



The Serpent Monte Carlo code: Status, development and applications in 2013



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ABSTRACT

The Serpent Monte Carlo reactor physics burnup calculation code has been developed at VTT Technical Research Centre of Finland since 2004, and is currently used in over 100 universities and research organizations around the world. This paper presents the brief history of the project, together with the currently available methods and capabilities and plans for future work. Typical user applications are introduced in the form of a summary review on Serpent-related publications over the past few years.

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1. Introduction

The work on a Monte Carlo reactor physics code currently known as Serpent was started at VTT Technical Research Centre of Finland nine years ago, and since its public release in 2009, the code has gathered an active user community of more than 250 users in 100 organizations in 28 countries around the world. The typical Serpent user is an M.Sc. or Ph.D. student, using the code for academic research and thesis work, the applications ranging from group constant generation and fuel cycle studies to research reactor modeling and coupled multi-physics calculations. The code is currently developed by a five-member team at VTT, supported by feedback and contributions from active users around the world.

This paper presents a general overview on the methods and capabilities developed in Serpent over the years, together with the current work in progress. Typical user applications are introduced in the form of a summary review on Serpent-related studies, most of which were published during the past two years. The following section presents the brief history of Serpent development, starting from the beginning in 2004.

2. History

The idea of developing a new Monte Carlo neutron transport code from scratch came from the fact that the general-purpose codes

available at the time were not particularly well suited for lattice physics applications, especially group constant generation. The reaction rate tallies required for the task had to be defined separately for each problem, and the results and the associated statistical errors combined after the calculation was completed. The large number of tallies increased the already prohibitively long running time, and the calculation of certain parameters, such as scattering matrices, diffusion coefficients and effective delayed neutron fractions lied completely beyond the standard tally capabilities. The fact that Serpent started out as a Monte Carlo lattice physics code can still be seen in both the structure of the code, and its applications.

2.1. PSG

Work on the predecessor of Serpent, carried out under the working title Probabilistic Scattering Game, or PSG, was started at VTT in 2004, and presented for the first time in an international conference in 2005 (Leppänen, 2005). The development rested on the idea of creating a simplified Monte Carlo code, dedicated to lattice physics applications. The work was therefore focused on neutron transport in reactor geometries, and the generation of homogenized group constants for deterministic reactor simulator calculations. The early work is summarized in a Doctoral Thesis, completed in 2007 (Leppänen, 2007).

It was realized early on that by narrowing down the scope of applications to homogenization and other assembly-level reactor physics calculations, it was possible to optimize the calculation routines and gain several factors in performance compared to

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general-purpose Monte Carlo codes.¹ This optimization relied heavily on several programming tricks and two features that are of particular importance: (1) Tracking routine based on the Woodcock delta-tracking method, and (2) The use of a single unionized energy grid for all microscopic and macroscopic cross sections. These methods are still in use, and brief technical descriptions are given in Section 3.

The interaction physics in PSG was based on ACE format cross section libraries, which meant that the results could be compared to reference MCNP calculations without additional uncertainties originating from the nuclear data. Even though there were still a lot of problems to be worked out, the results turned out to be in a relatively good agreement (Leppänen, 2007).

2.2. Serpent 1

The source code of PSG was completely re-written in 2007. The geometry routine was revised, and several problems in the interaction physics fixed, which brought the differences to MCNP calculations to within the range of statistical accuracy. Work on a self-contained built-in burnup calculation routine was started in 2008 (Leppänen and Pusa, 2009). Evaluation of different options for solving the Bateman depletion equations lead to the introduction of a novel matrix exponential solution based on the Chebyshev Rational Approximation Method (CRAM). This method was extensively studied over the following years (Pusa and Leppänen, 2010, 2012, 2013; Pusa, 2011, 2013a), and summarized in a Doctoral Thesis in 2013 (Pusa, 2013b). The name was changed from PSG to Serpent before the code was released to the OECD/NEA Data Bank in May 2009. Distribution via RSICC started one year later, in March 2010.

As the Serpent user community began to grow, also the flaws in the calculation routines started becoming more and more apparent. In general, the code was well adapted to two-dimensional lattice physics and burnup calculations, but when the geometries were extended from two to three dimensions, it turned out that the excessive memory usage due to the unionized energy grid approach posed serious limitations to the number of depletion zones. Similar limitations resulted from the fact that parallelization in PSG and Serpent 1 was based on the Message Passing Interface (MPI) – a distributed-memory technique, which meant that the overall memory demand was multiplied by the number of parallel tasks.

2.3. Serpent 2

To fix the problems resulting from the excessive appetite for computer memory, it was decided to re-write the source code one more time. The work started in October 2010, and the public release of Serpent 2 is scheduled for 2015. At the time of this writing the code is in a beta-testing phase, and available to licensed users of Serpent 1. Most of the essential features in the previous versions are already implemented, and work on entirely new capabilities, some of which are described in the following sections, is under way.

