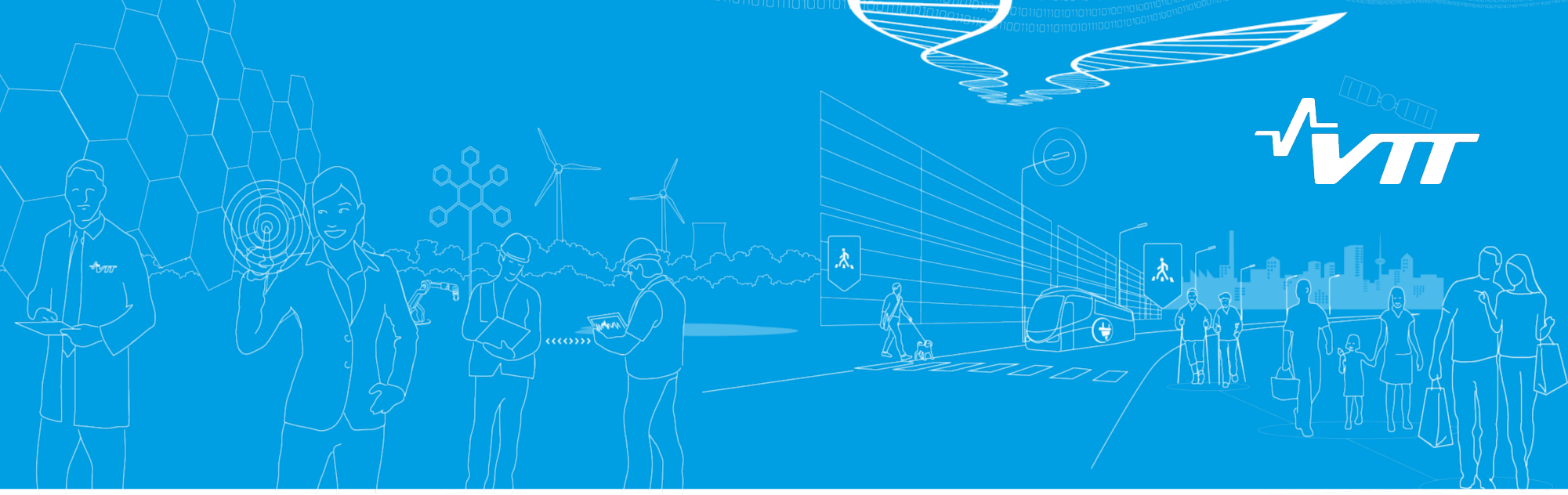

Introduction to Serpent

LPSC Grenoble, Feb. 26, 2015

Jaakko Leppänen

VTT Technical Research Center of Finland

Outline

- Serpent overview
- Monte Carlo method in spatial homogenization:
  - What is spatial homogenization?
  - Homogenization methods in Serpent 2
  - Automated calculation sequence of Serpent 2
  - Practical experience
  - Future work in spatial homogenization
- New applications:
  - CAD-based geometry type
  - Fusion neutronics
  - Photon transport mode

I - Serpent overview

Background

Development of Serpent started at VTT in 2004:

- Original idea: to create a simplified lattice physics code for spatial homogenization (topic of a D.Sc. Thesis completed in 2007[1])
- Specialized in assembly-level calculations: several tricks to speed-up the calculation,[2,3] automated calculation of group constants
- Automated burnup sequence based on the Chebyshev Rational Approximation method (CRAM)[4]

Serpent is not the only Monte Carlo code used for group constant generation, but in 2004 it was one of the first codes specifically developed for this purpose

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[1] J. Leppänen. "*Development of a New Monte Carlo Reactor Physics Code.*" D.Sc. Thesis, Helsinki University of Technology, 2007. (VTT Publications 640).

[2] J. Leppänen. "*Performance of Woodcock Delta-Tracking in Lattice Physics Applications Using the Serpent Monte Carlo Reactor Physics Burnup Calculation Code.*" Ann. Nucl. Energy **37** (2010), 715–722.

[3] J. Leppänen. "*Two Practical Methods for Unionized Energy Grid Construction in Continuous-Energy Monte Carlo Neutron Transport Calculation.*" Ann. Nucl. Energy **36** (2009), 878–885.

[4] M. Pusa. "*Numerical Methods for Nuclear Fuel Burnup Calculations.*" D.Sc. Thesis, Aalto University, 2013. (VTT Science 32).

Background

Serpent 1 was released for public distribution in 2009:

- Available free of charge for non-commercial research and educational use
- Distribution by OECD/NEA Data Bank and RSICC
- License for commercial use in preparation

Development is currently focused on Serpent 2:

- Available by request to registered users of Serpent 1
- Public release scheduled for 2016

Serpent 1 was developed primarily as a lattice-physics code, Serpent 2 is clearly a general-purpose rector physics code, with future applications also in radiation shielding and fusion neutronics

Developer team

Developer team at VTT:

- Jaakko Leppänen (misc. stuff)
- Maria Pusa (CRAM, deterministic solvers for homogenization)
- Tuomas Viitanen (TMS temperature treatment routine)
- Ville Valtavirta (multi-physics coupling)
- Toni Kaltiaisenaho (photon transport)

Development is focused on two topics:

