



Fun stuff with the built-in response matrix solver

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Outline

Background

Response matrix method

Weight window based variance reduction (skip)

Built-in response matrix solver in Serpent 2:

- ▶ Adjoint solution for variance reduction
- ▶ Forward k -eigenvalue solution to accelerate source convergence

Future plans

Background

A built-in response matrix solver was implemented in Serpent 2.1.27 (Sept. 2016):

- ▶ Adjoint solution for calculating importance meshes for variance reduction
- ▶ Presented at M&C 2017 in April¹
- ▶ Methodology revised and multi-group mode added in version 2.1.29

The solver is still under development, and k -eigenvalue criticality source mode was added in version 2.1.30:

- ▶ Improved source guess to accelerate fission source convergence
- ▶ Paper submitted to PHYSOR 2018

Question: In addition to these two applications, is there any other potential use for this built-in solver?

¹J. Leppänen, T. Viitanen, and O. Hyvönen, O. "Development of a Variance Reduction Scheme in the Serpent 2 Monte Carlo Code." In proc. M&C 2017, Jeju, Korea, Apr. 16-20, 2017.

Response matrix method

The response matrix method provides a deterministic solution to the transport problem in the form of interface currents over spatially discretized cells.

The method is based on the preservation of particle balance inside each cell and the continuity of current through its boundaries by means of various coupling coefficients, such as:

- ▶ Current transfer coefficients $\alpha_{i,j}$, which determine the fraction of inward current that passes through the cell from boundary i to boundary j
- ▶ Source coefficients s_j , which determine the fraction of source particles that exit the cell through boundary j
- ▶ Response coefficients r_i , which determine the contribution of inward current through boundary i to a given response

These coefficients are easily calculated using the Monte Carlo method.

The response matrix solution preserves the results of the Monte Carlo simulation, not only to within statistics, but to within the accuracy of floating point arithmetics!

Response matrix method

The solution proceeds by iterations, during which the particle currents are passed through the geometry until their contribution becomes negligible.

Two solution modes have been implemented in Serpent 2:

Adjoint solution – Essentially a backwards iteration that tracks the currents in inverse order starting from the responses

k -eigenvalue solution – Forward iteration that converges the fission source distribution (very similar to a Monte Carlo criticality source simulation)

The coupling coefficients required for the solution are obtained from a forward Monte Carlo simulation.

Currently implemented on a 1-, 2- or 3-dimensional Cartesian mesh, super-imposed over the geometry (adjoint solution also in cylindrical mesh).

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.

Weight window based variance reduction

The adjoint solution is used to obtain an importance mesh for variance reduction. The idea is best understood by considering the following concepts:

Physical reality – Infinite number of possible particle histories

Analog simulation – Randomly selected sample from the infinite number of possible particle histories

Implicit simulation – Sample from the infinite number of possible particle histories, selected in such way that the histories contribute to a specific result

In implicit simulation, each particle is assigned with a statistical weight, which is used as a multiplier for all tallies

Variance reduction techniques work by “cheating” in the analog game, and correcting the results by adjusting the particle weight

The idea is that the transport of particles may be manipulated, but the simulation remains unbiased as long as the transport of the statistical weight is preserved

Weight window based variance reduction

Favoring histories that contribute to a specific result is done by assigning importances to various events (collisions, boundary crossings, etc)

Particles can be encouraged to migrate towards higher importance by using a weight window mesh:²

- ▶ The geometry is covered by a mesh (Cartesian, cylindrical, unstructured, etc.)
- ▶ Each mesh cell is assigned with a minimum and maximum weight: W_{\min} , W_{\max}
- ▶ The bounding weights are inversely proportional to importance

When the particle enters the mesh cell, its weight w is compared to the boundaries:

- ▶ If $w < W_{\min}$ – Russian roulette: particle is either killed or its weight is increased
- ▶ If $w > W_{\max}$ – Splitting: the history is divided into multiple parts

After the operation all particles inside the mesh cell have weights between W_{\min} and W_{\max}

²The mesh can also include energy dimension.

Adjoint solution: importance

Forward and adjoint transport problems:

Forward problem – Calculate responses (physical reaction rates) induced by particles originating from a given source

Adjoint problem – Calculate contributions of various events (reactions, boundary crossings, etc.) to a given response

Solution to the adjoint problem provides the importances needed for forming the weight window mesh for variance reduction

Physical interpretation of importance: The average contribution of a particle at position (x, y, z) , traveling in direction (u, v, w) with energy E to given response f

Solving the adjoint problem using the Monte Carlo method essentially implies running the transport simulation backwards – the response matrix solver provides a solution that is equivalent with a backwards simulation.

