Multi-physics capabilities in Serpent 2

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Structure of this talk

1. Multi-physics with Monte Carlo neutronics
2. Multi-physics approach in Serpent 2
3. Some recent advances in multi-physics capabilities of Serpent 2
4. Examples.
5. Summary and future work.

Multi-physics with Monte Carlo neutronics

Background

- Monte Carlo neutron tracking is based on simulating the random-walk of individual neutrons.
- The physical laws are taken in account by basing the probability sampling distributions on cross sections:
  1. Macroscopic cross sections represent the interaction probability per traveled unit length. Used for:
     - Sampling the distance to the next collision site (exponential distribution)
     - Sampling the target nuclide in a collision
     - Scoring macroscopic reaction rate tallies (e.g. power)
  2. Microscopic cross sections represent the interaction probability between a neutron and a single target nuclide.
     - Sampling the reaction mode in a collision (after the target nuclide has been sampled)
     - Scoring microscopic reaction rate tallies (e.g. transmutation xs for burnup calculation)

Monte Carlo neutronics - Multiphysics

- In operating nuclear reactors, materials have complex temperature and density distributions.

- This creates some challenges for MC neutron tracking:
  1. Cross sections are material temperature and density dependent.
     - Temperature treatment of cross sections is non-trivial.
     - Density treatment of cross sections is straightforward.
  2. The path length sampling between interactions is based on the assumption that the material Σ_{tot} is constant over the sampled path:

     $$l = -log(\xi)/\Sigma_{tot},$$

     where ξ is a random number from the unit interval.
     - Can be taken in account by subdividing materials to even smaller zones (leads to some difficulties).
     - A better way to handle the problem is to use rejection sampling, where instead of material total cross section, a majorant cross section ($\Sigma_{maj} \geq \Sigma_{tot}$) is used to sample the path lengths and some of the sampled path lengths are rejected.

Multi-physics approach in Serpent 2

Multi physics capabilities

- The multi-physics capabilities of Serpent 2 rely heavily on three factors:
  1. The rejection sampling of neutron path lengths.
  2. The capability to handle the temperature dependence of microscopic cross sections on-the-fly by the Target Motion Sampling (TMS) temperature treatment[1,2,3].
  3. The capability to model continuously-varying density distributions[4]
- Combining these methods allows the <u>efficient</u> modeling of materials with arbitrarily refined temperature and density distributions.

[1] T. Viitanen and J. Leppänen. "Explicit treatment of thermal motion in continuous-energy Monte Carlo tracking routines." Nucl. Sci. Eng., 171: pp. 165 – 173 (2012).

[2] T. Viitanen and J. Leppänen,"Target motion sampling temperature treatment technique with elevated basis cross section temperatures." Nucl. Sci. Eng., 177 (2014) 77-89

[3] T. Viitanen and J. Leppänen, "Temperature majorant cross sections in Monte Carlo neutron tracking. Nucl. Sci. Eng." (Accepted for publication)

[4] J. Leppänen. "Modeling of Nonuniform Density Distributions in the Serpent 2 Monte Carlo Code". In: Nucl. Sci. Eng. 174 (2013), pp. 318–325.

The multi-physics coupling scheme

- The multi-physics coupling scheme in Serpent 2 operates on two levels[5]:
  1. Internal light-weight solvers for thermal hydraulics and fuel behavior.
  2. External coupling via a universal multi-physics interface.
- The main function of the multi-physics interface is to separate the state point information from the Monte Carlo geometry model:
  - For the tracking routine this means that the temperature and density distributions can be handled efficiently using the rejection sampling methodology and TMS.
  - For the user this means that the solution from the external coupling can be passed into Serpent without any modifications in the main input.

[5] J. Leppänen, T. Viitanen, and V. Valtavirta. "Multi-Physics Coupling Scheme in the Serpent 2 Monte Carlo Code". In: Trans. Am. Nucl. Soc. 107 (2012), pp. 1165–1168.

