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ON THE USE OF THE CONTINUOUS-ENERGY MONTE CARLO METHOD FOR LATTICE PHYSICS APPLICATIONS

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ABSTRACT

This paper is a general overview of the Serpent Monte Carlo reactor physics burnup calculation code. The Serpent code is a project carried out at VTT Technical Research Centre of Finland, in an effort to extend the use of the continuous-energy Monte Carlo method to lattice physics applications, including group constant generation for coupled full-core reactor simulator calculations. The main motivation of going from deterministic transport methods to Monte Carlo simulation is the capability to model any fuel or reactor type using the same fundamental neutron interaction data without major approximations. This capability is considered important especially for the development of next-generation reactor technology, which often lies beyond the modeling capabilities of conventional LWR codes.

One of the main limiting factors for the Monte Carlo method is still today the prohibitively long computing time, especially in burnup calculation. The Serpent code uses certain dedicated calculation techniques to overcome this limitation. The overall running time is reduced significantly, in some cases by almost two orders of magnitude. The main principles of the calculation methods and the general capabilities of the code are introduced. The results section presents a collection of validation cases in which Serpent calculations are compared to reference MCNP4C and CASMO-4E results.

1. INTRODUCTION

Monte Carlo neutron transport codes can handle complicated three-dimensional geometries, and the capability to use continuous-energy cross sections allows the modeling of neutron interactions at the microscopic level without major approximations. These capabilities make the calculation method well suited for its traditional applications, such as criticality safety analyses, shielding and dosimetry calculations, detector modeling and the validation of deterministic transport codes. The common factor in these applications is the need to model the physics of the transport process to within maximum accuracy, often regardless of the computational effort.

The computational challenges for lattice physics applications are often slightly different. The main goal is not to simulate neutron transport in a realistic system, but to produce source terms and interaction parameter by preserving the reaction rate balance at the macroscopic level. The calculations are carried out separately for each fuel assembly type and repeated to cover the local reactor operating conditions. The set of values is then used as the input data in full-core reactor simulator calculations. This multi-stage calculation scheme is based on the theory of homogenization [1, 2], and it is the standard approach to solving coupled large-scale reactor physics and dynamics problems.

Homogenization is a repetitive routine procedure that basically requires condensing isotopic high energy-resolution interaction parameters into a set of case-specific multi-group constants. The task also requires tracking the isotopic changes in the materials during the irradiation cycle. The main advantage of using Monte Carlo codes for homogenization is not so much the accuracy of the calculation method, but rather its versatility. The same code and cross section data can be used for modeling any fuel or reactor configuration without loosing the reliability of the calculation scheme. This is not always the case with deterministic lattice transport codes, which often rely on various application-specific methods.

The main reason why Monte Carlo codes are not more widely used for lattice physics applications is probably the prohibitively long running time, especially when burnup calculation is involved. Another reason is that most general-purpose codes are simply incapable of calculating all the input parameters required for full-core reactor simulator calculations. These challenges gave rise to the development of the Serpent code [3]. One of the main goals of the project is to show that most of the limitations can be lifted by using dedicated calculation techniques, and that the continuous-energy Monte Carlo method may become a viable option to deterministic transport codes within the near future.

This paper is a general overview of the capabilities and the calculation methods used in the most recent version of the Serpent code. Example validation calculations compared to other Monte Carlo and deterministic codes are presented in the results section.

2. HISTORY

The Serpent project was started at VTT Technical Research Centre of Finland in 2004, under the working title “Probabilistic Scattering Game”, or PSG. All publications dated before October 2008 refer to the code using this name. The main motivation at the time was to develop the capability to produce homogenized multi-group constants for deterministic nodal diffusion codes using the continuous-energy Monte Carlo method. This capability was considered essential for the modeling of next-generation reactor systems, as the applications generally lie beyond the capabilities of traditional LWR codes. It was also thought that the development of a dedicated Monte Carlo lattice physics code could extend the applications of the calculation method, and bring new possibilities for LWR analyses as well.

The early versions of the code were developed without burnup calculation capability, and the main focus was in the interaction physics and the production of homogenized multi-group constants. Significant effort had to be put especially in the calculation of diffusion coefficients, as the continuous-energy Monte Carlo method is not easily combined with the diffusion approximation. The early code development was also the topic of a doctoral thesis, completed in 2007 [4].