Adjoint solution: Variance reduction in action

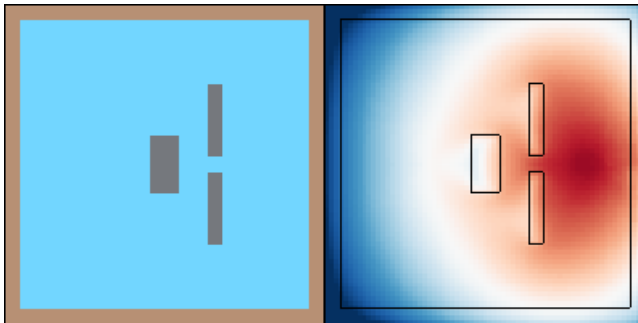


Figure 1 : Demonstration of a weight-window based variance reduction scheme. Photon point source in water, detector located behind three steel blocks. Left: analog simulation, Right: implicit simulation showing importance mesh (logarithmic color scheme).

Adjoint solution: Variance reduction in action

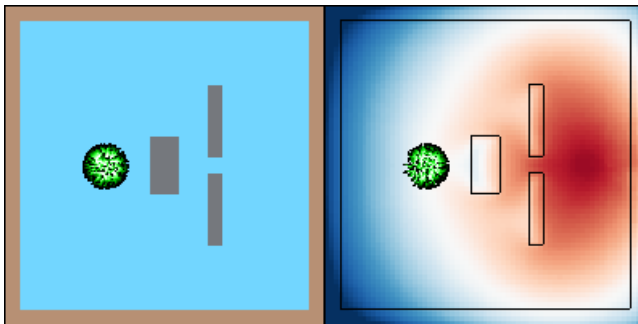


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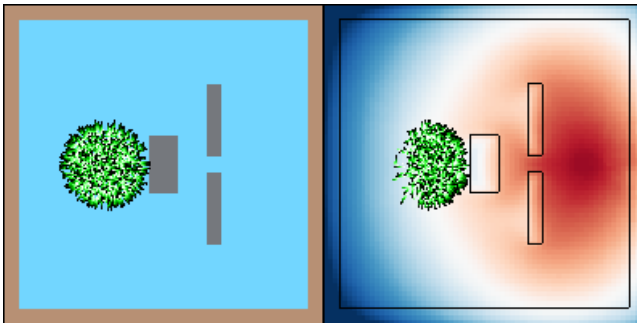


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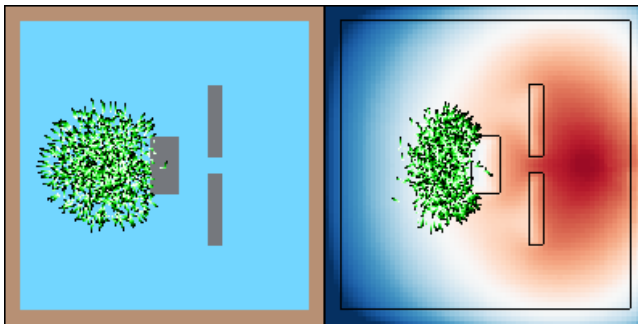


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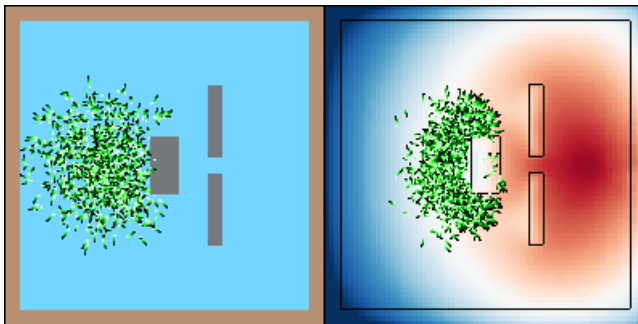