Internal solvers

- Internal multi-physics coupling is based on two light-weight solvers, integrated to Serpent 2 at source code level:

  COSY – A 3D system/component scale TH solver based on a porous-medium three-field flow model (not coupled to Serpent yet)

  FINIX – A thermo-mechanical fuel behavior module for the modeling of temperature feedback inside fuel pins in steady-state and transient conditions[6,7]

- The internal solvers are intended to provide good solutions to the coupled problem with a low computational cost.

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[6] T. Ikonen et al. "FINIX – Fuel Behavior Model and Interface for Multiphysics Applications." In proc. TopFuel 2013. Charlotte, NC, Sept. 15-19, 2013.

[7] T. Ikonen et al. "Module for thermomechanical modeling of LWR fuel in multiphysics simulations." Annals of Nuclear Energy (Accepted for publication).

External multi-physics interface

- Genuinely high fidelity solutions to coupled problems can be obtained by coupling state-of-the-art solvers to Serpent 2 via the universal multi-physics interface.
- Based on sequential exchange of input and output files. Not intended to be limited to any particular solver or code.
- Various formats[8,9,10]:
  1. Weighted average of point-wise values.
  2. Piece-wise constant distribution on a regular mesh
  3. User specified functional dependence
  4. Special interface for fuel performance codes
  5. Unstructured mesh based interface for CFD code coupling
- Current development focuses on the two latter formats.

[8] J. Leppänen. "Modeling of Nonuniform Density Distributions in the Serpent 2 Monte Carlo Code". In: Nucl. Sci. Eng. 174 (2013), pp. 318–325.

[9] V. Valtavirta et al. "The Universal Fuel Performance Code Interface in Serpent 2". In: TopFuel 2013. Charlotte, NC, Sept. 15-19, 2013.

[10] J. Leppänen et al. "Unstructured Mesh Based Multi-physics Interface for CFD Code Coupling in the Serpent 2 Monte Carlo Code". In: PHYSOR 2014. Kyoto, Japan, Sept. 28 - Oct. 3, 2014.

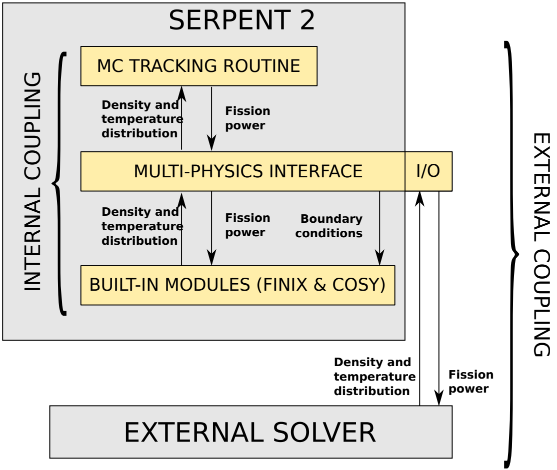


Figure: Multi-physics coupling scheme in Serpent 2

Complex geometries with unstructured mesh based multi-physics interfaces

Unstructured mesh based interface format

- Unstructured mesh based interface type for CFD code coupling:
  - Currently based on OpenFOAM mesh format
  - Support for tetra-, hexa- and polyhedral meshes
  - Adaptive search grid to speed up cell search routine
- Preliminary results presented at PHYSOR 2014[11] (in collaboration with Politecnico di Milano)

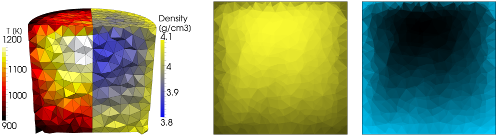


Figure: MSR model used for testing the unstructured mesh based interface. **Left:** Temperature and density distributions calculated by OpenFOAM. **Center:** Temperature distribution from Serpent 2 geometry **Right:** Density distribution from Serpent 2 geometry plot.

