Current Status and Recent Development of Serpent 2

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Contents

Current trends in Serpent development:

1. Traditional reactor physics and methodology for group constant generation
2. Coupled multi-physics applications
3. Methodology for radiation transport applications

The first two topics fall under Kraken development. Other presentations on new / rarely-used methodologies:

- Ville Valtavirta: Kraken - a Serpent based Finnish reactor analysis framework
- Riku Tuominen: Effect of energy deposition modelling in coupled steady state Monte Carlo neutronics/thermal hydraulics calculations
- Manuel García: Collision-based Domain Decomposition scheme for Serpent 2
- Danila Roubtsov: Serpent2 at CNL: ENDF/B-VIII.0 library ZED-2 benchmarks and Photonuclear Option
- Alexander Wheeler: Documenting and demystifying online processing features of Serpent
- ...

This presentation covers the recent progress on radiation transport capabilities.

Background: photon transport mode

VTT

Originally the main 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 neutron and photon heating may become important especially in fast transients

Development of photon physics routines:

- First introduced in 2015[1]
- Coupled neutron-photon transport mode in 2017[2]
- Photonuclear reactions in 2019[3]

Photonuclear reactions are not yet available in the publicly distributed version (2.1.31). For access and more information, contact: Toni.Kaltiaisenaho@vtt.fi.

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1 T. Kaltiaisenaho. “*Implementing a photon physics model in Serpent 2.*”. MSc Thesis, Aalto University. 2016.

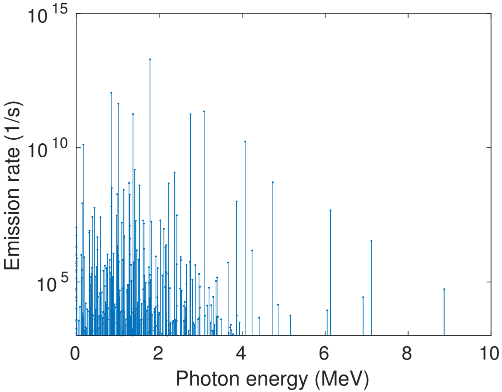
2 J. Leppänen et al. “*Implementation of a Coupled Neutron / Photon Transport Mode in the Serpent 2 Monte Carlo Code.*”. In proc. M&C 2017. Jeju, Korea, Apr. 16-20, 2017.

3 T. Kaltiaisenaho. “*Photonuclear Reactions in Serpent 2 Monte Carlo Code.*”. In proc. M&C 2019. Portland, OR, Aug. 25–29, 2019.

Background: photon transport mode

The physics routines in Serpent 2 provide the basic functionality for radiation transport transport calculations involving neutrons and photons:

- Photon interaction physics from 1 keV to 100 MeV + photonuclear reactions
- Prompt gammas in coupled neutron/photon mode
- Radioactive decay source mode for photons, neutrons and secondary bremsstrahlung produced by beta-decay[4]
- Photon-specific tallies: analog energy deposition, pulse-height detector, built-in response functions



[4] For the bremsstrahlung model, see: T. Kaltiaisenaho. "Implementing a beta bremsstrahlung source in Serpent.". VTT-R-00953-18, VTT Technical Research Centre of Finland, Ltd. (2018).

Background: advanced geometry types

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

- Most reactor geometries can be described using planes and cylinders
- Regular structures are easy to model using standard universes and lattices
- Special geometry type for HTGR fuels (particles and pebbles)[5]

Advanced types available for irregular and unstructured geometries:

- Mesh-based geometry type developed together with the OpenFOAM multi-physics interface was introduced in 2013[6]
- CAD-based geometry type based on STL file format implemented in 2014[7]

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

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5 V. Rintala et al. "*Modelling of Realistic Pebble Bed Reactor Geometries Using the Serpent Monte Carlo Code.*". Ann. Nucl. Energy **77** (2015), 223–230.

6 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.

7 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.

