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Abstract. Using virtual reality technology - a modern trend. The nuclear industry is no exception. This article provides an overview of mathematical models used to create virtual analogue of critical assembly Godiva in virtual reality. Godiva - there is a simple example that allows to hone techniques for creating more complex virtual analogues of nuclear reactors and nuclear facilities. Mathematical models include stationary and dynamic ones. The stationary model is based on data from calculations carried out using Monte Carlo programs such as MCU, Serpent and Geant4. An approach is also described that makes it possible to calculate the reverse multiplication from the values of the effective multiplication factor for various states of the subcritical assembly. The dynamic model allows one to calculate the neutron-physical characteristics of the supercritical assembly during fast processes such as a neutron burst. In conclusion, there are other examples of virtual analogs created using similar approaches.

1. Introduction

Virtual reality is an actively developing technology used in many areas of human activity. Now, with the help of virtual reality technology, a person can get a completely new experience of complete immersion in the worlds of computer games. In addition, this technology allows a person to see the interior of his future home or the interior of his new car, without getting up from his sofa. This technology opens up completely new possibilities in the field of education and training of specialists. With the help of virtual reality glasses, it becomes possible to create super-realistic simulators available to any organization in any part of the world. All you need is electricity. Now you can see physical phenomena inaccessible to the human eye. Now the teacher can clearly show students what radiation, radiation or electricity is. All this simplifies the assimilation of the material and raises the quality of education to a new level.

In this article, the authors want to present the approaches they use to create virtual analogues of nuclear research facilities - subcritical and critical assemblies, charged particle detectors [1]. To simulate stationary processes, spatial and energy distributions of particle fluxes, programs are used, the functioning of which is based on the Monte Carlo method. The authors use the MCU, Serpent and Geant4 programs.

- MCU (Monte Carlo Universal) [2], this is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in three-dimensional systems by means of the Monte Carlo method [3].

- Serpent is a continuous-energy multi-purpose three-dimensional Monte Carlo particle transport code [4]. It is widely used to simulate different reactor tasks [5-8].
- Geant4 (GEometry ANd Tracking) is a toolkit for simulating the passage of elementary particles through matter using Monte Carlo methods. Developed at CERN in the object-oriented programming language C ++. The first releases came out in 1998 [9, 10].

To simulate dynamic processes in the cores of nuclear reactors, the authors use programs for solving the transport equation in the point kinetics approximation, written by themselves.

The article will describe the mathematical models used to create Godiva's virtual critical assembly.

2. Godiva stationary model

Experiments on critical assembly imply measurements of various neutron-physical quantities using ionizing radiation detectors, that is, to reproduce a real experiment in virtual reality, it is necessary to know the characteristics of radiation fluxes from the active zone of the assembly. For example, when carrying out an experiment to determine the critical load of the stand with fuel, the neutron density is measured.

The simplest functional of the neutron field in a medium to be calculated using software systems is the effective multiplication coefficient. To reconstruct the readings of the system for measuring the neutron flux from the core, a mathematical model was developed that relates the effective multiplication coefficient to the required value of the neutron density.

2.1. Godiva construction

It is an experimental pulsed nuclear reactor built at Los Alamos National Laboratory. The spherical reactor core, divided into 3 parts, has a cylindrical opening inside and consists of highly enriched (up to 93.7%) uranium weighing 53 kg and 17 cm in diameter. For a short-term achievement of criticality, the parts are brought together, a cylinder of uranium is inserted into the opening, while in this device, and a self-sustaining nuclear chain reaction begins, accompanied by a burst of neutron and gamma radiation. A 3D model of a critical assembly is shown in figure 1.

To calculate the dependence of the multiplication factor on the distance between the hemispheres, we used the MCU and Serpent software packages. The dependence of the coefficient on the distance between the hemispheres is shown in figure 2.

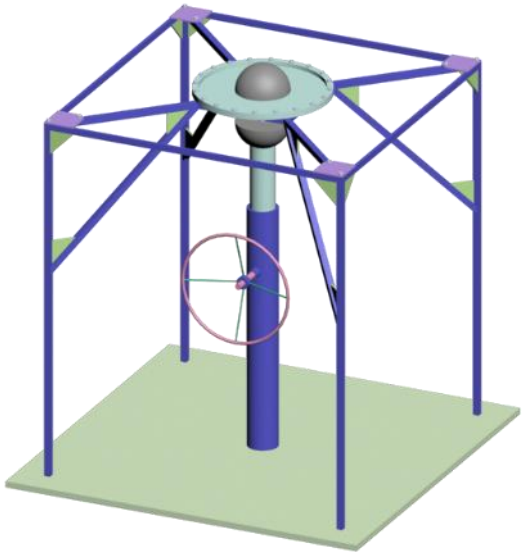

Figure 1. Three-dimensional model of the critical assembly.