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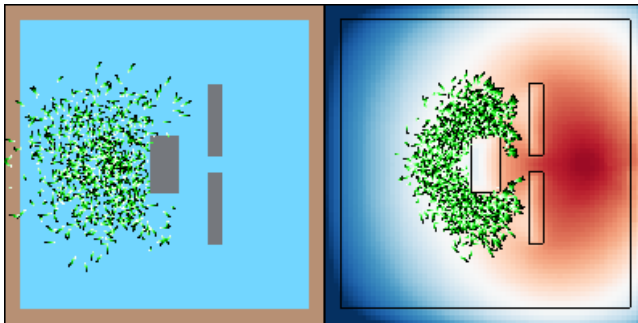


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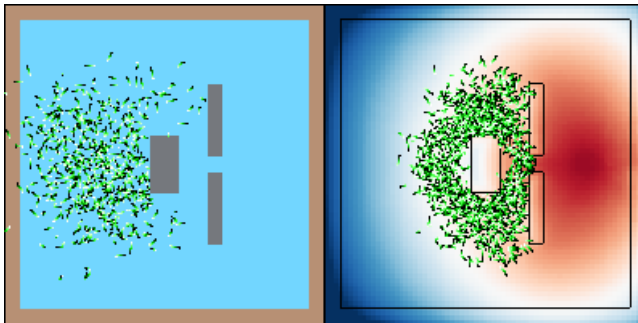


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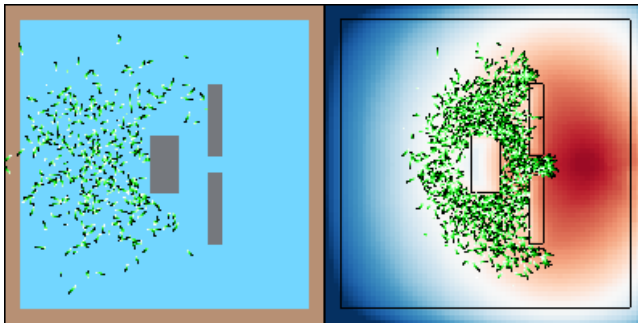


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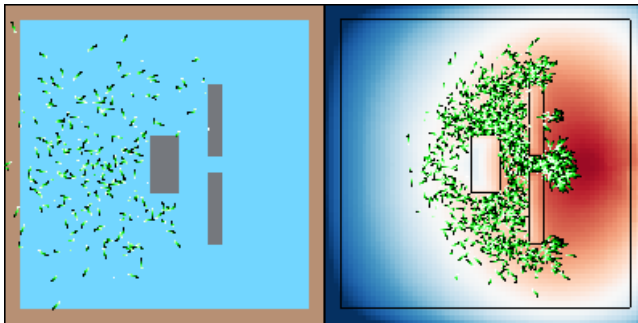


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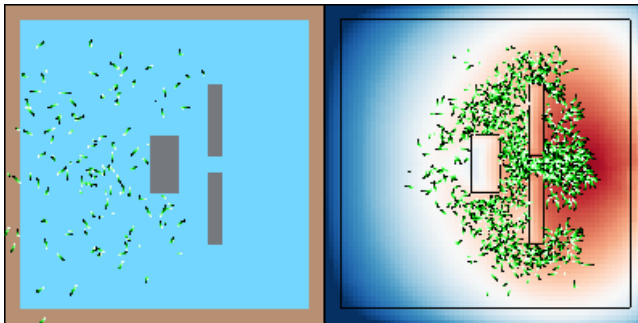


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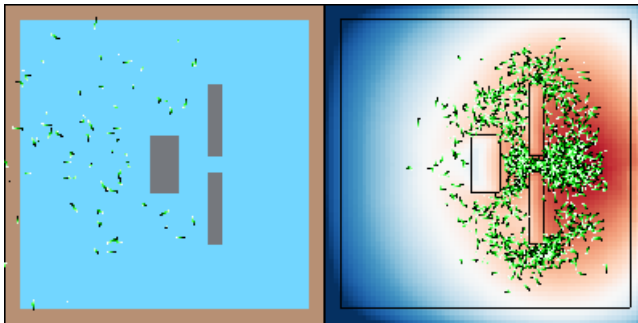


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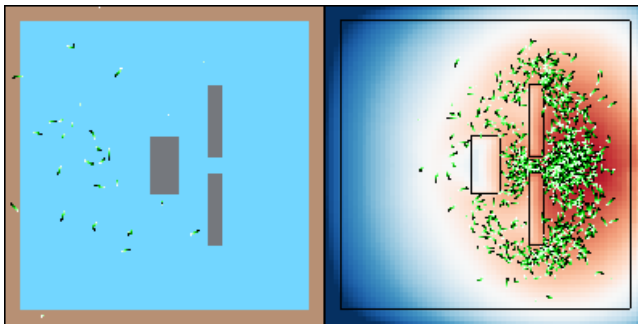