Background: advanced geometry types

The CAD-based geometry type in Serpent is based on the STL file format:

- Solid bodies constructed from triangulated surfaces
- Widely used for 3D printing – supported by most CAD tools
- Geometries consisting of one or several STL solids are handled as universes
- Background universe for undefined regions (no need to define empty space)
- Tracking routine can handle gaps between solids without problems
- Adaptive search mesh to speed-up geometry routine

The STL geometry type can be used in combination with other types (CSG, mesh-based, stochastic pebble/particle fuel model).

Background: advanced geometry types

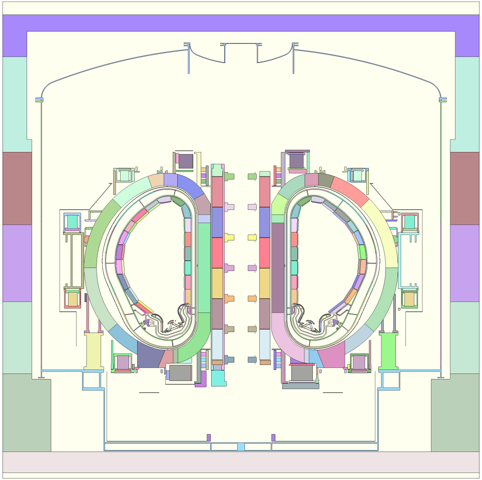

Figure 1: Serpent geometry plot of an STL geometry type Different CAD solids are plotted with different colors. (C-Lite model of the ITER fusion reactor comprised of 11 components, 1,548 solids, 1,842,576 points, 614,192 triangular facets).

Background: advanced geometry types

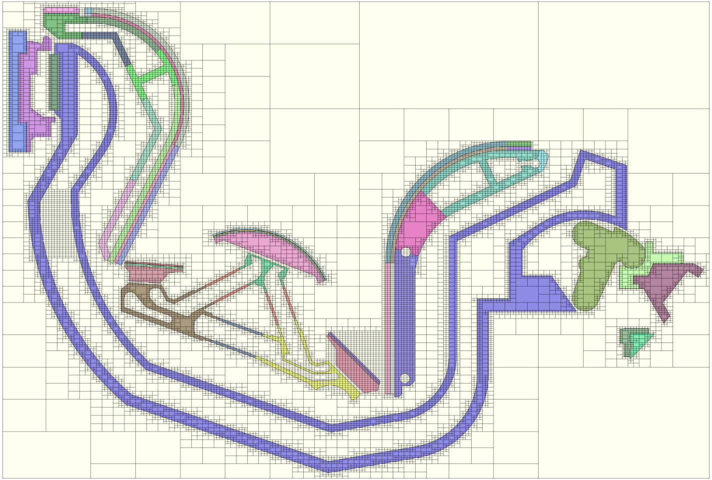

Figure 2: Serpent geometry plot of an STL geometry type (divertor cassette, part of the ITER C-Lite model). Different CAD solids are plotted with different colors. The search mesh is automatically adapted around the triangulated surface.