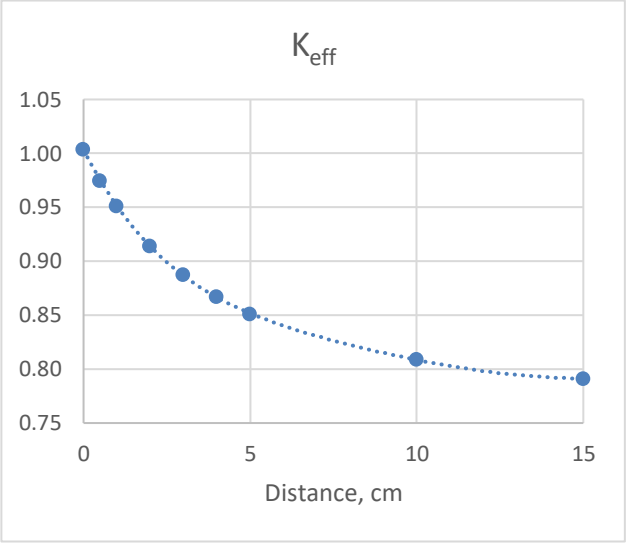

Figure 2. Dependence of the coefficient on the distance between the hemispheres.

It was also used to simulate neutron flux distribution around the critical assemblies for various distances between the hemispheres

2.2. Godiva stationary model

The simplest functional of the neutron field in a medium to be calculated using software systems is the effective multiplication coefficient. To reconstruct the readings of the system for measuring the neutron flux from the core, a mathematical model was developed that relates the effective multiplication coefficient to the required value of the neutron density.

The system of equations for the kinetics of a nuclear reactor in the point approximation has the form:

$$\frac{dn}{dt} = \frac{\rho - \beta}{\Lambda} n + \sum_{i=0}^{6} \lambda_i C_i + S\,; \tag{1}$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n - \lambda_i C_i, i = 1 \dots 6, \tag{2}$$

The components of the equation: n – neutron density, Λ – prompt neutron generation time, $\Lambda = \acute{\Lambda}/K_{eff}$, $\acute{\Lambda}$– prompt neutron lifetime in the reactor, K_{eff} – effective neutron multiplication coefficient; C_i , λ_i – concentration and decay constant of nuclei-emitters of the i-th group; β_i – fraction of delayed neutrons of the i-th group during fission (the ratio of the number of emitted delayed neutrons of the i-th group to the total number of emitted fission neutrons); β – total fraction of delayed neutrons; ρ – reactivity; S – neutron source power.

S can mean both an external source of neutrons and a source caused by secondary nuclear reactions with neutron emission: (γ,n), (α,n), spontaneous fission, etc. The solution to this system:

$$n = -S\frac{\Lambda}{\rho}. \tag{5}$$

In a point kinetics approximation, the stationary neutron density in the subcritical assembly is proportional to the power of the neutron source and inversely proportional to the reactivity of the subcritical assembly. The minus sign reflects the fact that the reactivity value in the subcritical assembly is negative.

If an ideal neutron detector is installed in the assembly, then N – the number of neutrons detected by it is proportional to the neutron density n:

$$N = C\left(K_{eff}\right) \cdot n\,, \tag{6}$$

The function $C\left(K_{eff}\right)$ takes into account the spatial distribution of neutrons and the efficiency of the detector. Almost all factors affecting the value of $C\left(K_{eff}\right)$, amenable to calculation (although often complex). However, this is not necessary, since the fundamental fact is that when approaching criticality $C\left(K_{eff}\right)$ approaches 1:

$$C\left(K_{eff}\right) \xrightarrow{K_{eff} \to 1} 1\,. \tag{7}$$

The inverse of the stationary neutron density has zero as its limit when the reactivity tends to zero:

$$\frac{1}{n} = \frac{-\rho}{S\Lambda} = \frac{1 - K_{eff}}{S\Lambda K_{eff}} = \frac{1 - K_{eff}}{S\acute{\Lambda}}\,; \tag{8}$$

$$\frac{1}{N} = \frac{1 - K_{eff}}{S\acute{\Lambda} C\left(K_{eff}\right)}. \tag{9}$$

