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UNÌC: Ultimate Neutronic Investigation Code

G. Palmiotti, M. Smith, C. Rabiti, M. Leclere
Nuclear Engineering Division

D. Kaushik, A. Siegel, B. Smith
Mathematics and Computer Science Division

Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

E. E. Lewis
Northwestern University
Department of Mechanical Engineering
Evanston, Illinois 60208

Email contact: GPalmiotti@anl.gov

ABSTRACT

A code called UNÌC is currently under development at Argonne National Laboratory (ANL). The aim of the code is to provide a neutronic solver with the same geometrical flexibility of Monte Carlo codes and without the approximations (homogenization and energy condensation) associated with the common multi-step approach currently used. Moreover, UNÌC will offer the capability of multi-resolution in phase space. At the moment, two methodologies are implemented: a second order spherical harmonics (P_N) form of the transport equation and the first order method of characteristics. To improve overall performance (per-processor and scalability to thousands of processors) and reduce memory requirements, we are developing some specialized implementations of key PETSc preconditioners and matrix objects.

Key Words: neutronics, P_n, method of characteristics, PETSc

1. INTRODUCTION

Current neutronics analysis requires two or more homogenization and energy group collapsing steps. Typically, the first step involves a local calculation to obtain the spectral self-shielding for the individual pin. The second step requires an assembly-level calculation to obtain the spectral self-shielding for each assembly and to produce homogenized parameters for each unique assembly in the reactor. These assembly-level cross sections are then used in a whole-core diffusion or transport calculation to obtain the flux solution for a targeted reactor system.

One of the major enhancements proposed for neutronics analysis is the elimination of the multi-step procedure for treating the energy variable. The objective is to exploit advances in both numerical and algorithmic efficiency, combined with increasing computing power offered by systems with several thousands of processors, in order to solve the neutron transport equation in a detailed three-dimensional geometry with thousands of energy groups. Such a deterministic approach would directly compete with Monte Carlo methods and should offer the additional advantage of a hierarchical treatment of the discretized variables. The ability to obtain the adjoint solution for sensitivity calculations is also directly achieved within this framework. This approach has been adopted for **UNÌC** (**U**ltimate **N**eutronics **I**nvestigation **C**ode) which is under development at Argonne National Laboratory.

2. MAIN FEATURES

UNÌC fundamentally has a flexible geometrical option, as in the case of Monte Carlo stochastic-based codes, by utilizing a general finite element decomposition combined with a large number of energy groups (upwards of 10,000). This approach should be able to reduce the spatial approximations and eliminate the lattice cross-section generation step thus directly accounting for energy and space resonance self-shielding effects. The intent is to enable analysis of advanced nuclear reactor designs, including fast reactor systems.

A key feature of UNÌC will be the ability to do multi-resolution. At the moment two methods are under development for the code. The first method, P_NFE, is based on the even-parity (second-order) form of the Boltzmann transport equation. The second is a method of characteristics (MOC) approach based on the first-order integral transport equation. Both methods share the use of unstructured three-dimensional mesh geometry along with a multigroup energy discretization. These and other future methods are intended for simultaneous use by space-angle-group coupling on the boundaries of a decomposed problem domain.

UNÌC will combine the advantages of various methods such as spherical harmonics, the method of characteristics, and/or discrete ordinates. While current reactor analysis tools use a form of the integral transport method (collision probability or method of characteristics) to handle the assembly and pin heterogeneity in one- or two-dimensions, one can envision a characteristics formulation being used locally to handle the pin heterogeneity in 3-dimensions while a spherical harmonics formulation is used for the remainder of the domain.

The key is to use flexible coding structures and develop a strategy for coupling the different methodologies (characteristics, spherical harmonics, etc.). To this end, we are using the variational nodal method developed for fast reactor analysis at Argonne [1]. This method splits the problem domain into large spatial “nodes,” or subdomains, and uses spherical harmonic interface approximations to couple the nodes. In our recent work, we generalized the spherical harmonic interface conditions, thereby allowing different methodologies to be used in each subdomain.