Depletion routines were added in the “version 2” of the code in 2008, the name was changed from PSG to Serpent, and a website was established for the project at http://montecarlo.vtt.fi. A limited pre-release version was also distributed to some research institutes for testing purposes. The official release was scheduled for January 2009, but the process was delayed for several months due to some unexpected export control issues. The code finally became publicly available in May 2009.

Serpent is licensed free of charge for non-commercial research and educational purposes. The main distributor of the code is the OECD/NEA Data Bank, and RSICC distribution is anticipated later this year. Bug fixes and minor updates in the source code are distributed to registered users by e-mail. The calculations presented in this paper were carried out using code version 1.1.2.

3. APPLICATIONS AND METHODS

The Serpent code is mainly intended for lattice physics calculations, similar to the presently-used second-generation deterministic lattice transport codes. At this stage of development the suggested applications include:

- Generation of homogenized multi-group constants for deterministic reactor simulator calculations
- Fuel cycle studies involving detailed assembly-level burnup calculations
- Validation of deterministic lattice transport codes

The transport capabilities of the continuous-energy Monte Carlo method naturally extend beyond the capabilities of traditional lattice physics codes. The simulation is not limited to two-dimensional assembly geometries, but the code can be used for modeling any three-dimensional full-core configuration as well. The interaction physics covers all reactor types, including both thermal and fast-spectrum systems.

3.1. Neutron Tracking and Interaction Physics

Serpent uses a combination of the conventional surface-to-surface ray tracing and the Woodcock delta-tracking method [5] for simulating neutron transport through the geometry. The delta-tracking method is essentially a rejection sampling technique that enables the random walk to be continued over several material regions without stopping the neutron at each boundary surface. This method has proven fast and efficient in lattice geometries, especially when combined with conventional techniques. The geometry routine is built on a universe-based approach, very similar to other Monte Carlo codes, such as MCNP [6] and KENO-VI [7] (the universe concept is equivalent with the unit definition in SCALE). This type of geometry model allows the description of practically any two- or three dimensional fuel or reactor configuration.

The interaction physics in Serpent is based on classical collision kinematics and ENDF reaction laws. The code reads continuous-energy cross sections from ACE format library files, which are also used by MCNP. The reaction cross sections are reconstructed using a single unionized energy grid for all nuclides [8]. This approach leads to a dramatic increase in efficiency, as the number of time-consuming grid search iterations is reduced to minimum. The speed-up is even more significant when modeling irradiated fuels, typically containing cross sections for over 200 actinide and fission product nuclides.

3.2. Burnup Calculation

Simulation of fuel depletion is a cyclic process that requires the calculation of isotopic one-group transmutation cross sections for each depleted material at each depletion step. This data

is combined with radioactive decay constants and fission yields, and formulated into a set of coupled first-order differential equations. Serpent has two optional methods for solving these depletion equations. The first option is the Transmutation Trajectory Analysis method (TTA), which is basically an analytical solution for the linearized depletion chains [9]. The second alternative, the Chebyshev Rational Approximation Method (CRAM) [10], is an advanced matrix exponential solution specifically developed for the Serpent code.

All parameters needed to form the depletion equations are automatically calculated and set up without additional user effort. The radioactive decay constant and fission yield data is read from standard ENDF format libraries and Serpent can be run as a completely stand-alone application without dependence to external depletion codes or pre-generated data sets.

3.3. Parallel Calculation Mode

Serpent has the capability to use the Message Passing Interface (MPI) for parallel calculation. Parallelization is implemented by dividing the neutron histories to several tasks and combining the results after the transport cycle. If the number of depleted materials is large in burnup calculation, the preprocessing and depletion routines between the burnup steps may take a significant fraction of the overall calculation time. To speed up the calculation, these processes are also divided into several tasks.

3.4. Output

Since Serpent is primarily intended as a lattice physics code, several assembly level parameters are calculated by default. This data includes:

- Effective and infinite multiplication factors calculated using analog and implicit estimators
- Homogenized multi-group reaction cross sections
- Group-transfer probabilities and scattering matrices
- Diffusion coefficients calculated using two fundamentally different methods
- P_n scattering cross sections up to order 5
- Assembly discontinuity factors for boundary surfaces and corners in square and hexagonal fuel lattices
- Assembly pin-power distributions
- Point reactor kinetics parameters
- Physical and effective delayed neutron fractions and decay constants in 6 or 8 precursor groups
- Normalized flux, power and reaction rates integrated over geometry
- Parameters for the six-factor formula
- Various parameters related to the Monte Carlo transport simulation

All result estimates are accompanied by the associated relative statistical errors.

