Geant4 in a new role - Reactor Physics

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Abstract. The accurate modeling of nuclear reactors is essential for design, regulation, safety analysis, operations and forensic analysis. There are two classes of approaches to modeling the neutronics of nuclear reactors. The first is deterministic, where the neutron transport equations are solved using a combination of approximations and numerical methods based on a space-time discretization. This approach currently dominates where computing speed and resource limitations apply. The second class of models is stochastic in nature. Here many statistically independent histories for each neutron event and all secondary events related to its interactions are tracked and various physical data are stored for later statistical analysis. This paper presents several results that establish the proof of principle in the stochastic Monte Carlo (MC) modelling of a nuclear reactor core using the Geant4 framework. The simulation is exercised in the context of a High Temperature Gas Cooled Reactor (HTGCR) with pebble fuel and helium coolant. MCNP and SERPENT are better known codes in this context, however Geant4 promises to be a significant additional coding framework. It has a modern C++ modular architecture, it is multi- threaded and trivially parallel on multiple nodes and the well documented source is readily available. Rather than being input file driven, the user modifies and extends the class structure. It has excellent engines for geometry, materials, physics, tracking, history recording, visualisation and the analysis is readily done with additional frameworks such as ROOT. In this paper we review the implementation of the following aspects in proof of principle form : the basic neutronics (thermalisation and containment), validation of the databases (elementary neutron induced reactions), scalability, thermal neutronics, geometrical discretisation for studying the spatial variation of physical parameters, time slicing and adaptation of Geant4 for correct intra-slice persistence, a scheme of integration with thermal hydraulics by workflow scheduling, the process of fission, burn, decay, and differential energy depositions for the various physics processes, criticality and core follow over multiple time steps. The benchmarking programme against MCNP and Serpent is also discussed.

1. Introduction

The accurate modeling of nuclear reactors is essential for design, regulation, safety analysis, operations and forensic analysis. In the most demanding case, the calculations must usually be sufficiently rapid that they are much faster than natural time for burn and decay processes while still being sufficiently accurate. There are two classes of approaches to modeling the neutronics of nuclear reactors. The first is deterministic, where the neutron transport equations are solved using a combination of approximations and numerical methods based on a space-time discretization [1]. Usually, compromises are made in the accuracy of the model in terms of the level of approximations used, the scale of the discretization and the level of geometric and material detail, in order to achieve a sufficiently fast speed of calculation. The error induced due to the compromises made is offset with often rather unsatisfactory

compensating modifications of the physical description or processes. The second class of models is stochastic in nature. Here many statistically independent histories for each neutron event and all secondary events related to its interactions are tracked and various physical data is stored for later statistical analysis [2–12]. The physics content manifests through the microscopic cross sections (probabilities) for each interaction. The thermal and material information is encoded into thermally averaged macroscopic cross sections, which are assembled together with the microscopic cross sections. The geometrical information is reconstructed using technical drawings of the system, essentially to the desired precision.

The full physics of the reactor are in this way encoded into probability distributions to be sampled on an event-by-event basis in the particle tracking and data extraction process, as various objects tracked are manifested in different regions of the reactor. The particle transport code, Geant4, developed for high-energy physics, has recently been extended to accommodate lower energy nuclear physics and energy scales down to the far sub-eV region. More recently it has been used in areas where several elements of the processes in a nuclear reactor are considered, for example, fission [13], thermal neutrons [14] and spallation [15–17].

The Monte Carlo space for neutronics in nuclear reactors currently has two main players MCNP [5, 6] and Serpent [7], among some others too. The former is very well benchmarked and widely used. It is a general neutron transport code, with far wider application than nuclear reactors. The latter is gaining popularity as a specialist nuclear reactor code. The interest in Geant4 arises as it is written in a modern object oriented language (C++) in contrast to MCNP. It also is a framework, in contrast to the previous mentioned codes, in that it is operated on the basis of user modified mandatory classes from templates, rather than preparation of input files. The user is therefore deeply integrated into the design of the simulation and its operation. Geant4 is open source code, again where the two previous examples are not. Geant4 is free, and MCNP is not. Geant4 has base elements in its geometry construction, materials definition, physics lists, data bases, tracking code and history analysis that are very well benchmarked in very many different scenarios. It is therefore interesting to investigate if it can be adapted also to the nuclear reactor context.

