COUPLING OF NEUTRONICS AND OPTIMIZATION CODES FOR RESEARCH REACTOR OPERATIONAL PARAMETERS

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ABSTRACT

Arbitrary Geometry Neutron Transport (AGENT) is an advanced computational environment that provides neutronics analysis and configuration of reactor systems of any design. The AGENT code methodology is based on the method of characteristics combined with a solid geometry modeler which enables an accurate treatment of exact geometries. Specifically, the AGENT modeling of the University of Utah TRIGA Reactor (UUTR) core is established as a computational system for predicting and determining the operational parameters of the UUTR. To better enhance experiments and research conducted with research reactors, an optimization software, DAKOTA (Design Analysis Kit for Optimization and Terascale Applications), has been coupled with AGENT. Sandia National Laboratories has released DAKOTA as open source and is readily available for use and implementation. This coupling of the two innovative codes allows for integrated analysis of the input parameter space and response functions of the UUTR operational parameters and under various experimental set-ups.

1. Introduction

The Utah Nuclear Engineering Program (UNEP) operates and conducts experiments and training with the University of Utah TRIGA Reactor (UUTR). The UUTR is licensed to operate up to 100 kW and is utilized by many different faculty and students at the university. AGENT is an advanced computational environment that provides neutronics analysis and configuration of reactor systems of any design. Specifically, the AGENT modeling of the UUTR core is established as a computational system for predicting and determining the operational parameters of the UUTR. Certain experiments and tests would be enhanced if specific UUTR parameters such as neutron flux could be obtained at designated experimental ports in the UUTR. The goal is to couple the UUTR modeled AGENT environment with an optimization code to be able to provide the UUTR operators and staff with a guide to rearrangement of the UUTR core materials to obtain desired core parameters. The initial goal that is undertaken is to link the neutronics code, AGENT, with the optimization code, Dakota, for development of this idea.

2. AGENT Methodology

The Arbitrary GEometry Neutron Transport (AGENT) code uses the theory of R-functions, which permits basic modeling of complex geometries, combined with the method of characteristics (MOC), which solves the neutron transport equation along characteristic

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neutron trajectories [1-5]. The AGENT code system is extensively benchmarked and in this case, it is evaluating the UUTR steady-state operation eigenvalue and flux distribution.

The 3-D modeling of a reactor steady-state with AGENT is constructed on 2-D/1-D coupled MOC equations through the neutron leakage term; general flow-chart of the AGENT methodology is depicted in Figure 1. In the AGENT methodology, the UUTR core is divided into 2-D radial planes, and therefore, a radial solution is obtained for each core plane configuration. A 1-D axial solution is then obtained for each pin region [3]. Figure 2 displays the 2-D/1-D coupling and Figure 3 demonstrates the basic parameters of the MOC discretization used by AGENT methodology.
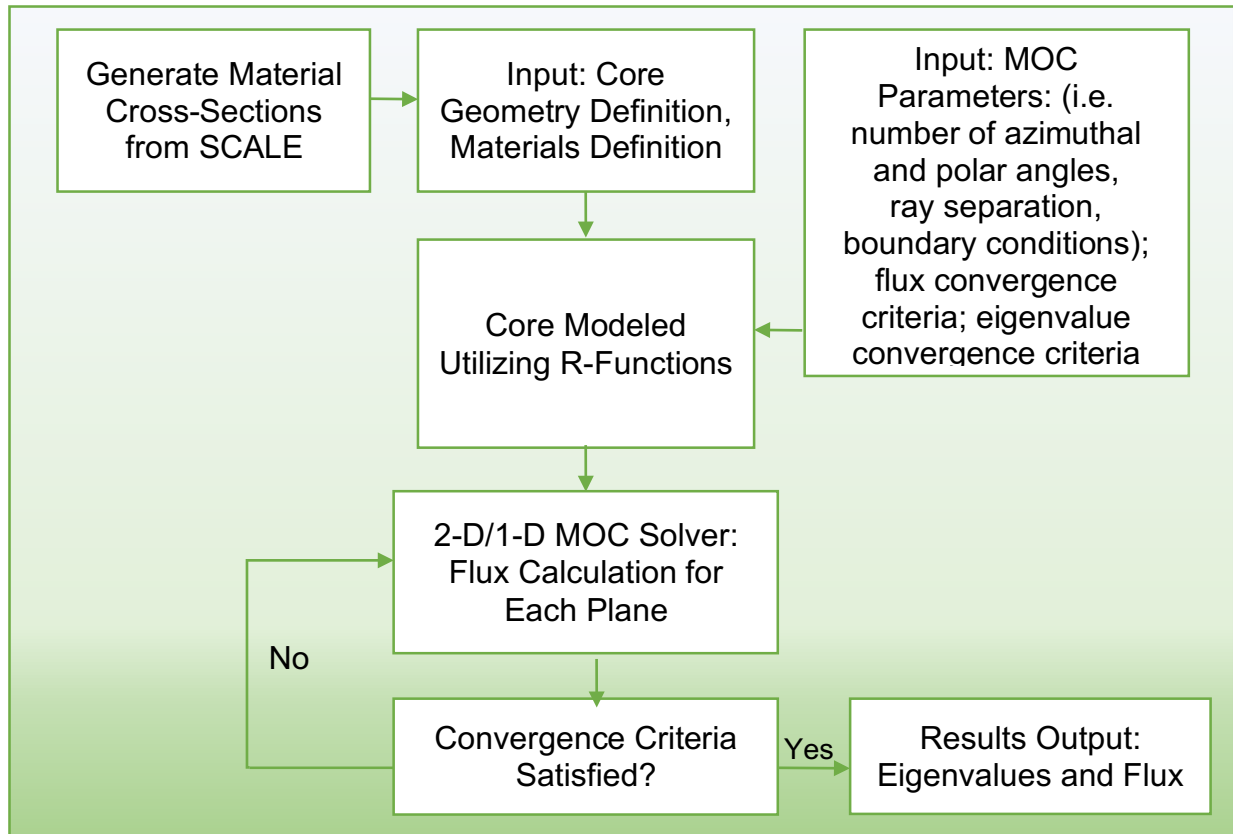

