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ACCURACY OF TITAN BASED ON A NEW OECD-NEA BENCHMARK OVER A RANGE IN PARAMETER SPACE

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ABSTRACT

TITAN, a 3-D deterministic transport code, has been recently developed by implementing a new hybrid discrete ordinate and characteristics approach. In this paper, the TITAN code is applied to solve the NEA/OECD benchmark problem on the accuracy of solution of 3-D transport codes over a range in parameter space. The parameter space contains 729 cases over six independent variable parameters with three possible values each. TITAN's block-oriented S_N solver is used to calculate all the cases in a batch run. Results for all the 729 cases in the parameter space are in good agreement with the Monte Carlo reference solution .

Key Words: TITAN, Hybrid, S_N, Characteristics, Benchmark

1. INTRODUCTION

Recently, we have developed a new 3-D deterministic code, TITAN [1]. TITAN uses a hybrid approach to solve particle transport problems with both the Discrete Ordinates method (S_N) [2-3] and Method of Characteristics (MOC) [4-5]. The Discrete Ordinates method and Method of Characteristics are two widely used deterministic method to solve the Linear Boltzmann Equation (LBE). TITAN integrates the two methods in one code. A block-oriented S_N solver and a block-oriented characteristics solver have been implemented. This allows users to apply preferred method to solve the LBE in different spatial blocks (coarse meshes) in a physical model.

TITAN has been benchmarked on various reactor physics problems, including the C5G7 MOX [6-7] and Kobayashi problems [8]. Recently we also apply TITAN to simulate the SPECT projection images [9-10], in which the Monte Carlo method is generally used. The results of the benchmarks show that TITAN has a higher computational efficiency as compared to the S_N method or Monte Carlo method, specifically for application to problems containing regions of low scattering.

In this paper, TITAN is used to solve a new NEA/OECD benchmark problem on the accuracy of solution of 3-D transport codes over a range in parameter space. [10] The remainder of this paper is organized as follows. In Section 2, a brief description of this benchmark problem is provided. We briefly discuss the TITAN code in Section 3. Calculation results are presented in Section 4. Conclusions and future work are given in Section 5.

2. BENCHMARK DESCRIPTION

This benchmark includes 729 cases for a simple geometry 1-group problem as shown in Figure 1.

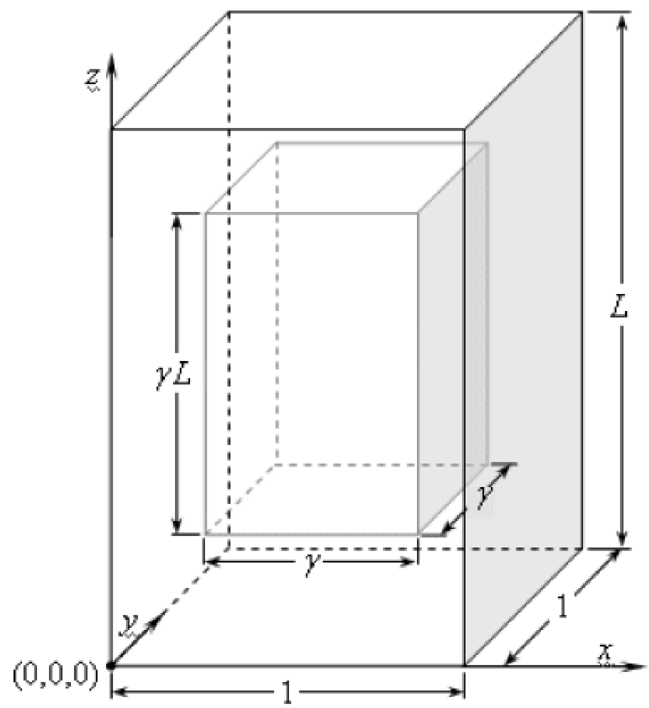

Figure 1. Geometric configuration of the benchmark problem.