Background: advanced geometry types

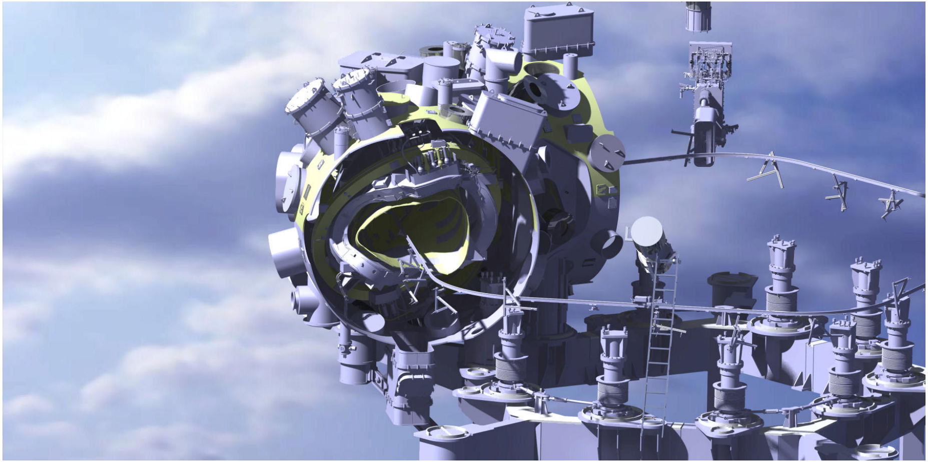

Figure 3: The next challenge: CAD-based model of the Wendelstein 7-X stellarator.

Background: variance reduction

Radiation shielding calculations using the Monte Carlo method require extensive use of variance reduction.

A weight-window based variance reduction scheme was first introduced in 2016:[8]

- Support for MCNP WWINP format weight-window mesh generated using some deterministic tool
- Built-in light-weight response matrix based importance solver[9]

The built-in solver obtains coupling coefficients for the response matrix method from a forward Monte Carlo simulation, and provides the importances (adjoint solution) for calculating the weight-window boundaries:

- Applicable to both photon and neutron transport problems
- Support for single and multiple detector responses and global variance reduction (GVR)
- Rectangular, cylindrical, hexagonal and self-adaptive octree mesh[10]

Examples and short tutorial at: http://serpent.vtt.fi/mediawiki/index.php/Variance_reduction

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[8] 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.

[9] J. Leppänen. "*Response Matrix Method–Based Importance Solver and Variance Reduction Scheme in the Serpent 2 Monte Carlo Code.*". Nucl. Technol. (2019, in press). DOI: 10.1080/00295450.2019.1603710.

[10] J. Leppänen and M. Jokipii. "*Global Variance Reduction Scheme with Self-Adaptive Weight-Window Mesh in the Serpent 2 Monte Carlo Code.*". In proc. M&C 2019. Portland, Oregon, USA, Aug. 25–29, 2019.

GVR and adaptive weight-window mesh

The response matrix method in a nutshell:

- Particle currents are passed through the geometry until their contribution becomes negligible
- Adjoint solution is obtained by backwards iteration that tracks the currents in inverse order starting from the responses
- The standard solution provides importances with respect to a single response, but the method can be extended to multiple responses[11]

Problems with large heavily shielded geometries:

- Particles may not reach the responses $\longrightarrow$ no coupling coefficients to enable running the response matrix solver
- Solution is to use global variance reduction (GVR), i.e. to gradually populate the entire geometry until sufficient statistics for generating the optimal mesh
- The importance mesh is generated by treating the flux inside each mesh cell as a separate response

The calculation proceeds by iterations between the Monte Carlo simulation and the importance solver.

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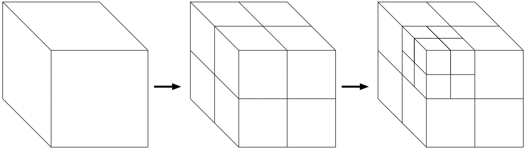
[11] Equal statistical contribution is obtained by weighting the responses with the inverse of the importance-weighted flux.

GVR and adaptive weight-window mesh

The response matrix solver was previously implemented on a on a 1-, 2- or 3-dimensional Cartesian, cylindrical and hexagonal mesh, super-imposed over the geometry.

However: The geometry of the system is defined by a topology matrix, which describes how the cells are connected to each other – the solution algorithm itself is completely dimensionless.

The methodology has now been extended to an adaptive rectangular mesh.



No changes required for the solution algorithm (only the topology matrix) $\longrightarrow$ practical challenges related to mesh generation.[12]

[12] Similar data structure is used in Serpent to speed-up handling of CAD-based geometry types.

GVR and adaptive weight-window mesh

An adaptive mesh is ideal for variance reduction problems in which the geometry consists of both heavily shielded structures and large volumes of empty space:

- Steep importance gradients in shielded parts $\longrightarrow$ high mesh resolution needed
- Flat distribution in low-density regions (air) $\longrightarrow$ refining the resolution only wastes memory

Question: How to construct the mesh?