Fig 1: General 3-D AGENT Methodology

The deterministic methods provide an explicit solution to the following steady-state neutron transport equation,

$$\Omega \cdot \nabla \Psi(\vec{r}, \Omega, E) + \Sigma_t(\vec{r}, E)\Psi(\vec{r}, \Omega, E) = Q(\vec{r}, \Omega, E) \tag{1}$$

where Ω is the solid angle, $\Psi(\vec{r}, \Omega, E)$ is the energy dependent neutron angular flux, $\Sigma_t(\vec{r}, E)$ is the total macroscopic neutron cross section, and $Q(\vec{r}, \Omega, E)$ is the total neutron source. These variables are functions of the distance $(\vec{r})$, the solid angle, and the energy (E). The first term in Eq (1) represents the leakage of neutrons from the region under consideration and the second term represents the loss of neutrons due to absorption and out-scattering. The neutron source term, Q, includes the source due to in-scattering, production reactions such as fission and any external sources.
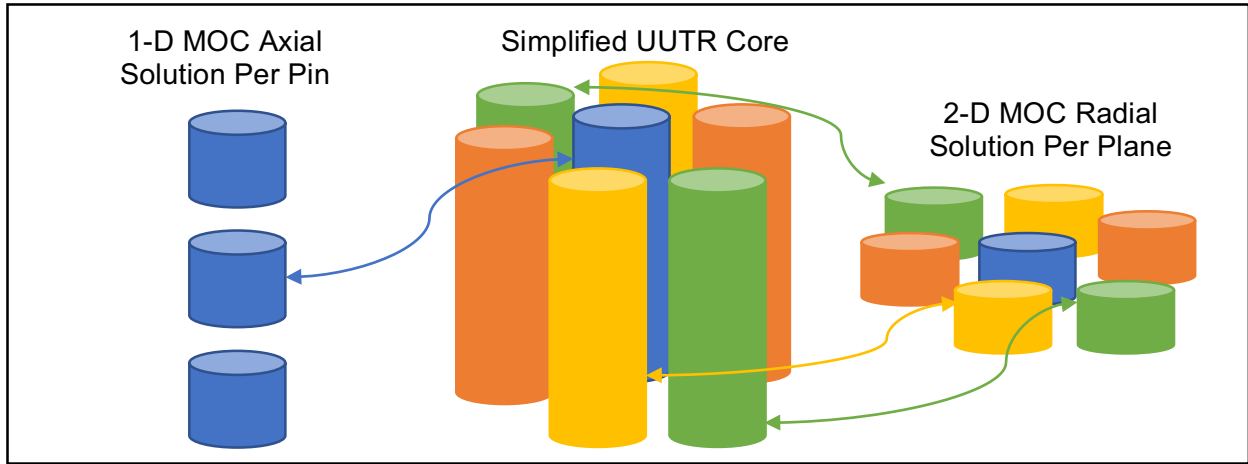
Fig 2: 2-D/1-D AGENT Coupling Solution for Evaluation of UUTR