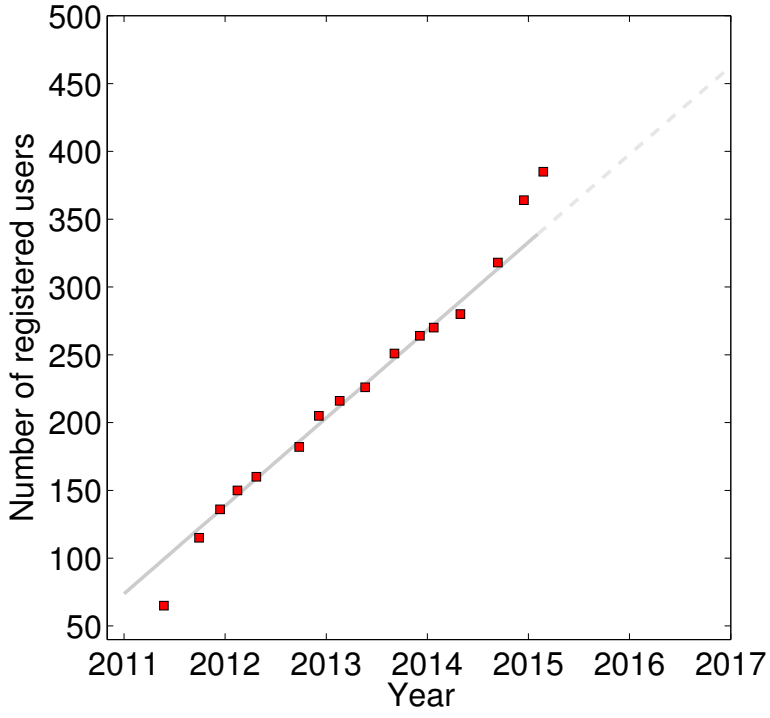
i) Advanced methods for spatial homogenization

ii) Coupled multi-physics calculations

User community

User community in numbers:

- 385 registered users in mailing list (44% Europe, 40% North America)
- 126 organizations (54% universities)
- 32 countries
- Typical user: M.Sc. or Ph.D. student
- 50 Theses on Serpent-related topics since 2007
- 200 scientific journal and conference papers since 2005



Serpent website: http://montecarlo.vtt.fi

Serpent discussion forum: http://ttuki.vtt.fi/serpent

User community

Group photos from International Serpent User Group Meetings: Dresden, 2011; Madrid, 2012; Berkeley, 2013; Cambridge, 2014.

II - Monte Carlo method in spatial homogenization

What is spatial homogenization?

Modeling of an operating nuclear reactor is a complicated task:

- Full-scale solution to neutron transport problem is computationally expensive
- Transport problem becomes non-linear when feedbacks from material temperatures and densities are taken into account
- Same applies to changes in fuel composition with increasing burnup

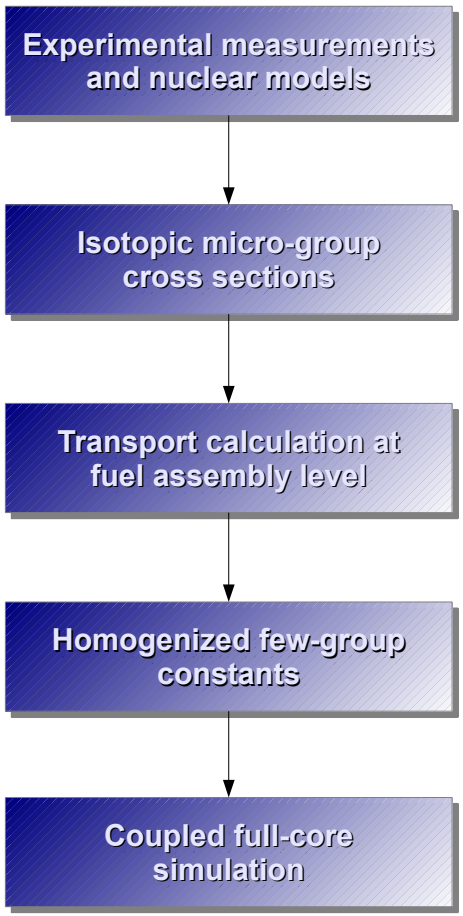
In practice, the solution to the coupled problem is obtained by iteration between:

- Solution of linearized transport problem
- Solution of heat transfer and coolant flow
- Solution of Bateman depletion equations

There exists high-fidelity solution methods for the independent problems (e.g. continuous-energy Monte Carlo and CFD), which can be combined for the solution of the coupled problem, but the approach is not practical for routine design and safety analyses

What is spatial homogenization?

Instead, the solution is obtained by gradually increasing the scale of the system, while simplifying the physics. The calculation sequence essentially consists of two parts:



i) Spatial homogenization:

- Interaction physics at the fuel assembly level is condensed into a set of representative group constants
- Geometry is homogenized, energy dependence condensed into few energy groups
- Local reaction rate balance is preserved
- Traditionally based on 2D transport calculation

ii) Full-core calculation:

- Group constants from spatial homogenization are used as the building blocks for a simplified full-core calculation
- In LWR applications typically based two-group nodal diffusion methods
- Neutronics solution is obtained at an acceptable computational cost, which enables iterative solution to the coupled problem

What is spatial homogenization?