Fission source entropies are available for convergence studies and user-defined detectors (tallies) can be set up for calculating various integral reaction rates. The output in the burnup calculation mode consists of isotopic compositions, transmutation cross sections, activities and decay heat data. The results are given both as material-wise and total values. Group

constants and all the other output parameters are calculated and printed for each depletion step.

All numerical output is written in Matlab m-format files to simplify the post-processing of the data. The code also has a geometry plotter feature and a reaction rate plotter, which is convenient for visualizing the neutronics in thermal systems.

3.5. Major Limitations

The optimization of the calculation routines for lattice physics applications results in some limitations in terms of generality. The delta-tracking method necessitates the use of the collision flux estimator for calculating integral reaction rates. The conventional approach is to use the track-length estimator, which has a better efficiency in small and optically thin cells and in regions of low collision density. For this reason the Serpent code is not well suited for detector and dosimetry calculations, at least to the extent of general-purpose Monte Carlo codes.

The unionized energy grid structure combines the energy points of all the constituent nuclides to avoid repeating the grid search for the partial grids. The drawback of the efficiency gain is that computer memory is wasted for storing redundant data. The memory demand easily grows to several gigabytes in burnup calculation, due to the number of actinide and fission product cross sections involved. The problem becomes even worse in the parallel calculation mode if several MPI tasks are sharing the same memory space. Serpent uses two methods, based on grid thinning and the double-indexing of the energy grids [8] to reduce the overall memory demand, and the problem is not considered a limiting factor for current workstations and computer clusters dedicated to numerical computing.

The most significant methodological flaw in the physics model is currently the lack of probability table treatment for unresolved resonances. It is generally known that the use of smooth averaged cross sections in the unresolved region may have a significant impact on the results, especially in fast reactor calculations. So far the code has mainly been used for LWR applications, in which the differences are not significant. The probability table sampling is not easily combined with the optimized routines using the internal unionized energy grid format, but the development of the methodology is under way.

4. EXAMPLE RESULTS

The Serpent code has mainly been validated by comparing the results to reference MCNP calculations. This is considered to be the best approach, since the capability to use the same ACE format cross section libraries eliminates all discrepancies originating from the fundamental interaction data. The main problem is that the reaction rate tallies in MCNP only allow the calculation of homogenized reaction cross sections, pin-power distributions and assembly discontinuity factors. Other group constants, such as diffusion coefficients, scattering matrices and effective delayed neutron fractions have to be validated by comparing to deterministic calculations. The discrepancies are inevitably larger, due to the fundamental differences in the data and the transport methods. It should also be noted that value of the diffusion coefficient in particular dependents on how it is defined, and it is not uncommon that the two methods used by Serpent yield values that differ by 30% [4]. This is not a

difference between a “correct” and an “incorrect” result, but due to the fact that the calculations are based on different interpretations of an approximation that is not particularly valid within the physical system.

The validation of the depletion routines becomes even more complicated, especially since the current MCNP version is not capable of burnup calculation. Some comparisons to coupled codes like Monteburns [11] have been carried out, but so far the main reference code has been the deterministic CASMO-4E [12]. The CASMO code is widely used for LWR analyses both in research and the industry, which makes it a valuable tool for Serpent validation as well.

The following subsections present a representative collection of validation calculations where Serpent is compared to MCNP4C and CASMO-4E results.

4.1. Criticality and Group Constant Generation

Effective multiplication factors and homogenized multi-group cross sections calculated by Serpent are compared to reference MCNP4C results. The calculations were carried out for six different geometry types with some variation in the parameters:

1. Hexagonal VVER-440 PWR fuel assembly with and without boron shim
2. Mixed 17 × 17 PWR UOX/MOX lattice
3. BWR fuel assembly with burnable absorber, different void fractions
4. Heavy water cooled and moderated CANDU cluster
5. Sodium-cooled fast reactor fuel assembly
6. Prismatic HTGR fuel block with and without burnable absorber

Since the intention was to compare the results of two calculation codes, the geometry dimensions and material compositions are not considered essential and hence not repeated here.

