GPU-based Method of Characteristics with CMFD Acceleration in Unstructured Mesh Geometry

Kyung Min Kim, Han Gyu Lee, and Han Gyu Joo*
Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826
**Corresponding author: joohan@snu.ac.kr*

1. Introduction

A need for flexible geometry handling in reactor core analyses has risen for designing advanced reactor systems, such as heat-pipe-cooled microreactors and molten salt reactors. Accordingly, neutronics codes that can deal with the unstructured mesh to represent a flexible geometry have been recently developed and used more widely. Among the deterministic transport codes are PROTEUS-MOC [1] which initially aimed at unstructured mesh geometry, and Griffin [2] based on the MOOSE framework [3]. Serpent [4] and PRAGMA [5] are representative Monte Carlo codes that recently introduced their own modules for processing unstructured meshes.

Unfortunately, processing flexible geometry demands more computing resources and runtime than conventional geometry because of large and complicated information. Moreover, flexible geometry handling is not prevalent as direct whole-core calculations take a long time to achieve sufficiently accurate solutions even in conventional lattice geometry. However, it can be alleviated by applying accelerators such as graphical processing units (GPUs). One of the pioneers of deploying GPUs in the main calculation is nTRACER [6], which has recently demonstrated a drastic performance enhancement made by adopting graphics processing units (GPUs) as an accelerator [7].

Motivated by such research, it can be posed that hardware acceleration can be applied even in the unstructured mesh geometry and enhance performance. In this sense, a new deterministic code is developed and presented here, which is named NuDEAL standing for Neutronics using Deterministic Finite Element Algorithms. NuDEAL aims to take full advantage of unstructured mesh representation and GPU acceleration to achieve practicality and flexibility simultaneously.

This paper states the technical treatment considered in the unstructured mesh geometry. Then, algorithms of NuDEAL involving the planar method of characteristics (MOC) and the coarse mesh finite difference (CMFD) method are briefly described. Preliminary results will be demonstrated with a benchmark problem to verify the soundness of the implementation.

2. Background and Methodologies

2.1. Representation of Unstructured Mesh

NuDEAL represents the extruded geometry which can be described as a 2D geometry. Here, the half-edge data structure [8] is employed to efficiently store and load the geometry data, which is widely used. It classifies geometry objects into four topological elements: vertices, edges, half-edges, and faces as shown in Fig. 1. Table I describes each topological element except for a half-edge has only a single pointer to the corresponding half-edge, a half-edge has all the relations to the other elements. This data structure provides efficient and natural ways to navigate the entire mesh, such as traversal around a face and traversal around a vertex. These are useful when finding ray-mesh intersections, which is a requisite for the MOC calculation.

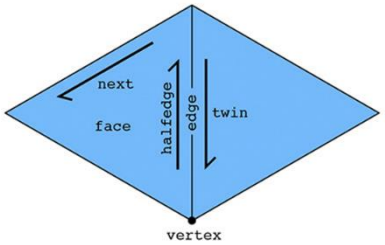

Fig. 1. A diagram of the half-edge data structure

Table I. Topological elements and their compositions

Element	**Composition**
Vertex	A half-edge
Edge	A half-edge
Face	A half-edge
Half-edge	Twin, next, vertex, edge, face

2.2. Planar Method of Characteristics

The basic theories and strategies regarding the GPU-based planar MOC are similar to those in [7]. Algorithm 1 briefly outlines the parallel ray tracing algorithm employed in NuDEAL. While other conventional MOC codes based on lattice geometry hierarchically store the ray data, the unstructured mesh geometry does not contain any explicit hierarchy. Hence, the ray data is organized with an indexing structure where the spatial rays are located outermost, and the energy group is indexed innermost, as illustrated in Fig. 2. The calculation of segment-average angular flux for each ray segment is performed using the incoming and outgoing angular flux relation. Here, the outgoing angular flux is cached to serve as an incoming one for the next segment, while the segment-averaged one for each polar angle is stored in register. The segment-averaged one is then accumulated to the region-wise scalar flux.

Another main difference from the lattice-based codes is the ray generation process. Since the modular ray approach [9] can no longer be applied, the back

projection method [10] is employed in NuDEAL to determine the ray distribution. However, discarding the modular ray leaves another consideration regarding the reflective boundary condition as reflected rays at the boundary are not consecutive anymore. Instead of using surface angular flux, which was initially suggested to determine reflected angular flux [11], NuDEAL employs track-wise interpolation which is more fine-grained.

Before performing the MOC calculation, ray intersections should be found to serialize the ray segment data. The traversal features of the half-edge data structure are used here, which makes it easy to find ray intersections. This procedure is briefly given in Algorithm 2. Once a ray finds the first incident face, all the intersections with the edges are gathered while traversing around that face, and the most proper one is chosen. An exception should be appropriately handled when the chosen intersection is a vertex or near the vertex. In this case, the next face can be found by traversing around the vertex. This sequence is repeated until a ray meets the boundary.