Traditional methods for spatial homogenization:

- Deterministic transport solution, for example, MOC or CP
- Two-dimensional infinite-lattice geometry
- Includes simulation of fuel burnup
- Repeated to cover all operating conditions within the reactor core

The result is a library of core-specific group constants, which are used as the building blocks for a full-scale simulation

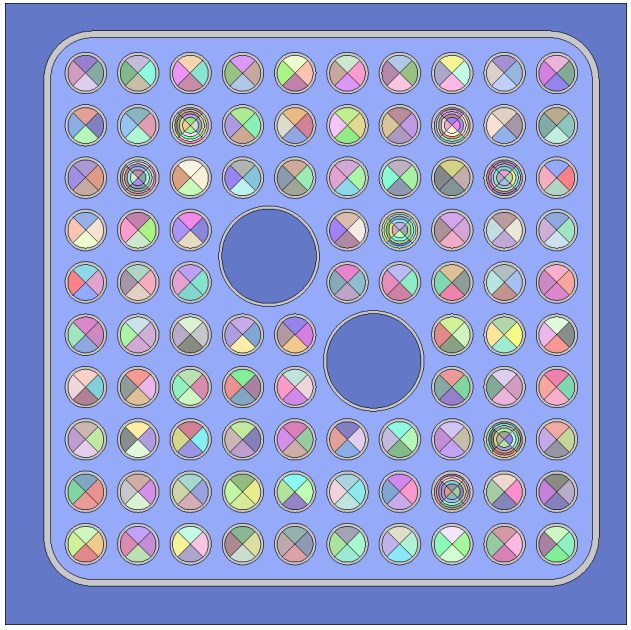


Figure 1: Typical 2D BWR assembly geometry used for spatial homogenization

What is spatial homogenization?

There is increasing interest in using continuous-energy Monte Carlo simulation for spatial homogenization, because of several advantages:

- The transport simulation is inherently three-dimensional, possibility to account for axial heterogeneity
- The best available interaction data can be used almost as-is, no need for additional processing to account for self-shielding effects, etc.
- The same code and cross section library can be used for modeling any fuel or reactor type
- The same code and cross section library can be used for the heterogeneous full-scale problem, which represents the best reference solution for the calculation scheme

In addition, the use of Monte Carlo for homogenization can open new possibilities in full-scale simulations (e.g. the response matrix method)

Monte Carlo method in homogenization

But there are also some major challenges:

- Burnup calculations and covering all state points requires a lot of CPU time
- All group constants are random variables, associated with a statistical error
- Calculation of certain parameters requires special tricks:
  - Diffusion coefficients (no physical equivalent in Monte Carlo simulation)
  - Leakage-corrected group constants (methodology developed for deterministic codes)
  - ADF's and pin-power form factors with non-zero net current boundary conditions (requires solution of homogeneous diffusion flux)
- Managing the calculation sequence becomes complicated

In general, the continuous-energy Monte Carlo method has a lot of potential for spatial homogenization, but a practical demonstration in routine use is yet to be accomplished

Homogenization methods in Serpent 2

Serpent was designed from the beginning for spatial homogenization, and the code has the capability to produce group constants for nodal diffusion reactor simulator calculations:

- Homogenized reaction cross sections
- Scattering matrices
- Diffusion coefficients
- Assembly discontinuity factors
- Form factors for pin-power reconstruction

Methods exist for the calculation of effective delayed neutron fractions, but the routines were not originally designed for homogenization

Homogenization methods in Serpent 2

The calculation is based on the preservation of local reaction rate balance and two built-in deterministic solvers:

i) B_1 critical spectrum calculation:

- Homogenized reaction cross sections are calculated using an intermediate micro-group structure (by default WIMS 69-group structure)
- B_1-equations are formed and solved by critical buckling iteration[5]
- The result is a leakage-corrected micro-group spectrum, which is used for collapsing the cross sections into group constants using the final macro-group structure (by default 2 energy groups)

ii) Homogeneous diffusion flux solver for ADF's and form factors:

- Based on the solution of two-dimensional diffusion equation in the homogenized region, using net currents as boundary conditions
- Used when homogenization is performed for assembly colorset or reflector (non-zero net current)
- Currently based on boundary conditions equivalent with what is used in ARES

[5] E. Fridman and J. Leppänen. "*On the Use of the Serpent Monte Carlo Code for Few-Group Cross Section Generation.*" Ann. Nucl. Energy **38** (2011), 1399–1405.