The main structural differences between Serpent 1 and Serpent 2 are found in the handling of cross section data and parallelization. The unionized energy grid approach developed for boosting the performance in lattice physics calculations was made optional,

and different optimization modes were introduced for large and small burnup calculation problems (Leppänen and Isotalo, 2012). Parallel calculation is based on the combination of MPI and OpenMP, which is a shared-memory parallelization technique that allows dividing the calculation into multiple threads within the same computational unit, without increasing the overall memory demand. Test calculations on a modern PC workstation with 96 GB of memory have shown that Serpent 2 can handle 200,000 depletion zones in burnup calculation, without limitations in parallelization.

Attaining good scalability in parallel calculation is a non-trivial task that requires a lot of optimization. The transport routine in Serpent 2 typically attains near-linear scalability at least up to 12 CPU cores, although the performance is extremely case-dependent. The situation becomes more complicated in burnup calculation, when certain processing routines require a non-negligible fraction of the overall calculation time. The poor scalability of these routines deteriorates the overall performance. Optimization is still under way, and comprehensive characterization of parallel scalability is yet to be done.

3. Methods and capabilities

Based on its methods and capabilities, Serpent is best characterized as a continuous-energy Monte Carlo reactor physics burnup calculation code. The neutron transport simulation can be run in external and k -eigenvalue criticality source modes, and a dynamic simulation mode for the modeling of short reactivity transients is under development. Work on gamma and coupled neutron-gamma transport simulation modes has been started, and is to be completed in 2014. The descriptions given below apply to Serpent 2, and some of the introduced features are not available in the previous version.

3.1. Geometry routine

The basic geometry routine in Serpent is based on a three-dimensional constructive solid geometry (CSG) model, which is a typical choice for Monte Carlo particle transport codes. The model is built from elementary quadratic and derived surface types, which are used to form two- or three-dimensional cells. The geometry can be divided into multiple levels using universes, transformations and repeated structures, such as square and hexagonal lattices. In addition to regular structures, an explicit stochastic geometry model is available for the handling of randomly-distributed particle fuels used in high-temperature gas-cooled reactors (HTGR's) (Leppänen, 2010a). The coordinates of individual fuel particles are read from a separate input file, and the distribution is modeled without approximations. The same geometry type can be used for the distribution of fuel pebbles in pebble-bed type reactors.

Particle tracking in Serpent relies on the combination of conventional ray-tracing based surface tracking and the rejection sampling based delta-tracking method.² The advantage of using delta-tracking in reactor calculations is that the neutron mean-free-path is typically long compared to the spatial dimensions of the geometry, and the fact that neutrons can be moved directly to their next (tentative) collision site without stopping the track at each boundary crossing can lead to a considerable speed-up in the transport simulation. LWR calculations typically gain about a factor of 2 in

¹ The running time of Serpent is often compared to MCNP, and it is true that the code can run significantly faster in lattice calculations involving a large number of tallies or irradiated fuels. This is the result of optimizing the calculation routines for group constant generation. However, the overall performance of a Monte Carlo code is a complicated issue, and extremely application-dependent. Therefore, the conclusions from one test case should *never* be extended to cover all imaginable applications.

² The delta-tracking method was originally proposed by Woodcock in 1965 (Woodcock et al., 1965), as an alternative to the conventional ray-tracing based surface tracking routine. The method is based on a rejection sampling algorithm that allows neutron tracks to be continued over several material boundaries without calculating the distances to the boundary surfaces.

performance, but in HTGR's with double-heterogeneous micro-particle fuel this factor can become as high as 10.

In order to avoid certain efficiency problems related to the presence of localized heavy absorbers, the transport routine switches to surface-tracking when the efficiency of the delta-tracking rejection sampling loop becomes low (Leppänen, 2010b). What remains as an inherent drawback of this approach is that the track-length estimate of neutron flux cannot be used for calculating reaction rate integrals, and all cell flux tallies in Serpent are based on the (potentially less-efficient) collision estimator. In practice it has turned out that the difference in efficiency is not significant in reactor calculations due to the high collision density in the regions of interest, but the methodology is poorly suited for shielding and other applications where reaction rates need to be calculated in regions located far or isolated from the active source.

3.2. Interaction physics

Serpent reads neutron interaction data from continuous-energy ACE format cross section libraries, which form the basis for the laws of physics in the transport simulation. Separate thermal scattering data can be used for important moderator materials, and probability table sampling is available in the unresolved resonance region. Nuclide temperatures can be adjusted using a built-in Doppler-broadening preprocessor routine (Viitanen, 2009), and the temperature dependence of resonant scattering kernels can be taken into account using the Doppler-broadening Rejection Correction (DBRC) method (Becker et al., 2009). A lot of recent work has been devoted to the development of an on-the-fly temperature treatment routine, which is briefly discussed in Section 3.4.