The dependence serves as the basis for the experimental method used for extrapolated estimation of the critical value of the parameter that changes during the approach to the critical state (fuel mass, reflector thickness or height). A safe procedure for approaching the critical state consists in measuring the neutron registration rate $N_{\text{ст}}^{i}$ after each change in the parameter and completion of the transient process, followed by plotting the dependence RM_i – the reverse multiplication of the neutron density in the assembly on the value of the variable parameter:

$$RM_i = \frac{N^0}{N^i}. \tag{11}$$

$$N^0 = S\Lambda. \tag{10}$$

Then, when the value of the effective multiplication factor tends to 1, this statement is true

$$RM_i = 1 - K_{eff}. \tag{11}$$

To determine the area of applicability of this formula, comparative calculations were carried out. In the MCU software package, the neutron flux densities were calculated at different distances between hemispheres in a certain region of space. This region of space was an ideal virtual detector. The results of calculating RM by both methods are shown in figure 3. Blue dots - calculation of RM for an ideal detector based on the simulation of the neutron flux density distribution. Green dots - forecast of the critical distance between hemispheres. Red dots - calculation of RM in the point kinetics approximation. The magnitude of the error of the data of the first method is significantly greater than that of the second method with similar time costs for the calculation.

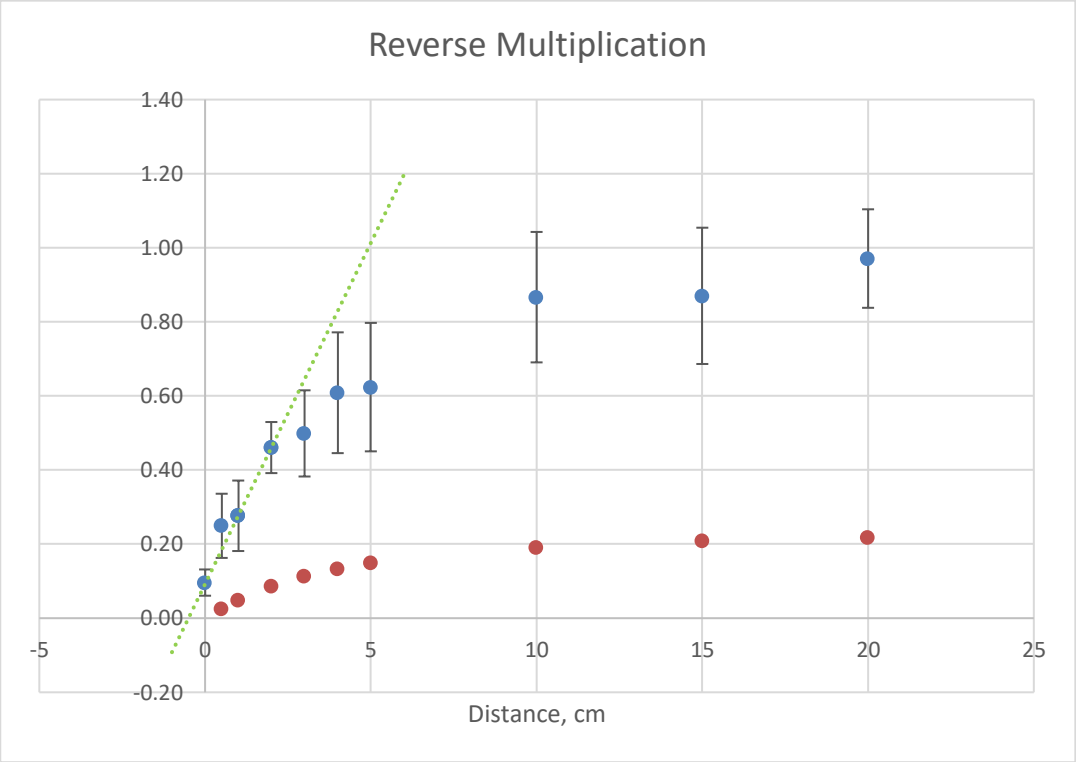

Figure 3. Dependence of RM on the distance between the hemispheres. Blue dots - calculation of RM for an ideal detector based on the simulation of the neutron flux density distribution. Green dots - forecast of the critical distance between hemispheres. Red dots - calculation of RM in the point kinetics approximation.