Homogenization methods in Serpent 2

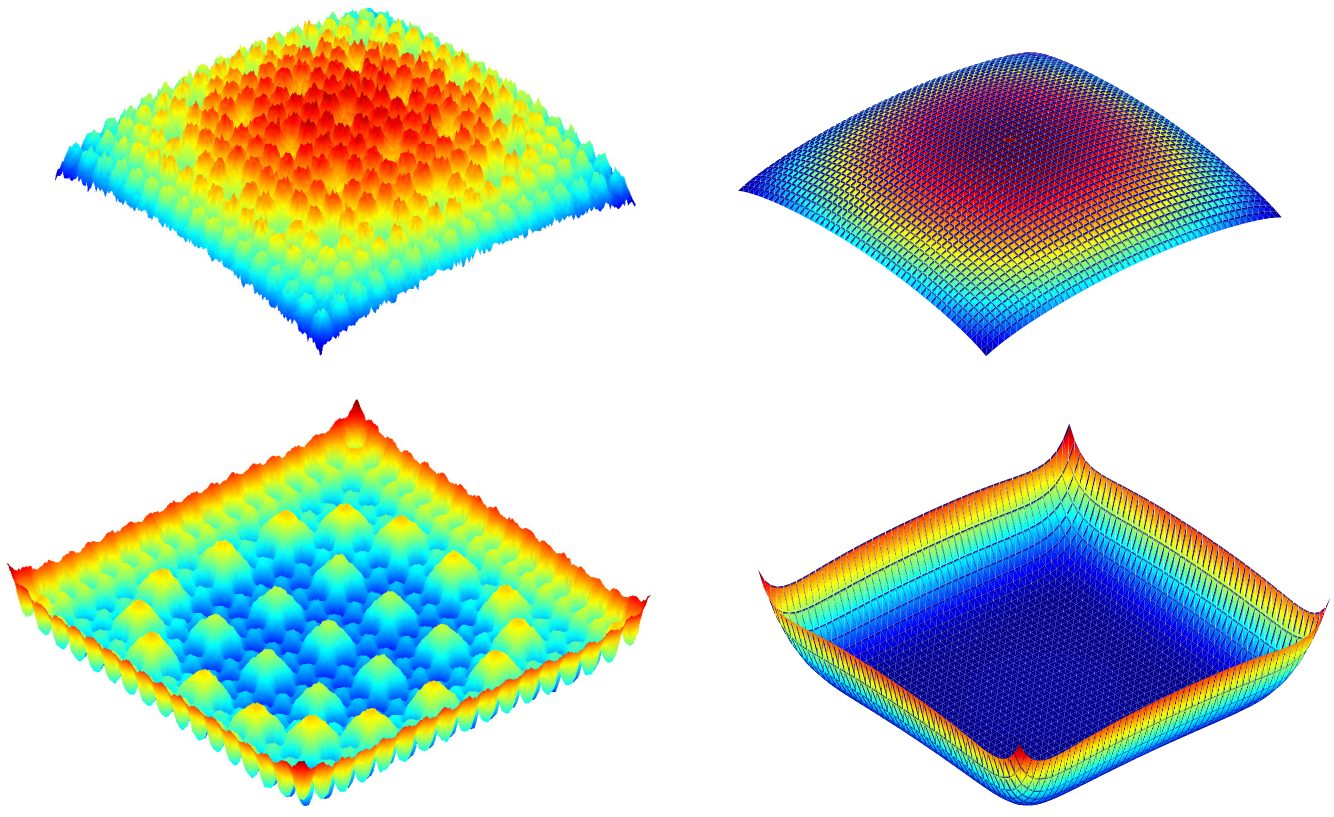


Figure 2: Example of heterogeneous and homogeneous flux calculated by Serpent 2 inside a single fuel assembly. Top left: fast heterogeneous flux, Top right: fast homogeneous flux, Bottom left: thermal heterogeneous flux, bottom right: thermal homogeneous flux.

Automated calculation sequence in Serpent 2

To simplify covering all state points in group constant generation, an automated calculation sequence is currently being developed for Serpent 2:

- Based on restart calculations, performed after the main burnup cycle
- Capable of handling branches to different state points
- Writes a separate output file, easily read by processing scripts[6]
- Covers only branch calculations, history calculations must be run separately
- Parallelization still handled similar to normal Serpent 2 calculation (separate branches not distributed to MPI tasks)

The work is still under way, and there is a separate topic for discussion at the Serpent forum: http://ttuki.vtt.fi/serpent

[6] A processing script called “SXSFit” is currently being developed for producing input data for nodal diffusion codes used at VTT (ARES, TRAB3D, HEXBU, HEXTRAN, Apros). The procedure involves converting the data into correct format and calculating polynomial coefficients for state-point dependencies.

Automated calculation sequence in Serpent 2

The calculation sequence is based on branches ('branch' card), used to inflict changes into original input file:

- Change in material density and temperature ('stp' entry)[7]
- Replace one material with another ('repm' entry)
- Replace one universe with another ('repu' entry)

And a coefficient matrix ('coef' card):

- Defines burnup points for which branch calculations are performed
- Defines combinations of branches run for each burnup point

In addition, state-point information can be passed directly into the output by defining variables

[7] The code automatically retrieves the correct cross sections from the directory file and performs Doppler-broadening on the data. Variations in moderator temperature can be inflicted by replacing the entire material.

Automated calculation sequence in Serpent 2

Input example 1: Independent variations

```
% -- Nominal state branch (do nothing):

branch nom

% -- Fuel temperature branches (change in material temperature):

branch fueH stp fuel24 -10.457 1600
branch fueC stp fuel24 -10.457 625

% -- Coolant boron concentration branches (replace material):

branch borL repm cool cool_loB
branch borH repm cool cool_hiB

% -- Control rod insertion branch (replace universe):

branch CR repu T R

% -- Coefficient matrix (13 burnup points, 3x3x2 branch combinations):

coef 13
0 5 10 15 20 25 30 35 40 45 50 55 60
3 nom fueH fueC
3 nom borL borH
2 nom CR
```