As mentioned in the previous section, Serpent has the option to reconstruct all cross sections using a single unionized energy grid (Leppänen, 2009). This approach has two major advantages. First, the energy grid search needed for interpolating microscopic cross sections between two tabulated values needs to be performed only once, each time the neutron scatters to a new energy. Second, several material-wise macroscopic cross sections can be pre-calculated, which avoids summing over the constituent nuclides during the transport simulation. The overall result is a considerable reduction in calculation time, which in extreme cases can amount to a factor of 10. The performance also becomes less dependent on the number of nuclides and tallies, which is important considering group constant generation and burnup calculations.

The drawback of energy grid unionization is that computer memory is wasted for storing redundant data points. The pre-calculated macroscopic cross sections increase the memory demand per material zone, which is why the method cannot be applied to large burnup calculation problems.

3.3. Burnup calculation

Burnup calculation in Serpent is based on self-contained built-in subroutines, without any couplings to external depletion solvers. Decay and transmutation paths are formed automatically, and the nuclides selected for the calculation without additional user input. Radioactive decay data and energy-dependent fission yields and isomeric branching ratios for neutron reactions are read from ENDF format data libraries. Division of irradiated materials into depletion zones is carried out automatically.

One-group transmutation cross sections required for forming the Bateman depletion equations are calculated during the transport simulation, or to speed up the calculation, after the simulation is completed by collapsing the continuous-energy cross sections with flux spectra collected separately for each burnable material. This spectrum-collapse method has been used in other Monte Carlo burnup calculation codes as well (Haeck and Verboomen, 2007;

Fridman et al., 2008a,b), and in Serpent it is implemented with a separate treatment in the unresolved resonance region.

Irradiation history can be divided into multiple intervals with different normalization, defined by power, power density, or total flux, fission or source rate. Depletion steps are given in units of time or burnup. Available depletion algorithms include the conventional Euler and predictor–corrector method with linear interpolation for the corrector calculation. Higher-order methods based on combinations of linear and quadratic interpolation and extrapolation (Isotalo and Aarnio, 2011b) are available in Serpent 2, together with sub-step solution (Isotalo and Aarnio, 2011c) for the intra-step reaction rates. Test calculations have shown that these advanced time integration methods can reduce the discretization errors for certain important nuclides, which allows increasing the burnup step length without compromising accuracy (Leppänen and Isotalo, 2012).

The Bateman depletion equations are solved using the CRAM matrix exponential method (Pusa, 2011), which has the capability to handle the full system of nuclides without approximations for short-lived isotopes, limitations for step length, or problems with numerical precision. The method has proven accurate and efficient, and well suited to burnup calculation problems containing a large number of nuclides and depletion zones (Isotalo and Aarnio, 2011a). Decay steps are handled using the linear chains method (Cetnar, 2006), which in the absence of neutron reactions provides an efficient analytical solution to the Bateman depletion equations.

The total number of nuclide concentrations tracked in a typical burnup calculation ranges from 1200 to 1600, including 250 to 300 actinides and fission products with cross sections. The output includes depletion zone-wise, material-wise and total nuclide concentrations, masses, activities, decay heat, ingestion and inhalation toxicities and spontaneous fission rates. The nuclides selected for the output are listed by the user, with an option to automatically include the most significant contributors to the different output categories (Viitanen and Leppänen, 2012c).

3.4. Multi-physics coupling scheme

One of the most significant on-going development projects for the Serpent code is related to multi-physics applications, in particular the coupling of Serpent 2 to CFD and system-scale thermal hydraulics and fuel performance calculations. The multi-physics coupling scheme (Leppänen et al., 2012) operates at two levels, based on: (1) Internal light-weight solvers for fuel behavior and thermal hydraulics, and (2) External coupling via a universal multi-physics interface.

The methodology relies heavily on a novel on-the-fly temperature treatment routine based on target motion sampling (TMS), which means that instead of conventional Doppler-broadening, the thermal motion of target nuclides is handled explicitly, by sampling the relative velocity at the event of collision (Viitanen and Leppänen, 2012a,b, 2013a,b, 2014). The method is currently limited to continuous-energy free-atom cross sections, and work on extending the capability to unresolved resonance probability table sampling and thermal bound-atom scattering is scheduled for the near future.

The implementation of TMS is based on a rejection sampling method, which enables the modeling of continuously-varying temperature distributions over material regions. Similar methodology is used to adjust macroscopic cross sections for the purpose of modeling non-uniform density distributions (Leppänen, 2013b). The capability to adjust local temperature and density makes it possible to pass state variables to the Monte Carlo transport simulation without any modifications in the geometry input. This forms the basis of the universal multi-physics interface, which supports several input formats, including an unstructured mesh for coupling

to CFD codes,³ and a separate interface format for fuel performance codes (Valtavirta et al., 2013).

