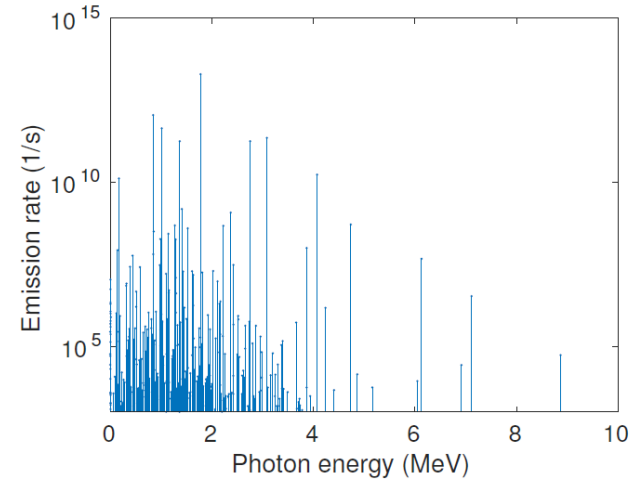
From T. Kaltiaisenaho, "Photonuclear reactions in Serpent 2 Monte Carlo code," Proc. M&C 2019, Portland, OR, USA, Aug. 25-29, 2019.

A very nice recent application of coupled neutron-photon transport for a shielding application:

Christoph Hauf (TUM) - [Simulations of the new shielding at SR8 with Serpent 2](#)

Radioactive decay source

- Neutrons and photons produced from decay reactions are not included in coupled neutron photon calculations.
- The radioactive decay source definition in Serpent generates a fixed source of neutrons, photons and secondary bremsstrahlung from beta-decay based on depleted material compositions.
- Useful for spent fuel shielding calculations as well as other shielding applications.



Photon line spectrum from a Serpent decay source definition

Nuclear data uncertainties

Deterministic approach

- Serpent includes collision history based sensitivity calculation capabilities.
- First order sensitivities of various responses such as k_{eff} and spectral indices to perturbations in etc. nuclear data simple to calculate.
- Can be combined with multigroup covariance data libraries during or after runtime.
- Utilized at VTT for uncertainty propagation and similarity analyses.
- Not applicable for depletion problems.

VTT – beyond the obvious

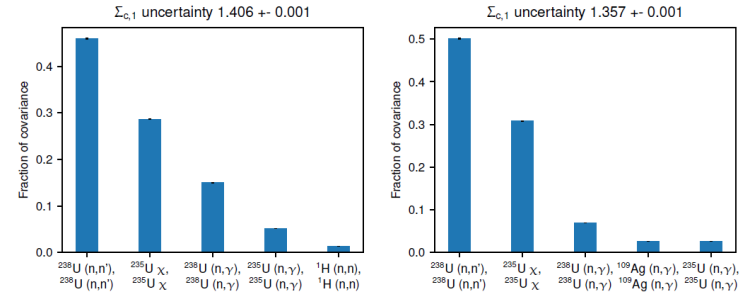
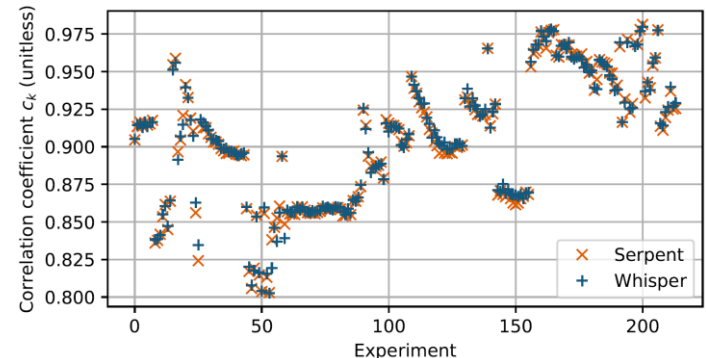