Automated calculation sequence in Serpent 2

Input example 2: Combined variations

```
% -- BOR 0 TFU 300 TMO 550:

branch BRA01
repm cool cool_0B
stp fuel24 -10.457 300
stp water -0.76971 550
var BOR 0.0 var TFU 300.0 var TMO 550.0

% -- BOR 750 TFU 600 TMO 550:

branch BRA02
repm cool cool_loB
stp fuel24 -10.457 600
stp water -0.76971 550
var BOR 750.0 var TFU 600.0 var TMO 550.0
...

% -- Coefficient matrix (13 burnup points, 21 branches):

coef 13
0 5 10 15 20 25 30 35 40 45 50 55 60
21 BRA00 BRA01 BRA02 BRA03 BRA04 BRA05 BRA06 BRA07
BRA08 BRA09 BRA10 BRA11 BRA12 BRA13 BRA14 BRA15
BRA16 BRA17 BRA18 BRA19 BRA20
```

Practical experience

The methodology has been tested by Serpent users with different code sequences and reactor types, for example:

- Serpent-DYN3D: VVER-440,[8] HTGR,[9] SFR,[10] PWR[11]
- Serpent-PARCS: PWR,[12,13] SFR,[14] RBWR[15,16]

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[8] S. Duerigen and E. Fridman. "*The Simplified P3 Approach on a Trigonal Geometry of the Nodal Reactor Code DYN3D.*" Kerntechnik **77** (2012), 226–229.

[9] S. Baier et al. "*Extension and application of the reactor dynamics code DYN3D for Block-type High Temperature Reactors.*" Nucl. Eng. Design **271** (2014), 431–436.

[10] E. Fridman and E. Shwageraus. "*Modeling of SFR Cores With Serpent-DYN3D Codes Sequence.*" Ann. Nucl. Energy **53** (2013), 354–363.

[11] M. Daeubler, J. Jimenez, and V. Sanchez. "*Generation and Application of Interface Discontinuity Factors in the Reactor Simulator DYN3D.*" In proc. ICAPP-2014. Charlotte, NC, 2014.

[12] M. Hursin et al. "*Comparison of Serpent and CASMO-5M for Pressurized Water Reactors Models.*" In proc. M&C 2013. Sun Valley, ID, 2013.

[13] N. Brown et al. "*Neutronic performance of uranium nitride composite fuels in a PWR.*" Nucl. Eng. Design **275** (2014), 393–407.

[14] L. Ghasabyan. "*Use of Serpent Monte Carlo Code for Development of 3D Full-Core Models of Gen-IV Fast-Spectrum Reactors and Preparation of Group Constants for Transient Analyses with PARCS/TRACE Coupled System.*" M.Sc. Thesis, Royal Institute of Technology. 2013.

[15] A. Hall et al. "*Advanced Neutronics Methods for Analysis of the RBWR-AC.*" Trans. Am. Nucl. Soc. **108** (2013), 771–774.

[16] A. Hall et al. "*Advanced Methods Development for Equilibrium Cycle Calculations of the RBWR.*" In proc. ICAPP-2014. Charlotte, NC, 2014.

Practical experience

At VTT, Serpent has been used with two code sequences:

- Serpent-ARES: MIT BEAVRS Benchmark (PWR)[17,18]
- Serpent-TRAB3D: EPR initial core[19]

The validation of Serpent-ARES using the BEAVRS Benchmark is an on-going project:

- Phase I: proof-of-concept with HZP calculations (completed)
- Phase II: Testing of group constant parametrization with HFP initial core calculations (preliminary results)
- Phase III: Testing of fuel cycle simulation (on-going)

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[17] J. Leppänen, R. Mattila, and M. Pusa. "*Validation of the Serpent-ARES Code Sequence Using the MIT BEAVRS Benchmark – Initial Core at HZP Conditions.*" Ann. Nucl. Energy **69** (2014), 212–225.

[18] J. Leppänen and R. Mattila. "*On the Practical Feasibility of the Continuous-energy Monte Carlo Method for Spatial Homogenization.*" In proc. PHYSOR 2014. Kyoto, Japan, Sept. 28 - Oct. 3, 2013.

[19] V. Sahlberg. "*Development of Serpent 2 – TRAB3D code sequence.*" Special Assignment, Aalto University, 2014. (VTT-R-04538-14).

Practical experience

Lessons learned from earlier calculations:

- It is possible to reach a good level of accuracy for power distribution at both assembly and pin level
- Homogenization of assemblies located at the core-reflector boundary required special treatment
- Continuous-energy Monte Carlo seems like a feasible option for group constant generation, although the computational cost is still high

Recent results for HFP initial core and burnup calculations:

- Critical boron concentrations and control rod bank worths for HZP consistent with benchmark values and 3D Serpent reference calculation
- Good results for HFP radial and axial power distribution compared to a reference 3D Serpent calculation[20]
- Boron dilution curve consistent with benchmark result

[20] ARES calculation was run first, and the resulting fuel temperature and coolant temperature and density distributions fed to Serpent via the universal multi-physics interface.

Practical experience

Table 1: Critical boron concentrations for HZP core (ppm).

Configuration	ARES	Ref.	A-R
ARO	978	975	2
D	916	902	14
C,D	818	810	8
A,B,C,D	682	686	-4
A,B,C,D,SE,SD,SC	492	508	-16

Table 2: Control rod bank worths for HZP core (pcm).