The internal solvers include a light-weight 3D component-scale thermal hydraulics solver, developed under working title COSY, and a temperature-feedback module based on the FINIX thermo-mechanical fuel behavior model and interface (Ikonen, 2013; Ikonen et al., 2013). The internal models are intended to be used either separately, or in combination with external coupling, to speed up the convergence of the coupled solution. The FINIX module can also be used to obtain the temperature distributions and dimensions of fuel rods in transient conditions, which together with a dynamic neutronics simulation mode (Leppänen, 2013a) allows the modeling of fast reactivity excursions.

A topic partly related to multi-physics applications is the development of gamma and coupled neutron/gamma transport routines, to be completed in 2014. One of the main motivations for this capability is the explicit handling of gamma heating, which provides a source term for direct heat deposition in coolant and structural materials.

3.5. Output

The methods used in Serpent for homogenization have been developed and revised over the years. The code calculates automatically all input parameters needed for nodal diffusion calculations, including homogenized few-group reaction cross sections, scattering matrices and cross sections up to Legendre order 7, diffusion coefficients, poison cross sections, assembly discontinuity factors and assembly-wise power distributions for pin-power reconstruction. Homogenization in a leakage-corrected flux spectrum is available using a semi-deterministic approach, based on the solution of the multi-group B_1 equations (Fridman and Leppänen, 2011). Some recent work has been focused on the calculation of assembly discontinuity factors for reflectors and other regions without zero net-current boundary conditions (Fridman et al., 2013a; Canepa et al., 2013; Leppänen et al., 2014b), and the methodology will be implemented in Serpent 2 as an internal subroutine within the near future.

Another recently-added feature in Serpent 2 is the calculation of adjoint-weighted effective delayed neutron fractions and point kinetics parameters using the iterated fission probability (IFP) method (Leppänen et al., 2014a). User-defined flux tallies based on the collision estimator can be used for calculating integral flux and reaction rates in cells, materials and universes, or over a superimposed Cartesian, hexagonal, cylindrical or spherical mesh.⁴ The available response functions include microscopic and macroscopic cross sections from the material compositions or separate ACE format dosimetry libraries.

All main output files are written in Matlab m-file format, to simplify the post-processing of results. The geometry can be visualized with a built-in plotter routine, and the neutronics using track plots and reaction rate mesh plots produced during the transport simulation.

4. Applications, on-going and future work

As mentioned above, Serpent started out as a Monte Carlo lattice physics code, with the main purpose of generating homogenized group constants for deterministic reactor simulator

calculations. The applications have considerably diversified along with the growing user community, and the following subsections present a summary review on the work carried out by Serpent users, together with some outlines for future development.

4.1. Homogenization

The main motivation for using the continuous-energy Monte Carlo method for reactor analysis is its inherent capability to handle geometry and interaction physics without major approximations. When used for spatial homogenization, Monte Carlo codes also have the advantage of being able to model the full-scale heterogeneous problem, which represents the best available reference solution for the calculation scheme. Serpent-generated group constants have been validated in particular for the Serpent-DYN3D code sequence, at the Helmholtz-Zentrum Dresden-Rossendorf (HZDR). Test calculations involving various PWR (Fridman and Leppänen, 2011, 2012; Fridman et al., 2013a,b; Duerigen and Fridman, 2012) and SFR (Fridman and Shwageraus, 2013; Fridman et al., 2013c; Rachamin et al., 2013) cores have shown good agreement in both full-scale comparisons to three-dimensional Serpent calculations and assembly-level comparisons to deterministic lattice transport codes HELIOS 1.9 and ECCO/ERANOS 2.1.

Other similar comparisons include full-scale calculations with Serpent-PARCS at the Paul Scherrer Institute (PSI) (Hursin et al., 2013) in Switzerland, the Royal Institute of Technology (KTH) (Ghasabyan, 2013) in Sweden, and University of Michigan (Hall et al., 2013) and Brookhaven National Laboratory (BNL) (Brown et al., 2013b) in the U.S. In addition, Serpent has been coupled to in-house transport code TNXY for full-scale comparisons at the Instituto Politécnico Nacional and Instituto Nacional de Investigaciones Nucleares in Mexico (Gómez et al., 2012). Assembly-level comparisons to CASMO-5 have been performed at PSI (Hursin et al., 2013; Canepa et al., 2013), comparisons to WIMSD at Institut Josef Stefan (IJS) (Čalić et al., 2012a) in Slovenia, comparisons to DRAGON at the École Polytechnique de Montréal (Harrisson and Marleau, 2012) and comparisons to TRITON-NEWT and BOXER at BNL (Brown et al., 2013a).

At VTT, Serpent 2 is currently being validated in sequence with the ARES code (Leppänen et al., 2014b). ARES is a LWR core simulator, developed at the Finnish Radiation and Nuclear Safety Authority (STUK) for the purpose of independent safety analyses of Finnish power reactors, and based on the two-group nodal diffusion method and a three-dimensional Analytic Function Expansion Nodal Model (AFEN) (Mattila, 2002). Additional studies involving in-house fuel cycle and transient simulator codes HEXBU, HEXTRAN-3D and TRAB-3D are in preparation. Serpent is also used for group constant generation in a VTT research project involving the development of a multi-group diffusion model for the APROS system code.