The MOC uses the integro-differential form of the neutron transport equation, Eq (1), and solves along the straight lines throughout the geometry in a finite number of directions [5]. The parameterization transforms the neutron transport equation into its characteristic form:

$$\frac{d\Psi(\vec{r}' + s\Omega, \Omega, E)}{ds} + \Sigma_t(\vec{r}' + s\Omega, E)\Psi(\vec{r}' + s\Omega, \Omega, E) = Q(\vec{r}' + s\Omega, \Omega, E) \tag{2}$$

The geometrical domain to use Eq. (2) is divided into zones in which the flux, source and cross sections are assumed to be constant or flat. In addition to spatial discretization, the energy variable is subdivided into groups and the flux solution is sought for each energy group. After dividing up the solid angle and the neutron energy range, Eq. (2) in energy group g moving in direction Ω_m may be written as [6],

$$\frac{d\Psi_{g,m}(\vec{r})}{ds} + \Sigma_{g,i}\Psi_{g,m}(\vec{r}) = Q_g(\vec{r}) \tag{3}$$

Equation (3) is analytically integrated along a characteristic line segment and provides the angular flux in a zone i as,

$$\Psi_{g,m,i,k}(s) = \Psi_{g,m,i,k}(0)e^{-\Sigma_{g,i}s} + \frac{Q_{g,i}}{\Sigma_{g,i}}\left(1 - e^{-\Sigma_{g,i}s}\right) \tag{4}$$

where $\Psi_{g,m,i,k}(0)$ is the incoming angular flux and $Q_{g,i}$ is the average source in zone i [5]. $Q_{g,i}$ is the sum of the scattering source and the fission source and is expressed as,

$$Q_{g,i} = \frac{1}{4\pi}\left[\sum_{\acute{g}} \Sigma_{s,\acute{g}\rightarrow g,i}\bar{\phi}_{\acute{g},i} + \frac{\chi_{g,i}}{k_{eff}}\sum_{\acute{g}} v\Sigma_{f,\acute{g},i}\bar{\phi}_{\acute{g},i}\right] \tag{5}$$

where $\Sigma_{s,\acute{g}\rightarrow g,i}$ represents the macroscopic scattering cross section from group $\acute{g}$ to group g, $\chi_{g,i}$ represents fission neutron energy distribution, k_{eff} represents the multiplication constant which is the ratio of the total neutron production rate to the total neutron loss rate, $\Sigma_{f,\acute{g},i}$ represents the macroscopic fission cross section, and v represents the number of neutron

released per fission interaction. $\bar{\phi}_{\acute{g},i}$ is the zone i averaged scalar flux in group $\acute{g}$ [6]. Figure 3 shows how the angular flux in a zone i along the line segment of length s is calculated.

MOC Parameters

m = azimuthal angle
i and j = materials
δ = ray separation
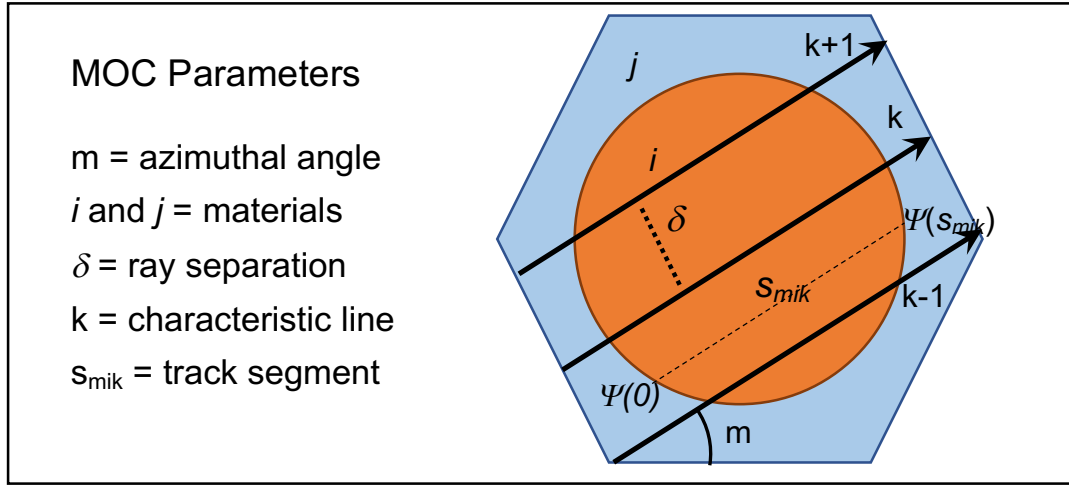k = characteristic line
s_{mik} = track segment