Algorithm 1. Parallel ray tracing kernel.

```
for each ray parallel do
  for each group g parallel do
    for each segment s ∈ ray do
      for each polar angle p do
        Save outgoing angular flux on cache
        Accumulate angular flux change on register
      end for
    Atomically accumulate region-wise scalar flux
    end for
  end parallel for
end parallel for
```

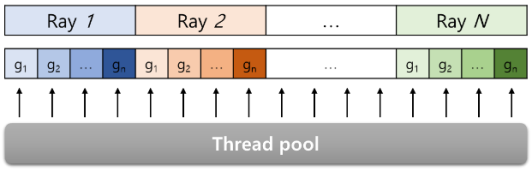

Fig. 2. Ray data structure configuration.

Algorithm 2. Finding ray-mesh intersections.

```
for each parallel_ray do
Find an incident face for parallel_ray
  repeat
    h ← face.half_edge
    repeat
      Calculate intersection point p with h
      Gather p into points
      h ← h.next_half_edge
    until h = face.half_edge
    intersection ← min(points)
    if intersection is a vertex v
      Find next face by using v
    else
      face ← intersection.face
  until face is a boundary
end for
```

2.3. Coarse Mesh Finite Difference

For the CMFD acceleration, NuDEAL follows a coarse mesh generation scheme implemented in the PROTEUS-MOC [12]. This scheme requires only a stencil grid that is used to partition the fine mesh to compose the coarse mesh. Any arbitrary stencil grid is accepted, as illustrated in Fig. 3. After overlaying the stencil over the fine mesh, the coarse mesh is generated by partitioning the fine mesh so that a coarse mesh element includes several fine mesh elements by measuring the centroid distance. Since the fine mesh elements become a subset of the coarse mesh counterpart, the relationship is defined, which maps the fine mesh to the coarse mesh. This is used to extract the partial neutron current from the MOC calculation.

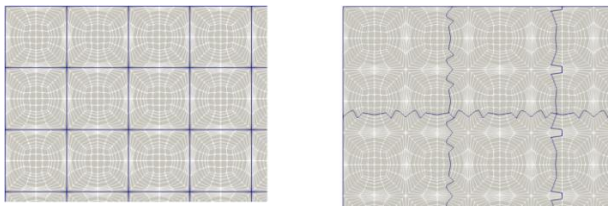

Fig. 3. Coarse mesh generated by the partitioning algorithm.

However, the accumulated neutron current can raise an imbalance within a coarse mesh cell because a ray track might pass around a vertex. This imbalance leads to an inconsistency between MOC and CMFD solutions, so the CMFD does not work as an acceleration method properly. This issue is resolved by introducing a pseudo absorption cross section (PAXS) [13], defined in each CMFD cell as the following equation:

$$\Sigma_p \equiv \frac{\bar{q}V - \sum_k J_k \Delta A_k}{\bar{\phi}V} - \Sigma_r \,. \qquad (1)$$
$$\tilde{\Sigma}_r \leftarrow \Sigma_r + \Sigma_p$$

In equation (1), $\bar{q}$ is the volumetric neutron source, $\bar{\phi}$ is the average neutron flux, Σ_r is the homogenized macroscopic removal XS, and J_k is the net neutron current at surface k. The PAXS defined in equation (1) ideally becomes zero when the solution sufficiently converges. However, it is not the case because the contribution of the neutron current is ambiguous at vertices. Therefore, the PAXS is generated from the MOC solution and interpreted as an equivalence factor in the CMFD formulation, which forces the neutron balance from the higher-order solution to be satisfied. Then, the PAXS is directly involved in the CMFD formulation modifying the removal reaction rate by added with the original removal XS. Introducing the PAXS was at first devised to resolve the inconsistency between MOC and CMFD in the discontinuous finite element framework, but it was revealed that it also works well in this type of inconsistency [14].

3. Preliminary Results and Discussion

The need for PAXS is examined for the single assembly problem from the C5G7 benchmark [15], as illustrated in Table II. The listed eigenvalues were obtained by the CMFD calculation after tightly converging the MOC fission source error to 10^{-10}. The inconsistency becomes severer as the coarse mesh granularity gets finer. This is due to the imbalance between the solved flux and the accumulated neutron current. Therefore, applying PAXSs is a mandatory prescription in unstructured mesh representation.

The C5G7 2D core problem is adopted to demonstrate the comprehensive soundness of the code. Note that the volume correction method [16] is applied during the mesh generation phase to compensate for the fuel volume reduction due to the linear-order mesh representation. The calculation conditions are described in Table III.