The capability to produce high quality reference results for the deterministic full-scale calculation becomes particularly valuable in the modeling of novel reactor concepts, and other systems where experimental data is scarce or not available at all (Fridman and Shwageraus, 2013; Fridman et al., 2013c; Rachamin et al., 2013; Ghasabyan, 2013; Hall et al., 2013; Brown et al., 2013a,b; Harrisson and Marleau, 2012, 2013; Shen, 2012a,b,c; Aufiero et al., 2013b). The advantages of continuous-energy Monte Carlo calculation also become apparent when used to support the development of deterministic transport methods (Duerigen and Fridman, 2012; Scopatz and Schneider, 2012; Jareteg et al., 2013; Baier et al., 2014). Moving from two- to three-dimensional methods in homogenization becomes important in the modeling of complicated systems, and practically a necessity when generating group constants for next-generation

³ The unstructured mesh based interface currently supports OpenFOAM file format, and work on CFD General Notation System (CGNS) format support is under way.

⁴ Due to the use of delta-tracking, surface crossings are not recorded during the transport simulation. This prohibits the use of the track-length estimator for calculating volume-integrated reaction rates and complicates the calculation of surface tallies. Serpent has a user-defined surface current tally, but the methodology is subject to certain limitations.

fuel and reactor types with strong axial heterogeneities (Herman et al., 2011). A good example of extending the conventional methods of homogenization to three dimensions is the introduction of axial discontinuity factors in nodal diffusion calculations performed for Resource-Renewable BWR (RBWR) cores, with alternating seed and blanket layers inside the fuel assemblies (Hall et al., 2013; Fridman et al., 2013a).

4.2. Burnup calculation

The capability to model the evolution of nuclide compositions in irradiated materials is absolutely essential for homogenization. All studies referenced above, however, were carried out without burnup. This is mainly due to the fact that the entire methodology is still under development, and validating the code sequences for initial core configurations is the logical first step. Further, Monte Carlo burnup calculations are computing-intensive, and covering all state points requires branch and coefficient calculations, which cannot be done using the currently available built-in capabilities.⁵ Therefore, most of the assembly-level burnup calculations carried out using Serpent have so far been focused on validating the code for later use.

It should be pointed out, however, that in addition to neutronics, the results of burnup calculations are always subject to discrepancies originating from decay and fission yield data, depletion algorithm, subdivision of depletion zones and the number of nuclide concentrations tracked in the burnup simulation. Validation of burnup calculation codes, both Monte Carlo and deterministic, requires a systematic approach, which is complicated by the fact that radionuclide assay data is scarcely available and subject to experimental uncertainties. Examples of international validation effort include the various benchmarks coordinated by the Working Parties of the OECD/NEA Nuclear Science Committee.⁶

Serpent burnup calculations were compared to WIMSD5, TRITON-NEWT, Monteburns and MCNP-ACAB in a study carried out at the Universidad Politécnica de Madrid (Martinez et al., 2011), using the OECD/NEA Burnup Credit Benchmark Phase-1B from the 1990's as the test case. Another already completed NEA benchmark on plutonium recycling was chosen for a study carried out at IJS (Čalić et al., 2012b). Validation of Serpent using several VVER-440 and VVER-1000 burnup calculation benchmarks is currently under way at the TUV SUD Industrie Service GmbH, Germany (Lötsch, 2013). Other code-to-code comparisons have been carried out with Serpent at VTT (comparison to CASMO-4E) (Leppänen and Pusa, 2009), University of Genova (comparison to Monteburns) (Chersola et al., 2014), University of Zagreb (comparison to DRAGON, FA2D and TRITON-NEWT) (Grgic et al., 2012), University of Cambridge (comparison to WIMS) (Harris, 2013), and INVAP, Argentina (comparison to Condor) (Ferraro and Villarino, 2011). BWR assembly burnup calculations with and without control rods have been performed at the Instituto Politécnico Nacional and Instituto Nacional de Investigaciones Nucleares in Mexico (Silva et al., 2013), and the next phase of the study involves comparison to CASMO-4.

Similar to group constant generation, extending assembly-level burnup calculations from two- to three- dimensional geometries is a prerequisite for the modeling of advanced fuel types with strong axial heterogeneities. It turns out, however, that the same calculation schemes that work well in closely-coupled two-dimensional systems exhibit instabilities and Xe-135 driven oscillations in larger and more loosely-coupled geometries (Dufek and Gudowski, 2006; Dufek and Hoogenboom, 2009; Dufek et al., 2013b). Any results from a simulation where the neutronics state of the system is oscillating are practically useless for the purpose of homogenization, since the parametrization of group constants is based on fixed state points. These problems have been studied recently, and methods based on forced equilibrium xenon calculation and new burnup algorithms have shown good results in stabilizing the oscillations (Isotalo et al., 2013; Dufek et al., 2013a; Kotlyar and Shwageraus, 2013).