Fig 3: Basic Parameters of the MOC Discretization

The set of characteristic lines give the ray map and is generated per number of selected azimuthal directions and intersections of each ray with each surface in the domain as seen in Figure 3. Polar directions are treated somewhat different in that a geometrical correction is applied to the length of the segment, $s_{m,i,k}$, in Eq. (4) instead of producing a set of characteristic lines [6]. The spatial discretization permits for an adaptable range of neutron trajectories by specifying the number of azimuthal angles, polar angles, and the distance between the neutron tracks [4].

A 3-D substitute method uses 2-D planar solutions coupled with 1-D axial solutions. The 2-D/1-D combination approach begins by dividing the UUTR into a user-defined number of axial planes as shown in Figure 2 [5]. The axial one-dimensional solutions are based on the MOC and found for each pin region. The 2-D planar solution is based on the MOC as discussed in the previously [4]. Hursin *et al* [5] and Kim *et al* [7], demonstrates the methods used to calculate the coupled 2D/1D AGENT equations:

- 2-D Radial MOC equation coupled with axial leakage:

$$\frac{d\Psi(\vec{r}^{2D}, \Omega, E)}{ds} + \Sigma(\vec{r}^{2D}, E)\Psi(\vec{r}^{2D}, \Omega, E) = q(\vec{r}^{2D}, E) - TL^{Axial}(\vec{r}^{2D}, \Omega, E) \qquad (6)$$

- 1-D Axial Diffusion equation coupled with radial leakage:

$$\frac{d\Psi^{1D}_{g,m(polar),i,k}}{ds_{m(polar),i,k}} + \Sigma^{1D}_{t,g,i}\Psi^{1D}_{g,m(polar),i,k} = q^{1D}_{g,i} + S1^{1D}_{g,m(polar),i,k} - TL^{Radial}_{g,m(polar),i} \qquad (7)$$

where:

$$TL^{Axial}(\vec{r}^{2D}, \Omega, E) = \frac{cos\theta}{h_z}[\Psi^{Top}(\vec{r}^{2D}, \Omega, E) - \Psi^{Bottom}(\vec{r}^{2D}, \Omega, E)] \qquad (8)$$

$$TL^{Radial}_{g,m,i} = \frac{sin\theta cos\varphi}{h_x}\left[\Psi^{S_2}_{g,m(polar),i,k} - \Psi^{S_4}_{g,m(polar),i,k}\right] + \frac{sin\theta sin\varphi}{h_y}\left[\Psi^{S_3}_{g,m(polar),i,k} - \Psi^{S_1}_{g,m(polar),i,k}\right] \qquad (9)$$

The MOC equations are solved as a fixed source problem with only the transverse leakage changing from one iteration to the next. A converged solution, in terms of angular flux and

leakages, gives the computation a new eigenvalue. The fission source for both equations is then updated [4].

3. DAKOTA Methodology

The Dakota (Design Analysis Kit for Optimization and Terascale Applications) project started in 1994 as an internal research and development activity at Sandia National Laboratories in Albuquerque, New Mexico [8]. Sandia National Laboratories has released the Dakota software as open source and is thus readily available for use and implementation. A key Dakota advantage is access to a broad range of iterative capabilities through a single, relatively simple, interface between Dakota and AGENT. Trying a different iterative method or meta-algorithm typically requires changing only a few commands in the Dakota text input file and starting the new analysis. It does not require intimate knowledge of the underlying software package integrated in Dakota, with its unique command syntax and interfacing requirements. In addition, Dakota will manage concurrent executions of neutron interaction computational model in parallel, whether on a desktop or high-performance cluster computer.

