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Status of Serpent Monte Carlo code in 2024

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Abstract. The Serpent Monte Carlo code has been in public distribution for 15 years, and has a large international user basis with both research and commercial applications. Serpent is currently developed as part of the Kraken multi-physics framework, which has dedicated capabilities for core-level reactor physics analyses. In Kraken, Serpent can be used either as a high-fidelity neutronics solver, or for generating homogenized group constants for the Ants nodal neutronics code. The neutron and photon transport modes in Serpent enable using the code also for various stand-alone applications beyond reactor physics, such as radiation shielding and fusion neutronics. This paper presents a review of the current status and capabilities of Serpent, corresponding to the latest release 2.2.1. The main features are introduced, with references to publications with more detailed methodological descriptions.

1 Introduction

Serpent is a continuous-energy Monte Carlo neutron and photon transport code, with built-in capabilities for fuel depletion, group constant generation, multi-physics coupling and variance reduction. The development started at VTT Technical Research Centre of Finland in 2004, and the first version was released to public distribution five years later. The latest version 2.2.1 was published in March 2023. Distribution for non-commercial research is handled by two data centres: the OECD/NEA Data Bank and RSICC. Commercial use is enabled with a separate license agreement. In addition to personal licenses, an educational group license ("Professor license") is available to universities for teaching purposes and academic work.

The previous overview of features and capabilities in Serpent was published more than ten years ago [1]. The purpose of this paper is to provide a status update, with references to recent publications. Major developments during the past ten years include incorporating Serpent into VTT's Kraken computational multi-physics framework, improved methodologies for group constant generation, and implementation of a photon transport mode, variance reduction capabilities and advanced geometry types.

This paper is divided into two main parts. Section 2 describes the capabilities of Serpent for high-fidelity and reduced-order reactor physics applications as part of Kraken. Section 3 provides an overview of other features and capabilities relevant for applications beyond reactor physics. The final section is left for summary and discussion. It should be noted that this paper is not intended to be a comprehensive methodological description, but rather an overview pointing out some of the highlights considered relevant by the developer team. More information can be found on the Serpent website and in the Serpent Wiki[1].

2 Reactor physics applications

Serpent has been developed with a pragmatic approach and focus on reactor physics applications since the beginning of the project. Neutron interaction data is obtained from standard ACE format libraries, which support all major reaction modes and provide separate models for thermal scattering and unresolved resonance probability table sampling. Doppler-broadening Rejection Correction (DBRC) is available as a separate model for resonance scattering at low energy.

Serpent has a built-in fuel depletion solver, which combines neutron reactions with ENDF radioactive decay and fission yield data. The Bateman equations are solved using the Chebyshev Rational Approximation Method (CRAM) [2]. Burnable materials can be automatically divided into depletion sub-zones to improve spatial resolution. In addition to solid fuels, the depletion solver enables the modeling the continuous material streams in molten salt reactors.

The standard geometry model relies on a three-dimensional universe-based constructive solid geometry type (CSG), which is sufficient for most reactor

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[1] Serpent website – https://serpent.vtt.fi/serpent/; Serpent Wiki – https://serpent.vtt.fi/mediawiki/

applications involving regular structures. For micro-particle fuel types and pebble-bed reactors Serpent features an explicit geometry model that enables describing the geometry without major approximations [3]. Fragmented fuel and other stochastic heterogeneous configurations can be modeled using a geometry type based on Voronoi tessellation [4]. More complicated core structures can be modeled using CAD and mesh-based geometry types, as discussed in Section 3.2.

Serpent can be used for coupled reactor physics applications either as a high-fidelity neutronics solver, or for generating homogenized cross sections for a reduced-order transport code. The approach at VTT relies on the Kraken computational framework, which handles the two-way coupling to thermal hydraulics and fuel behavior solvers.

2.1 Kraken computational framework

Kraken [5] is VTT's multi-physics, multi-scale computational platform, intended for solving the coupled reactor physics problem. Kraken features a driver module and an interface for the exchange of input and output data between the physics solvers, together with pre-and post-processing capabilities. The coupling is intended to be code-agnostic, but the default configuration includes neutronics, thermal hydraulics and fuel behavior solvers developed at VTT. The computational sequences are illustrated in Figure 1.