Bank	Serpent 3D	ARES	Ref.	A-S	A-R
D	781 (5)	754	788	-27	-34
C	1244 (5)	1203	1203	-41	0
B	1199 (6)	1134	1171	-65	-37
A	538 (6)	526	548	-12	-22
SE	497 (5)	420	461	-77	-41
SD	785 (6)	782	772	-3	10
SC	1120 (6)	1095	1099	-25	-4

Practical experience

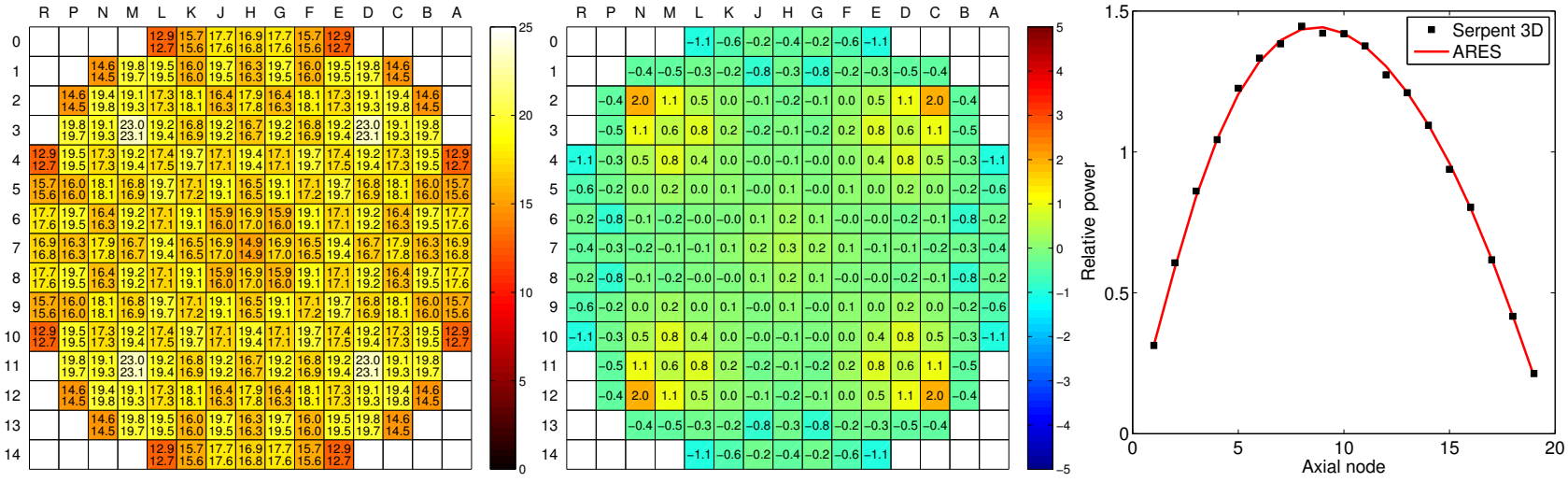

Figure 3: HFP radial and axial power distributions calculated using Serpent-ARES compared to reference 3D Serpent calculation. Left: Assembly powers (MW). Center: Relative differences in assembly powers (%). Right: Axial power peaking.

Practical experience

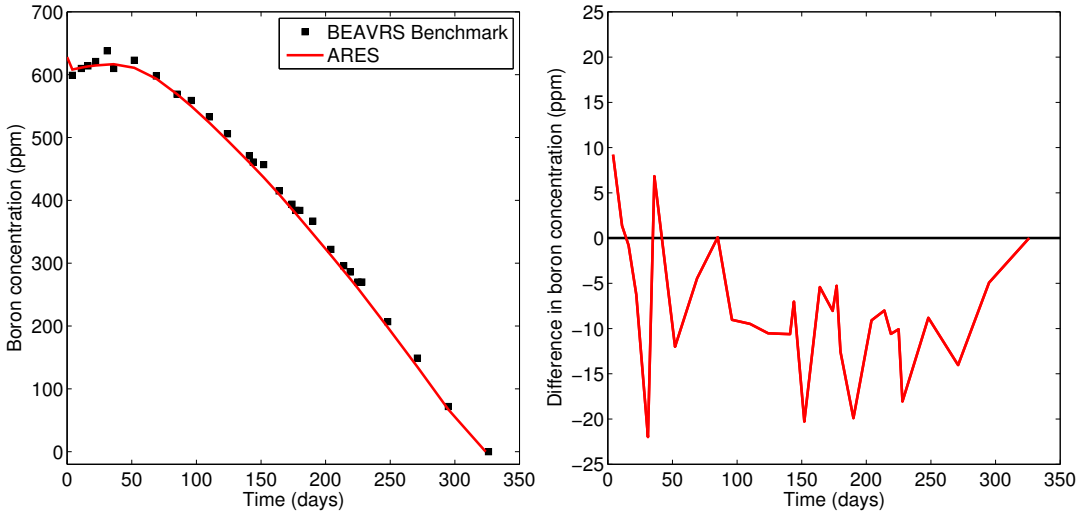

Figure 4: Boron dilution curve calculated by ARES for the first operating cycle in the BEAVRS benchmark compared to experimental data.