Table IV compares the obtained eigenvalues with the reference, in which the difference between them is only 3 pcm. The flux distributions in the fast and thermal energy groups are illustrated in Fig. 4 and Fig. 5, respectively. The fission source distribution is also depicted in Fig. 6. These demonstrate that high-resolution flux distributions can be obtained.

A wall time for each calculation procedure is listed in Table V. A number parenthesized beside the MOC wall time indicates the number of fission source iterations. Note that this examination is not strict because this calculation was performed on a personal computer, and a single GPU, NVIDIA GeForce GTX 1080, was used. Nevertheless, the computing time result demonstrates that the GPU-accelerated MOC method is efficient enough even in the unstructured mesh representation. Furthermore, this result also shows the effect of CMFD acceleration. The number of fission source iterations was reduced by 35 times, and the corresponding wall time of the MOC calculation was also drastically reduced. Consequently, the calculation can be completed in less than 20 seconds, and this computing time shows the feasibility of GPUs deployed in MOC calculations under flexible geometry.

Table II. Effects of PAXS on calculation consistency.

Coarse mesh stencil grid	w/ PAXS	w/o PAXS	Diff. (pcm)
1×1	1.3336115	1.3336115	0.00
3×3		1.3336087	-0.28
9×9		1.3335636	-4.79
27×27		1.3329712	-64.03

Table III. Calculation conditions for the C5G7 2D problem.

Ray spacing (cm)	0.05
# azimuthal / polar angles	16 / 4
# ray segments	23,891,009
# flat source regions	189,584
# CMFD cells	2,601

Table IV. Eigenvalue results for the C5G7 2D core problem

MCNP (Reference)	**NuDEAL (Diff. in pcm)**	
	w/o CMFD	w/ CMFD
1.18655 (±0.00003)	1.18652 (-3)	

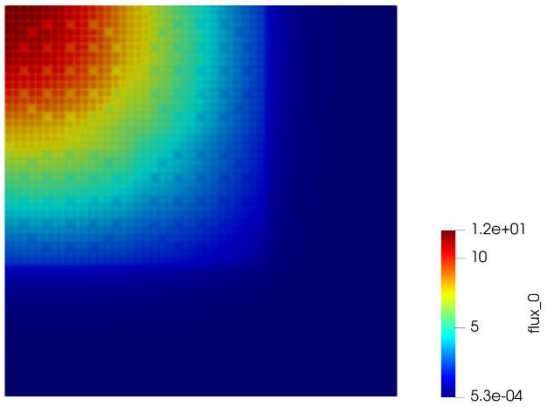

Fig. 4. Fast-group flux of the C5G7 2D problem.

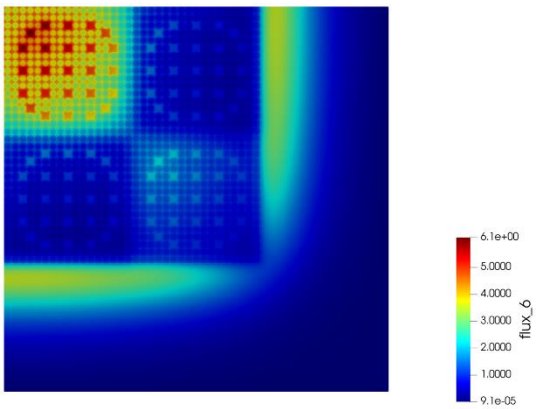

Fig. 5. Thermal-group flux of the C5G7 2D problem.

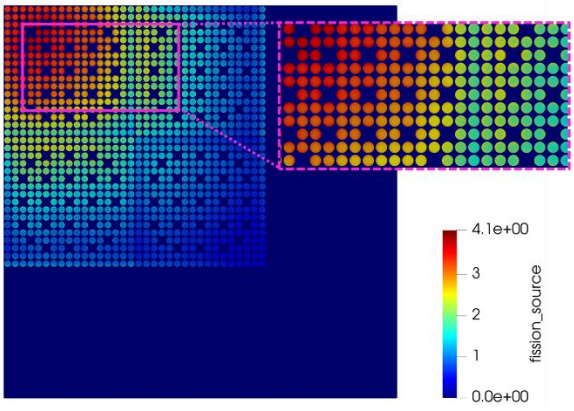

Fig. 6. Fission source distribution of the C5G7 2D problem.

Table V. Computing time and number of iterations

Composition	w/o CMFD	w/ CMFD
Initialization	9s	9s
MOC	144s (249)	3.5s (7)
CMFD	-	2.5s
Total	153s	16s

4. Conclusions

NuDEAL, a deterministic neutronics code targeted for unstructured and flexible geometries, started to be developed, and its soundness in implementation and consistency was demonstrated in this work. The unstructured mesh geometry was represented with the efficient half-edge data structure. This data representation helps initialize the MOC calculation in the mesh geometry by making it easy to find ray-mesh intersections. The CMFD acceleration was also successfully formulated with the PAXS and coupled with the planar MOC calculation. These series of implementations were verified with the C5G7 2D core problem, which shows a good agreement in eigenvalue and fine-grained flux distributions. Although the examination was preliminary, the feasibility of the GPU-accelerated MOC calculation in the unstructured mesh was demonstrated, in which the C5G7 2D problem can be solved less than 20 seconds on a personal computer.

