Serpent 2 beta-testing and hot topics for future development

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Jaakko Leppänen, VTT

Outline

- Current status of Serpent 2:
  - Comparison to Serpent 1 – what has been implemented, what is still missing
  - Entirely new features and capabilities
- Near-future work:
  - Multi-physics
  - Other topics
- Collaboration and student exchange
- Demo

Serpent 2 beta testing started in January 2012, and the test group consist of 54 users
Public distribution is scheduled for 2013-2014

Current status of Serpent 2

- The development of Serpent 2 started in October 2010
- Two goals were set for re-writing the source code:

  1. To remove the memory limitations and extend burnup calculation capability all the way to full-core problems involving hundreds of thousands of depletion zones
  2. To remove memory limitations related to parallelization using MPI

- The work continues, but for the main part these goals can now be considered achieved:

  1. Optimization modes for small and large burnup calculation problems[1]
  2. Parallelization based on combination of OpenMP and MPI

[1)] J. Leppänen and A. Isotalo. *"Burnup Calculation Methodology in the Serpent 2 Monte Carlo Code."* In Proc. PHYSOR-2012. Knoxville, TN, 15-20 April, 2012.

Current status of Serpent 2

- Serpent 2 has the capability to perform most of the tasks of Serpent 1:
  - Neutron physics and Doppler-broadening pre-processor are fully implemented
  - All Serpent 1 geometries should work with Serpent 2
  - Burnup calculation routine should produce the same result (to within statistics)
  - Group constant generation produces most of the same parameters as Serpent 1
  - Detector capabilities are more or less the same
- However:
  - The calculation routines have not been as thoroughly validated, and there will still be major changes in future updates
  - The calculation routines in Serpent 2 are less optimized, so it is expected that the simulation runs ~20% or so longer (in debug mode there is at least a factor of 2 difference in calculation time)

Current status of Serpent 2

- What is still missing in Serpent 2:
  - Some group constants (ADF's, pin-power distributions)
  - Xe-135 iteration
  - Alpha-eigenvalue mode
  - Soluble absorbers
  - Some experimental features (k-eff iterations using leakage corrections)
  - Externally-coupled burnup calculation mode
  - Some cut-offs are not used or are based on different criteria
- Some of these features will not be implemented in Serpent 2 (because they were bad ideas in the first place)

There is no separate manual for Serpent 2, new features are documented at the discussion forum (for password, contact: Jaakko.Leppanen@vtt.fi)

Current status of Serpent 2

- New features intended to make life easier for the user:
  - Union operator for cell definitions
  - Material mixtures
  - Extended mesh plotter capabilities (coupling to detector responses, etc.)
  - New random number generator that allows reproducibility in (OpenMP) parallel mode
  - Improved universe symmetry options
  - Improved division to depletion zones
  - MC volume calculation routine produces input lines for geometry model
  - New options for burnup inventory (important nuclides, pre-defined isotope lists, option to reproduce different output without re-running the simulation)
  - Pre-defined material compositions
- These are features that should have been implemented in Serpent 1 (but were not, because of the complexity of the source code)

Current status of Serpent 2

- Entirely new capabilities:
  - Advanced time-integration methods for burnup calculation (presentation by A. Isotalo)
  - Photon transport simulation
  - On-the-fly temperature treatment (“Doppler-broadening”) routine, with capability to model continuously-varying temperature distributions (presentation by T. Viitanen)
  - Internal temperature feedback module (presentation by V. Valtavirta)
  - Capability to model continuously-varying density distributions
  - Multi-physics interface
- Some of the new capabilities are not visible to the user (transit from analog to implicit Monte Carlo)
- Some of the new capabilities are not documented, because they still require a lot of work (photon transport)

NUMPS (Numerical Multi-Physics) Project

- A Major research grant was received from the Academy of Finland for the multi-physics coupling of Monte Carlo neutronics and CFD
- Four-year project started in September 2012, that more than doubles our funding for Serpent-related work
- 110 to 130 person-months of extra work, divided between neutronics (Maria Pusa, Tuomas Viitanen, Ville Valtavirta) and thermal hydraulics (Ville Hovi, Joona Kurki)
- Neutronics part covers on-going work with Serpent + new topics related to sensitivity and uncertainty analysis
- Thermal hydraulics part covers work on CFD code PORFLO (in-house code at VTT), or the development of a new code from scratch (to be decided)