A fixed source is located at (0,0,0) corner in this box-in-box model with two materials. The 729 cases are constructed by independently varying each of six variables, including L, γ, σ_1, c_1, σ_2, and c_2, where L is the height of the outer box, γ is the fraction of inner box height to the outer box. σ_1, c_1, σ_2, and c_2 are the total cross sections and scattering ratios for the two materials. Each variable has 3 possible values (see Table 1). Therefore, the total number of combinations is 729 cases (3^6=729). 23 quantities [10] are specified by the benchmark to report, numbering as 1.a, 1.b; 2.a to 2.h; and 3.a to 3.m. These quantities include some average fluxes at certain locations, and net leakage for some surfaces. The benchmark is designed to test the performance of a transport code over a broad range of parameter values, instead of just one set of input parameters.

Table I. Range of Parameters Comprising the Suite of Benchmark problem

Parameter	Possible Values		
L	0.1	1.0	5.0
γ	0.1	0.5	0.9
σ_1	0.1	1.0	5.0

c_1	0.5	0.8	1.0
σ_2	0.1	1.0	5.0
c_2	0.5	0.8	1.0

3. THE TITAN CODE

TITAN uses a hybrid S_N and ray-tracing method approach to solve the Linear Boltzmann Equation. TITAN allows user to choose a preferred method in a given region within the same problem model. Generally, ray-tracing method is used in low-scattering medium region, while S_N method is applied for the remainder of the model. In this benchmark, however, only TITAN's S_N solver is used. The scattering ratio parameter varies from 0.5 to 1.0 for the two materials used in this benchmark. While TITAN's characteristics solver is specially designed for low-scattering media. The S_N solver is more efficient for this problem model.

4. TITAN MODELING AND RESULTS

Figure 2 shows the TITAN model for this benchmark.

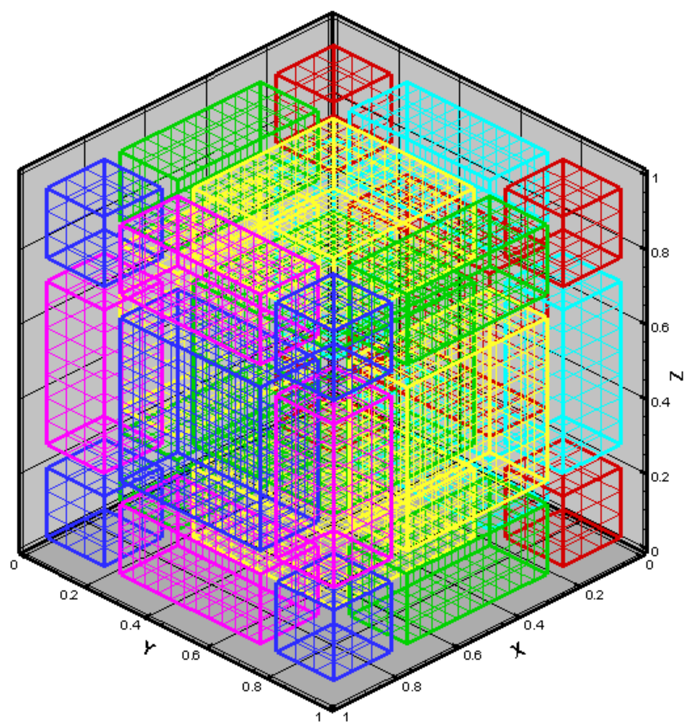

Figure 2. TITAN 3x3x3 coarse-mesh model of the benchmark problem

For all cases, the model has 3x3x3 coarse meshes. The inner box in Figure. 1 is represented by Coarse Mesh (2, 2, 2). The rest of the coarse meshes cover different regions within the outer box but outside of the inner box. The source region is located at Coarse Mesh (1, 1, 1). The coarse mesh boundaries are determined case by case by the variables L and γ. The number of fine meshes for each coarse mesh is also determined case by case based on the size of the individual coarse mesh and the material mean free path.

Due to the large number of cases, we wrote a Python script to drive the TITAN code to perform a batch run for all cases with the S_N method. Spatial meshing varies depending on the parameters of the individual case (L, γ, and mean free path). Our Python script automatically adjusts the mesh size in each region case by case. A control variable, called 'meshing factor,' can be specified in the script's input file. This factor allows users to adjust the overall number of meshes for each batch run. For example, the script will determine a total number of 1,728 meshes for Case 111111 if the meshing factor is 2, while a meshing factor of 3 will result in 5,832 meshes for the same case. Note that cases are numbered by six digits, with each digit representing the choice of three possible values for each variable (L, γ , σ_1 , c_1 , σ_2 , and c_2). Therefore, cases are numbered from 111111 to 333333, and Case 111111 denotes the case with L=0.1, γ=0.1, σ_1=0.1, c_1=0.5, σ_2=0.1, and c_2=0.5 (See Table I), while Case 333333 denotes the case with L=5.0, γ=0.9, σ_1=5.0, c_1=1.0, σ_2=5.0, and c_2=1.0.