The effective multiplication factors are presented in Table 1. All calculations were carried out using cross section libraries based on the JEFF-3.1 evaluated nuclear data file. To reduce the level of statistical noise, a total of 10 million active neutron histories were simulated in each case. The results show that the differences between the codes are well within the range of statistical accuracy.

The multiplication factor can be considered a necessary, although somewhat insufficient indicator of the validity of the calculation methods. For a more detailed analysis, the homogenized total, fission, capture and scattering cross sections were calculated and compared. The group structure used in the calculations was based on four energy groups:

Group 1 (fast fission)	0.821 MeV	$< E <$	20 MeV
Group 2 (slowing-down)	5.5 keV	$< E <$	0.821 MeV
Group 3 (resonance)	0.625 eV	$< E <$	5.5 keV
Group 4 (thermal)	0	$< E <$	0.625 eV

Table 1. Comparison of criticality eigenvalues between MCNP4C and Serpent. The relative statistical errors and differences are in per cent.

#	Case	MCNP4C		Serpent		Diff.
1a	VVER-440 assembly, 650 ppm boron	1.26845	(0.015)	1.26844	(0.014)	-0.001
1b	VVER-440 assembly, no boron	1.34237	(0.014)	1.34261	(0.014)	0.018
2	Mixed PWR UOX/MOX lattice	1.07120	(0.018)	1.07117	(0.017)	-0.003
3a	BWR+Gd assembly, 25% void fraction	1.07570	(0.018)	1.07556	(0.020)	-0.013
3b	BWR+Gd assembly, 50% void fraction	1.06058	(0.018)	1.06021	(0.020)	-0.035
3c	BWR+Gd assembly, 75% void fraction	1.04095	(0.017)	1.04100	(0.021)	0.005
4	CANDU cluster	0.91923	(0.015)	0.91932	(0.016)	0.010
5	SFR assembly	1.14196	(0.015)	1.14179	(0.016)	-0.015
6a	Prismatic HTGR fuel block without BA	1.76607	(0.008)	1.76639	(0.007)	0.018
6b	Prismatic HTGR fuel block with BA	1.45063	(0.015)	1.45091	(0.016)	0.020

Table 2. Comparison homogenized 4-group reaction cross sections between MCNP4C and Serpent in the CANDU case. The relative statistical errors and differences are in per cent.

Parameter	*g*	MCNP4C		Serpent		Diff.
Σ_{tot}	1	2.32978E-01	(0.057)	2.33028E-01	(0.009)	0.022
	2	3.50815E-01	(0.028)	3.50802E-01	(0.003)	-0.004
	3	3.54947E-01	(0.014)	3.54931E-01	(0.002)	-0.005
	4	4.17002E-01	(0.042)	4.16998E-01	(0.002)	-0.001
Σ_{fiss}	1	2.32997E-03	(0.064)	2.33038E-03	(0.047)	0.018
	2	5.65098E-05	(0.036)	5.65262E-05	(0.032)	0.029
	3	5.29534E-04	(0.041)	5.29111E-04	(0.048)	-0.080
	4	4.96685E-03	(0.042)	4.96800E-03	(0.030)	0.023
Σ_{capt}	1	7.85075E-04	(0.089)	7.85556E-04	(0.059)	0.061
	2	1.34275E-03	(0.045)	1.34267E-03	(0.037)	-0.006
	3	5.14724E-03	(0.051)	5.14402E-03	(0.044)	-0.062
	4	4.84072E-03	(0.042)	4.84157E-03	(0.028)	0.018
Σ_{scatt}	1	2.29863E-01	(0.075)	2.29913E-01	(0.069)	0.022
	2	3.49415E-01	(0.049)	3.49403E-01	(0.003)	-0.004
	3	3.49270E-01	(0.042)	3.49257E-01	(0.002)	-0.004
	4	4.07194E-01	(0.052)	4.07189E-01	(0.003)	-0.001

The results for the CANDU calculation (case 4) are presented as an example in Table 2. The capture cross section consists of all (n,0n) reaction modes. The scattering cross section is the sum of elastic and all inelastic two-body collisions. All differences between the codes are below 0.1%. Other similar comparisons to MCNP using the same ACE libraries usually give equally consistent results.