For the initial test case the built-in Dakota evolutionary algorithm, coliny_ea, is used. This is a minimum optimization tool that applies the following steps as depicted in Figure 4:

1. Chooses an initial population randomly and executes the function evaluations on these individuals.
2. Performs selection for parents based on relative fitness.
3. Applies crossover and mutation to generate new individuals from the selected parents.
4. Executes function evaluations on the new individuals.
5. Performs replacement to determine new population
6. Returns to step 2 and continues the algorithm until convergence criteria is satisfied or iteration limits are exceeded.
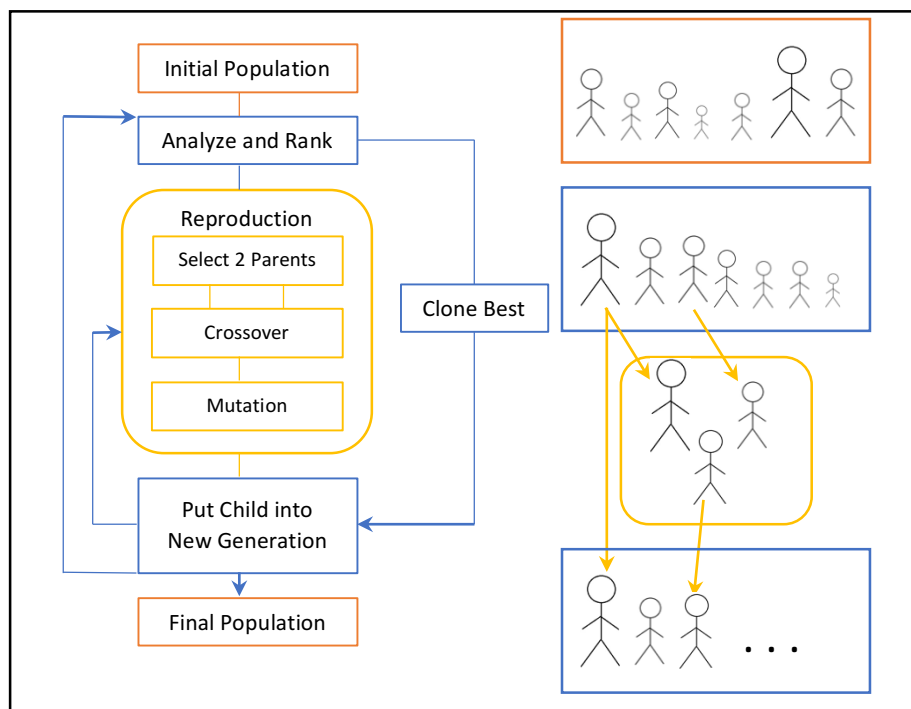

Fig 4: Dakota Evolutionary Algorithm

4. Coupling of DAKOTA and AGENT

The initial testing completed on the coupling of Dakota and AGENT were basic trials to see if proper coupling and operation occurred. The initial trial runs entailed having Dakota change the AGENT UUTR input file by varying only the central cavity with different fuel elements and materials and then send the results back to Dakota so that it can evaluate the response and determine a different material to be substituted in the centre of the UUTR. Because there are only eleven different materials, the optimization algorithm only changed the eleven different materials and then organized the results by minimizing k_{eff}. The coupling flowchart between Dakota and AGENT is given in Figure 5. Dakota runs AGENT with eleven different trials, each time varying the central cavity in the UUTR for 11 different materials. Normally the central cavity is empty and only contains the reactor tank water. The trial runs were also conducted with all three control rods fully inserted into the core. The AGENT simulation parameters are provided in Table 1. Table 2 gives the varied cell material and the subsequent k_{eff} calculated by AGENT and fed back to Dakota in the post-processing portion of the coupling.
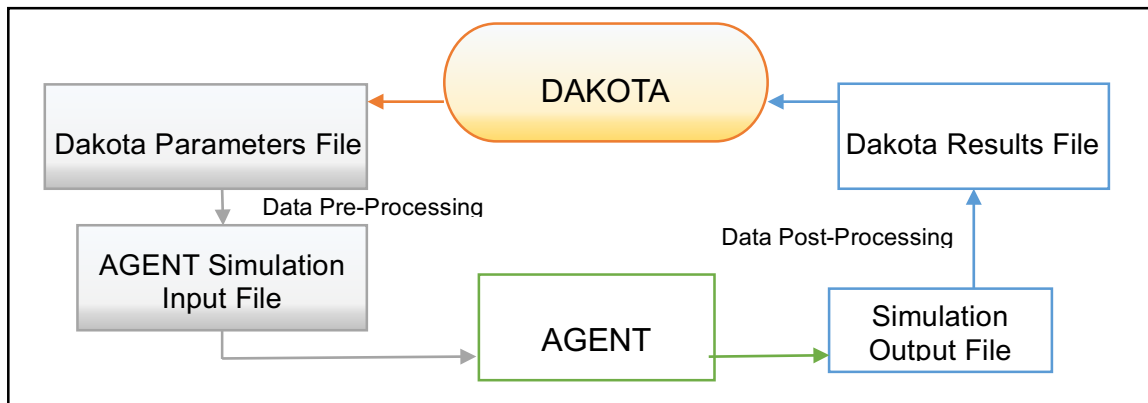