The graph shows that the calculation of the RM from the data based on the simulation of the neutron flux density distribution has significant uncertainty and can give an incorrect result - an underestimated value of the reactivity of the critical assembly. This is a consequence of the large magnitude of the error. The values obtained using the previously described technique accurately predict the onset of the critical state of the assembly when the distance between the hemispheres becomes equal to zero. However, these data are proportionally less in absolute value than they should be. Therefore, it is necessary to determine the proportionality coefficient between the obtained dependences of RM. By multiplying the RM value by the obtained coefficient, it will be possible to calculate the ideal RM dependence.

3. Godiva dynamic model

A dynamic model was developed to describe the transition process in a bare sphere, which describes neutron kinetics and thermomechanics.

3.1. Feedback kinetic model

A point kinetics model with an unlimited number of groups of delayed neutron emitters was chosen as a model for describing the dynamics of neutron fission; the user determines this number independently, depending on the required accuracy. Consideration of feedbacks on fuel temperature and its density is provided. The system of equations describing the model is presented below.

$$\begin{cases} \dfrac{dW(t)}{dt} = \dfrac{\rho(t)-\beta}{\Lambda} W(t) + \sum\limits_{i=1}^{N} \lambda_i C_i(t) + \tilde{S}(t) \\ \dfrac{dC_i(t)}{dt} = \dfrac{\beta_i}{\Lambda} W(t) - \lambda_i C_i(t) \\ m_T c_T \dfrac{dT_T(t)}{dt} = W(t) - k_T (T_T(t) - T_T(0)) \\ \gamma_T(t) = \dfrac{1}{\mu}(T_T(t) - T_T(0)) + \gamma_T(0) \\ \rho(t) = \rho_0 + \alpha_{T_T}(T_T(t) - T_T(0)) + \alpha_{\gamma_T}(\gamma_T(t) - \gamma_T(0)) \end{cases} \tag{12}$$

Where μ is the coefficient of volumetric expansion of the fuel material, kT is the coefficient of thermal conductivity of t he fuel material, is the power of the source multiplied by a constant linking the thermal power and the neutron flux. Zero time is the moment of the beginning of the transient process. The concentration of delayed neutron emitters at the initial moment can be calculated by the formula:

$$C(0) = \frac{\beta W(0)}{\Lambda \lambda} \tag{13}$$

This value has the meaning of the thermal power provided by the delayed neutrons. In order to correctly apply this model, it is necessary to list its limitations:

- Similarity and time independence of the spatial distributions of neutron density, which implies the symmetry of the transient processes without any local inhomogeneities;
- The temperature of the coolant changes little during the transient. Otherwise, one more feedback must be taken into account - on the temperature of the coolant, but in order to correctly take into account the heating of the coolant, it is necessary to take into account many other factors, for example, the geometry of the model, the flow regime of the coolant, the change in the density of the coolant, which greatly complicates the model.

To solve the neutron kinetics equations, the implicit Runge – Kutta [11] method of the second order was used.

The principle of the method is to calculate the predicted value of the function in order to then iteratively refine this value until the loop exit condition is met. Expression for calculating the forecast:

$$\tilde{y} = y_{i-1} + (x_i - x_{i-1}) f(x_{i-1}, y_{i-1}) \tag{14}$$

An expression to clarify the value of a function:

$$y_i = y_{i-1} + (x_i - x_{i-1}) \frac{f(x_{i-1}, y_{i-1}) + f(x_i, \tilde{y}_i)}{2} \tag{15}$$

Loop exit condition:

$$\left| \frac{y_i - \tilde{y}_i}{y_i} \right| < \varepsilon \tag{16}$$

Where ε is the relative error specified by the user. The implicit method was chosen because such methods provide a significant advantage in the required number of operations for stiff systems of ordinary differential equations.