As the third example, the flux spectra integrated over the prismatic HTGR fuel block are compared in Figure 1. The two curves are completely overlapping, and the difference shows only statistical noise.

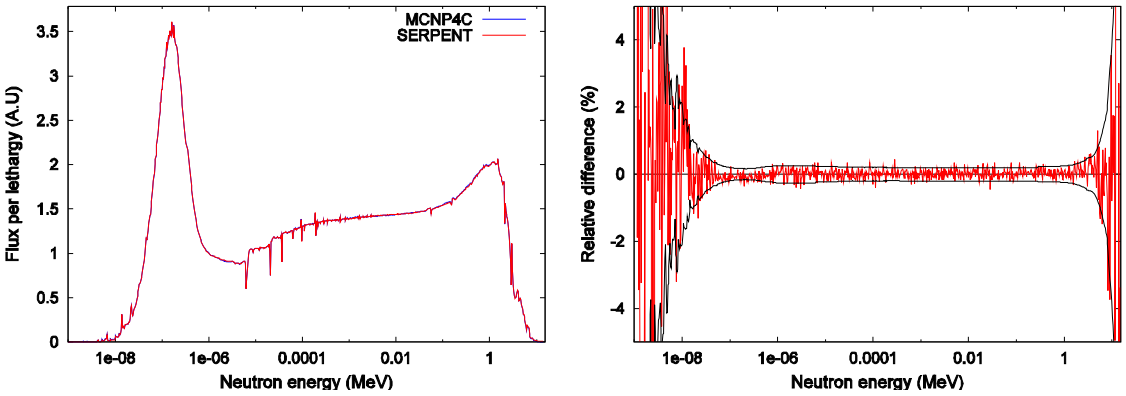

Figure 1. Flux spectra in the prismatic HTGR fuel block without burnable absorber calculated using MCNP4C and Serpent. The figure on the right shows the relative differences compared to the statistical 95% confidence intervals of the MCNP calculation.

4.2. Burnup Calculation

The depletion capability was included in the Serpent code no earlier than 2008, and the validation is still under way. The most comprehensive test case carried out so far is a 17 × 17 PWR burnup calculation with burnable absorber [13]. The geometry is divided into 65 separate depletion zones, including 10 annular rings for each burnable absorber pin. Comparison to reference CASMO-4E results shows consistent evolution for k-eff and the depletion of U-235 and gadolinium isotopes. Some small discrepancies are observed in the buildup rates of Pu-239 and the main fission product poisons. The differences are most likely to originate from several factors, such as the microscopic neutron capture cross section of U-238 and the special Xe-135 treatment used by the CASMO code. The infinite multiplication factors as function of fuel burnup are plotted in Figure 2. The Serpent calculations were repeated using the two methods available for the solution of the depletion equations.

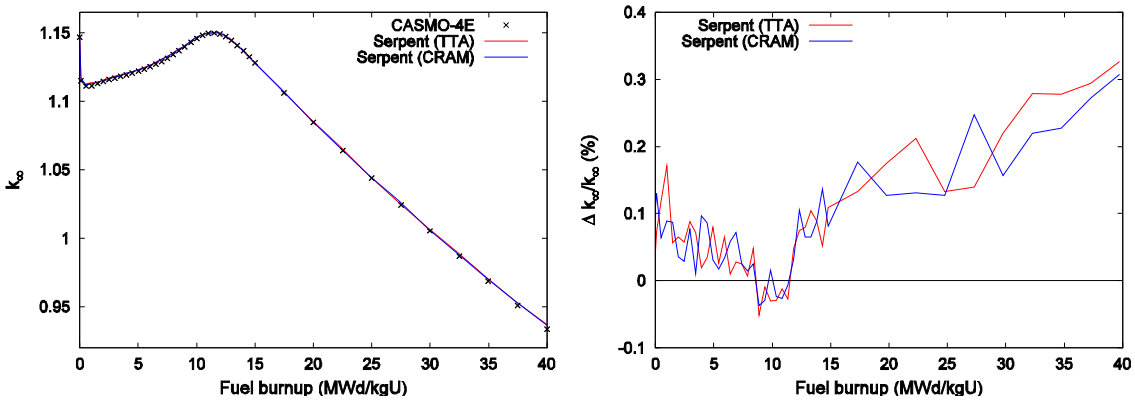

Figure 2. Effective multiplication factors as function of fuel burnup in a PWR assembly burnup calculation. Comparison between Serpent and CASMO-4E. The relative differences are plotted on the right.