In this work, the application of the Geant4 framework to a new area, that of gas-cooled reactors, is investigated. This approach promises the capacity for a much higher degree of detail in the geometry and material definitions as well as the physics modeling detail. The advent of massively parallel high-performance computing will make it more feasible in terms of the speed of the calculations. The design and manufacturing of small modular reactors will be affordable and feasible for developing countries to meet their energy needs and requirements.

1.1. Gas Cooled Reactors and the TRISO particle fuel

We consider a HTGCR with pebble fuel, helium cooled and graphite moderated. In the simulation below, the fuel characteristics are borrowed from the Pebble Bed Modular Reactor (PBMR) fuel definition [18, 19]. The discrete element of the fuel is about 12000 low enriched uranium triple coated isotropic (LEU-TRISO) particles, each of about 1 mm diameter, all distributed within a spherical graphite matrix of diameter 50 mm. The TRISO particle innermost sphere is a kernel of uranium dioxide. There are subsequent layers of porous carbon, pyrolytic carbon, silicon carbide and then finally pyrolytic carbon again. The first layer acts as a buffer, and the three subsequent layers are primary containment. The 50 mm fuel sphere has a final pure carbon layer, bringing it to a 60 mm outside diameter. The whole is then sintered and annealed and then accurately machined to finish it off.

For the purposes of the proof of principle calculations, the pebbles were chemically homogenised simply as fresh fuel mass fractions with PBMR data to yield uranium dioxide 4.248%, silicon carbide 0.759% and carbon at 94.992%. In a full neutronics treatment, they would of course be subject to a state dependent homogenisation to respect various requirements

such as reaction rates and/or boundary fluxes. In this work we note that the depletion of the fuel and the production of actinides and fission fragments and all their progeny can in principle be tracked and stored for each time slice of operation, so that the composition of the fuel can be modified and followed as in a normal reactor. The dimensions of the fuel sphere could also be modified to respect thermal effects.

1.2. Event Generation and time slices

A summary of the event flow is shown in Figure 1. A time slice consists of neutronic processes and isotope decay events. Neutron events are created either by sampling a neutron density file or reading the previous time slices neutron n-Tuple. The neutrons are tracked, and lead to energy deposits and the creation of isotopes via neutron capture and fission. Reactions that occur within the time slice are simulated, and final isotopes stored in order to update the isotope inventory. Isotope decay events are created by sampling the isotope inventory. The isotope inventory is updated either by recording the simulated daughter isotopes at the end of the time slice, or via a deterministic calculation based on pre-calculated branching ratios. The 3D map of energy deposits, binned according to the appropriate mesh, will then be input to the thermal transport code for the next time slice.

In a standard simulation, Geant4 simulates all particles until their end, for example when they are destroyed or come to rest. For supercritical reactors, the simulation will never terminate. In order to simulate a reaction for a time slice only, a custom physics process was added to the Geant4 physics list, which culls all particles at the end of the time slice. All particles that are not neutrons deposit their kinetic energy at their current position. Neutrons do not deposit kinetic energy, as it is understood that they will be recreated with the same energy at the beginning of the next time slice, so this energy is not lost. The custom particle culling process has priority over the standard radioactive decay process. This means that decays of short-lived isotopes that occur within the time slice are simulated. In this implementation, at the end of the time slice, the radioactive decay process is interrupted, and longer-lived isotopes that are present at the end of the time slice can be culled from the simulation and recorded in order to update the isotope inventory for the next time slice. Each time slice is therefore a Geant4 run, with an updated geometry / materials inventory that has tracked burn and decay and thermal effects. The neutronic code can link to a thermal hydraulic code through the concept of work-flow scheduling, based on the handover of updated state information between timeslices. A reactor time scale is of the order of a minute when it is critical, so time slicing in the millisecond scale is sufficient for this workflow scheduling. Figure 1 suggests where the handover of the updated state information between timeslices would occur.