Neutronics calculations in Kraken are based on Serpent. In the reduced-order sequence, Serpent is used to produce homogenized group constants for the multi-group nodal neutronics program Ants, which solves eigenvalue or fixed-source steady-state, depletion and time-dependent problems for rectangular or hexagonal core geometries [9–11]. Hexagonal cores can also be modeled with a triangular nodal geometry [12]. The nodal diffusion solution is based on combination of the flux expansion nodal method (FENM) and analytic function expansion nodal method (AFEN). Ants supports pin power reconstruction and microscopic depletion of nodal nuclide compositions [13,14].

The fuel behavior solution is provided by the SuperFINIX [15] core-level fuel behavior solver, which delegates the modeling of individual or representative fuel rods to the FINIX [16] fuel behavior module. In steady state and fuel cycle simulations the core-level thermal hydraulics solution can be obtained using the time-independent two-phase closed-channel porous-medium thermal hydraulics solver Kharon, which was originally developed as a placeholder for more advanced methodology. Time-dependent simulations and problems requiring more accurate modeling of mixing phenomena has been handled using an OpenFOAM based solver applying the porous-medium approximation.

The core physics model in Kraken can also be coupled to system-scale simulations via external boundary conditions. At VTT, the external coupling is typically established to the Apros process simulator [17], but Kraken has also been coupled to TRACE [18,19].

2.2 High-fidelity sequence

When used as part of the high-fidelity calculation sequence in Kraken, Serpent is coupled to the other physics solvers via the multi-physics interface in the Cerberus module. Temperature and density distributions are brought into the Monte Carlo simulation from the coupled solvers, and heat deposition from neutron and photon interactions passed into the opposite direction. Features and capabilities enabling such coupling are discussed in the following.

2.2.1 Universal multi-physics interface

The multi-physics coupling scheme was implemented in Serpent several years before developing the Kraken framework [20]. The methodology is based on the complete separation of state-point information from the geometry description. Density and temperature distributions are super-imposed over the geometry, and no modifications, such as material sub-division, are required in the underlying model. The methodology supports various interface types, including an unstructured OpenFOAM format polyhedral mesh [21] and a special interface type for fuel performance coupling [22].

Most interface formats rely on spatially discretized distributions, but since the methodology is based on a rejection sampling algorithm, temperatures and densities may also exhibit continuous changes. Density variations are accounted for by applying a simple multiplier to the underlying material density [23], but variations in temperature involve more physics.

2.2.2 On-the-fly temperature treatment of cross sections

The ACE data format provides continuous-energy cross sections for neutron interactions. In addition, cross sections in the unresolved resonance region can be handled by probability table sampling, and molecular and lattice binding effects by specific thermal scattering cross sections and $S(\alpha, \beta)$ scattering laws. Each data type is pre-generated for a specific temperature. In multi-physics calculations, however, the temperature has to be adjustable to account for local variation.

The methodology applied in Serpent for continuous-energy cross sections relies on the target motion sampling (TMS) method [24]. The energy and direction of motion of the target nuclide are sampled from a Maxwellian based distribution for every neutron collision. A coordinate transformation made to the target-at-rest frame of reference then allows using cross sections generated for the corresponding temperature. Temperature treatment for thermal scattering data relies on interpolation between fixed temperatures [25]. Similar interpolation has been implemented in the development version 2.2.2 for unresolved resonance probability table sampling.

2.2.3 Domain decomposition

The default optimization mode in Serpent uses pre-generated macroscopic total cross sections to avoid the costly operation of summing over nuclides each time a new track length is sampled from a material [26]. This results