In reactor physics applications, tracking the isotopic composition of the irradiated fuel is usually a means towards the actual results, rather than the final outcome of the study. Core design and safety analyses, often involving burnup calculation as an intermediate step, are discussed in the following section. Burnup calculations are also needed for fuel cycle studies, involving next-generation reactor technology designed for breeding fissile material or burning nuclear waste. A good example is a recent study carried out at the Universidad Politécnica de Madrid, in which Serpent was used for evaluating the effects of deploying Gen-IV SFR's in the Spanish nuclear fleet (Ochoa et al., 2013a).

4.3. Core design and safety analyses

Due to their inherent capability to model complicated three-dimensional systems, Monte Carlo codes are an attractive option for full-scale reactor physics calculations as well. In practice, however, the applications are limited by the sheer extent of the task, and the modeling of large power reactor cores requires millions of reaction rate tallies and months or even years of CPU time. In 2010, Hoogenboom, Martin and Petrovic set up a well-known benchmark problem for evaluating the performance and capabilities of Monte Carlo codes in the modeling of full-size reactor cores (Hoogenboom et al., 2010). The calculations were also carried out using Serpent (Leppänen, 2010c). A more recent full-scale PWR benchmark problem was introduced by the MIT Computational Reactor Physics Group in 2012 (Horelik and Herman, 2012). The BEAVRS benchmark was set up for the validation of high-fidelity neutron transport codes in comparison to experimental data. A detailed three-dimensional Serpent model of the BEAVRS benchmark core was constructed for the purpose of validating the Serpent-ARES code sequence (Leppänen et al., 2014b). The results were found to be in good agreement with experimental data as well.

Even though Monte Carlo codes cannot yet be considered practical design and analysis tools for full-scale LWR simulations, they are widely used for modeling small research reactors and other closely-coupled systems. Serpent has been used for modeling the TRIGA Mark II type F1 reactor at VTT (Barray, 2012), and two research groups at the Idaho National Laboratory (INL) are benchmarking the code for the modeling of their Advanced Test Reactor (ATR) (Lyons, 2013; DeHart et al., 2013; Nigg et al., 2013), and the High-temperature Engineering Test Reactor (HTTR) operated by the Japan Atomic Energy Agency (JAEA) (Ortensi et al., 2010a,b).

When measured in units of neutron mean-free-path, fast reactors are small compared to large LWR cores, which makes Monte Carlo codes viable candidates for their design and safety analyses. Serpent has been extensively used in the European Lead-Cooled Training Reactor (ELECTRA) project (Wallenius and Fokau, 2009; Wallenius et al., 2012, 2013; Suvdantsetseg et al., 2012; Alhassan

⁵ Work on an automated burnup sequence for group constant generation was started in late 2013. At the time of this writing there exists at least two wrapper scripts that can be used to automate the procedure for the Serpent-PARCS coupling – Python-based SerpentXS, developed at MIT (see: <http://canes.github.io/SerpentXS/index.html>), and Matlab-based S2P, developed at PSI. (Ghasabyan, 2013) In addition, the Python for Nuclear Engineering (PyNE) package developed as a collaboration project between several universities in the U.S has a built-in module for Serpent support (Scopatz et al., 2012).

⁶ See, for example, the OECD/NEA WPNCs Burnup Credit Criticality Safety Benchmarks at <http://www.oecd-nea.org/science/wpncs/buc/> and WPRS benchmarks on LWR and HTGR depletion calculations at <http://www.oecd-nea.org/science/wprs/egrpans/>.

et al., 2013; Bortot et al., 2013; Wolniewicz et al., 2013), initiated at KTH. Other fast reactor applications include modeling and depletion analyses of both experimental (Juutilainen, 2008) and conceptual (Tesinsky et al., 2012b,a, Zhang et al., 2013a,b; Ochoa et al., 2013a,b; Aufiero et al., 2013b) lead- and sodium-cooled fast reactors and accelerator-driven systems (Antolin et al., 2013; Rintala et al., 2012; Korkmaz et al., 2013).

A systematic approach to the core design process of fast reactors has been studied at the University of California, Berkeley, using the Assembly Design and Optimization Tool (ADOPT) – a modular code system developed in a recently completed Ph.D. project (Qvist and Greenspan, 2012, 2013; Qvist, 2013). The ADOPT code couples together assembly and core level neutronics, structural and thermal hydraulics analyses, and carries out several automated tasks, such as equilibrium cycle search using the FAST-BEAU wrapper tool. Serpent is used for performing various neutronics calculations as a part of the automated sequence.

