Status and development of 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. Recent work.
4. Current capabilities, limitations and future work.

Multi-physics with Monte Carlo neutronics

Monte Carlo neutronics

- 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.
  - Path lengths and interactions in the random walk are sampled based on the physical cross sections.

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 efficient modeling of materials with arbitrarily refined temperature and density distributions.

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[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 at two levels[5]:
  1. Internal light-weight solvers for thermal hydraulics (COSY) and fuel behavior (FINIX[6,7]).
  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.

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[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.

[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 (submitted).

Multi-physics interface formats

- 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.

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[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.

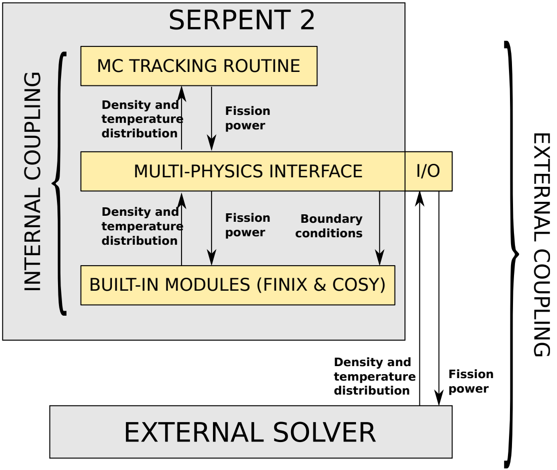

Figure: Multi-physics coupling scheme in Serpent 2

Recent work

New multi-physics 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 submitted to PHYSOR 2014[11] (in collaboration with PoliMi)

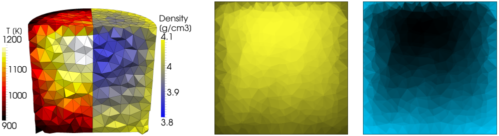

Figure: MSR model used for testing the unstructured mesh based interface. **Left:** Temperature and density distributions calculated by OpenFOAM. **Center:** Temperature distribution from Serpent 2 geometry **Right:** Density distribution from Serpent 2 geometry plot.

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[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
- Current implementation is limited to OpenFOAM format but CGNS based implementation is under development.

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

Irregular geometry types

- 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 submitted to PHYSOR 2014[12] (in collaboration with PoliMi)
  2. Stereolitography (STL) format solid models – support for CAD-based geometries.

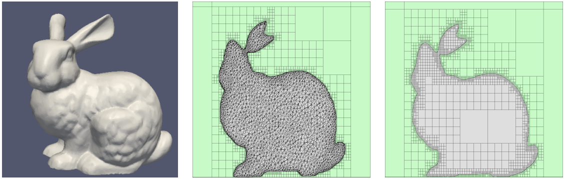

Figure: Left: Original 3D CAD model of the Stanford Critical Bunny, Center: Geometry plot of OpenFOAM mesh-based model, Right: Geometry plot of STL model

[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

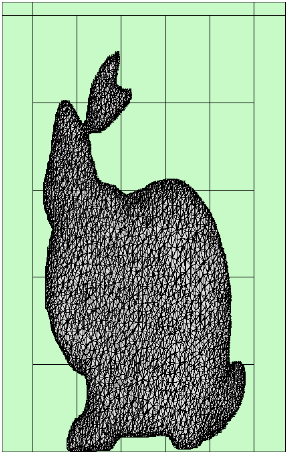

Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5

Irregular geometry types - Adaptive search mesh

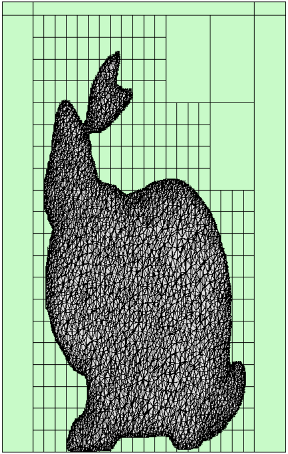

Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4

Irregular geometry types - Adaptive search mesh

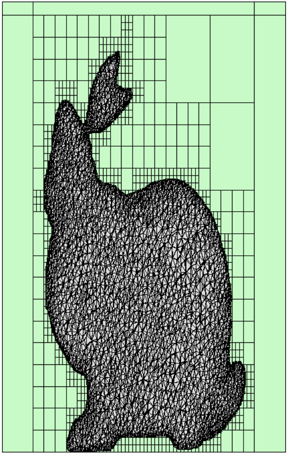

Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4, 3x3x3

Irregular geometry types - Adaptive search mesh

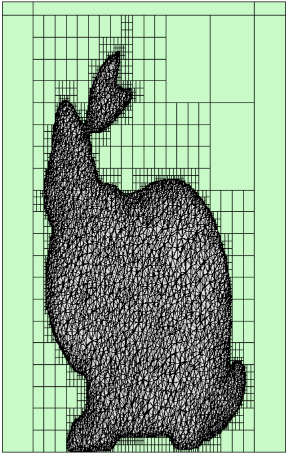

Figure: Adaptive search mesh on an irregular geometry. Mesh dimensions on different levels: 5x5x5, 4x4x4, 3x3x3, 2x2x2

Neutron recoil energy response function

Response function -10

```
det 1 dm cool ...  dr -10 void
```

- For calculating kinetic energy deposition straight to coolant / structural materials.
- Tallies the energy difference between incoming and outgoing neutron in scattering reactions.