Future work in spatial homogenization

Recent work on spatial homogenization has been funded from the KÄÄRME project in the SAFIR 2014 Finnish National Research Programme on Nuclear Power Plant Safety:

- Main parts of the methodology were completed
- Proof-of-concept type demonstration that the Monte Carlo method can be used for group constant generation

The work continues in the MONSOON project of SAFIR 2018:

- Development of Serpent into a practical tool for group constant generation
- Comprehensive validation using fuel cycle and transient simulator codes used at VTT (ARES, TRAB3D, HEXTRAN, HEXBU, PARCS)
- Development of new methodologies: 3D methods in homogenization, fuel-performance and thermal hydraulics coupling in assembly-level calculations, new options for group constant parametrization

III - New applications

New applications

The second major development area is coupled multi-physics applications, which will be covered in Ville's presentation. Other topics include:

- Development of a CAD-based geometry type
- Methodology for fusion neutronics
- Photon transport mode

These are all still very much beta-features, and not documented or fully available in the distributed version

New applications: CAD based geometry type

Serpent was originally developed as a reactor physics code:

- Transport simulation limited to neutrons
- Calculation routines optimized for lattice calculations
- Built-in burnup routine
- No variance reduction techniques

Increasing interest to extend the scope of applications to new fields:

- Radiation shielding
- Fusion neutronics
- Medical physics (?)

New applications require development in transport physics (new particle types) and variance reduction, but also in tracking routine and geometry models

New applications: CAD based geometry type

Serpent is originally based on the CSG geometry type. The implementation of two new types is currently under way:

OpenFOAM mesh based geometry type:

- By-product of an unstructured mesh-based multi-physics interface for CFD code coupling (Ville's presentation)
- Presented at PHYSOR 2014[21]

CAD based geometry type:

- Based on the stereolithography (STL) format
- Presented at ANS Winter Meeting 2014[22], paper in M&C 2015[23]

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[21] 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.

[22] J. Leppänen. "*Development of a CAD Based Geometry Model in Serpent 2 Monte Carlo Code..*" Trans. Am. Nucl. Soc. **111** (2014), 663–667.

[23] J. Leppänen. "*CAD-Based Geometry Type in Serpent 2 – Application in Fusion Neutronics.*" In proc. M&C 2015. Nashville, TN, April 19–23, 2015 (accepted).

New applications: CAD based geometry type

The CAD based geometry type in Serpent is based on the Stereolitography (STL) format:

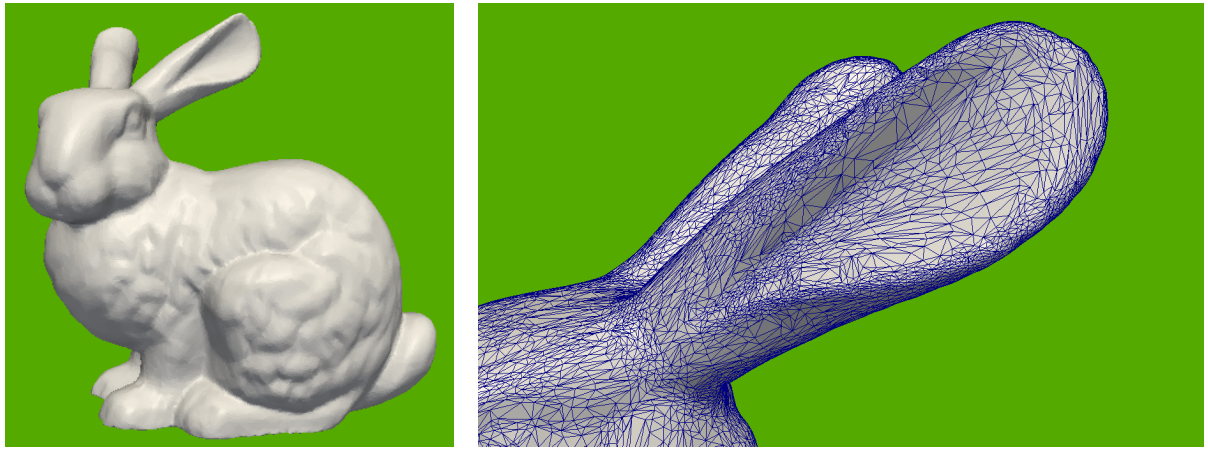
- One of the simplest geometry types used by computer-aided design (CAD)
- Based on the triangulation of curved surfaces
- Supported by most CAD tools because of its use in 3D printing

What this means for Serpent:

- New universe type, in which material cells are defined by STL solids
- Completely different cell search routine (based on ray tests)
- Capability to model complicated, arbitrarily-shaped bodies without conversion to CSG
- Potential applications in radiation shielding, fusion neutronics, engineering and space applications, etc. (especially when combined with the new photon transport mode)

New applications: CAD based geometry type

First test case (presented at ANS Winter Meeting 2014) was a toy problem:



- Stanford critical bunny: 3D model of a high-enriched uranium bunny (Godiva composition)
- Single STL solid
- Triangulated surface consists of 45,916 points and 91,840 triangular facets
- Demonstrated that the geometry routine works and is efficient

New applications: CAD based geometry type

Recent work (to be presented at M&C 2015 in April) focused on fusion neutronics:

- Full-scale CAD model of the ITER fusion reactor (C-Lite)
- 11 components, 1548 STL solids
- 441,056 points, 625,662 facets