[11] J. Leppänen et al. "Unstructured Mesh Based Multi-physics interface for CFD Code Coupling in the Serpent 2 Monte Carlo Code." In proc. PHYSOR 2014. Kyoto, Japan, Sept. 28 - Oct. 3, 2014

Unstructured mesh based interface type

- The mesh is constructed of:
  1. List of points that are used to map the underlying geometry
  2. List of 2D faces formed by combining three or more adjacent points
  3. List of 3D cells formed by combining four or more faces
- This interface type is considered the best way to pass TH information from CFD codes into Serpent tracking routine because:
  1. The mesh can be arbitrarily refined
  2. Temperature and density distributions are passed into Serpent without loss of information
  3. The same structure can be used for passing power distributions back to the CFD code

Unstructured mesh based interface type

Unstructured mesh based interface (type 7)

```
7 <mat> 1
<output_file>
<rho0> <T0>
<msh_split> <msh_dim> <s0> <sz1> ...  <sz_dim>
<points_file>
<faces_file>
<owner_file>
<neighbour_file>
<density_file> <dm>
<temperature_file> <tm>
<mapping_file>
```

See the complete input/output description at the discussion forum:
http://ttuki.vtt.fi/serpent/viewtopic.php?f=24&t=1765

Example:
OpenFOAM interface

Irregular geometry types

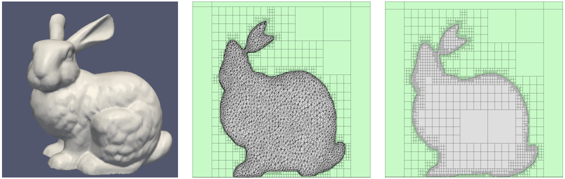


Figure: Left: Original 3D CAD model of the Stanford Critical Bunny, Center: Geometry plot of OpenFOAM mesh-based model, Right: Geometry plot of STL model

- Serpent 2.1.19 introduced two options for modeling complex irregular geometry types
  1. OpenFOAM mesh-based geometry – by-product of the OpenFOAM mesh-based multi-physics interface, paper presented at PHYSOR 2014[12] (in collaboration with Politecnico di Milano)
  2. Stereolitography (STL) format solid models – support for CAD-based geometries.
- Efficient neutron tracking in highly refined cell based geometries is possible because of the Woodcock delta-tracking method in Serpent.