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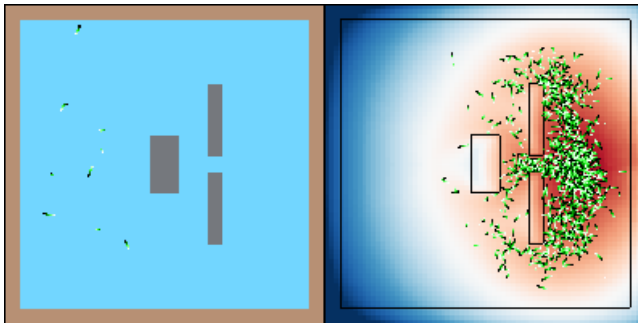


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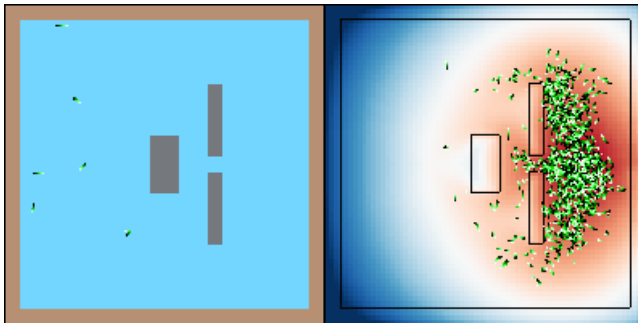


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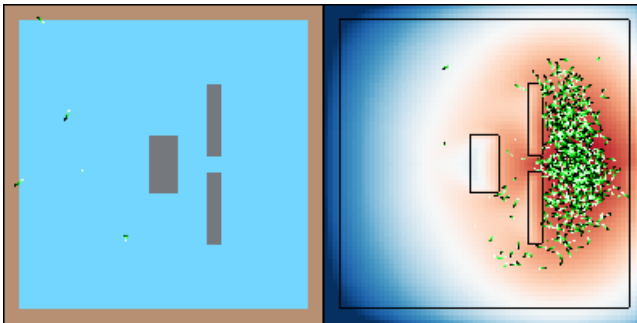


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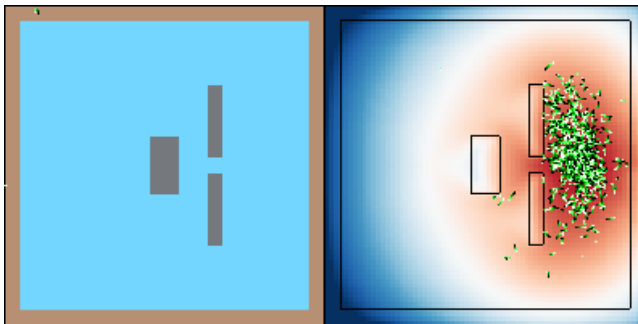


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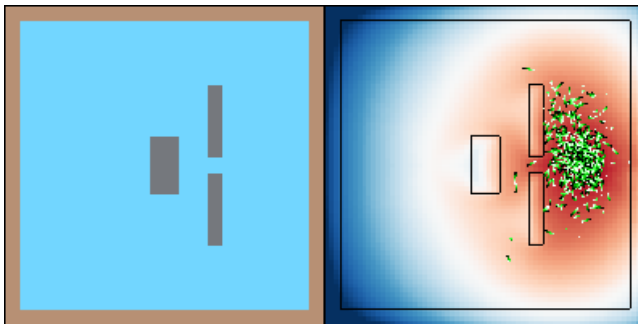


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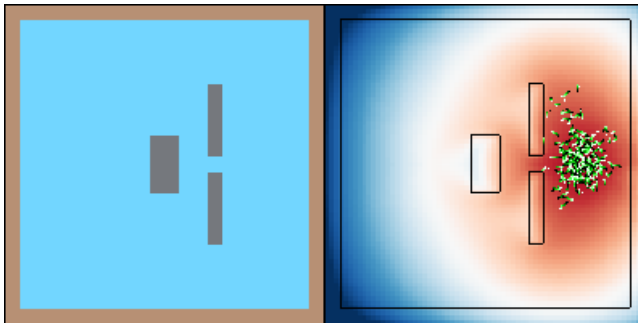