The context of the simulations described here is a fictitious "cigar reactor" designed to have a length longer the the neutrino mean free path (λ_{mfp}), but to be as small as possible otherwise, so that certain aspects of the physics can be captured, while the calculations are not too resource intensive.

2. Simulation Results

Figure 2 below shows a fictitious cigar reactor (1m cylinder, with radius 9 cm) with 80 pebbles and a superimposed thermal gradient (ranging from a minimum of 300K to a maximum of 1200K). There is no shielding between the pebbles. The aim of this simulation is to validate the neutron thermalisation behaviour and the correct operation of the thermal macroscopic cross sections. To see this, note the neutron flux distribution as a function of energy (inset) can be histogrammed and the energy-time behaviour (main graph) can be recorded locally. One sees fast neutrons rapidly thermalise to the local temperature as revealed by the quasi Maxwellian distributions that result from the long-time behavior for each individual neutron. The temperature recovered from the Maxwellian is 353 ± 29 K, for Probe 1 and 884 ± 65 K

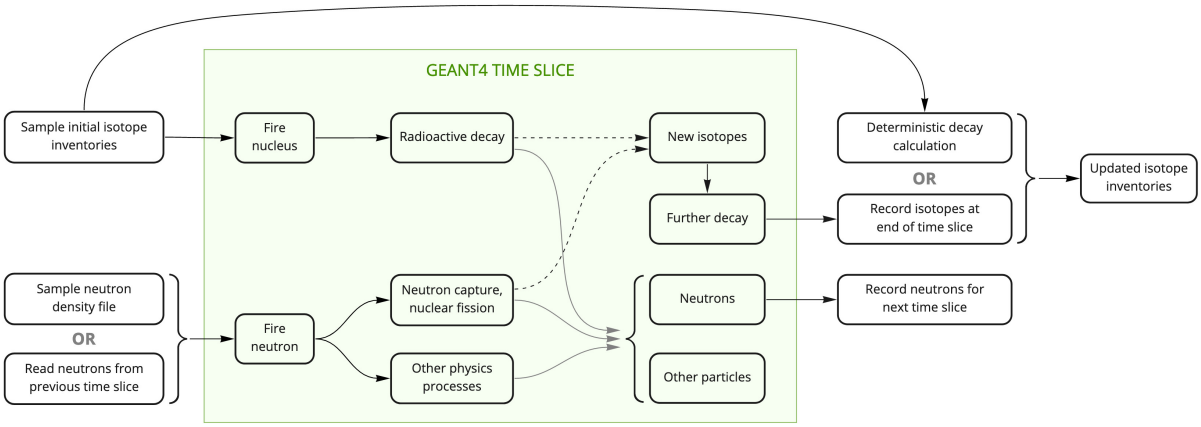

Figure 1. Event flow for a time slice, including both neutron and isotope decay events.

for Probe 2. This matches the temperatures superimposed in the simulation. The differences from the ideal Maxwellian behaviour are expected and accounted for by the energy dependent absorption cross sections and also the energy dependent leakage due the energy dependence of the length of the neutron mean free path. The boundaries were modelled with reflection considering an adjustable albedo as a new Geant4 class to simulate an effective much larger reactor while using a more constrained geometry. A special geometric discretization was placed over the reactor defining virtual local regions where local information could be recovered from the Geant4 simulation.