[12] 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

Irregular geometry types - Adaptive search mesh

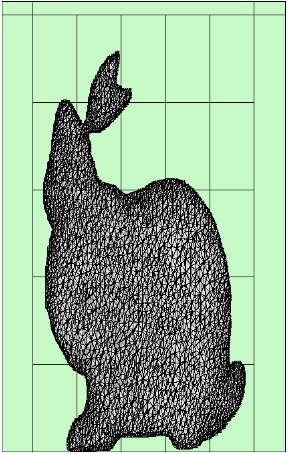


Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5

Irregular geometry types - Adaptive search mesh

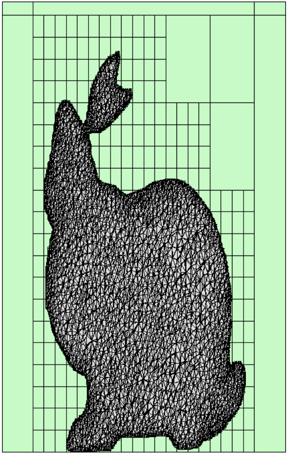


Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4

Irregular geometry types - Adaptive search mesh

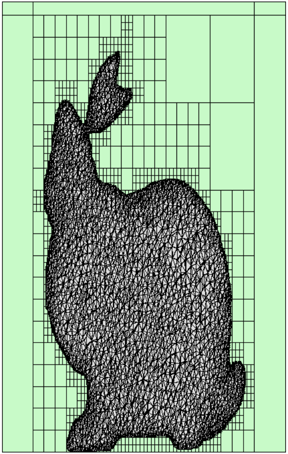


Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4, 3x3x3

Irregular geometry types - Adaptive search mesh

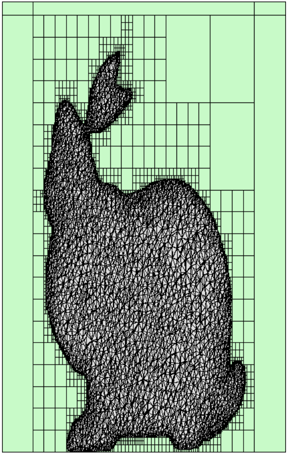


Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4, 3x3x3, 2x2x2

Example:
Mesh based geometry

Standardized coupled calculation sequence

- Multi-physics calculations require sequential and iterative solving of power distribution and coupled fields.
- Running multiple separate Monte Carlo calculations will waste some time on initialization, XS loading, fission source convergence etc.
- Solution:
  - Update state-point information without restarting the whole calculation.
  - Tallies cleared after each iteration to yield separate neutronics solutions.
  - Fission source carried over to next iteration.
- Program flow control is easy with internal coupling.
- In case of external coupling a wrapper code (user implemented) with two-way signaling is used. (POSIX-signals or file based signals)
  - SIGUSR1 = Solution updated, iterate current time point.
  - SIGUSR2 = Move to next time point.
  - SIGTERM = Calculation completed.

Standardized coupled calculation sequence

Solution relaxation

- Relaxation can be applied to flux/power solution for a stable solution scheme[13,14].
- Convergence check can be done in Serpent or in wrapper program.

[13] J. Dufek and W. Gudowski, "Stochastic Approximation for Monte Carlo Calculation of Steady-State Conditions in Thermal Reactors", *Nucl. Sci. Eng.*, **152**, 274-283 (2006)

[14] J. Dufek and J. E. Hoogenboom, "Description of a stable scheme for steady-state coupled Monte Carlo-thermal-hydraulic calculations", *Ann. Nucl. Energy*, **68**, 1-3, (2014)

Standardized coupled calculation sequence
Universality

- Standardized coupled calculation sequence for Serpent 2 agnostic of external solver.
- Same iteration scheme used regardless of
  - Coupling type: internal / external.
  - Solver type: TH / CFD / Fuel behavior.
  - Calculation type: Steady state, transient, depletion.

Coupled calculation sequence

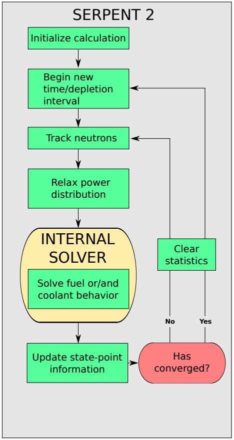


Figure: Schematic illustration of coupled calculation sequence with internal coupling.

Coupled calculation sequence

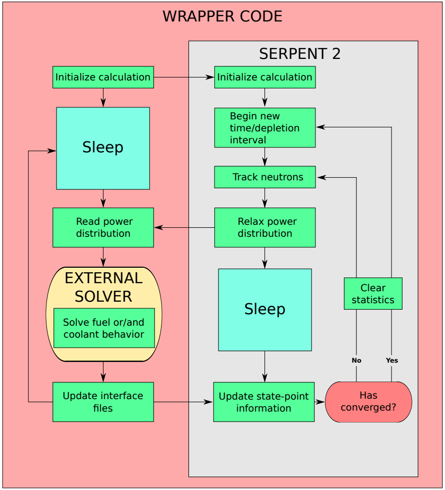


Figure: Schematic illustration of coupled calculation sequence with external coupling. POSIX signalling is used between wrapper code and Serpent 2.

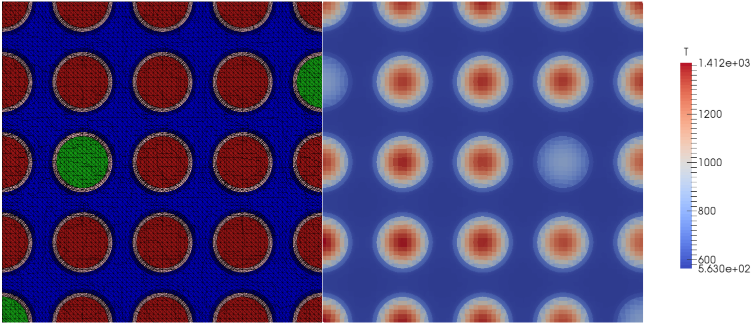
Example:
Coupled calculation with OpenFOAM interface