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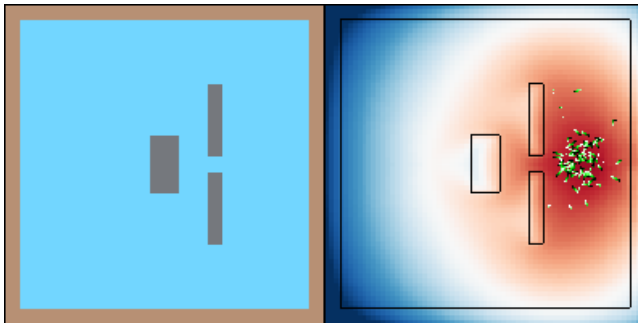


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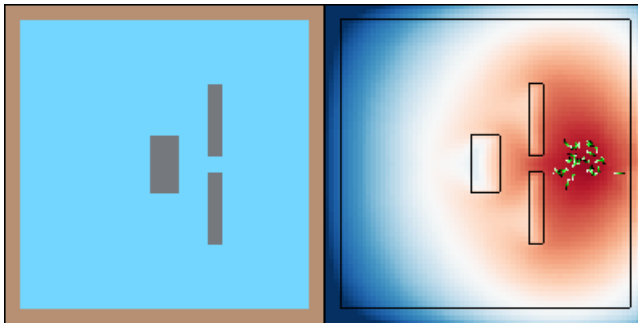


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Adjoint solution: Ex-core dosimetry calculation

The built-in response matrix solver was used in the M&C 2017 paper in a test case involving an ex-core dosimetry calculation with variance reduction:

- ▶ Activation of surveillance chains positioned outside the core barrel in a VVER-440 pressurized water reactor
- ▶ 2 cm diameter spherical detector, 8 material samples: ^{54}Fe , ^{58}Ni , ^{63}Cu , ^{46}Ti , ^{93}Nb (two reactions), ^{59}Co , ^{58}Fe
- ▶ Transport simulation run in external source mode with fissions switched off
- ▶ Source distribution obtained from the HEXBU-3D core simulator code
- ▶ Cartesian $50 \times 50 \times 70$ importance mesh produced using the built-in response matrix based solver

The calculations are related to a feasibility study of using Serpent for the evaluation of structural integrity of the Loviisa-1 and -2 reactor pressure vessels. The results are, for the main part, proprietary.

Adjoint solution: Ex-core dosimetry calculation

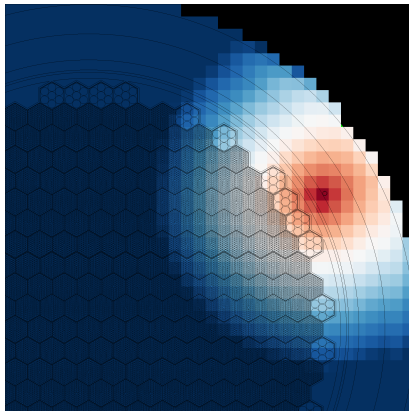


Figure 2 : Serpent geometry plot showing a quadrant of the VVER-440 reactor core, together with the importance mesh produced by the built-in response matrix based solver. The color scheme is logarithmic, and extends from blue (low importance) to red (high importance). The importance peaks at the position where the detector is located.

Adjoint solution: Ex-core dosimetry calculation

Table 1 : Results of the VVER-440 ex-core dosimetry calculation. The first three columns provide the detector materials, reactions and threshold energies, followed by the relative difference between the results (the actual results are proprietary) given by analog and implicit simulations, relative statistical errors and figure-of-merits. The last column shows the gain in computational efficiency (ratio of FOM's). Differences and statistical errors are in percent.⁴