This work will be the #1 hot topic in Serpent development for the next four years

Near-future work on multi-physics

- Monte Carlo:
  - Time-dependent neutron transport simulation
  - Gamma heating from coupled neutron / photon simulation
- On-the-fly temperature routine:
  - Extending the methodology to unresolved resonance region and bound scattering
  - Compatibility with reaction rate estimators, optimization
- Temperature feedback module:
  - Effect of thermal expansion
  - Axial heat conduction and other geometries (fuel plates / spheres)
  - Extending the methodology to burnup calculation
  - Dynamic heat conduction

Near-future work on multi-physics

- Multi-physics interface:
  - Temperature distributions and / or boundary conditions for the internal temperature feedback module
  - Coupling to fuel performance codes (revisiting previous work on Serpent / ENIGMA coupling)
  - Interface based on unstructured mesh for coupling with CFD codes (CGNS format?)
- **NOTE**: The multi-physics interface is not being developed only for our own purposes:
  - Testing and feedback from users is extremely valuable
  - Coupling should not be limited to any specific application, code or reactor type

If you are planning to couple Serpent to anything, please contact me first!

Other near-future topics

- Generation of new cross section libraries (gamma transport, heating / gas production reactions, new evaluations)
- Burnup calculation routines (with Aalto University and KTH):
  - Advanced time integration methods
  - Stability analysis for the burnup schemes
- Processing routines for fuel cycle analysis:
  - Fuel shuffling and reload, control rod movement, boron shim, etc.
  - Restart capability and branch calculations
  - On-line reprocessing for MSR (with Politecnico di Milano)
  - Equilibrium fuel cycle analysis (with UC Berkeley)

Other near-future topics

- Gamma transport:
  - Implementing missing photon interaction physics (emission of secondary photons)
  - Radioactivity source based on material compositions
  - Coupled neutron / photon transport simulation
  - Energy deposition from gamma heating
- Variance reduction:
  - Standard VR techniques for shielding calculations (photon and neutron transport)
  - Weight windows for the energy variable (better statistics for fast reactor group constant generation)
  - Implicit methods for delayed neutron emission
- Sensitivity and uncertainty analysis, convergence analysis, etc.

Collaboration – user contributions

- Like always, user feedback and contribution is extremely welcome!
- We are in particularly interested in work related (but not limited) to:
  - Multi-physics coupling
  - Validation of burnup calculation routines, especially compared to experimental data
  - Large burnup calculation problems (thousands of depletion zones)
  - Parallelization, especially in large clusters (hundreds of CPU's)
  - Validation of photon transport routines
  - All errors and unexpected behaviour
  - Ideas on how to make the code better and more user-friendly

  MCNP is still the best reference code for Serpent, due to the capability to use the same ACE format data libraries (differences are expected to be within statistics)

- Contacts via discussion forum (http://ttuki.vtt.fi/serpent/) or e-mail

Collaboration – student exchange at VTT

- We are looking into the possibility of hosting one or two students at VTT for Serpent-related work:
  - Graduate or undergraduate level
  - For a period of few months to half a year
  - Existing assignment, or we can come up with something new
- VTT will provide workspace, computer, etc. and help with practical arrangements
- The student and university are responsible of salaries and travel and living costs
- If the funding involves a student exchange program, the work can be carried out in collaboration with Aalto University (if this helps, VTT is not a university)

New features in Serpent 2 (demo)

- Cool and useful stuff:
  - Pre-defined material compositions (“-comp “ command line option)
  - Track plotter (“-tracks” command line option)
  - Universe symmetries
  - New mesh plotter capabilities
- Tools for running large burnup calculation problems:
  - Automated division into depletion zones
  - Automated volume calculation using MC
- Multi-physics interface