Viable options:

- Manually – probably the optimal solution, but labor intensive (currently not supported)
- Iteratively, i.e. based on previous transport solutions (several viable criteria) – promising, but not always the best solution
- Density based, i.e. by probing the geometry with random tracks before starting the transport simulation – suitable for problems where the geometry is clearly divided into solid structures and empty space

User input consist of the split criteria, most importantly density limits and minimum mesh cell dimensions.[13]

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[13] Mesh cells can also be split based on importance gradients and number of neighbors.

Demonstration (from M&C 2019): Test case

Test case:

- CAD-based model of two adjacent hot-cell units at VTT's Centre for Nuclear Safety
- Geometry consists of lead shielding, stainless-steel support structure, lead-glass windows and concrete floor
- 370 GBq point isotropic ^{60}Co source, placed inside the second hot-cell unit
- The task is to calculate dose rate at four positions outside the shielded walls

Challenges:

- Geometry consists of heavy lead shielding and large volumes of air
- Unable to generate weight-window mesh from analog simulation (poor statistics)

Solution: use adaptive mesh for optimal resolution and apply multiple GVR iterations to populate the entire geometry before generating the final mesh.

Demonstration (from M&C 2019): Test case

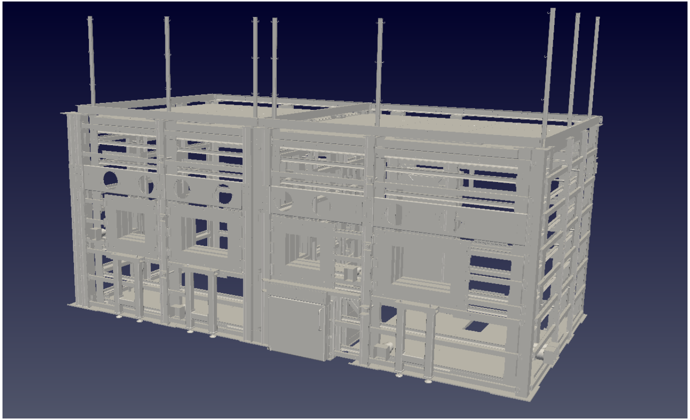

Figure 4: CAD-based geometry model of the stainless-steel support surrounding two adjacent hot-cell units.

Demonstration (from M&C 2019): Test case

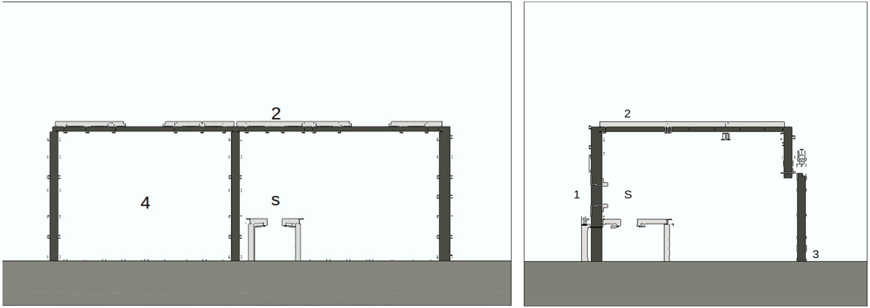

Figure 5: Geometry plot showing source and detector positions. Absorbed dose rates were calculated using inside 5 cm diameter spherical detectors (dtl detector type) and ANSI-standard flux-to-dose conversion factors.