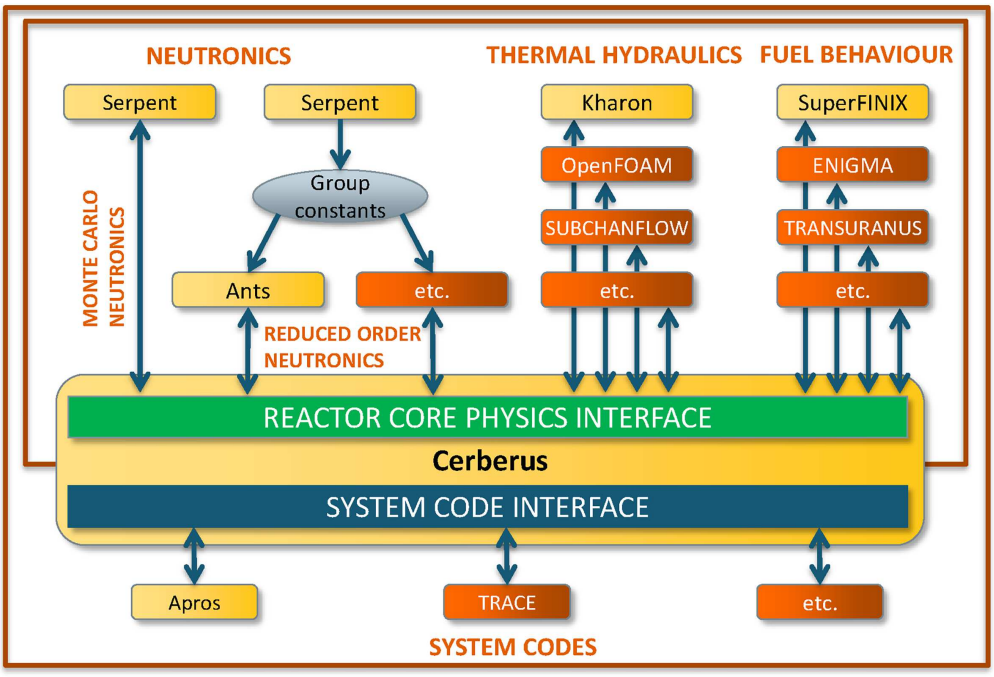

Fig. 1. The Kraken computational framework. Data transfer is handled through the driver module Cerberus, which also handles the external coupling to system-scale simulations. The default configuration is based on modular solvers developed at VTT (yellow). Various third-party solvers (orange) have also been coupled to Kraken, such as the SUBCHANFLOW [6,7] sub-channel thermal hydraulics code, and the TRANSURANUS [8] fuel performance code.

in a large memory footprint for burnup calculation, which increases along with the number of burnable materials. Burnup calculations involving tens of thousands of depletion zones can still be run by reducing the optimization.

Full-core burnup calculation problems, however, are beyond the conventional methodology. The number of depletion zones is increased to millions, and even storing the nuclide compositions requires an excessive amount of computer memory. The solution is to use domain decomposition, which means that the geometry is divided between computational nodes, each operating within its own memory space. Neutrons crossing a domain boundary are transferred to another node on-the-fly during the transport simulation.

Domain decomposition in Serpent relies on a collision-based approach [27]. Instead of using boundaries fixed to the geometry, the domains are assigned on material basis. Neutrons are transferred to another node when a collision occurs in a material belonging to a foreign domain. The division is applied to burnable materials only, based on their location in the global geometry. Limiting the decomposition to fuel materials reduces the computational overhead, since the vast majority of collisions typically take place in the moderator, for which the material data is shared by all nodes.

2.2.4 Fission source convergence acceleration

Full-core calculations are often troubled by slow fission source convergence, which results in a significant share of computing time lost to simulating inactive population cycles. The convergence is monitored using Shannon entropy, but Serpent also features an option to reduce the number of inactive cycles by applying an improved initial source distribution. The solution relies on the response matrix method, with coupling coefficients obtained from the Monte Carlo simulation [28]. A similar solver is also used for variance reduction (see Sect. 3.3).

2.2.5 Dynamic simulation mode with delayed neutron precursor tracking

Coupled steady-state and burnup calculations can be run as time-independent criticality source simulations, but the time-dependence of neutron histories is explicitly followed in external source and dynamic simulations. The difference in time scales between prompt fission chains and delayed neutron emission becomes a challenge especially in transients, where the system remains close to criticality. For this reason, precursor decay is treated separately from prompt fission chains in the dynamic simulation mode.