4.3. Running Time

The running times for the group constant calculations presented in Section 4.1 are listed in Table 3. All calculations were run in the same 3.0 GHz Intel Xeon PC workstation without parallelization. It is shown that the Serpent code is significantly faster in the LWR cases, but especially in the HTGR calculations. The two main factors behind the efficiency are the unionized energy grid format and the Woodcock delta-tracking method. The advantages of delta-tracking become pronounced in geometries containing regions that are small compared to the neutron mean-free-path. The HTGR fuel matrix with microscopic fuel particles is a good example of such geometry type.

Another factor in the comparison of running times is that the MCNP code tends to slow down significantly as the number of nuclides and reaction rate tallies is increased. This is shown even in group constant calculations, as the code runs noticeably faster without the tally definitions. The real significance of optimization becomes apparent in burnup calculation, when the transmutation cross sections of several hundred actinide and fission product isotopes need to be tallied. The transport cycle in Serpent typically slows down by less than a factor of 1.5 in the burnup calculation mode. When the overall running time in an LWR assembly burnup case is compared to a coupled code like Monteburns, the difference is not a factor of 5 or 6, but closer to a factor of 40 to 80. Based on the values in Table 3, the difference may become even more significant in HTGR calculations.

The PWR burnup calculation case in Section 4.2 was completed in 15 hours when the irradiation history was divided into 42 burnup steps with predictor-corrector calculation and 3 million neutron histories were simulated for each step. If multiple cases were run simultaneously on different machines and the calculation repeated to cover all assembly types and operating conditions in a reactor core to produce group constants for a simulator calculation, the task could still be completed within a reasonable time frame.

Table 3. Comparison of running times (in minutes) between MCNP4C and Serpent in the group constant calculations. The last column is the ratio of the values.

#	Case	MCNP4C	Serpent	M/S
1a	VVER-440 assembly, 650 ppm boron	196.5	16.8	11.7
1b	VVER-440 assembly, no boron	189.7	17.0	11.2
2	Mixed PWR UOX/MOX lattice	111.3	16.9	6.6
3a	BWR+Gd assembly, 25% void fraction	186.2	25.3	7.3
3b	BWR+Gd assembly, 50% void fraction	203.9	24.6	8.3
3c	BWR+Gd assembly, 75% void fraction	231.8	24.3	9.6
4	CANDU cluster	235.3	31.6	7.5
5	SFR assembly	297.3	17.1	17.4
6a	Prismatic HTGR fuel block without BA	1023.3	22.5	45.4
6b	Prismatic HTGR fuel block with BA	4822.0	100.8	47.8

3. CONCLUSIONS

The Serpent code is being developed at VTT Technical Research Centre of Finland in an effort to extend the use of the continuous-energy Monte Carlo method to lattice physics applications, including fuel cycle analyses and homogenized group constant generation for deterministic reactor simulator codes. The main advantage of the method in reactor physics calculations is the capability to model any fuel or reactor configuration using the same fundamental interaction data without major approximations.

The main limiting factor for most widely-used general-purpose Monte Carlo codes is the prohibitively long running time, especially when the codes are used in a coupled burnup calculation sequence. It has been shown that this limitation is not a necessity, and that the dedicated calculation methods used in the Serpent code can reduce the overall running time to an acceptable level. Detailed LWR assembly burnup calculations can be completed in less than 24 hours on a single-processor PC workstation, and the development in computer capacity and parallel clusters suggests that the continuous-energy Monte Carlo method may become a viable alternative to deterministic transport codes within the near future.

The production of homogenized multi-group constants also requires some specialized calculation techniques. The Serpent code is able to produce all input parameters needed in deterministic nodal diffusion calculations, which is the standard approach to solving coupled full-core reactor physics and dynamics problems. This data has been validated by comparison to other Monte Carlo and deterministic transport codes that are known to perform well in the reference calculations. So far the Serpent code has shown good consistency in the test cases.

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