3. MESH GENERATION

As part of the UNÌC effort, several mesh generators have been evaluated and incorporated into UNÌC. This has been done in order to simplify the exchange of data for neutron transport calculations and provide detailed data for the high resolution display of results in a post-processing module. The CUBIT package [2], developed at the Sandia National Laboratory, is the primary mesh generation tool used for neutronic analysis at this point, although ultimately we anticipate a specific package will be developed for modeling the reactor geometries.

Initial results using CUBIT mesh generation have been successful for reactor analysis, but several potential problems arose that need to be addressed. Currently, CUBIT can use hexahedron and tetrahedron elements with serendipity, and Lagrangian basis functions, that ensure accurate treatment of the curved geometry in nuclear reactors (volume fractions must be preserved). As is the case with most mesh generators, the focus was on development for structural mechanics or computational fluid dynamics. In these fields, a fine discretization of the geometry is needed due to the rapidly changing parameters (flow velocity, pressure, stress, strain, etc.). For neutronics, these meshes are typically too fine and thus substantial effort is required in CUBIT to generate a "coarse" mesh applicable for the resolution needed in neutron transport. Future development will focus on a procedure which strictly controls the mesh generation via user input, thereby saving computational time and providing a convenient way to control the geometry and mesh creation process.

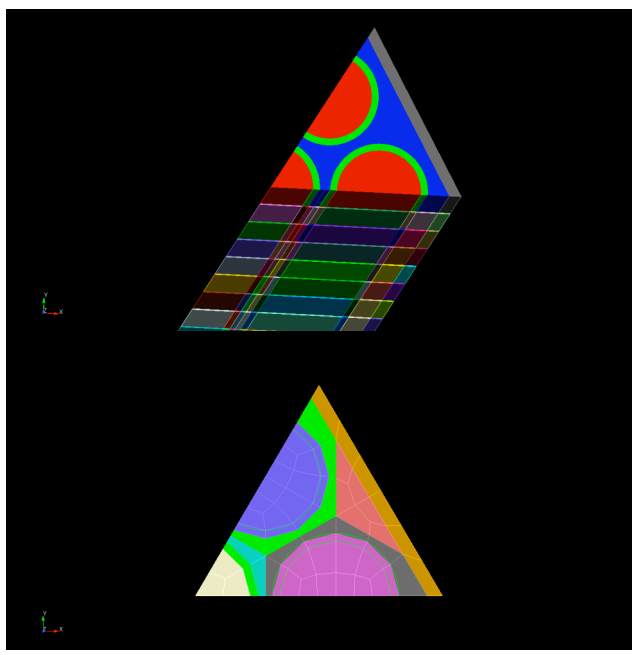

Figure 1. 3D Geometry in CUBIT with Blocks, and Associated 2D Cross Section Meshing.

One such approach to accomplish this was the development of a translator between the MCNP [3] geometry input file (combinatorial geometry) and the ACIS [4] CAD geometry description. This translator imports the MCNP combinatorial geometry input file and recursively generates solid geometry model exporting the result into a standard CAD format file. One such format,

ACIS (*.sat, *.acis and *.sab files), has widespread use and is quite portable. Future development is focused on auxiliary input which will directly control the meshing process.

Figure 1 shows the solid model geometry for a test problem consisting of a pin subset from a fast reactor design with the associated coarse mesh created by CUBIT using the converter code.

4. THE P_NFE SOLVER

At present the P_NFE option, based on a finite element discretization of the space variable and spherical harmonics expansion of the angular variable, is well-developed – a companion paper [5] gives a comprehensive description of the methodology adopted in P_NFE. The current solver is focused on steady state multigroup eigenvalue and/or fixed source problems for one, two, and three dimensional Cartesian geometries. In order to solve the large linear systems arising in this process, we employ preconditioned conjugate gradient method from PETSc (Portable, Extensible Toolkit for Scientific computation [6]. This library features distributed data structures - index sets, vectors, and matrices - as fundamental objects. Iterative linear and nonlinear solvers, implemented in as data structure-neutral a manner as possible, are combinable modularly, recursively, and extensibly through a uniform application programmer interface. Portability is achieved through MPI, but message-passing detail is not required in user code.