The most urgent of remaining works is to develop a 3D solver that is stable and accurate enough. Instead of the conventional 2D/1D approach, the low-order 3D solver will be coupled with the planar MOC to enhance stability. Then, an elaborate parallelization scheme and domain decomposition method for both high- and low-order solvers should be introduced without losing scalability. The microscopic XS library and the corresponding resonance treatment method will be subsequently developed.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2021M2D6A1048220).

REFERENCES

[1] A. Marin-Lafleche, M. A. Smith, and C. Lee, "PROTEUS-MOC: A 3D DETERMINISTIC SOLVER INCORPORATING 2D METHOD OF CHARACTERISTICS," in *International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering (M&C2013)*, 2013, pp. 2759–2770.

[2] C. Lee *et al.*, "Griffin Software Development Plan," ANL/NSE-21/23, INL/EXT-21-63185, Jun. 2021.

[3] D. Gaston, C. Newman, G. Hansen, and D. Lebrun-Grandié, "MOOSE: A parallel computational framework for coupled systems of nonlinear equations," *Nuclear Engineering and Design*, vol. 239, no. 10, pp. 1768–1778, Oct. 2009.

[4] J. Leppänen and M. Aufiero, "DEVELOPMENT OF AN UNSTRUCTURED MESH BASED GEOMETRY MODEL IN THE SERPENT 2 MONTE CARLO CODE," in *International Conference on Physics of Reactors (PHYSOR 2014)*, Sep. 2014.

[5] J. Im, M. J. Jeong, N. Choi, K. M. Kim, H. K. Cho, and H. G. Joo, "Multiphysics Analysis System for Heat Pipe Cooled Micro Reactors Employing PRAGMA-OpenFOAM-ANLHTP," *Nuclear Science and Engineering*, 2023.

[6] Y. S. Jung, C. B. Shim, C. H. Lim, and H. G. Joo, "Practical numerical reactor employing direct whole core neutron transport and subchannel thermal/hydraulic solvers," *Ann Nucl Energy*, vol. 62, pp. 357–374, 2013.

[7] N. Choi, J. Kang, H. G. Lee, and H. G. Joo, "Practical acceleration of direct whole-core calculation employing graphics processing units," *Progress in Nuclear Energy*, vol. 133, Mar. 2021.

[8] D. E. Muller and F. P. Preparata, "Finding the intersection of two convex polyhedra," *Theor Comput Sci*, vol. 7, no. 2, pp. 217–236, 1978.

[9] B. M. Kochunas, "A Hybrid Parallel Algorithm for the 3-D Method of Characteristics Solution of the Boltzmann Transport Equation on High Performance Compute Clusters," University of Michigan, 2013.

[10] G. Palmiotti *et al.*, "UNİC: Ultimate Neutronic Investigation Code," in *Joint International Topical Meeting on Mathematics and Computations and Supercomputing in Nuclear Applications (M&C+SNA 2007)*, Apr. 2007.

[11] C. Rabiti, M. A. Smith, W. S. Yang, D. Kaushik, and G. Palmiotti, "Parallel method of characteristics on unstructured meshes for the UNIC code," in *International Conference on the Physics of Reactors (PHYSOR 2008)*, Sep. 2008.

[12] A. M. Hsieh, "Development of Transient Analysis Capability of PROTEUS-MOC for Micro-reactor Applications," University of Michigan, 2022.

[13] Y. S. Jung and W. S. Yang, "A consistent CMFD formulation for the acceleration of neutron transport calculations based on the finite element method," *Nuclear Science and Engineering*, vol. 185, no. 2, pp. 307–324, Feb. 2017.

[14] A. Hsieh and W. S. Yang, "Implementation of CMFD Acceleration Scheme in PROTEUS-MOC," in *Transactions of the American Nuclear Society*, Jun. 2017, vol. 116, pp. 1140–1143.

[15] OECD Nuclear Energy Agency., *Benchmark on deterministic transport calculations without spatial homogenisation : a 2-D/3-D MOX fuel assembly benchmark*. Nuclear Energy Agency, Organisation for Economic Cooperation and Development, 2003.

[16] D. R. Gaston, "Parallel, Asynchronous Ray-Tracing for Scalable, 3D, Full-Core Method of Characteristics Neutron Transport on Unstructured Mesh," Massachusetts Institute of Technology, 2020.