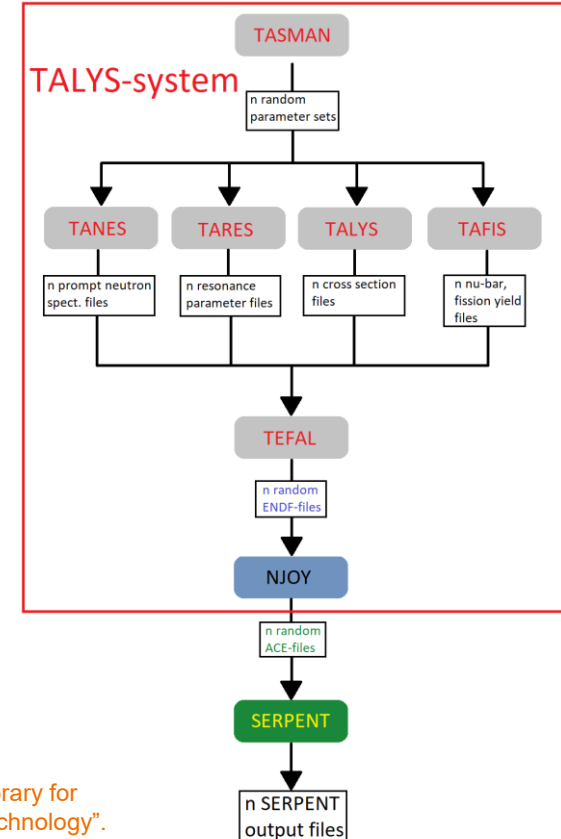
Figure 9. **TMI1 assembly at HZP**: Top contributors (as a fraction of the total covariance) to the uncertainty of the fast capture cross section for the unrodded (left) and the rodded (right) geometries. From http://montecarlo.vtt.fi/download/VTT-R-04681-18_web.pdf



Correlation coefficients between target application (VVER-1200 spent fuel wet storage) and various ICSBEP benchmarks evaluated by Serpent and Whisper (MCNP) using ENDF/B-VII.1 data.

Stochastic approach

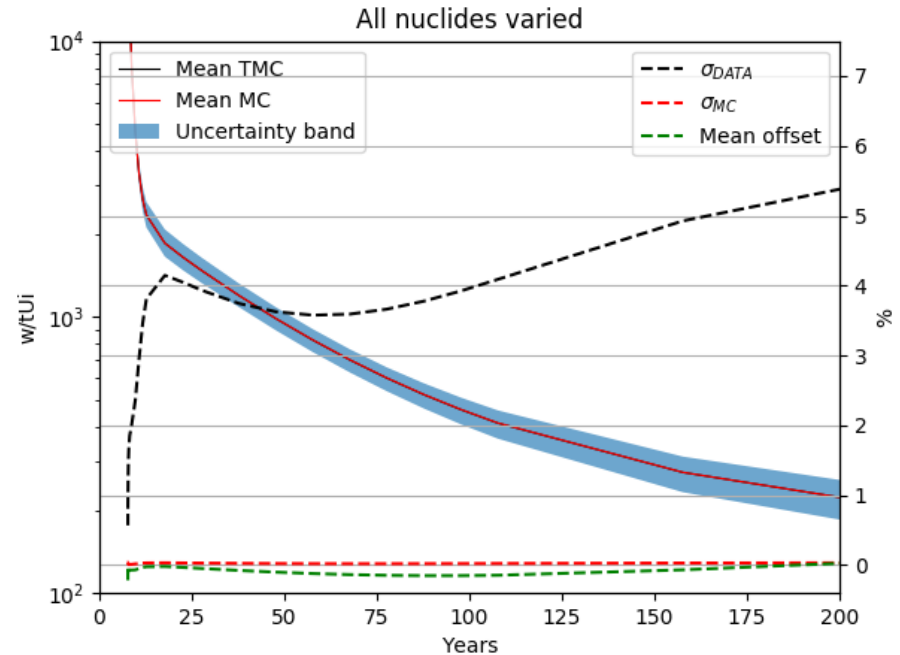
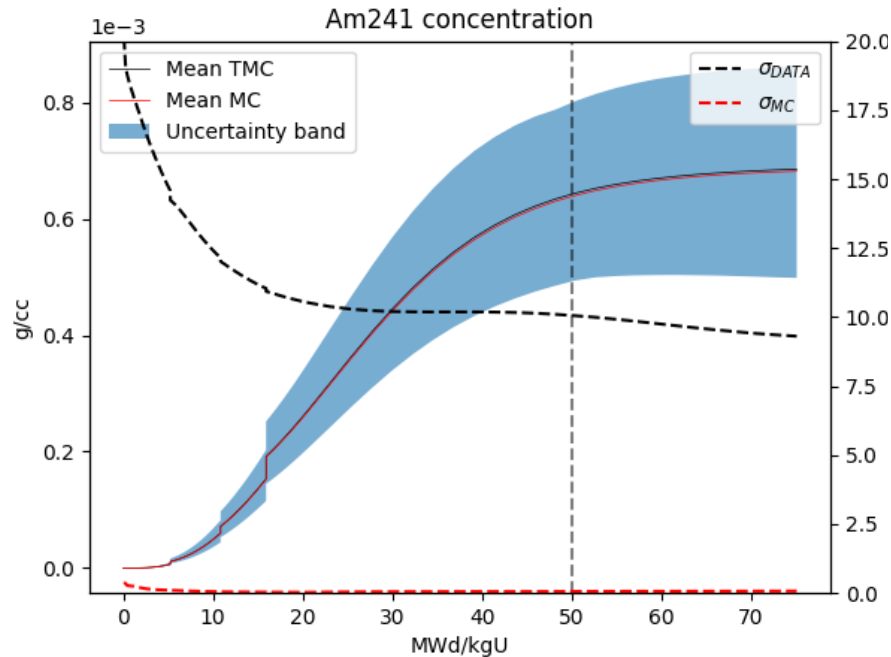
- Utilize T6 to generate randomized nuclear data files [*].
- Assign a random combination of the random data files for a Serpent run
- 500 files for 88 nuclides have been produced.
 - 0 K, 300 K, 600K, 900 K and 1200 K temperatures
- Random fission yield files have been included
 - Adopted from TENDL – website
- Pre-/postprocessing and visualization set up.
- It is now straightforward to propagate data uncertainties through Serpent at VTT, although computationally expensive.