Serpent adapts the dynamic Monte Carlo method [29] to track delayed neutron precursors either as point-wise particles, or as concentrations on a spatial mesh [30]: a snapshot of the live neutron population and delayed neutron precursors is saved from a criticality source simulation as the starting point of the dynamic simulation. During the transient, delayed neutrons are emitted from the decaying precursors, new precursors are produced in an implicit manner and population control is applied for both neutrons and delayed neutron precursors at user chosen time intervals to manage the number of tracked particles. Time-dependent transformations can be used to modify the geometry of the calculation model during the

simulation. This allows, for example the velocity or acceleration based extraction of control rods or rotation control drums to initiate reactivity transients or to model a reactor SCRAM. At the moment, delayed neutron precursors are not affected by such transformations, but allowing their movement for e.g. molten salt fueled reactor applications or VVER-440 fuel followers is a possible future research topic.

2.2.6 Advanced energy deposition modes

More than 80% of energy released in fission is deposited locally as the kinetic energy of the fission fragments. The remaining share is divided between fission neutrons, prompt gamma radiation and energy released in radioactive decay. In addition, a non-negligible amount of energy is released in other neutron reactions, especially radiative capture. The simplest model in Monte Carlo simulations is to assume that all this energy is deposited immediately at the fission site. This is a fairly good approximation for steady-state and burnup calculations, when the behavior mostly depends on total power.

More detailed representation of fission energy deposition can be accomplished by accounting for direct neutron and gamma heating explicitly. The direct neutron heating component requires no additional physics models, but the contribution of gamma heating necessitates running the simulation in coupled neutron-photon transport mode (see Sect. 3.1). The various physics options are implemented into four energy deposition modes [31]. The most accurate mode handles direct neutron and photon heating with prompt and delayed fission gammas. This method requires additional data, which is appended to the end of standard ACE-format data libraries.

2.3 Reduced-order sequence

Generation of homogenized multi-group constants has been one of the main applications for Serpent since the beginning of the project. With Kraken development, the methodology has been further tailored for the needs of the Ants nodal neutronics code, but Serpent has been widely used for producing group constant data also for other other nodal codes, such as DYN3D, PARCS and SIMULATE.

The main advantage of continuous-energy Monte Carlo simulation in group constant generation is its versatility. This method can be used for modeling any fuel or reactor type, without application-specific limitations. The drawbacks are related to high computational cost and the fact that the calculation of certain parameters, such as diffusion coefficients and leakage-corrected cross sections requires special treatment. The related methods and capabilities are discussed in the following.

2.3.1 Generation of multi-group constants

Serpent has the capability to produce all homogenized group constants required by Ants for nodal diffusion calculations [32]. Multi-group reaction cross sections, poison cross sections, assembly discontinuity factors and pin-power form factors are obtained using standard Monte Carlo tallies. Scattering matrices combine homogenized cross sections with analog estimates of group-transfer probabilities. Multiple options are available for calculating the diffusion coefficients: the out-scatter approximation, the cumulative migration method (CMM) [33,34], and a user-defined transport correction factor applied to the total cross section (TRC). The last two options correspond to the in-scattering approximation, which is relevant especially for hydrogen. The transport correction factors can be obtained for individual isotopes and temperatures from data produced with a separate Serpent calculation. Diffusion coefficients are also obtained from B_1 and P_1 critical spectrum iterations (see Sect. 2.3.2).

Serpent can also calculate homogenized multi-group microscopic cross sections for user-defined nuclides and reactions [14]. In Ants, these parameters are utilized, for example, to track the densities of ^{239}Pu and its precursors to correct the group constants for spectral effects in fuel burnup [35]. The current methodology is limited to reaction cross sections, and cannot be applied to microscopic diffusion coefficients or scattering matrices.

Group constants can be generated for both physical universes and universes super-imposed over the physical geometry. This capability is utilized in evaluating radial reflector constants for Ants: group constants and boundary conditions for discontinuity factor calculation can be evaluated for all reflector positions from a single 2D core-level calculation.

2.3.2 Critical spectrum calculations

The infinite lattice models typically used for fuel assembly group constant generation fail to account for the spectral effects from the streaming of neutrons between assemblies in the reactor geometry. Critical spectrum methods try to account for these effects by introducing a leakage correction to the neutron balance.