Demonstration (from M&C 2019): Work flow

The calculations were divided in multiple parts:

1. Generation of adaptive mesh, analog Monte Carlo simulation, first GVR iteration
2. Monte Carlo simulation using weight-window mesh from previous step, second GVR iteration
3. Monte Carlo simulation using weight-window mesh from previous step, generation of optimal mesh for the four detectors
4. Monte Carlo simulation using weight-window mesh from previous step, calculation of final results

Notes:

- The final octree mesh was comprised of 816,214 cells
- Weight-window generation was performed using 100 million photon histories per iteration (running times: 34/37/98 min), final calculation with 1 billion histories (running time: 197 min)
- Analog reference results were calculated using 50 billion photon histories (running time: 7.9 days)
- Preparation of adaptive mesh and running the response matrix solver took only a few minutes in total

All calculations were run on a 28-core 2.6 GHz Intel Xeon cluster node.

Demonstration (from M&C 2019): Mesh generation

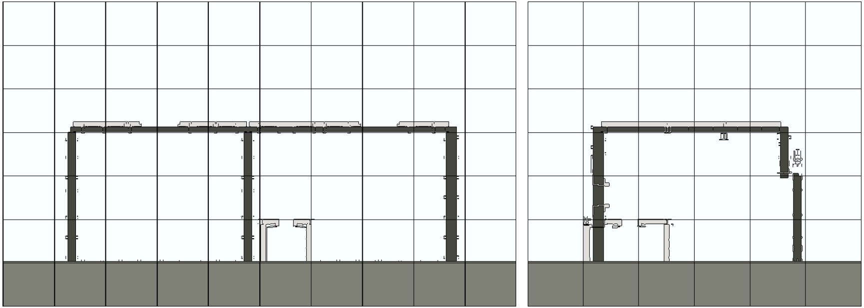

Figure 6: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

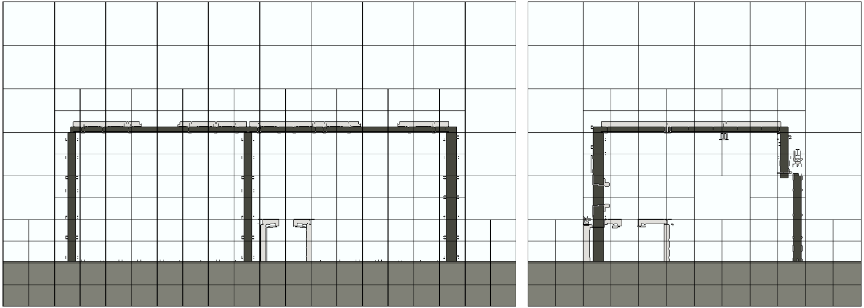

Figure 7: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

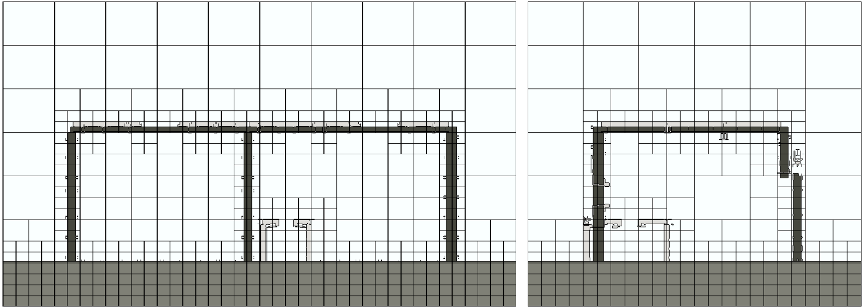

Figure 8: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

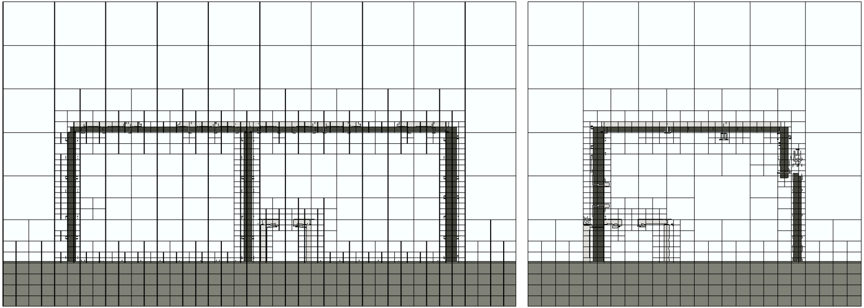

Figure 9: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

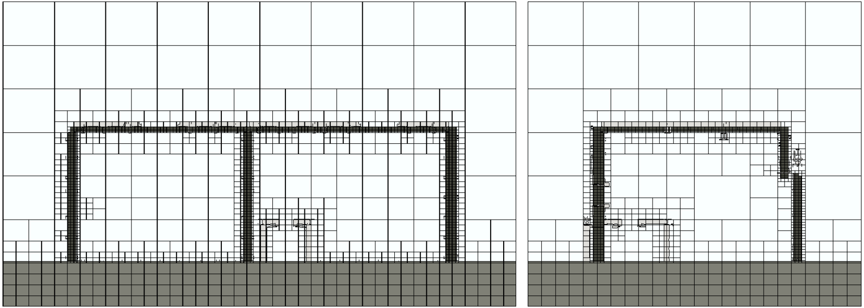

Figure 10: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

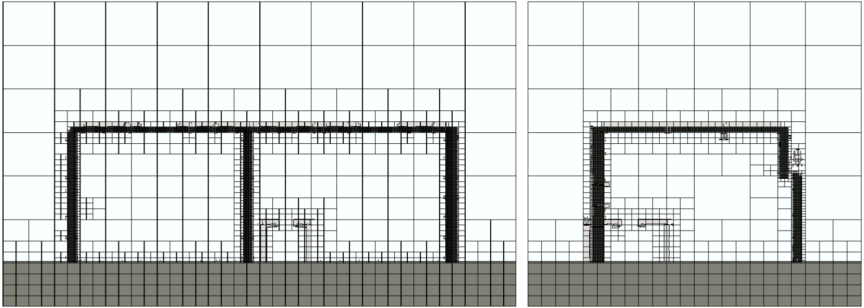

Figure 11: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

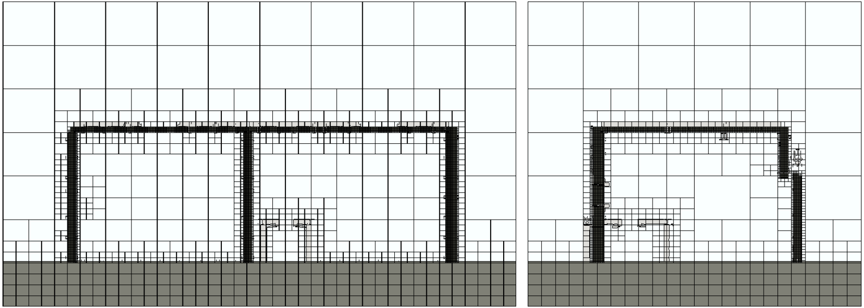

Figure 12: Octree mesh adapted around the heavily shielded parts of the geometry.

Demonstration (from M&C 2019): Mesh generation

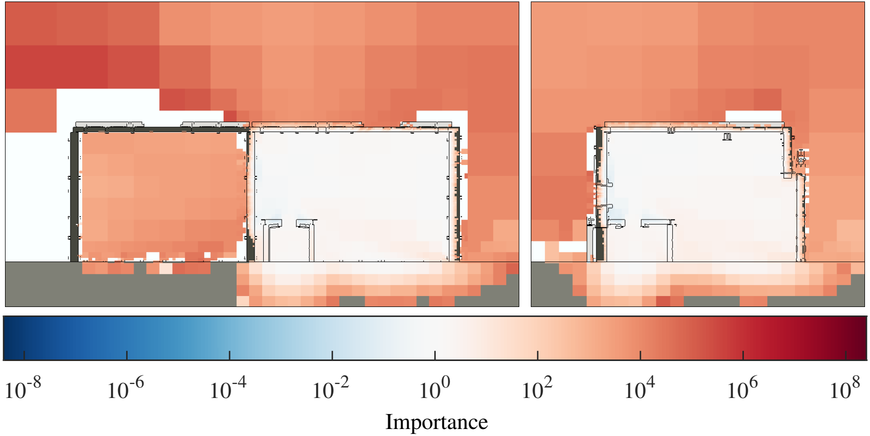

Figure 13: Weight-window mesh after 1st GVR iteration.

