Current status and future plans for Serpent 2

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Background

Serpent has been developed since 2004, mainly as a reactor physics code for very specific applications:

1) Traditional reactor physics applications, including spatial homogenization, criticality calculations, fuel cycle studies, research reactor modeling, validation of deterministic transport codes, etc.

2) Multi-physics simulations, i.e. coupled calculations with thermal hydraulics, CFD and fuel performance codes

In recent years there has been significant effort to broaden the scope to neutron and photon transport simulations for radiation dose rate calculations, shielding and fusion research.

This presentation summarizes the current status of Serpent 2 and outlines some of the near- and long-term plans for future development.

Photon transport mode

The original motivation for expanding to photon transport was to simulate gamma heating in multi-physics calculations:

- Accurate deposition of fission energy requires accounting for direct and indirect components of prompt and delayed heating
- Prompt indirect neutron and photon heating may become important especially in fast transients

Development of photon physics routines:

- First introduced in version 2.1.24 in 2015[1]
- Radioactive decay source mode including discrete photon spectra in 2.1.24
- Coupled neutron-photon transport mode in version 2.1.29[2]
- More about recent developments in Toni's presentation

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[1] T. Kaltiaisenaho. "*Implementing a photon physics model in Serpent 2.*" M.Sc. Thesis, Aalto University. 2016.

[2] J. Leppänen et al. "*Implementation of a Coupled Neutron / Photon Transport Mode in the Serpent 2 Monte Carlo Code.*" In proc. M&C 2017. Jeju, Korea, Apr. 16-20, 2017.

Photon transport mode

Accurate heat deposition models with gamma heating remain as one of the major near-term development goals.

However, the photon transport mode and other related capabilities have also enabled expanding the applications of Serpent from reactor physics to new fields, in particular:

- Radiation shielding and dose rate calculations
- Fusion applications

The built-in burnup calculation routine combined with the radioactive decay source mode allows performing radiation transport calculations involving irradiated fuel and/or activated materials with very little additional effort.

Challenges:

- Geometries are often complicated and irregular
- Shielding calculations require extensive use of variance reduction

One of the major limitations is the lack of user basis – Serpent is still used almost exclusively for reactor physics applications!

Complex geometries

The basic CSG geometry type used in Serpent is great for reactor applications:

- Most reactor geometries can be described using planes and cylinders
- Regular structures are easy to model using standard universes and lattices

Advanced types available for irregular and unstructured geometries:

- Mesh-based geometry type developed together with the OpenFOAM multi-physics interface was introduced in version 2.1.13 in 2013[3]
- CAD-based geometry type based on STL file format implemented in version 2.1.22 in 2014[4]

Even though these capabilities have been available for several years, they have not been widely used!

Implementing a voxel-based geometry model is also an option if medical applications become important at some point.

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[3] J. Leppänen and M. Aufiero. "*Development of an Unstructured Mesh Based Geometry Model in the Serpent 2 Monte Carlo Code.*" In proc. PHYSOR 2014. Kyoto, Japan, Sept. 28 - Oct. 3, 2014.

[4] J. Leppänen. "*CAD-based Geometry Type in Serpent 2 – Application in Fusion Neutronics.*" In proc. M&C + SNA + MC 2015. Nashville, TN, Apr. 19-23, 2015.

Variance reduction

A weight-window based variance reduction scheme was first introduced in version 2.1.27 in 2016.[5]

Two options:

1) Read MCNP WWINP format weight window mesh generated using some deterministic tool

2) Apply a built-in light-weight response matrix based solver

Challenges and on-going work:

- Support for multi-dimensional WWINP mesh
- Efficient source sampling routine
- coupled neutron-photon transport simulations
- Multi-group support for built-in solver

More about the built-in solver in my second presentation.

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[5] J. Leppänen, T. Viitanen, and O. Hyvönen. "*Development of a Variance Reduction Scheme in the Serpent 2 Monte Carlo Code.*" In proc. M&C 2017. Jeju, Korea, Apr. 16-20, 2017.

Future plans for reactor applications

Serpent has been used for group constant generation for several years now with varying degree of success:

- Good results form several Serpent-DYN3D calculations performed for different reactor types
- Reasonably good results from Serpent-ARES calculations
- Not so good results with VTT's in-house codes

Lesson learned: The capability to perform spatial homogenization using the Monte Carlo method is not enough to guarantee the quality of reduced-order calculations.

Instead of trying to make VTT's legacy codes work with Serpent, we decided to start developing a new nodal diffusion solver specifically designed to use Serpent-generated cross sections.

Another important reason is the education of new experts – hands-on code development is the best way to learn!

New computational framework "Kraken"

The new computational framework "Kraken" consists of independent modular solvers, coupled together via a common core-level multi-physics interface.