Serpent features both deterministic and Monte Carlo based methods for critical spectrum calculations. In the Monte Carlo approach [36,37], the leakage correction is applied directly into the transport simulation by adding or removing neutrons from the population to obtain balance between the source and loss terms according to the fundamental mode (FM) buckling iteration. The energy dependence of the correction term corresponds to the estimated diffusion coefficient. The correction is automatically applied to all results, including reaction rates calculated for burnup calculation.

The deterministic approach relies on an intermediate multi-group structure. Multi-group cross sections obtained from the Monte Carlo simulation are used for formulating the critical spectrum equations. The solution provides the leakage-corrected flux spectrum, which is used to condense the multi-group cross sections into the final few-group structure. The methodology is applied to the group constants only, whereas the cross sections used in the burnup calculation are condensed using the infinite flux spectrum. The effects of using critical spectrum or

infinite spectrum data for lattice burnup calculations was investigated in reference [37].

The calculation was originally based on the B_1 critical spectrum method [38]. It was later pointed out, however, that the diffusion coefficients produced in this way are generally not suitable for LWR simulations [39]. The methodology in Serpent was therefore revised by introducing additional P_1 and fundamental mode (FM) solutions[2]. An example comparison of Ants results with infinite spectrum and FM group constants is presented in reference [13].

2.3.3 Automated calculation sequence

To accurately describe the homogenized properties of the fuel in a reduced order solver, group constants need to be generated taking into account both historical and momentary conditions of the fuel. Independent calculations accounting for conditions that persist for an extended period of time are called history variations. Each history variation corresponds to a separate burnup calculation. Momentary changes in the operating conditions are accounted for with branch variations, which are invoked by performing restarts at different burnup points.

Serpent provides an automated calculation sequence for generating full sets of group constants. This reduces the manual effort for handling the input files and executing the computationally expensive calculations. The variations can be defined as separate input options without the need to re-write entire material or geometry definitions. These variations can then be applied as history or branch variations in automatically executable sequences. The calculation involves a large number of relatively fast independent runs, making it well suited for large computer clusters. The methodology enables automatically distributing the calculations between different computer nodes. The procedure has been utilized, for example, in the group constant calculations of reference [42].

2.3.4 Point-kinetics parameters

Calculation of point-kinetics parameters, such as delayed neutron fractions and neutron generation times requires weighting with adjoint flux. Since the adjoint solution is not easily obtained from a continuous-energy Monte Carlo simulation, the calculation typically relies on approximations. In Serpent, the effective point-kinetics parameters are calculated using the iterative fission probability (IFP) method [43].

3 Other neutron and photon transport applications

Serpent can also be used for various applications beyond reactor physics, such as radiation shielding and fusion neutronics. These simulation tasks often involve complicated irregular geometries and calculation sequences comprised of multiple parts. Such sequences are not automated in the same sense as the two-way coupling when Serpent is used as the high-fidelity neutronics solver in Kraken, but they do involve repeating the transport simulation with small changes in the input files. The capability to generate a radiation source or a weight window mesh without third-party tools can reduce both the user effort and the risk of human error. Some of the key features and capabilities are described in the following.

3.1 Photon physics model

The photon physics model in Serpent covers photo-atomic reactions up to 100 MeV energy, and includes the four main interaction modes: Rayleigh scattering, Compton scattering, photoelectric effect and electron-positron pair production, as well as the generation of secondary photons via atomic relaxation, and electron and positron bremsstrahlung [44]. This level of physics is considered sufficient for modeling gamma radiation emitted in radioactive decay.

Serpent also supports coupled neutron-photon transport simulations [45]. Secondary photons produced in neutron reactions can be written into a source file, or included directly in the transport simulation. Typical applications for the coupled neutron-photon transport mode include reactor shielding, and multi-physics calculations run with a detailed energy deposition model (see Sect. 2.2.6).

The burnup routine in Serpent enables obtaining isotopic compositions for irradiated fuel and activated materials. The output from a previous burnup or activation calculation can be directly used with a radioactive decay source mode, which combines the isotopic compositions to radioactive decay data and photon and neutron emission spectra from ENDF format files. The decay source also works with user-defined radioactive materials.

3.2 Advanced geometry types

The standard CSG geometry type is not always ideal for modeling complicated irregular systems. Construction of large complex geometries requires considerable user effort, and is prone to input errors and computational bottlenecks. As an alternative to CSG, Serpent enables importing CAD- and mesh-based models. All geometry types operate at the universe level, which allows using different types for different parts of the modeled system.