3.2. Thermo-mechanical model

In order to more accurately describe the transient process in a multilayer sphere with gaps, it is necessary to take into account the expansion of each spherical shell separately, as well as track the coincidence of the shell radii and start solving a new problem with different radii. It makes no sense to take into account the angular distribution, since the system under study is spherically symmetric. Thus, the system of equations describing heat transfer in a spherical layer is as follows:

$$\begin{cases} \dfrac{dT}{dt}(r,t) = a\Delta T(r,t) + f(r,t) \\ T(r,0) = T_0(r) \\ \dfrac{dT}{dr}(R_1,t) = 0 \\ \dfrac{dT}{dr}(R_2,t) = 0 \\ r \in [R_1, R_2] \\ t \in [0, \tau] \end{cases} \tag{17}$$

As can be seen from the equations, the shells are thermally insulated, since the time during which the flash occurs (less than a millisecond) is too short for heat transfer to pass through the gaps, therefore, until the sphere expands and the gaps between the shells disappear, the heat transfer between the shells can be neglected. The calculation of the kinetics must be carried out in each shell separately, distributing the power of the internal heat sources in proportion to the stationary distribution of the internal sources of neutrons. Temperature feedbacks are taken into account in each shell; they should have an insignificant positive effect, since nuclear fission in the resonant energy region will increase as a result of the Doppler effect on ^{235}U, the content of which is very high. However, the expansion feedback will be lagging, because the power of internal sources at the periphery is much less than inside, and K_{eff} decreases due to an increase in leakage, which grows following the surface area during thermal expansion of the peripheral shell. The physical characteristics must be recalculated for each object at each time step. To solve the problem of unsteady heat conduction (17), it is advisable to use an implicit

scheme, which leads to a system of linear algebraic equations that form a tridiagonal matrix [12]. To solve a system of linear equations, it is advisable to use the matrix sweep method. In contrast to the explicit method, the implicit one ensures the absolute stability of the solution, which is important when solving rigid ODE systems. To solve problem (17), the numerical scheme for solving this problem looks as follows:

$$\begin{cases} \frac{T_0^j - T_0^{j+1}}{\Delta r} = 0 \\ \dots \\ \frac{T_i^{j+1} - T_i^j}{\Delta t} = \frac{T_{i-1}^{j+1} - Tu_i^{j+1} + T_{i+1}^{j+1}}{\Delta r^2} + \frac{1}{r}\frac{T_{i+1}^{j+1} - T_i^{j+1}}{\Delta r} + f_i^{j+1} \\ \dots \\ \frac{T_{Nr-1}^j - T_{Nr}^{j+1}}{\Delta r} = 0 \\ i = 1, Nr \\ j = 1, Nt \end{cases} \quad (18)$$

Where i is the index of the step along the radius, j is the step in time, Δr is the step along the radius, Δt is the step in time, Nt is the number of steps in time, Nr is the number of steps along the radius.

3.3. Test calculation of neutron burst

To determine the input characteristics of the calculation, the MCU and Serpent programs were used. These programs are considered to be precision programs, however, both packages were used in this work, since they use different constant libraries. The results of modelling the reference state are presented in the table 1.

Table 1. Input data for the transient state simulation.

	MCU	Serpent
Iinitial reactivity	3.78E-3	3.56E-3
Prompt neutron lifetime (s)	5.74E-09	
Specific heat ($J(Kkg)^{-1}$)	117.72	
Assembly mass (kg)	53.7	
Initial temperature (K)	300	
Reactivity coefficient for fuel temperature (K^{-1})	5E-7	1.35E-7
Volume reactivity coefficient (m^{-3})	-1.20E2	-1.15E2

Also, as a result of calculations, a relative change in the density of energy release was obtained depending on the radius. The graph of this dependence is shown in figure 4.