The angular quadrature order is fixed for all cases. Based on our test run results, high order quadrature is not necessary for some c=1.0, or 0.8 and larger size cases. However, it is required for some low scattering cases to overcome the ray-effect. We performed two batch runs :

1. Serial run with Legendre-Chebyshev quadrature S_{50} (~2500 directions) and a meshing factor of 2. Number of total meshes ranges from 1,728 for Case 111111 to 22,400 for Case 333333
2. Parallel run (20 CPUs) with Legendre-Chebyshev quadrature S_{60} (~3600 directions) and a meshing factor of 3. Number of total meshes ranges from 5,832 for Case 111111 to 75,600 for Case 333333.

The benchmark requires the participant deterministic codes to calculate 23 quantities for each case. These quantities, numbered as 1.a, 1.b, 2.a to 2.h, and 3.a to 3.m, include some averaged scalar fluxes over some specific regions, and the net leakages through some specific surfaces. Detail specifications for each quantity can be found in Ref. 10. The benchmark also provides refined Monte Carlo solutions as reference. Instead of calculating these quantities in the Python script, we added a post-processing subroutine directly in the TITAN source code to evaluate these 23 quantities. Figure 3 shows the relative errors for Quantity 1.a for all cases compared to the Monte Carlo reference solution. Note that Quantity 1.a is the scalar flux averaged over the region in parallelepiped 1 not in 2. As shown in x axis of Figure 3, we also re-number all the cases from 1 to 729 as from 111111 to 333333.

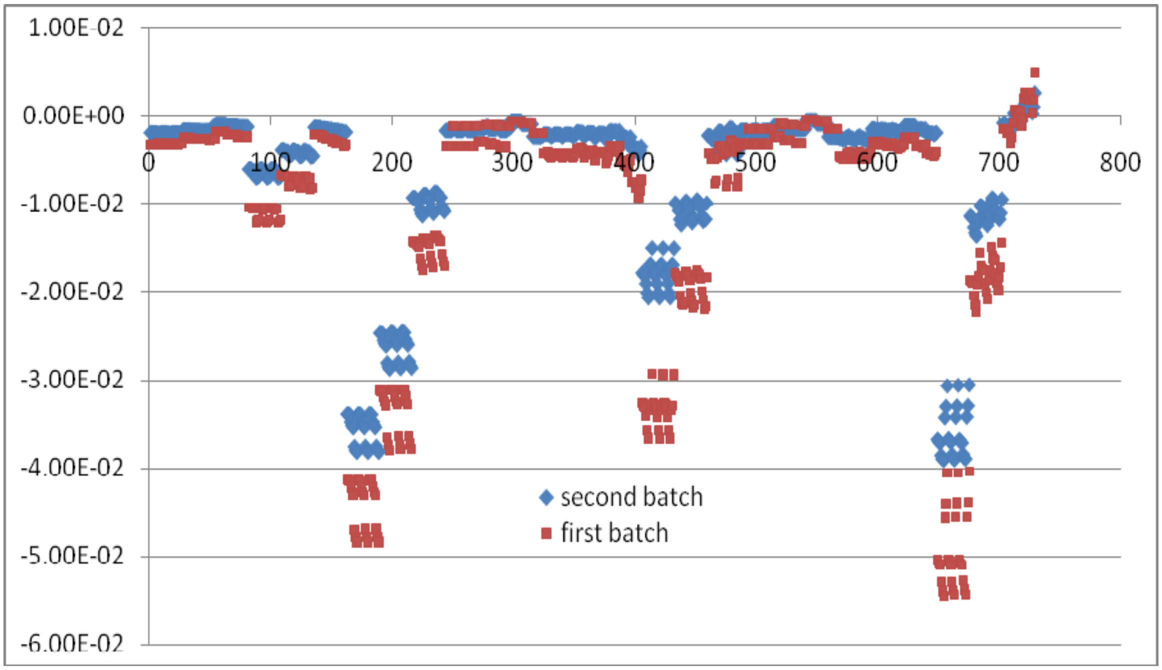

Figure. 3 TITAN to MCNP relative errors for Quantity 1.a for all cases.