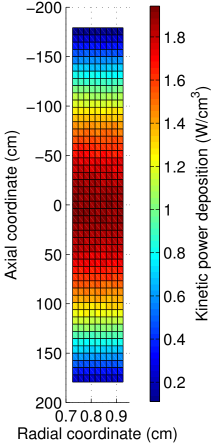

Figure: Kinetic power density deposited in coolant in an axially finite pin-cell calculation.

Dynamic simulation with fuel temperature feedback

First results presented in PHYSOR 2014[13]

- Time dependent simulation mode[14] 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.

[13] 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.

[14] 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

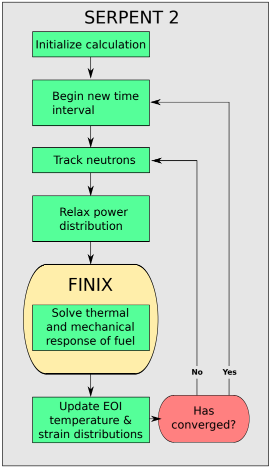

Figure: Schematic illustration of the sequential and iterative solution procedure for time-dependent coupled modeling with the Serpent-FINIX code system

Dynamic simulation with fuel temperature feedback

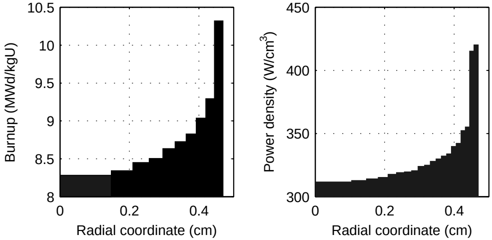

Figure: Radial burnup distribution (left panel) for the fuel pellet in the Serpent-FINIX calculation and the resulting radial power density distribution (right panel) at the onset of the transient.

- 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

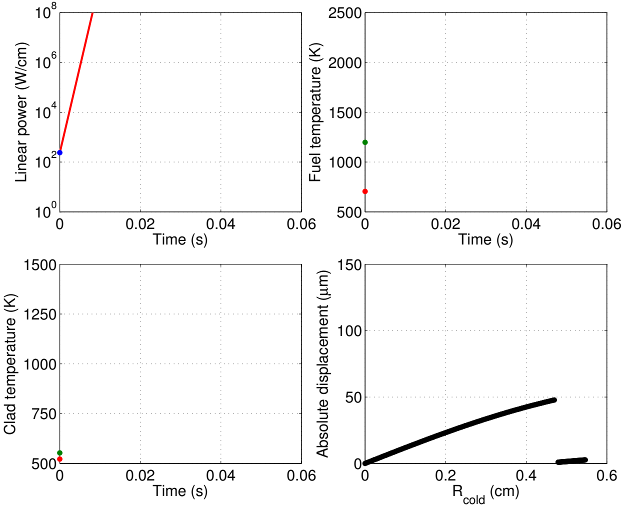

Figure: Conditions at the onset of the transient (exponential growth of power indicated by red line). Red dots correspond to outer surface, green dots to inner.

Movie time

Dynamic simulation with fuel temperature feedback

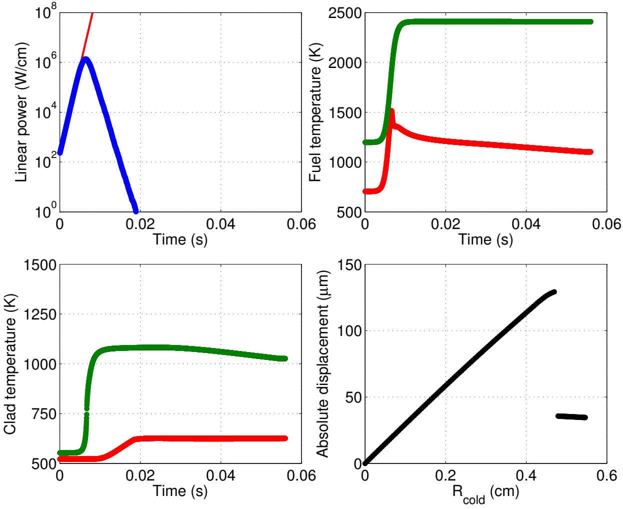

Figure: Development of the conditions during the transient (exponential growth of power indicated by red line). Red dots correspond to outer surface, green dots to inner.