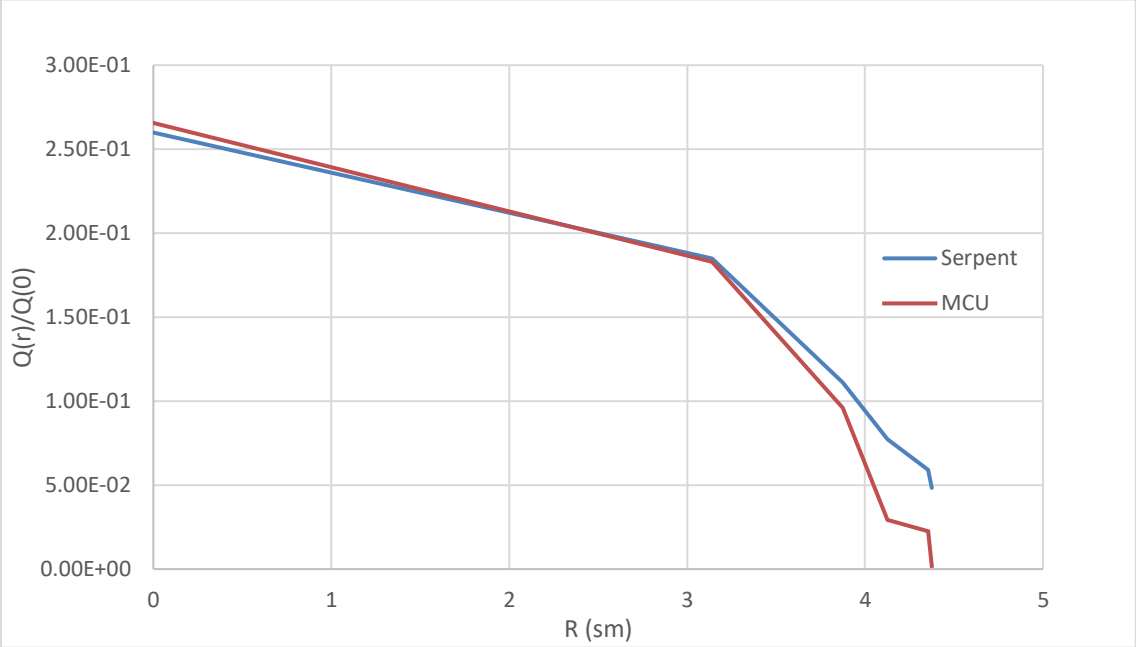

Figure 4. Relative dependence of the power of internal heat sources on the radius.

Then, using the obtained dependence, the transient process was simulated. The graphs of the dependences of the number of divisions and the average temperature in the installation on time are shown in figures 5 and 6.

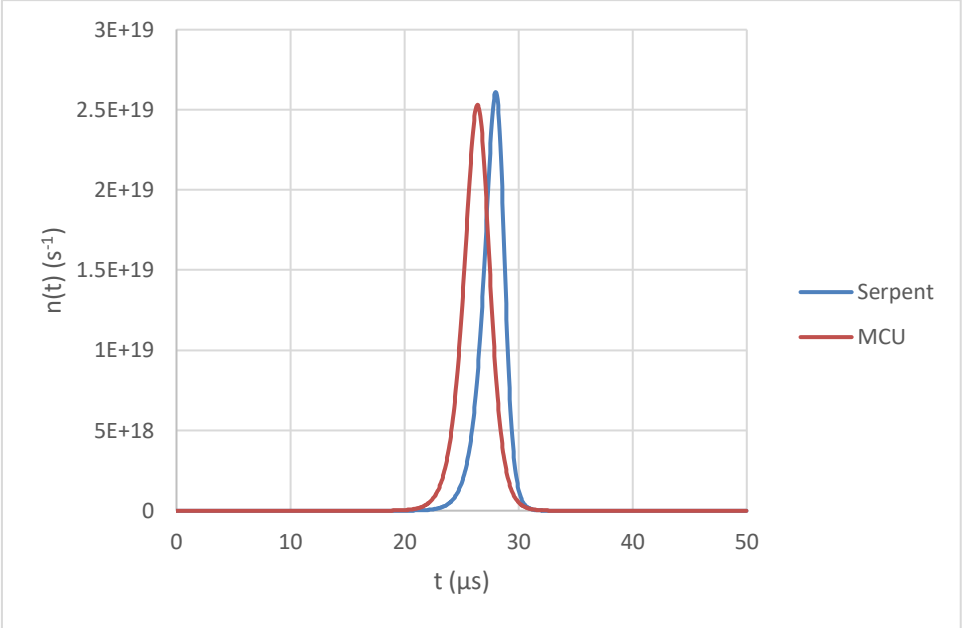

Figure 5. Time dependence of the reaction rate of the Godiva sphere.