The parallelization of unstructured mesh codes is complicated by the fact that no two interprocessor data dependency patterns are alike. Further, the user-provided global ordering may be incompatible with the subdomain-contiguous ordering required for high performance and convenient *single program multiple data* (SPMD) coding. We use one of many flavors of MeTiS [7] to partition the unstructured grid. We follow the ``owner computes'' rule under the dual constraints of minimizing the number of messages and overlapping communication with computation. Each processor “ghosts” its stencil dependences on its nearest neighbors, in our case with a one-level halo. We enforce a local ordering on the locally-owned nodes; ghost nodes get ordered after contiguous owned nodes. This strategy saves CPU cycles, since it avoids searches while deciding if a node is local or not, and the memory flag that would otherwise be required to distinguish a local or ghost node. Next, scatter/gather operations are created between local sequential vectors and global distributed vectors, based on runtime connectivity patterns. Finally, matrix vector products needed for the iterative groupwise linear systems are translated into local and nonblocking communication tasks.

Currently we are working on optimizing the parallel performance, memory allocation, and some custom preconditioners. We anticipate good performance of the PETSc solver technology for the parallel solution of all second order methods (P_N, S_N, and angular finite element).

5. THE MOC SOLVER

As mentioned, the other primary solver currently under development in the UNÌC code is based on the method of characteristics (MOC). The current geometrical decomposition has been applied to unstructured tetrahedral meshes with additional development for hexahedral elements underway. A finite element mesh discretization presents a great degree of modeling flexibility in

three-dimensional geometries when compared with that of combinatorial geometry and allows for a straightforward approach for defining the discrete source distribution. As is known, an important component of the computational expense of the MOC method is the calculation of the spatial intersection points of the characteristic lines (rays) which traverse the domain. The current ray tracing process begins by choosing an angular cubature on the unit sphere and defining a set of starting points on the boundary of the domain. Every ray that enters the problem domain will cross several elements in the domain and the intersection point for each ray with each element crossed must be computed as shown in Fig. 2. In Fig. 2, the box represents the problem domain while the triangle represents the triangular surface of some element within the domain where the intersection is being calculated for the various rays.

For a finite element discretization, a marching scheme develops through the domain where the element to element connection information is required to determine which element is entered upon the exit from an adjoining element. Since all of the elements are the same throughout the domain, the actual intersection calculations become regular thereby greatly reducing the problem of coding different types of procedures for different types of surfaces.

Within each tetrahedron the ray tracing is carried out by finding the intersections with the surface triangle using the highly efficient Moller-Trumbore algorithm [8]. This process has proven to be very effective due to the simple and repetitive structure of the finite element method.

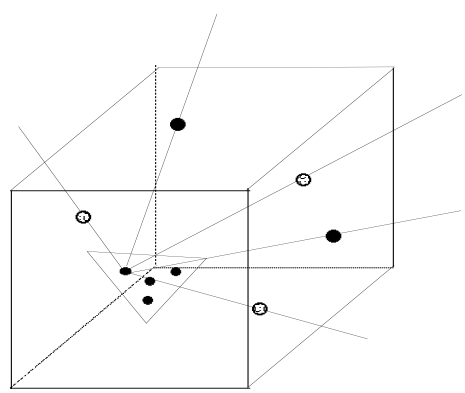

Figure 2. Ray Tracing Procedure.

Our current approach for defining the starting trajectory points on the exterior boundary of the domain is to apply an effective equal ray density distribution on the problem domain surface. Based upon the targeted ray density, each element surface on the boundary is subdivided into a number of equal area triangles which meets the ray density constraint and the centroid of these sub-triangles is taken as the starting point for the ray trajectories. As one would expect, the sub-triangles defined on the surface are easy to construct, but this approach can lead to a distribution of starting points which is not generally regular due to the fundamental differences in the boundary element surface areas. The primary drawback of this approach is that it does not control the number or density of rays very well. A better approach would be to define a set of rays which guarantees that every element in the domain is intersected for every angular direction in the cubature. In the literature, a ray casting or back projection method is typically used.

In the ray casting approach, the starting points are laid out in a regular grid on a plane which is perpendicular to the angular direction and outside of the problem domain. The intersection points with the domain boundary are then computed (ray casting) and the ray tracing process becomes the same as that already used. This additional "ray casting" calculation results in the method being more expensive than the current one while only providing a minor improvement in the distribution of points. In effect, although it guarantees an equal distribution of the rays, it does not guarantee that every element in the domain will be crossed by at least one ray.