Realized couplings

	Internal coupling	External coupling
Fuel behaviour	FINIX	ENIGMA
Thermal hydraulics		SUBCHANFLOW
CFD	OpenFOAM*	OpenFOAM PORFLO ANSYS CFX
Solid mechanics	OpenFOAM*	PRESTO

Serpent - OpenFOAM test assembly

- Ongoing Master's thesis work by Riku Tuominen at VTT.
- Building up in-house expertise for coupled calculations with OpenFOAM.
- A simple test case for development of the OpenFOAM interface.



Example:
Dynamic simulation with fuel temperature feedback

“Blind” transient analysis:

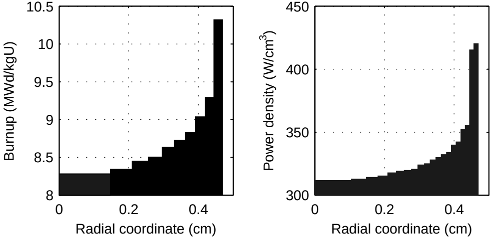


Figure: Radial burnup distribution (left panel) for the fuel pellet in the Serpent-FINIX calculation and the resulting radial power density distribution (right panel) at the onset of the transient.

- TMI-1 pin-cell with realistic nuclide distribution at 8.84 MWd/kgU.
- System held critical at HFP (233 W/cm) by soluble absorber.
- To onset the transient, coolant boron concentration reduced from 970 ppm to 860 ppm
  - Instantaneous reactivity insertion of 1865 pcm.
- Free evolution of neutronics and fuel behavior for 56 ms.

Dynamic simulation with fuel temperature feedback

First results presented in PHYSOR 2014[15]

- Time dependent simulation mode[16] in Serpent 2 used to model prompt-super critical conditions.
- Two way coupling of fission power and fuel behavior.
- Time dependent fission power tallied by Serpent.
- Time dependent fuel behavior solved by internal fuel behavior module FINIX.

[15] V. Valtavirta et al. "Simulating Fast Transients with Fuel Behavior Feedback with the Serpent 2 Monte Carlo Code". In: PHYSOR 2014. Kyoto, Japan, Sept. 28 - Oct. 3, 2014.

[16] J. Leppänen. "Development of a Dynamic Simulation Mode in the Serpent 2 Monte Carlo Code". In: M&C 2013. Sun Valley, ID, May 5-9, 2013.

Dynamic simulation with fuel temperature feedback

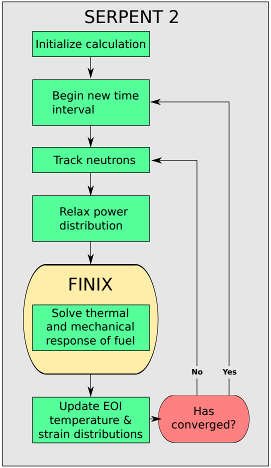


Figure: Schematic illustration of the sequential and iterative solution procedure for time-dependent coupled modeling with the Serpent-FINIX code system

Dynamic simulation with fuel temperature feedback

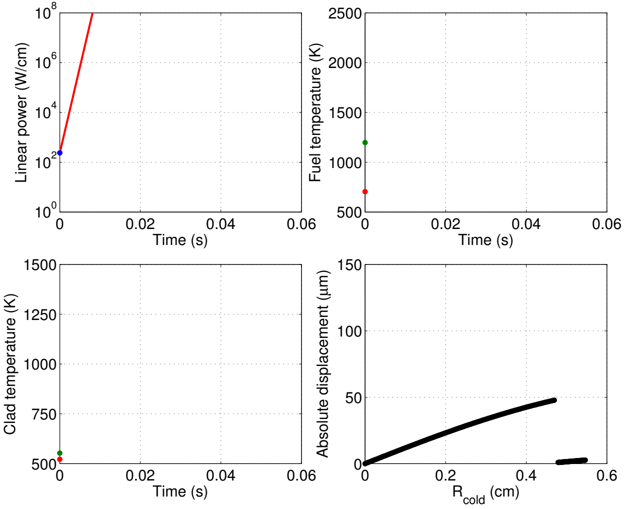


Figure: Conditions at the onset of the transient (exponential growth of power indicated by red line). Red dots correspond to outer surface, green dots to inner.