Demonstration (from M&C 2019): Mesh generation

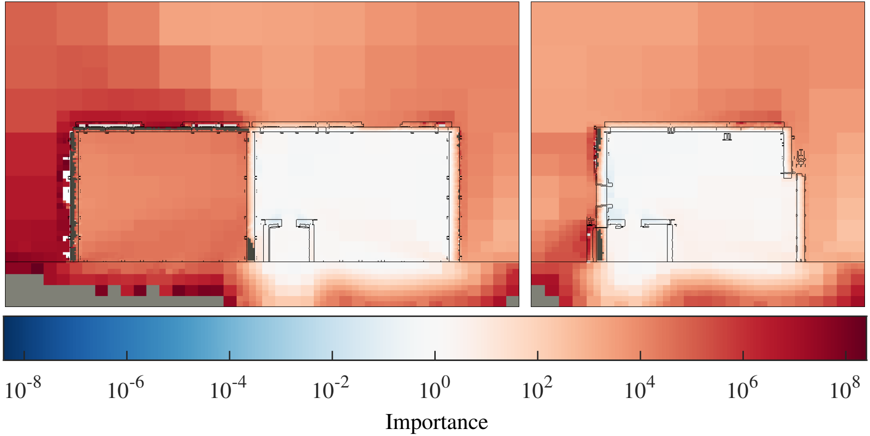

Figure 14: Weight-window mesh after 2nd GVR iteration.

Demonstration (from M&C 2019): Mesh generation

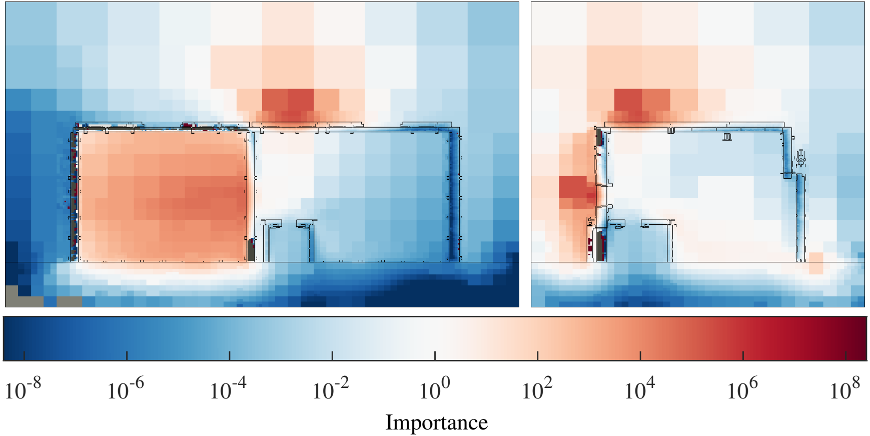

Figure 15: Weight-window mesh optimized for the 4 detectors.

Demonstration (from M&C 2019): Results

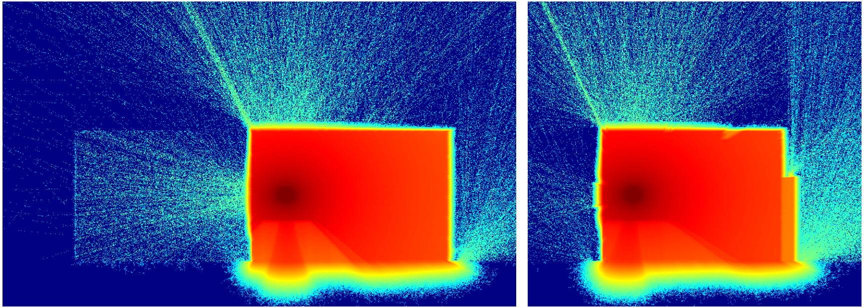

Figure 16: Serpent 2 mesh plots showing radiation dose rate distributions in an analog simulation. The distributions are in 2D, i.e. integrated over the third dimension. The color scale is logarithmic.