The more common option is the back projection method. In this approach, the entire mesh is projected onto the plane which is perpendicular to the angular direction and outside of the problem domain. This approach yields the minimal set of points required to guarantee that at least one ray in each angular direction will pass through each element. However, it requires the same effort as the ray casting process with the additional cost of generating the starting points via a mesh generation on the surface. In two-dimensions this approach has proved feasible since the back projection leads to one-dimensional meshing (line segments) which can be easily be translated into the minimal set of starting points. In three-dimensions this leads to a triangular mesh on the plane which is vastly more expensive to obtain. In future implementations of the code where parallel ray tracing is used, the back projection and ray casting approaches may prove to be better options for efficiently defining the starting points.

6. RESULTS ON ABR BENCHMARK

We have applied UNÌC to a small simplified problem derived from the ongoing design work of the Advanced Burner Reactor [9]. The intention was to check the validity of the results using the two methods implemented in the code, rather than obtaining physically meaningful solutions. Based upon the information obtained from the ABR design group, we have defined the simplified problem shown in Fig. 3 through Fig. 5.

As can be seen, the problem assumes one-sixth symmetry. An unrealistic duct wall was incorporated to simulate the necessary effects in a comparable computational fluid dynamics simulation and has minimal effects on the neutronics problem. Axially the configuration has 80 cm of active core zone with 20 cm lower reflector and upper reflector where structural steel replaces the fuel pin inside the pin clad. The fission gas plenum (1.5 m) and upper structural detail (~20 cm) were neglected from this study. Reflected boundary conditions are assumed in the radial plane and vacuum boundary conditions are assumed at the upper and lower boundaries. Typical metal fuel densities were used. Due to memory limitations on the available serial machines, a five energy group structure was implemented for the cross sections where 850 degree K nominal fuel temperatures were assumed in the MC^2-2 cross section generation code [10]. In the future, as computational capabilities allow, the energy group structure will be refined with a targeted goal of ~1000 groups.

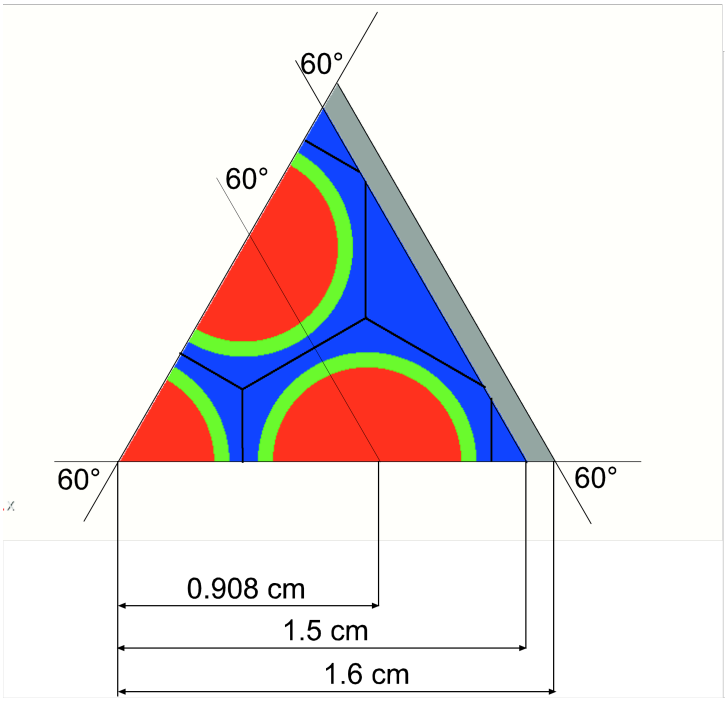

Figure 3. Benchmark Radial Geometry.