Detector	Reaction	E_{\min}	Diff.	Err _{ana}	Err _{vr}	FOM _{ana}	FOM _{vr}	Gain
Iron-54	$^{54}\text{Fe} (n,p) ^{54}\text{Mn}$	2.2 MeV	2.4	3.2	0.7	1.07E-02	6.85E+00	× 642
Nickel-58	$^{58}\text{Ni} (n,p) ^{58}\text{Co}$	1.8 MeV	2.7	2.9	0.6	1.38E-02	8.92E+00	× 645
Copper-63	$^{63}\text{Cu} (n,\alpha) ^{60}\text{Co}$	4.7 MeV	-0.7	8.9	2.1	1.41E-03	7.50E-01	× 533
Titanium-46	$^{46}\text{Ti} (n,p) ^{46}\text{Sc}$	3.7 MeV	2.3	5.7	1.3	3.47E-03	1.92E+00	× 555
Niobium-93	$^{93}\text{Nb} (n,n') ^{93m}\text{Nb}$	0.8 MeV	1.4	1.2	0.3	7.41E-02	5.02E+01	× 678
Cobalt-59	$^{59}\text{Co} (n,\gamma) ^{60}\text{Co}$	-	0.1	1.3	0.1	7.15E-02	1.90E+02	× 2666
Niobium-93	$^{93}\text{Nb} (n,\gamma) ^{94}\text{Nb}$	-	-1.2	2.4	0.2	1.91E-02	6.11E+01	× 3195
Iron-58	$^{58}\text{Fe} (n,\gamma) ^{59}\text{Fe}$	-	0.3	1.0	0.1	1.20E-01	2.85E+02	× 2370

⁴The calculations were run in a single 20-core 2.2 GHz Intel Xeon cluster node. The reference analog simulation was run for two wall-clock months (1478 hours) and the implicit simulation with variance reduction for 68 hours. Transport simulation for producing the importance mesh took 3 hours. The response matrix solution converged in less than 30 seconds.

Acceleration of source convergence

Criticality source simulations run for systems with high dominance ratio are often subject to slow fission source convergence:

- ▶ Typical for large LWR cores where neutron migration length is short compared to the dimensions
- ▶ A large number of inactive cycles (~ 100 – 200) may be required to converge the fission source
- ▶ Source convergence can be monitored using the Shannon entropy⁵

Running inactive cycles wastes CPU time, because any results collected before the source has converged have to be discarded.

The number of inactive cycles depends on the initial guess used for fission source distribution – computational cost can be reduced by providing a better initial guess.

Question: How to obtain the source distribution before the Monte Carlo simulation is actually run?

⁵In Serpent 2 this is switched on by “set his 1”.

Eigenvalue solution: Obtaining the source distribution

The response matrix method can be used to provide a spatial source distribution with coupling coefficients obtained from a short Monte Carlo particle transport simulation (single source cycle).

Problems:

- 1) The directional distribution of sampled source neutrons is completely lost
- 2) The energy distribution of sampled source neutrons is completely lost
- 3) The accuracy of the spatial distribution of sampled source neutrons is limited by the mesh resolution
- 4) The coupling coefficients used in the response matrix solution are obtained from an unconverged Monte Carlo simulation

The first two issues are not major limiting factors (isotropic ^{235}U fission source is a good approximation).

Eigenvalue solution: Obtaining the source distribution

Resolution of the spatial distribution can be improved by refining the mesh, but the price is paid in increased computational cost.

Solution: Calculate intra-cell form factors that can be used to reconstruct the high-resolution source distribution without added computational cost.

The last problem is addressed by iterating between Monte Carlo (MC) and response matrix (RMX) solutions:

- ▶ Start by running a MC simulation using a uniform source distribution to obtain coupling coefficients for the RMX solver
- ▶ Obtain a converged source distribution from the RMX solver
- ▶ Run another MC simulation using the previous source distribution and obtain another set of coupling coefficients for the RMX solver
- ▶ Repeat iterations N times ($N \sim 3-5$)

After the iterations have been completed, the Monte Carlo criticality source simulation is started from an initial guess that approximates the converged source distribution.

Eigenvalue solution: Test calculations

The implemented methodology is demonstrated in the following by single-assembly and full-core PWR calculations. The test cases were adopted from the MIT BEAVRS benchmark:⁶

- ▶ Single-assembly model with control rods 1/4 inserted
- ▶ Full-core model with sub-critical, critical and super-critical variants
- ▶ Fission source entropy monitored separately in axial (z) and radial (x,y) dimensions
- ▶ Comparison to calculations with uniform initial source guess

⁶N. Horelik, B. Herman, M. Ellis, S. Kumar, J. Liang, B. Forget and K. Smith. *"Benchmark for Evaluation and Validation of Reactor Simulations (rev. 2.0.1)."* MIT Computational Reactor Physics Group, 2017.