Fig 5: AGENT and Dakota Coupling Flowchart

Parameter	AGENT
Number of Azimuthal Angles	24
Number of Polar Angles and Scheme	2, Leonard-McDaniel
Ray Separation (cm)	0.05
Number of Boundary Edges per Core Face	264
Geometry Submeshing	6 Triangles per Hexagonal Fuel Rod
Flux and Eigenvalue Iteration Margin	10^{-6}
Initial Eigenvalue	1.0

Tab 1: AGENT Simulation Parameters for the UUTR Full 3-D Core Model

Trial Run of Dakota	Central Cavity Material	k_{eff}
1	1 – Stainless Steel Clad Fuel (New)	0.98249
2	2 – Stainless Steel Clad Fuel (Old)	0.98206
3	10 – Safety Control Rod	0.96285
4	11 – Shim Control Rod	0.96285
5	9 – Regulating Control Rod	0.97355
6	8 – Water	0.97664
7	4 – Reflector	0.97644
8	3 – Aluminium Clad Fuel	0.98265

9	5 – Water Rod	0.97669
10	7 – Heavy Water	0.97501
11	6 – Graphite	0.97732

Tab 2: Dakota/AGENT Initial Coupling Test Run Results

Thermal energy neutron scalar flux (10^{-6} ~ 0.125 eV) from Trial Run 2 and 3 are plotted in Figures 6 and 7. The difference can be seen by changing the central element from fuel to control rod.
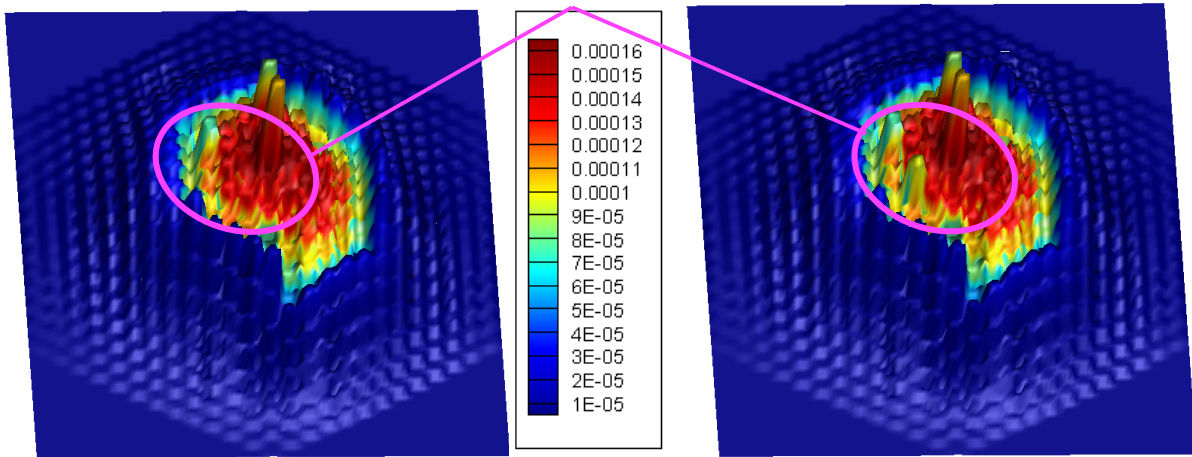

Fig 6: UUTR Thermal Scalar Flux for Trial Run 2; Fig 7: UUTR Thermal Scalar Flux for Trial Run 3

5. Conclusion and Future Work

Research reactors are used to carry out various experiments and tests. AGENT, a deterministic neutron transport code, is capable of modelling research reactors and outputs parameters such as flux and k_{eff}. In order to better achieve experiments and tests that require specific core parameters, AGENT is coupled with the optimization code Dakota. This allows a researcher to input requested values and the coupling of Dakota and AGENT can then output the arrangement of core materials to achieve the required core parameters. It has been proven that various core materials can be altered and expected results are achieved from AGENT when Dakota alters particular core materials. This was demonstrated by modelling the UUTR in AGENT and having Dakota modify the central area material of the core, achieving expected k_{eff} values. Future work will include expanding the ability of Dakota to achieve a specific flux value in an experimental port in the research reactor by altering the fuel and reflector elements around and near the experimental port.

6. Acknowledgement

7. References

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