Figures. 4 and 5 compare relative errors of Quantities 2.a and 3.a. Quantity 2.a the net leakage over the left boundary, and Quantity 3.a is averaged scalar flux over a fraction of the source region (coarse mesh 1)

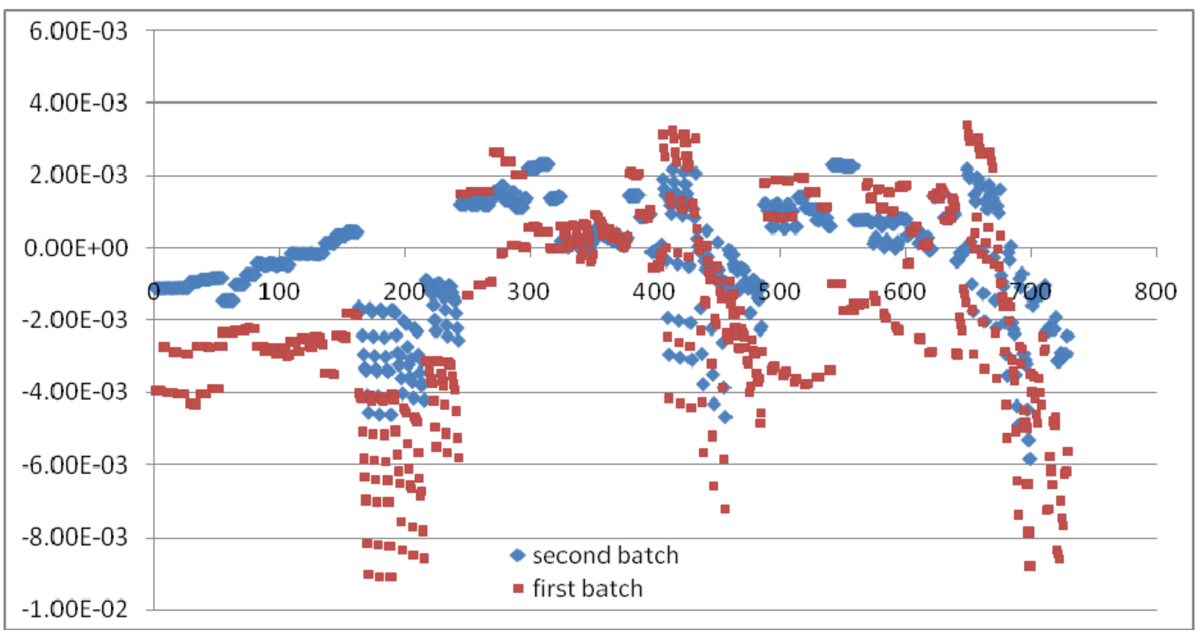

Figure. 4 Relative Difference between TITAN and MCNP for Quantity 2.a for all cases.