Movie time

Dynamic simulation with fuel temperature feedback

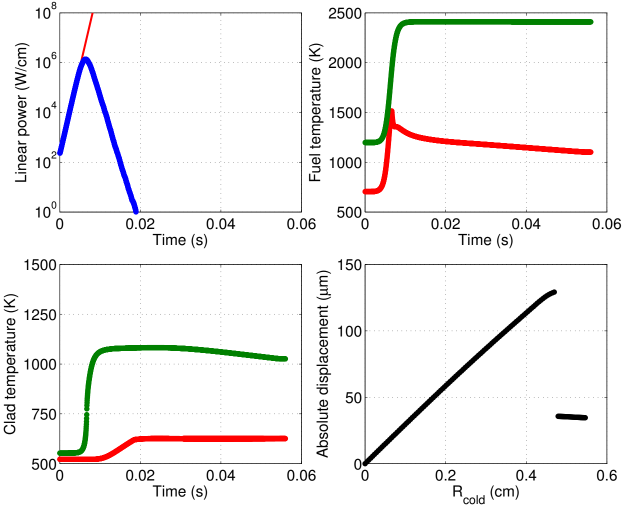


Figure: Development of the conditions during the transient (exponential growth of power indicated by red line). Red dots correspond to outer surface, green dots to inner.

Summary and future work

Summary 1/2

- The multi-physics coupling scheme in Serpent 2 is based on two internal solvers

  COSY – A 3D system/component scale TH solver based on a porous-medium three-field flow model (not coupled to Serpent yet)

  FINIX – A thermo-mechanical fuel behavior module for the modeling of temperature feedback inside fuel pins in steady-state and transient conditions

  and a universal multi-physics interface for external coupling.

- Internal solvers are lightweight, intended for fast "sufficiently accurate" solutions.

- Truly high-fidelity CFD / TH or fuel performance solutions can be coupled to Serpent 2 using the multi-physics interface with various input-formats.

Summary 2/2

- The main advantage of the multi-physics interface in Serpent 2 is the separation of the state-point information from the geometry model
  - The tracking routine can handle the temperature and density distributions efficiently using TMS and rejection sampling.
  - The user can include realistic temperature and density fields in their calculation without modifications to the main input.
- The multi-physics coupling scheme is still under development and suffers from several limitations:
  - The TMS method cannot adjust temperatures of ures probability tables or S(α, β) scattering laws (cannot model temperature distributions in water).
  - The internal COSY solver for thermal hydraulics has not yet been coupled to Serpent.
  - The internal FINIX solver for fuel behavior is coupled, but not yet included in the distributed version.
  - The dynamic simulation mode is limited to fast transients due to the lack of a model for delayed neutron emission.
  - Gamma heating is not yet included in the transport simulation.
  - The unstructured mesh based interface is limited to OpenFOAM file format.

Future work

- What's next:
  - Extend TMS to ures probability table sampling.
  - Implement a method to adjust temperatures of thermal scattering libraries.
  - Model for delayed neutron emission in time dependent simulations.
  - Internal coupling of COSY thermal hydraulics solver.
  - Distribute the FINIX fuel behavior solver (prob. under a separate license).
  - Allow deformation of mesh during coupled calculation.
- Testing the multiphysics coupling with various external codes, in steady state, depletion and time-dependent calculations.
- Future work will also focus on optimizing the coupled calculation sequence, i.e. iterations, solution relaxation, stability, parallelization of the coupled calculation sequence, performance, etc.

Thank you for your attention!

Questions and comments are well appreciated.

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