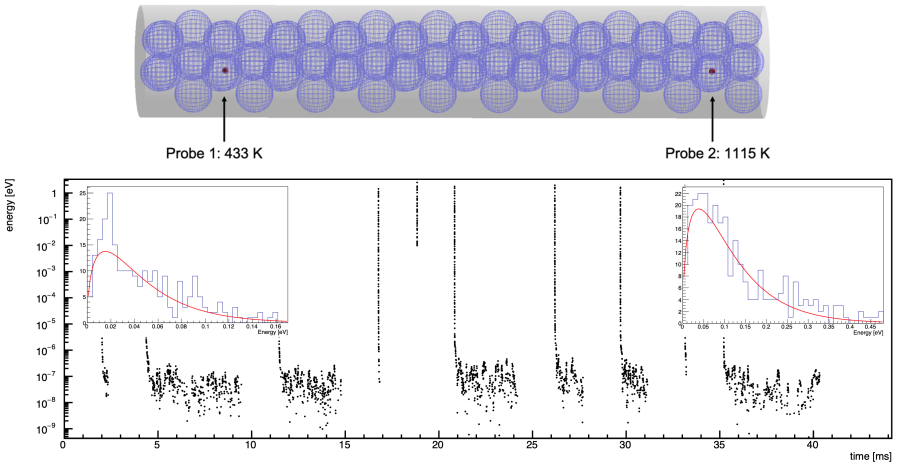

Figure 2. Top: Fictitious cigar reactor with a superimposed thermal gradient. Bottom: The neutron flux distribution as a function of energy (inset) and energy-time (main graph) showing the thermalisation to a quasi Maxwellian distribution where the local temperature is recovered.

The energy deposition per pebble would also depend on temperature through the doppler broadening of the resonance reactions, dominated by the high energy depositions of fission and neutron capture. Part of the physics background is cross section dependence on the CoM which is affected by the thermal motion of the target nuclei as seen in the Laboratory frame. Figure 3 shows this behaviour is effectively modelled, using the same cigar shaped reactor with the superimposed thermal gradient as mentioned above.

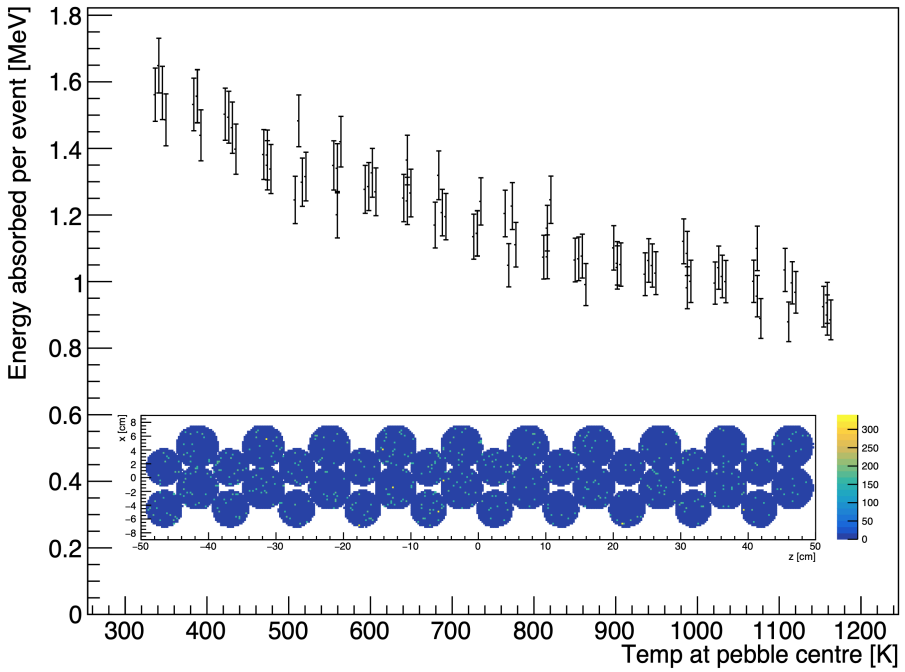

Figure 3. Validation of increased energy deposition per pebble as function of temperature.