[*] A.J. Koning et al. (2019)
 “TENDL: Complete Nuclear Data Library for
 innovative Nuclear Science and Technology”.
 Nuclear Data Sheets 155, 1-55.

Application of stochastic approach to decay heat predictions

Uncertainty in decay heat > 3.5 % due to nuclear data when cooling time > 15 y



Plans for SAFER2028

The SAFER2028 framework in Finland

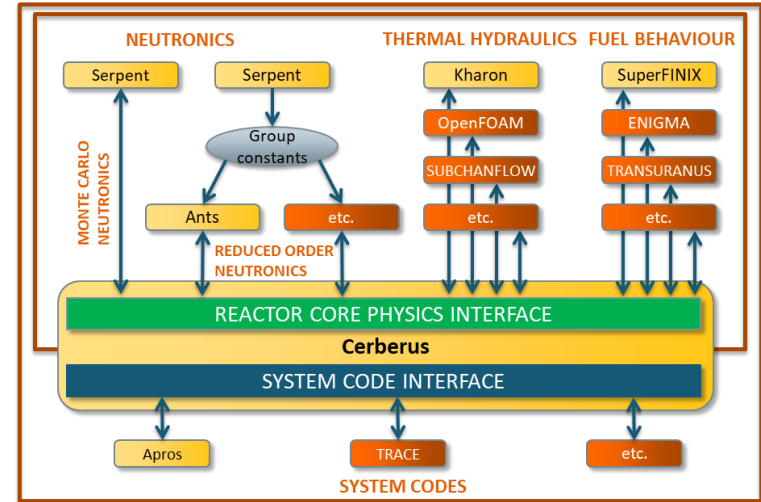
- The national nuclear safety research in Finland is largely funded from the national Nuclear Waste Management Fund.
- The next programme period starts in 2023 and extends 3+3 years until 2028.
- Some nuclear data related tasks in submitted project applications:
 - Nuclear data uncertainty propagation.
 - Nuclear data processing, testing, validation and simplification at VTT.

Nuclear data uncertainty propagation

- Main interests in Finland are on final disposal of LWR fuel in the Finnish deep geologic repository.
- Uncertainty of decay heat is the main specific question.
- Propagation of uncertainties to lattice burnup calculation results is straightforward with T6 stochastic approach:
 - Resulting uncertainties often “seemingly” too large (same with deterministic/sensitivity approach).
- How to handle dependencies/covariances between different assemblies / axial positions in operating full core reactors:
 - Lattice calculations independent of each other.
 - Requires 3D full core burnup calculations:
 - Monte Carlo is very expensive.
 - Monte Carlo group constant generation for two-step chain is also quite expensive.

Nuclear data processing, testing, validation and simplification (SYNTY project)

- Reactor analysis framework at VTT being modernized.
- Nuclear data comes in through Serpent:
 - High fidelity neutronics with direct Monte Carlo solution.
 - Two step Serpent-Ants neutronics solution.
- Good point in time to also revisit nuclear data processing, testing and validation in a structured manner.
- Some applications require simplified chains, that should be produced in a consistent manner between different base libraries.
- Work planned for setting up a modern nuclear data processing “framework” at VTT.



A schematic representation of the plans for the completed **Kraken** framework. Finnish solver modules developed at VTT are shown in yellow, while potential state-of-the-art third party solvers to be coupled are shown in orange.

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