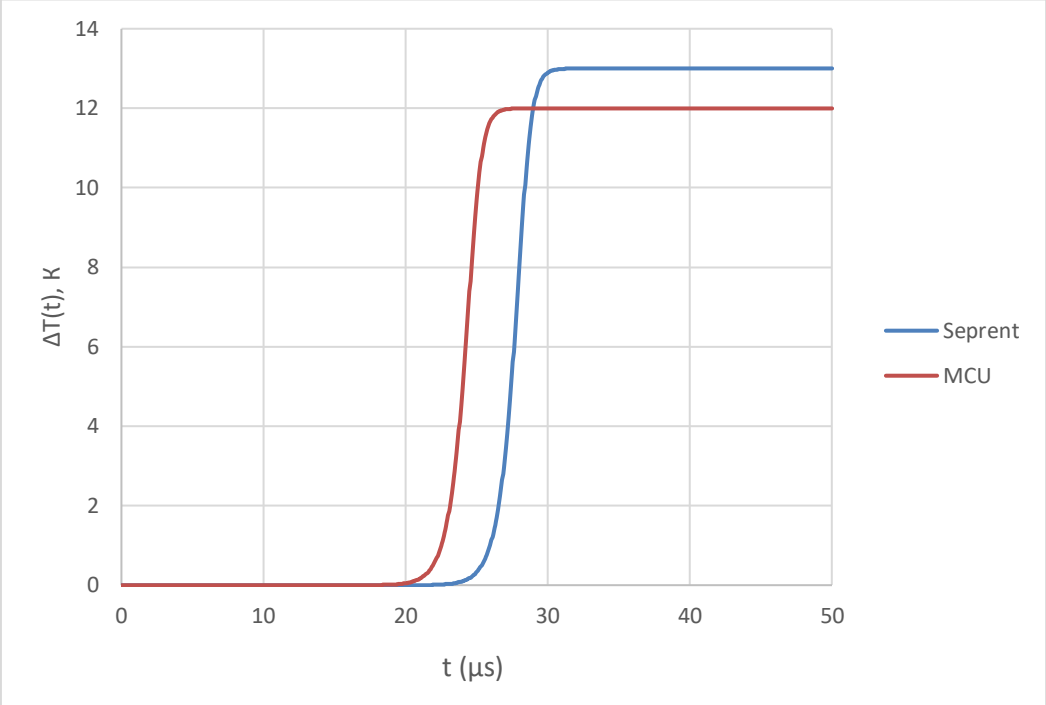

Figure 6. Time dependence of the average temperature of the Godiva sphere.

The results obtained upon completion of the calculation are shown in the table 2.

Table 2. Transient simulation results.

	MCU	Serpent	Experiment data [13]
Peak time (μs)	27.4	28.2	29.5
Relative peak size	2.53E19	2.61E19	2.68E19
Total fission yield	2.74E15	2.96E15	3.10E15
Average temperature at the moment of peak (K)	312	313	315
Relative expansion	7.9E-4	8.2E-4	6E-4

As it follows from the simulation results, the chain reaction decays faster when using the input parameters calculated using the MCU package. This can be explained by the fact that the coefficient of reactivity for volumetric expansion, calculated using the MCU in modulus is less than in Serpent.
In general, the simulation results using the developed code are very close to the experimental results, especially considering the fact that the calculation is performed on the order of a few seconds (1.25 s on one Intel Core i7 8750H core). This computation time is satisfactory for obtaining a virtual analogue response when performing a virtual experiment.

4. Conclusion

The main idea of this article is to draw attention to the idea of virtual analogs of physical installations. In the future, the use of virtual analogs will raise education and training of specialists to a new level. In addition to the Godiva virtual critical assembly described in the article, the authors are also developing other projects. For example - a visualizer of extensive air showers. The data for visualization were

obtained during simulation in such software systems as Geant4 or from real experiments. The functionality of the visualizer is shown in figures 7 and 8.

Figure 7. Visualization of extensive air shower.

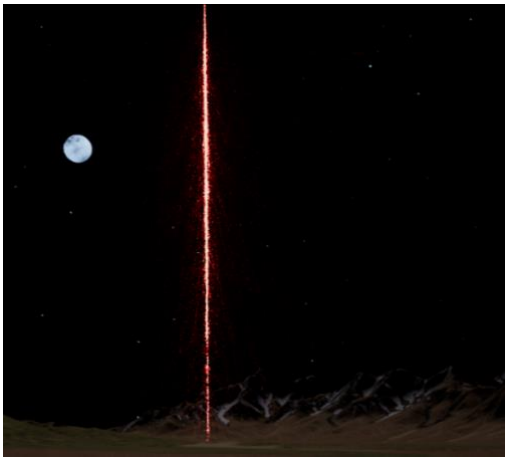

Figure 8. Visualization of extensive air shower.

In the future, this project will be used to train students and demonstrate scientific results.

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