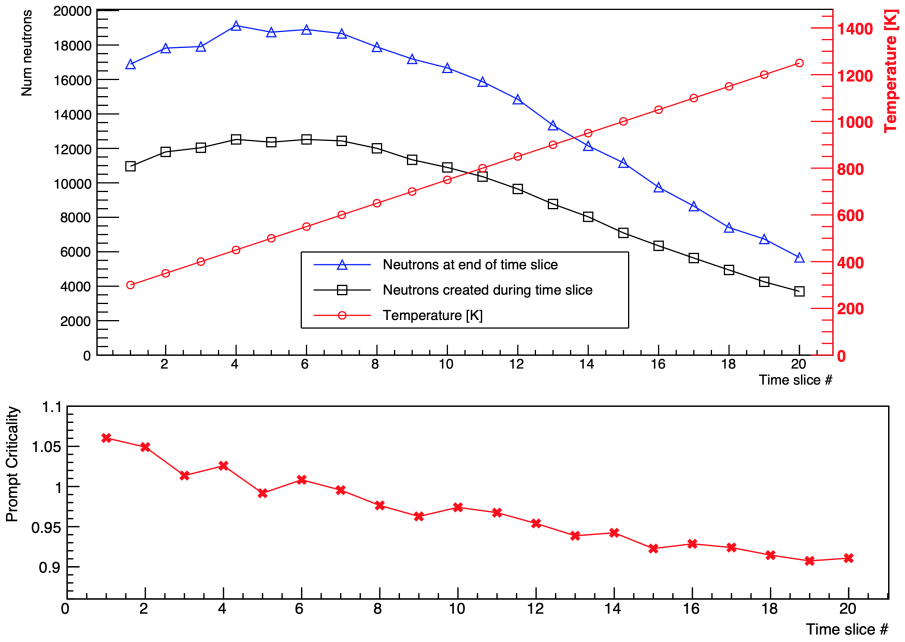

Figure 4. Numbers of neutrons per generation (top) and prompt criticality (bottom) for 20 time slices, with temperature rising by 50K per time slice, from 300K to 1200.

Up to this point, we have only presented results from a single time slice. We now demonstrate the simulations ability to follow and evolve a neutron population. A simulation was set up where the initial temperature and pressure throughout were 300 K and 100 atmospheres respectively. 10,000 neutrons with an energy of 26 meV (roughly corresponds to 300 K) from random positions

and random directions within pebbles. The uranium-235 enrichment was set to 18%, in order to get the criticality of this particular simulation geometry near 1. The neutron population was then followed through 20 consecutive 2 ms time slices. At the end of each time slice, neutrons were stored, then fired again with same position, energy and momentum in the next time step. At each time step, the temperature was increased by 50 K everywhere. This is not meant to represent a realistic reactor scenario, but rather to emphasise the response of the system to temperature changes. The helium density was adjusted in each time slice to maintain a constant pressure of 100 atmospheres as the temperature rose. Figure 4 shows the number of neutrons at the end of each time slice, the number of neutrons created during each time slice, and the prompt criticality calculated for each time slice. All neutrons were prompt, as the simulation did not include delayed neutrons. Figure 4 shows how the neutron population grows at low temperatures, then starts to shrink for at higher temperatures. Based on a comparison between the change in number of neutrons in each time slice, and the criticality (which is calculated based on number of parents and daughters), each 2 ms time slice corresponds to an average of 1.51 neutron generations.

3. Conclusions

In this paper we reviewed the implementation of the following aspects in proof of principle form as preliminary results towards the stated longer term goal: the basic neutronics, geometrical discretisation for studying the spatial variation of physical parameters, time slicing and adaptation of Geant4 for correct inter-slice persistence, a scheme of integration with thermal hydraulics by workflow scheduling, validation of the thermal macroscopic cross section behaviour, the process of fission, burn, decay, and differential energy depositions for the various physics processes, criticality and core follow over multiple time steps. The next step is to validate to other stochastic codes such as MCNP, SERPENT, and to deterministic codes, such as OSCAR for the SAFARI Reactor in South Africa, where there is also experimental data available. Then it would be interesting to select and implement a thermal hydraulic code. It will be necessary to introduce event biasing to improve the variance in rare processes without affecting the physics performance overall.

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