Eigenvalue solution: Single-assembly case

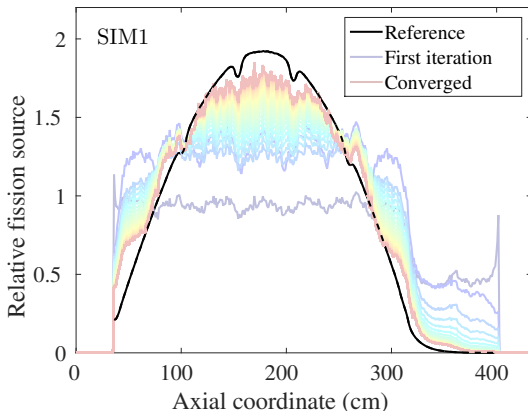


Figure 3 : Axial fission source distributions in the single-assembly test case. The colored curves show the solutions produced by the outer iterations of the response matrix solver, and the black curve the converged distribution obtained from a Monte Carlo simulation. Control rods are inserted 1/4 of the active fuel height, and the small dents in the shape result from reduced moderation near fuel spacers.

Eigenvalue solution: Single-assembly case

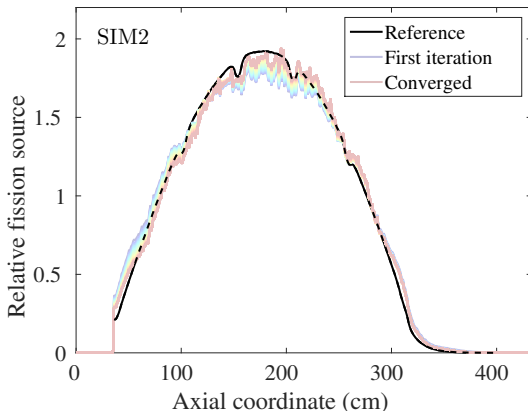


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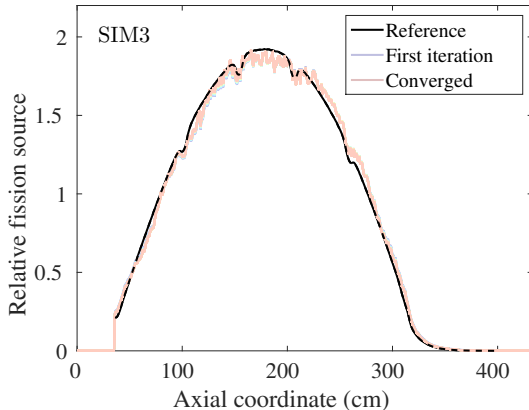


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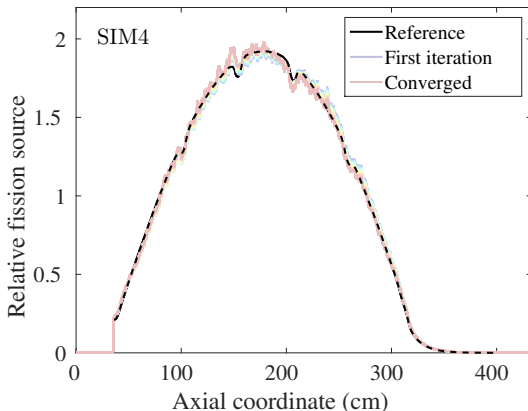


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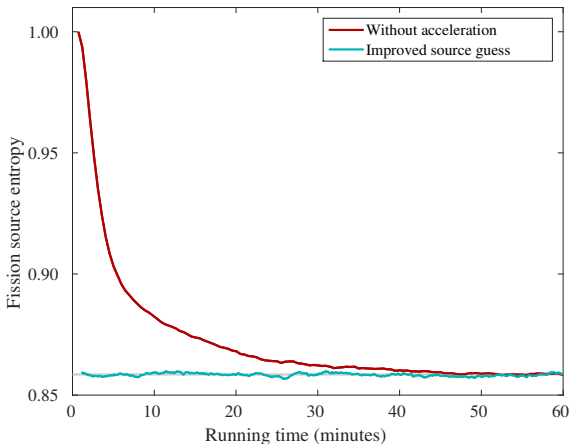


Figure 4 : Axial fission source entropy in the single-assembly test case with and without the improved source guess. The running time takes into account the time required for running the response matrix solver.