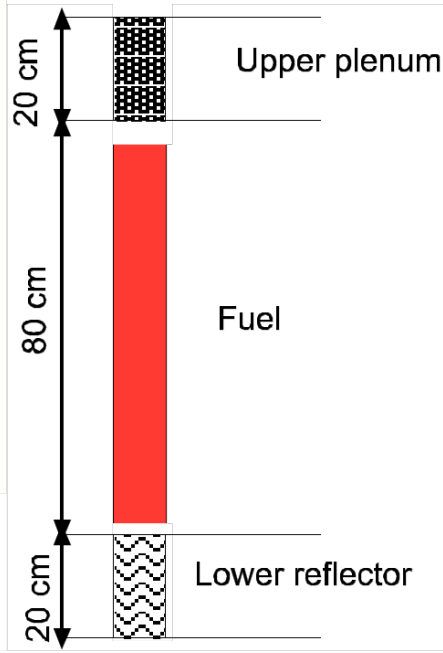

Figure 4. Benchmark Axial Geometry.

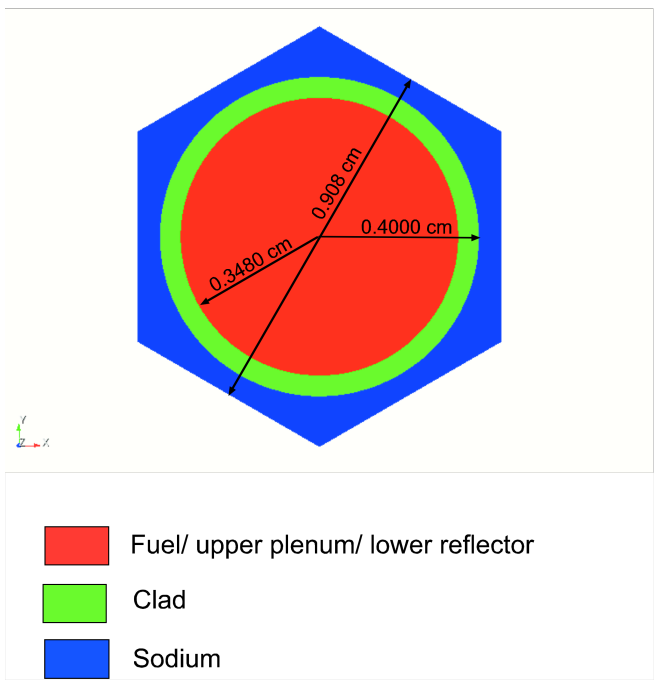

Figure 5. Benchmark pin radial geometry.

A reference solution was obtained by running the Monte Carlo code MCNP in multigroup mode using the 5 group set of cross sections. Twenty-five million histories were used to obtain an

eigenvalue of 1.45637 ± 0.00012. Table I shows the comparable solutions using the P_NFE option in UNÌC up to a P_{15} angular approximation. Figure 6 shows the power distribution at several different axial heights also obtained using the P_NFE option in UNÌC. Approximately 2000 spatial degrees of freedom are implemented in the linear hexahedral finite element mesh while 8000 were used for the quadratic hexahedral mesh (uniform meshes of 5 cm were used in the axial direction). Further increases in the number of spatial degrees of freedom did not lead to any significant changes in the results and no optimization study was performed to determine the optimal spatial approximation. From Table I, we can infer that full angular convergence is not present, which additional work in two-dimensions proved. In short, the residual error is attributable to the streaming of neutrons through the narrow sodium channel surrounding the fuel pin. This leads to an angular discontinuity in the flux, and thus a very large number of spherical harmonics are required to obtain an accurate solution. It is likely that this type of problem will worsen as more energy groups are used; hence the focus on development of a MOC option. A difference between the linear and quadratic spatial meshes is also observable as the angular approximation is refined. This is due to the general behavior of first order spatial approximations in the second order (double derivative) form of the transport equation which has been noted in the literature. The use of cubic and higher order Lagrange meshes has proven to provide virtually no advantage over the quadratic mesh approximation, especially with the current difficulties constraining the coarseness of the mesh.

Table I. Computed Eigenvalues for Benchmark Problem Using P_NFE Option.