As mentioned in Section 3.1, the delta-tracking based geometry routine in Serpent is particularly well suited to the modeling of high-temperature gas-cooled reactors with tristructural-isotropic (TRISO) particle fuel. The explicit stochastic geometry model developed for HTGR calculations has been used together with discrete-element methods (DEM) for pebble packing in the modeling of the ASTRA experimental facility in an on-going study at Lappeenranta University of Technology, Finland (Suikkanen et al., 2010, 2014). Similar coated micro-particle fuel has been envisioned for liquid salt cooled reactors (Gentry et al., 2013; George et al., 2013) and high-performance research reactors, (Hidayatullah and Kim, 2013) but also for accident tolerant fuel types for conventional LWRs (Shapiro et al., 2013).

There has been some considerable recent interest from various research groups around the world on the modeling of Molten Salt Reactor (MSR) physics with Serpent. Particularly interesting work has been carried out at the Politecnico di Milano, involving continuous refueling and removal of fission products, and the modeling of delayed neutron precursor drift with the fluid flow (Fiorina et al., 2013, 2014; Aufiero et al., 2013a, 2014).

Other novel reactor concepts modeled using Serpent include the Autonomous Corium Reactor, (Johns and Tsvetkov, 2012) based on molten metal fuel, and various Small Modular Reactor (SMR) designs, which cover a wide range of low-power water, gas and liquid metal cooled reactor types. An innovative example of such reactor concept is the super-critical CO₂ cooled High Temperature Integrated Multi-Modular Reactor (HT-IMMR) (Tsvetkov et al., 2011). Serpent has been used at the Texas A&M University for various neutronics and depletion analyses of thermal (Patel and Tsvetkov, 2013a,b) and fast (Patel and Tsvetkov, 2012) HT-IMMR core configurations.

4.4. Multi-physics applications

The multi-physics capabilities introduced in Section 3.4 are still work in progress, and it will take several years before the methodology is completed. Some preliminary work has involved 2D assembly-level calculations using an earlier steady-state version of the internal temperature feedback module (Valtavirta, 2012; Valtavirta et al., 2014). The multi-physics interface has been used to couple Serpent 2 to the ENIGMA fuel performance code (Valtavirta et al., 2013). Serpent is also one of the two Monte Carlo neutronics codes officially included in the High Performance Monte Carlo Reactor Core Analysis (HPMC) project within the 7th European Union Framework Programme, aiming at the full-scale coupling of high-fidelity neutronics and thermal hydraulics.

The explicit stochastic geometry model intended for HTGR calculations offers in itself the possibility to pass pebble-wise power

distributions to an external thermal hydraulics solver. Coupling to CFD calculations with the porous medium approximation is currently being studied at Lappeenranta University of Technology.

4.5. Uncertainty propagation

The unprecedented modeling precision of continuous-energy Monte Carlo codes has lead to situations where manufacturing tolerances and flaws in the evaluated nuclear data libraries become the dominant sources of uncertainty for the final application. Deterministic characterization of these uncertainties is a non-trivial task, in part because of the stochastic nature of the Monte Carlo simulation. Instead, the development of computer capacity and parallel calculation has enabled the implementation of brute-force stochastic methods for Monte Carlo based uncertainty analysis.

The Nuclear Research and Consultancy Group (NRG) has developed an automated sequence called Total Monte Carlo (TMC) (Koning and Rochman, 2008), in which the whole calculation chain from nuclear data evaluation to the continuous-energy Monte Carlo simulation is repeated multiple times, while varying some of the input parameters fed to the physics models. The resulting deviations in the response can be used to characterize the corresponding uncertainty in the final result. The TMC method has also been used with Serpent, for both transport and burnup calculations (Alhassan et al., 2013; Rochman et al., 2012, 2014; Helgesson et al., 2014).

Monte Carlo burnup calculations are subject to unknown statistical errors, even without uncertainties originating from the nuclear data. This is because the solution of the Bateman depletion equations is based on one-group transmutation cross sections that are accompanied by statistical errors. The result is that the material compositions become random variables after the first depletion step, and all information on the associated standard deviations is lost in the process. These uncertainties can be characterized by a similar brute-force approach, by repeating the calculation multiple times with a different random number sequence (Wyant, 2012; Wyant and Petrovic, 2012, 2013). At the moment, this is the only way to estimate the uncertainties propagating along the burnup calculation chain.

Serpent has also been used in the context of the Uncertainty Analysis in Best-Estimate Modeling (UAM) for Design, Operation and Safety Analysis of LWRs benchmark (Ivanov et al., 2012), which aims at propagating uncertainty through all stages of coupled neutronics/thermal hydraulics calculations. Karlsruhe Institute of Technology (KIT) has provided Monte Carlo reference solutions calculated using Serpent for the pin-cell and lattice physics exercises of the benchmark (Mercatali and Sanchez, 2013). In addition, Serpent together with the TMC methodology has been used by NRG for the depletion exercises (Cabellos, 2012).

5. Serpent user community

The Serpent code was released at the OECD/ NEA Data Bank in May 2009, and the user community has grown from 35 registered users at the end of 2009 to about 250 in September 2013. The code is currently used in 100 organizations, 58 of which are universities, in 28 countries around the world. The typical code user is an M.Sc. or Ph.D. student, using Serpent for academic research and thesis work. The role of Serpent as a research tool is also seen in the publications. Of the 70 or so references to Serpent-related work listed in the previous section, the vast majority deals with novel calculation methods or next-generation reactor technology. Most of the studies were dated no longer than two years ago, or are still in the process of being published.