Eigenvalue solution: Full-core case

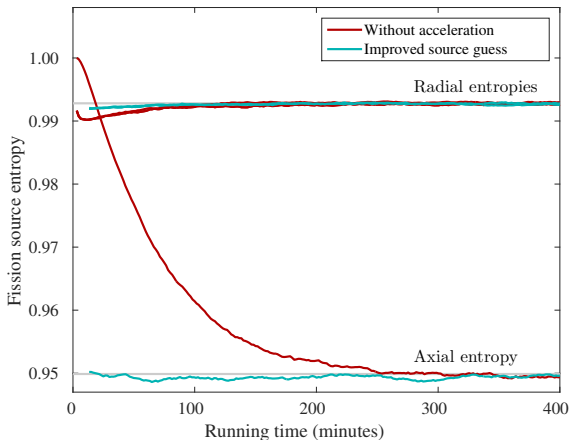


Figure 5 : Fission source entropies in the full-core test case with and without the improved source guess. The running time takes into account the time required for running the response matrix solver. Critical core configuration.

Eigenvalue solution: Full-core case

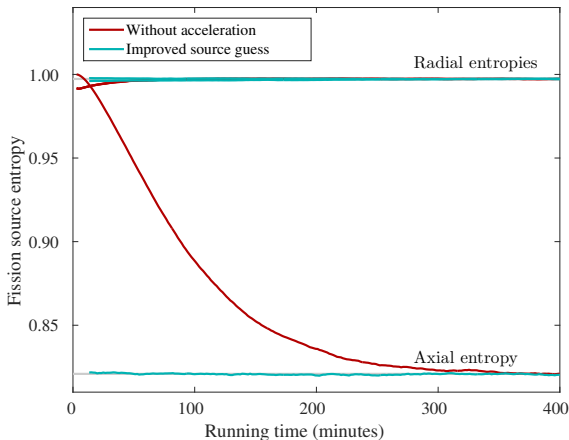


Figure 6 : Fission source entropies in the full-core test case with and without the improved source guess. The running time takes into account the time required for running the response matrix solver. Sub-critical core configuration.

Eigenvalue solution: Full-core case

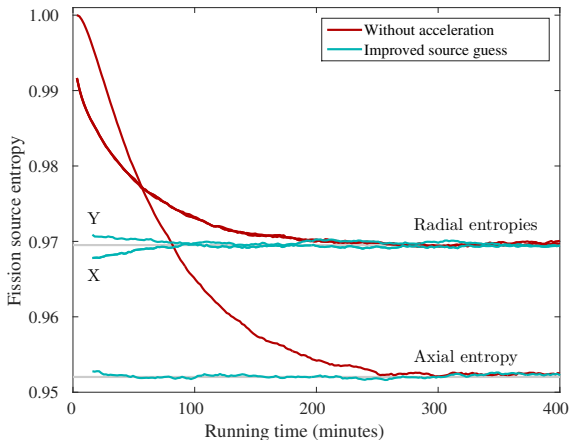


Figure 7 : Fission source entropies in the full-core test case with and without the improved source guess. The running time takes into account the time required for running the response matrix solver. Super-critical core configuration.

Eigenvalue solution

The response matrix solver is easy to apply and requires only a handful of parameters from the user:

- ▶ Mesh definition
- ▶ Convergence criteria for the response matrix solver
- ▶ Number of iterations between MC and RMX solutions

However:

- ▶ Getting sufficient statistics for the coupling coefficients requires large population size (1M and 10M were used in the test cases)
- ▶ Selection of mesh parameters affects the quality of solution (the best results were obtained by method of trial and error)
- ▶ The solution is subject to stochastic uncertainty, and the source distribution may be off by pure chance (see the radial entropies in the super-critical case)

Future work

Topics for future work on the built-in response matrix solver:

- ▶ Improve the implementation of multi-group adjoint solution
- ▶ Multiple responses and global variance reduction
- ▶ Implement support for hexagonal mesh
- ▶ Extend the source sampling routine to cylindrical and hexagonal mesh
- ▶ Figure out a convergence criterion for the outer iterations in eigenvalue mode
- ▶ Implement an iterative variance reduction scheme based on an adaptive mesh
- ▶ Testing, testing, testing...

Other ideas:

- ▶ Application in time-dependent simulations?
- ▶ Calculation of adjoint-weighted parameters?
- ▶ Etc...

Thank you for your attention!

Questions? - Jaakko.Leppanen@vtt.fi