P_N	Linear Hexahedral Mesh	Quadratic Hexahedral Mesh
1	1.38406	1.38447
3	1.41759	1.41887
5	1.43025	1.43242
7	1.43638	1.43936
9	1.43987	1.44355
11	1.44203	–
13	1.44346	–
15	1.44446	–

Table II shows the results obtained using the MOC option in UNÌC for standard S_N cubature of the angular approximation. The combined effect of a flat source approximation and the use of tetrahedral elements lead to 450000 elements being defined in the calculation. Figure 7 shows the cross section of the geometry used for this calculation. We anticipate a reduction in the number of elements of ~10 can be achieved if hexahedral elements are used. Additional gains can be achieved by implementing a linear spatial source approximation which is currently being studied. From Table II, the MOC code yields solutions which are in remarkably good agreement with the Monte Carlo reference solution. However, further investigation is required to understand the lack of systematic convergence with respect to refinements in the S_N cubature.

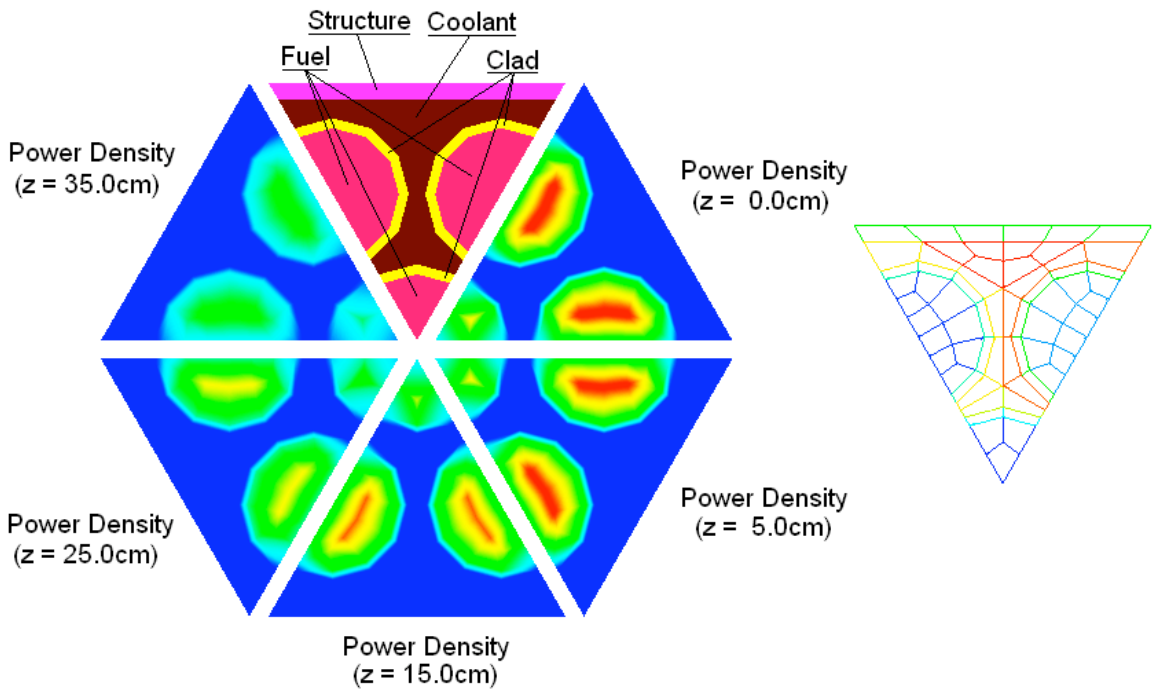

Figure 6. Power Distribution at Different Heights (z=0.0 is Midplane) For the Benchmark Problem Using P_NFE.