The STL geometry routine had to be almost completely re-written (Serpent 2.1.23), but the results turned out to be pretty good:

- Geometry passed all “sanity checks”[24]
- Volumes of all solids accurately preserved
- Reasonable running time: 10^9 neutron histories simulated in 56 hours on a 12-core 3.47 Intel Xeon workstation
- No physically relevant results yet, because of simplified representations of neutron source and material compositions

[24] Except for one solid, which had a geometry error resulting from conversion to STL

New applications: CAD based geometry type

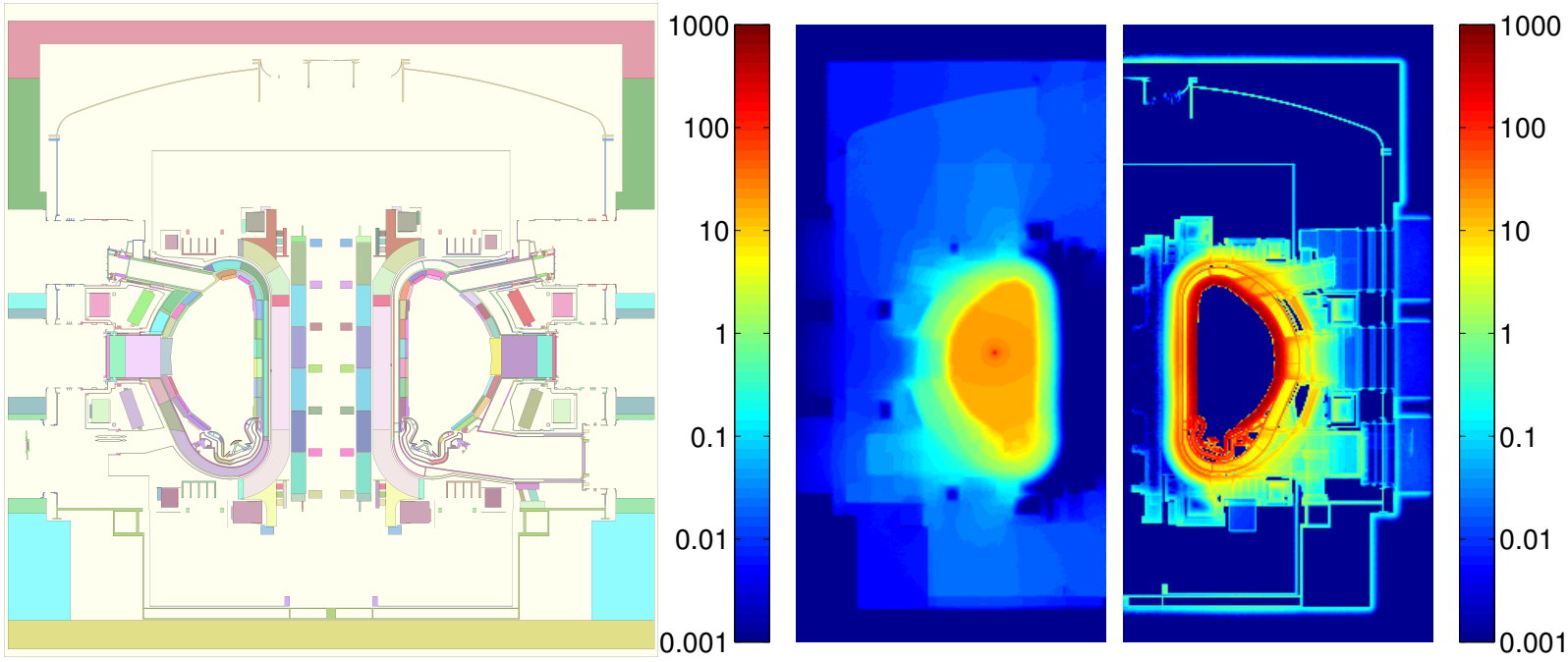


Figure 5: Left: Serpent geometry plot of the ITER C-Lite model. Right: flux (left half) and total collision rate (right half) calculated by Serpent.

New applications: Fusion neutronics

The applications for the CAD based geometry model are most likely found outside the scope of reactor physics. At VTT, work will be focused on fusion neutronics:

- VTT's fusion team was merged with reactor physics team at the beginning of 2014 $\Rightarrow$ synergy
- D.Sc. project (Paula Sirén) was started in late 2014:
  - First task: Development of a fusion neutron source based on the output of plasma simulation codes
  - Followed by: Material activation studies, DPA calculations, tritium breeding, radiation shielding,[25] etc.
  - Long term goals: coupling of Serpent into VTT's APROS system code for fusion power plant simulations

Feedback and contributions from user community are welcome!

[25] After the photon transport simulation is completed

New applications: Photon transport mode

Photon physics routines are completed, but not yet available in the publicly distributed version:

- Carried out as an M.Sc. project (Toni Kaltiaisenaho)
- Physics model somewhat different from MCNP6 (not entirely based on ACE format cross section libraries)
- To be included in update 2.1.23 or 2.1.24

First planned applications:

- Coupled neutron-photon transport mode for gamma heating in multi-physics applications
- Radiation shielding calculations in a dry spent fuel storage (KATVE project in the SAFIR 2018 Finnish National Research Programme)
- Radiation shielding calculations in fusion applications (combined to material activation)


TECHNOLOGY FOR BUSINESS