Capability to run two types of code sequences:

I) **Reduced-order sequence** – based on a reduced-order (e.g. nodal diffusion) neutronics solution and spatial homogenization, intended for routine design and safety analyses

II) **High-fidelity sequence** – based on a heterogeneous (Monte Carlo) transport solution, intended for best-estimate analyses and validation of reduced-order methods

Both sequences share the same input (as much as possible) and they can be coupled to the same modular thermal hydraulics and fuel performance solvers

The entire core physics framework can be coupled to system-scale analyses via a second power plant level interface

New computational framework “Kraken”

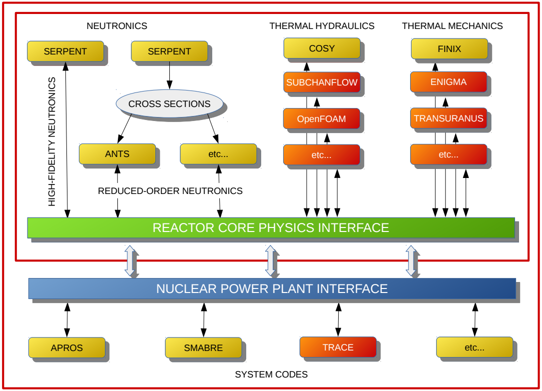


Figure 1 : Overview of the new computational framework for core physics calculations. All modular solvers operate on a common platform that couples the physical solutions together via a core-level multi-physics interface, and to external boundary conditions via the NPP interface. Most of the modular solvers will be interchangeable, so that the code sequence can be tailored to the specific needs of each application.

Kraken: Reduced-order calculation sequence

Reduced order methods rely on the conventional multi-stage calculation scheme and spatial homogenization.

Nodal diffusion codes are the “workhorses” applied to routine fuel cycle simulations and transient safety analyses.

Several widely-used codes (Simulate, PARCS, DYN3D, etc.) have been succesfully applied for this purpose for decades.

Approach in Kraken:

- Group constant generation using Serpent
- New AFEN/FENM-based nodal diffusion solver “Ants”, capable of handling square and hexagonal geometries and steady-state and transient solutions
- Other reduced-order methods will be studied in the future

The continuous-energy Monte Carlo method can also be used to provide the ideal reference solution for verifying the reduced-order methodology.

Kraken: High-fidelity calculation sequence

High-fidelity methods apply a direct solution to the heterogeneous neutronics problem, without spatial homogenization or other intermediate steps.

The methods are computationally too heavy for routine design and safety analyses, but can be used for some specific best-estimate type calculations and validation of reduced-order methods.

High-fidelity multi-physics calculations were extensively studied in the SA-NUMPS project in 2012-2016:

- Direct coupling of Serpent to thermal hydraulics, CFD and fuel performance codes
- State-point information passed via a universal multi-physics interface
- Coupling successfully established with OpenFOAM, Finix and Enigma

The development of the high-fidelity sequence continues where the NUMPS project was left off, and the same interfaces and coupling algorithms will be used with the reduced-order sequence.

High-fidelity methods have been extensively studied within the Serpent user community as well.

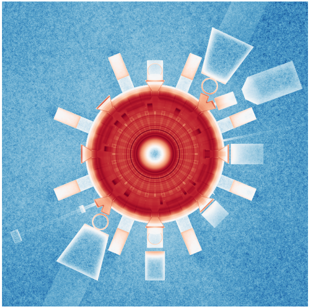
What is it good for?

The objective is that the new computational framework could eventually handle all core physics calculations carried out at VTT either independently or coupled to system codes.

Example applications:

- 3D transient safety analyses and fuel cycle simulations for large LWR cores (PWR, BWR and VVER) using the reduced-order sequence
- Full core calculations for SMR's and small research reactors using both high-fidelity and reduced-order methods
- Research projects involving Gen-IV reactors
- Educational use at universities
- Specific applications that require unconventional methodologies
- Production of source terms for severe accident, radiation shielding and final disposal analyses

What is it good for?



There are also various transport applications in which a coupled solution is not necessarily required:

- Criticality safety
- Radiation transport
- Fusion neutronics
- Modeling of low-power research reactors

These applications often involve complicated and irregular geometries that can only be handled using Monte Carlo particle transport codes.

Serpent has a lot of potential for these applications, and development of Kraken strongly supports these efforts.

National and international collaboration

The ambitious development goals cannot be achieved without close collaboration at both national and international level:

- Education of new experts requires close collaboration with universities
- VTT lacks the practical experience and understanding of how reactors are operated and what is important / interesting to the nuclear industry
- Close interaction with regulators ensures that the tools and methods are sufficiently validated and demonstrated to be used for reactor core safety analyses
- Similar methods are developed around the world, and being part of the international community is important for keeping up with the latest innovations

The success of Serpent largely results from its large international user basis, which has contributed significantly to code development and validation.

For the same reason the new computational framework will be developed as open-access software, to be distributed free of charge for non-commercial use.

The VIRNE project

The “Virtual research environment for nuclear engineering” (VIRNE) is a project proposal submitted to the Academy of Finland in September 2017:

- Research consortium with Lappeenranta University of Technology
- Total volume 104 person-months in 2018–2022
- Involves the development of a virtual national infrastructure for the computational modeling of nuclear reactors for research and educational purposes
- Methodology is based on the Kraken framework and computational models of current and emerging reactor technologies
- Applications range from class-room demonstrations of physical phenomena and virtual laboratory exercises to independent research projects and BSc, MSc and doctoral theses

The funding decision will be made in June 2018, but regardless of its success or failure, the VIRNE project proposal will be used as a roadmap for future work.

Thank you for your attention!

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