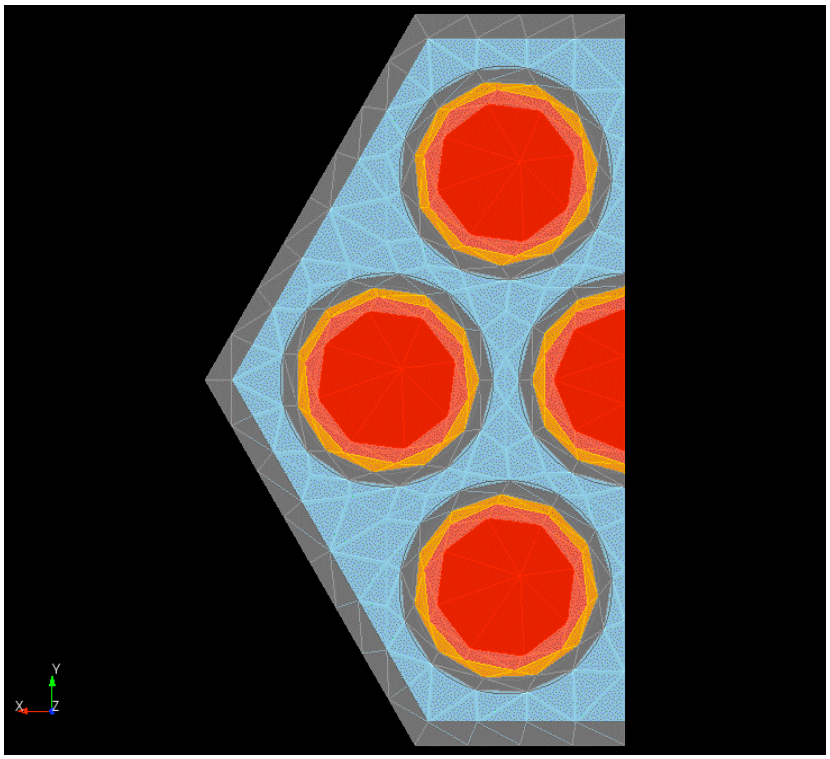

Figure 7. Two-dimensional Cross Section of meshes in the MOC Calculations.

Table II. Computed Eigenvalues for Benchmark Problem Using the MOC Option.

	S_n cubature order (Carlson Level Symmetric)			
Number of rays by angle	S_8	S_{10}	S_{12}	S_{14}
306355	1.45232 (-406)*	1.45654 (17)*	1.45740 (102)*	1.45621 (-16)*

***difference (pcm) vs. Monte Carlo Reference Calculation (1.45637 ± 0.00012).**

In the near future we expect to perform a full assembly (217 pins) ABR problem followed by a full core calculation. We hope to develop the capability such that up to 1000 groups can be used in a relatively short amount of time. With regard to coupled neutronics and computational fluid dynamics work, the short term goal is to solve the single fuel assembly problem coupling UNÌC and the NEK5000 thermal-hydraulics code [11].

7. CONCLUSIONS

A long-term project focused on advanced simulation of the nuclear fuel cycle is underway at ANL. One component of the overall code suite is a comprehensive neutronic code which fundamentally includes geometrical flexibility, multi-resolution, and self-adaptivity capabilities as well the use of a large number of groups such that modern multi-step procedures of group collapse and homogenization are avoided. Currently, two solvers of the transport equation have been developed and implemented in UNÌC: one is based on the second order form of the Boltzmann equation using a spherical harmonics angular approximation while the second one is based on the first order integral form of the transport equation using the method of characteristics.

In this work we have demonstrated the application of these codes to a simple, but difficult benchmark problem such that the numerical methodologies adopted can be verified. Although a large amount of work remains such that an efficient, every-day tool is developed, the current results do show promise. Many areas of development are foreseen for future work which include:

- Performance optimization of UNÌC on large scale parallel machines with tens of thousands of processors.
- Use of superior algorithms to reduce memory requirements needed in the solution of very large problems. We have estimated that upwards of 50 petabytes of data will be required in the case of 10,000 energy groups in a full reactor analysis.
- Implementation and use of improved iteration strategies: use of diffusion synthetic acceleration for inner iteration, Tchebychev polynomial acceleration of the outer iterations, and energy group rebalance techniques for upscattering iterations.
- Extended second order formulations to include discrete ordinate methods and possibly triangular angular finite elements.

- Development of a coupled methodology in space (and eventually energy) for simultaneous use of the various transport methodologies implemented in UNÌC.
- Multi-resolution: use of different methodologies in energy and angle.
- Self-adaptivity to automatically establish best meshing and/or angular discretization.
- Fine Grained Energy Treatment: use of spectral methods, efficient local collapsing (transparent to user).
- Calculation of adjoint, higher eigenfunctions, and the inhomogeneous solution: use of FAS (Full Approximation Scheme) [12], or Arnoldi method [13] for more than one eigenvalue, and simultaneous solution of forward and adjoint.

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