The CAD-based geometry type relies on the STL file format, which is used for various 3D applications and supported by most CAD tools. The geometry is comprised of solid volumes defined by tessellated surfaces. The computational cost of the tracking routine is considerably reduced by an adaptive search mesh laid on top of the CAD components [46].

The CAD solids are surface models without any internal structure. For applications requiring spatial sub-division it is possible to use a mesh-based model instead [47]. The geometry type is based on the same OpenFOAM polyhedral mesh that is also used by the multi-physics interface (see Sect. 2.2.1).

[2] For general descriptions of the critical spectrum methods, see references [40,41].

3.3 Variance reduction

Variance reduction is commonly needed for radiation transport and shielding applications. The approach in Serpent relies on standard weight window methodology, and can be applied for both neutrons and photons. The weight-window mesh can be read from MCNP WWINP format files [48], which also enables using state-of-the-art deterministic tools for the task.

Serpent also features a built-in light-weight importance solver based on the response matrix method [49], which has the advantage that the procedure is considerably streamlined since there is no need to generate additional input for an external solver. Weight window mesh generation can also be run iteratively, using the global variance reduction technique [50]. This methodology has shown good performance, especially for heavily shielded geometries.

3.4 Sensitivity and uncertainty analysis

Serpent can evaluate first order generalized perturbation theory equivalent sensitivities of responses to a wide range of perturbations using the collision history approach [51–53]. Typical results include sensitivities of k_{eff}, time constants or detector ratios to perturbations in cross sections, other nuclear data or material densities. The evaluated sensitivities can be tallied using an energy binning to evaluate multi-group sensitivity data or using a spatial binning to evaluate the sensitivities on a spatial mesh.

If multi-group covariance matrices are provided in ASCII or COVERX format, Serpent can apply the Sandwich rule during neutron transport to propagate the nuclear data uncertainties to the responses included in the sensitivity calculation [54].

4 Summary and discussion

The Serpent code has been developed for 20 years, originally for the purpose of practical and relatively straightforward reactor physics calculations. During this time, improvements in computational performance and parallel computing have enabled increasingly challenging applications for the Monte Carlo method, such as simulations with multi-physics coupling.

In recent years, the focus in Serpent development has been in the Kraken multi-physics framework, in which Monte Carlo simulations are used either for generating group constants for the Ants nodal neutronics code, or to provide a high-fidelity transport solution for the coupling. The main advantage of the method in spatial homogenization is its applicability to any fuel or reactor type. Full-core Monte Carlo simulations are not likely to replace traditional methods in routine reactor analysis tasks any time soon, but they can already be considered a valuable addition. In Kraken, the reduced-order calculation sequence can be conveniently verified by comparison to a reference full-core Serpent simulation.

The applications of Serpent have also been expanded to new fields, such as fusion research and radiation shielding. This has been made possible by the implementation of a photon transport mode, advanced geometry types and variance reduction capability. These calculations also often involve complicated sequences, albeit without two-way coupling. The approach taken in Serpent development is to rely on built-in methodology as much as possible. The capability to perform all steps with a single code and only minor changes to the input files reduces user effort and risk of human error.

The features and capabilities described in this paper correspond to Serpent version 2.2.1, released in March 2023. New methods implemented in future updates include, for example, on-the-fly temperature treatment for unresolved resonance probability table sampling, multi-particle and beta decay source sampling, and physics routines for photo-nuclear reactions. New cross section libraries based on the most recent ENDF/B and JEFF evaluated nuclear data files with support for the advanced energy deposition modes are also being planned, and more effort will be devoted to code validation.

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Conflicts of interest

The authors declare that they have no competing interests to report.

Data availability statement

This article has no associated data generated and/or analyzed/Data associated with this article cannot be disclosed due to legal/ethical/other reasons.

Author contribution statement

Jaakko Leppänen: Software, Methodology, Writing – original draft, Supervision; Ville Valtavirta: Software, Methodology, Writing – original draft; Antti Rintala: Software, Methodology, Writing – original draft; Riku Tuominen: Software, Methodology, Writing – original draft.

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