Demonstration (from M&C 2019): Results

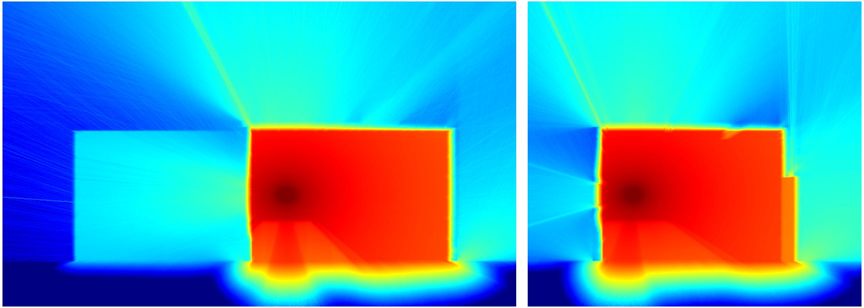

Figure 17: Serpent 2 mesh plots showing radiation dose rate distributions using variance reduction. The distributions are in 2D, i.e. integrated over the third dimension. The color scale is logarithmic.

Demonstration (from M&C 2019): Results

Detector results were compared to the analog reference calculation. Computational performance was evaluated using the figure-of-merit:

$$FOM = \frac{1}{\sigma^2 T}$$

where σ is the standard deviation of the evaluated tally and T is the wall-clock running time.

Table 1: Results of dose rate calculations with and without variance reduction. The mean values are accompanied by relative statistical errors in parentheses. The last two columns show the relative differences and gain in computational performance (ratio of VR to analog figure-of-merits), respectively.

Detector position	Absorbed dose rate [μGy/h]		Rel.	FOM
	Analog simulation	Adaptive WW-mesh	diff.	ratio
Outside the front window	1.22 (0.10)	1.15 (0.01)	-0.06	4079
Above the cell	3.14 (0.06)	3.41 (0.01)	0.08	555
On floor, near the back door	30.42 (0.02)	29.74 (0.01)	-0.02	82
Center of adjacent cell	0.31 (0.18)	0.33 (0.03)	0.08	1090

GVR and adaptive weight-window mesh

Lessons learned from preliminary studies:

- The developed methodology fulfills its purpose: easy to use built-in solver for (not the most challenging) variance reduction problems
- Significant improvement in computational performance
- Even though the calculation had to be divided into multiple parts, the amount of additional manual work was minimal
- Finding the optimal mesh parameters requires some trial and error (learning curve)

Potential pitfalls:

- Since the coupling coefficients are obtained from a Monte Carlo simulation, poor statistical accuracy is also reflected in the importance mesh
- One of the drawbacks of the response matrix method is large memory footprint – even though adaptivity reduces the mesh size, the calculation required some 12 GB of memory
- A geometry-based adaptation works for compact systems, but not necessarily for large geometries
- Atomic density may be a sufficient split criterion for photons, but not necessarily for neutrons

Potential radiation transport applications for Serpent 2

Serpent has a lot of potential for radiation transport applications, for example:

- Back-end of the nuclear fuel cycle (storage, transportation and final disposal of spent fuel, decommissioning of reactors)
- Industrial applications involving radioactive sources
- Shielding design (hot cells, sources, reactors, accelerators, space applications)
- Medical applications of radiation (radiotherapy, medical imaging)
- Dose rate calculations involving complicated source terms (e.g. radioactive fallout)

Serpent is still used almost exclusively for reactor physics, and radiation transport is a relatively new application for us as well, so all user feedback is greatly appreciated!

The end – thank you for your attention!

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