Communication between the developer team and Serpent users is handled via e-mail, website⁷ and an interactive discussion forum⁸. Annual Serpent user group meetings have been organized since 2011. The first three international meetings were held in Dresden, Germany; Madrid, Spain; Berkeley, California, and the fourth meeting will be hosted by the University of Cambridge in September 2014.

Feedback from Serpent users has proven extremely valuable for the development work. This is in particular the case for Serpent 2, which is still in a beta-testing phase. In addition to discovering bugs and problems, Serpent users have been actively participated in envisioning new features and capabilities, and validating the calculation routines.

Even though Serpent is not an open-source project, some significant development at source code level has also been carried out outside the developer team. Master's and doctoral students at Helsinki University of Technology⁹ have contributed with a built-in Doppler-broadening preprocessor routine (Viitanen, 2009), development of advanced time-integration methods for burnup calculation (Isotalo and Aarnio, 2011b,c; Isotalo, 2013), and a built-in temperature solver for fuel pins in 2D lattice calculations (Valtavirta, 2012; Valtavirta et al., 2014). Work is currently in progress on the development of new methods for calculating diffusion coefficients with Monte Carlo (Dorval, 2013). The iterated fission probability method for the calculation of adjoint-weighted delayed neutron fractions and point kinetics parameters was implemented in Serpent 2 at the Politecnico di Milano (Leppänen et al., 2014a), and work on methods for continuous reprocessing and delayed neutron precursor tracking with fuel flow in molten salt reactors is under way (Aufiero et al., 2013a, 2014).

Serpent users have also contributed in the project in the form of various driver, conversion and utility scripts. Two Serpent-PARCS wrappers, SerpentXS and S2P were already mentioned in Section IV.2, together with the more universal PyNE project. An interactive geometry plotter¹⁰ was developed some time ago at KTH, and a more recent project is under way at HZDR. Due to the similarities in Serpent and MCNP input syntax, various automated scripts have been written to simplify the conversion of existing complicated MCNP models into Serpent input format. Unfortunately, none of these conversion scripts are currently available in the public domain.

Funding for Serpent development mainly comes from two public national resources – the Finnish National Research Programme on Nuclear Power Plant Safety (SAFIR-2014) and the Academy of Finland Numerical Multi-physics project (NUMPS). At the international level, Serpent development receives funding from the HPMC project within the 7th EU Framework Programme, and international collaboration is recognized as one of the key performance indicators for Serpent development in the national projects as well.

6. Summary and conclusions

During its nine years of development, the Serpent code has evolved from a simplified Monte Carlo lattice transport code into a versatile reactor physics calculation tool, with applications ranging from group constant generation to fuel cycle analysis, reactor modeling and coupled multi-physics calculations. By October 2013 the code had users in 100 universities and research organizations around the world, and the growing user community has taken an active role in the project. User feedback has proven an

invaluable resource for code validation, as well as the development of new features and capabilities.

The development of the most recent version of the code, Serpent 2, started in October 2010, and the work is still in progress. The efforts are divided between two major fields of applications: (1) Advanced methods for spatial homogenization, and (2) Coupled multi-physics calculations. Topics falling into the first category include development of deterministic diffusion solvers for the purpose of calculating assembly discontinuity factors and pin-power reconstruction for geometries homogenized without zero net-current boundary conditions, and an automated burnup sequence capable of performing branch and coefficient calculations. Work on multi-physics applications is still at a relatively early stage, and near-future topics include completing and testing the universal multi-physics interface, and the implementation of internal solvers for fuel behavior and thermal hydraulics.

One important topic intentionally left beyond the scope of this paper is the performance of Serpent in computing-intensive applications. Such tasks include, for example, group constant generation for deterministic fuel cycle simulations, in which a large number of assembly burnup calculations need to be performed to cover all state points within the reactor operating cycle, and coupled multi-physics calculations, involving iteration between neutronics and thermal hydraulics. The fact is that, even though Serpent was specifically designed for these applications, such calculations have not yet been put to practice in full scale. This is in part due to the lack of computational resources – a problem that is anticipated to resolve itself along with the development in computer hardware. Another practical limitation is the fact that the parallelization routines in Serpent are still under development, and even the scalability tests performed so far have been limited to tens, or hundreds of CPU cores at most. Pushing the boundaries to the realm of supercomputing is therefore considered another challenge left for future work.

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⁷ <http://montecarlo.vtt.fi>.

⁸ <http://ttuiki.vtt.fi/serpent/>.

⁹ Helsinki University of Technology was merged with Helsinki School of Economics and University of Art and Design into Aalto University in 2010.

¹⁰ See: <https://github.com/andreif/serpent-plotter>.

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