Dynamic simulation with fuel temperature feedback - comments

- Development version of code based on 2.1.15 was used.
- Simulated population of 200 000 neutrons
- Calculation time 12 wall-clock-days with 12 Intel Xeon X5690 cores.
  - Mean generation time at onset 11.6 μs vs neutron tracking time 26 000 μs
- Main results are the proof-of-concept.
  - The size and shape of a power peak can be calculated from the initial conditions using coupled continuous energy 3D Monte Carlo neutronics.
  - Fuel performance safety parameters can be assessed at the same time.

Dynamic simulation with fuel temperature feedback - limitations

- Coolant properties are not updated during the simulation.
  - Gamma heating cannot be calculated yet.
  - Direct energy deposition to coolant by scattering could not be included (code version base was 2.1.15)
- TMS temperature treatment currently cannot handle S(α, β) scattering in water.
  - Applicability limited to transients without strong moderator temperature feedback.
- Delayed neutrons are not handled by the dynamic mode at the moment, which limits the applicability to fast transients.

Current status and future work

Current status - features

- Arbitrarily refined temperature and density distributions can be taken in account in neutron tracking in an efficient manner.
- Several interface formats for coupling of different types of codes.
- Complex irregular geometries can be modeled (OpenFOAM mesh / STL).
- Dynamic simulation mode for simulation of fast transients.
- Direct energy deposition to coolant/structural materials can be tallied.
- Users have successfully coupled several codes to Serpent 2.

Current status - 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 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 (probably not TMS based, but a method developed by Andrew Pavlou at Rensselaer Polytechnic Institute for MCNP)
  - Implement CGNS support for CFD interface.
  - Internal coupling of COSY thermal hydraulics solver.
  - Sorting out the distribution of FINIX fuel behavior solver.
- A large amount of the work so far has focused on the methods to pass data through the interface as well as taking it in account in the neutron tracking.
- Future work will focus more on the coupled calculation sequence, i.e. iterations, solution relaxation, stability, parallelization of the coupled calculation sequence, performance, etc.
- Currently no internally or externally coupled TH / CFD solver in-house at VTT. Makes testing harder. Upcoming Master's thesis student.

Standardized coupled calculation sequence (WIP)

- Multi-physics calculations with Monte Carlo neutronics require sequential and iterative solving of power distribution and system response.
  - Standardized coupled calculation sequence for Serpent 2 agnostic of external solver.
- Similar iteration scheme used regardless of
  - Coupling type: internal / external.
  - Solver type: TH / CFD / Fuel behavior.
  - Calculation type: Steady state, transient, depletion.
- Neutron tracking does not care about coupling type, solver type or calculation type.
- Coupled calculation sequence needed in any case for internal coupling.

Standardized coupled calculation sequence (WIP)

Solution relaxation

- Relaxation can be applied to flux/power solution for a stable solution scheme[15,16].
  - Handle flux relaxation internally in Serpent (already needed for internal solvers).
  - Possibility to use either constant or growing neutron population in iteration scheme.
- Convergence check can be done in Serpent or in wrapper program.

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[15] 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)

[16] 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 (WIP)

Program flow

- Running multiple separate Monte Carlo calculations will waste some time on initialization, XS loading, inactive cycles etc.
  - Update state-point information without restarting the whole calculation.
  - Tallies cleared after each iteration to simulate separate neutronics solutions.
  - Initial 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 POSIX-signaling is used. Initial tests without iteration in[17].
  - SIGUSR1 = Solution updated, iterate current time point.
  - SIGUSR2 = Move to next time point.

[17] V. Valtavirta *et al.*, "The Universal Fuel Performance Code Interface in Serpent 2", *In proc. 2013 Fuel Performance Meeting TopFuel*, Charlotte, USA, (2013)

Coupled calculation sequence

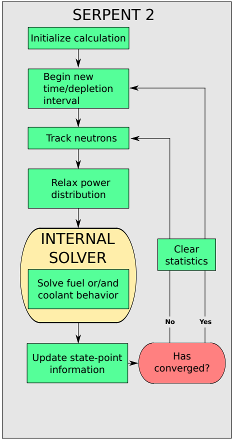

Figure: Schematic illustration of coupled calculation sequence with internal coupling.

Coupled calculation sequence

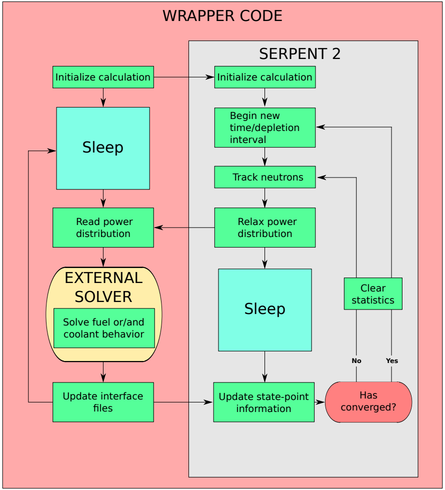

Figure: Schematic illustration of coupled calculation sequence with external coupling. POSIX signalling is used between wrapper code and Serpent 2.

Thank you for your attention!

Questions and comments are well appreciated.

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TECHNOLOGY FOR BUSINESS