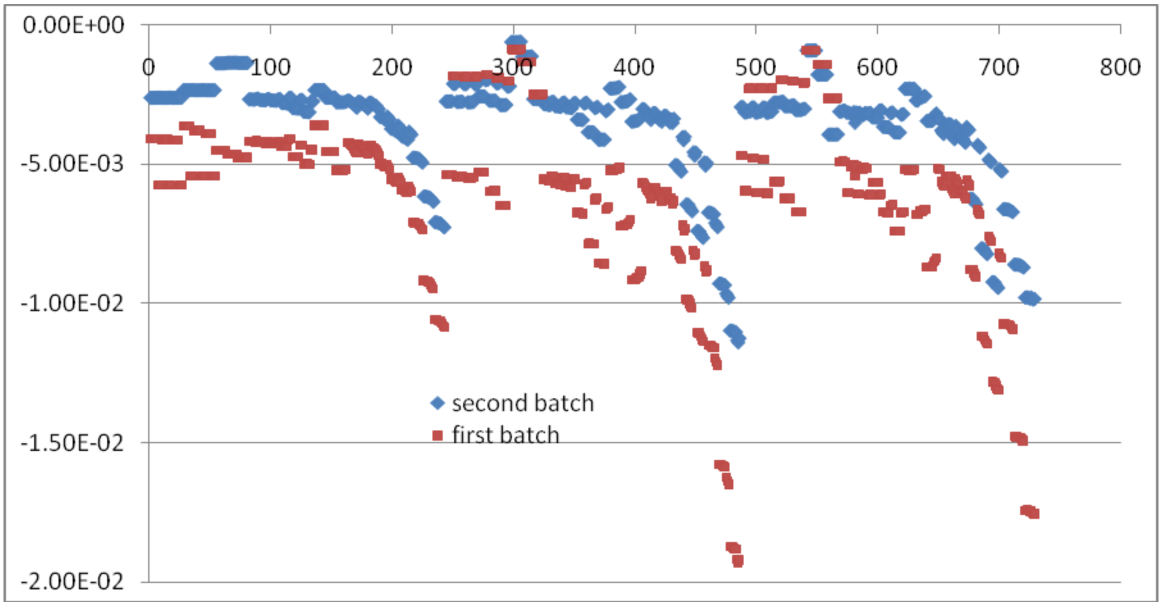

Figure. 5 Relative Difference between TITAN and MCNP for Quantity 3.a for all cases.

Figures 3, 4 and 5 show that the relative errors of Quantities 1.a, 2.a and 3.a for all the cases are below 5% comparing to the MCNP reference solution. Similar relative errors are observed for most of other quantities. The high quadrature order (S_{50} and S_{60}) we used in this benchmark contributes to the relatively high accuracy. We also noticed that the solutions for the second batch (Parallel run: quadrature order S_{60}; meshing factor 3) are improved compared to the first batch (Serial run: quadrature order S_{50}; meshing factor 2) because of the higher quadrature order and finer meshing for the second batch.

However, TITAN also experiences some difficulties at some quantities due to ray-effect for some cases. Among the worst quantities are 3.h and 3.i, which are the average fluxes at the corners far from the source region. Figures 6 and 7 compare the relative errors for Quantities 3.f and 3.i.

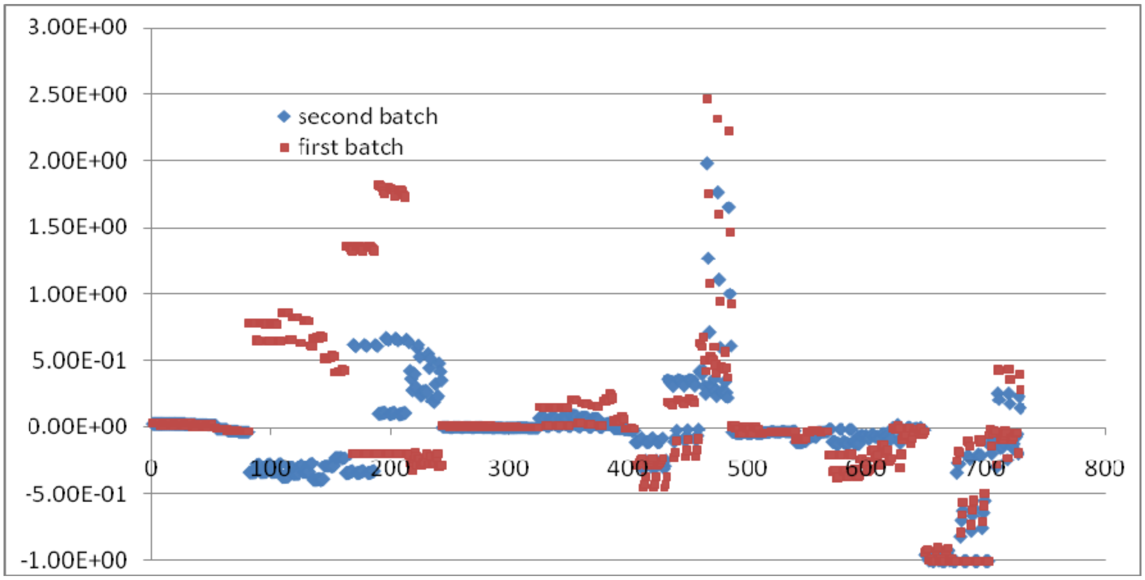

Figure. 5 Relative Difference between TITAN and MCNP for Quantity 3.h for all cases.

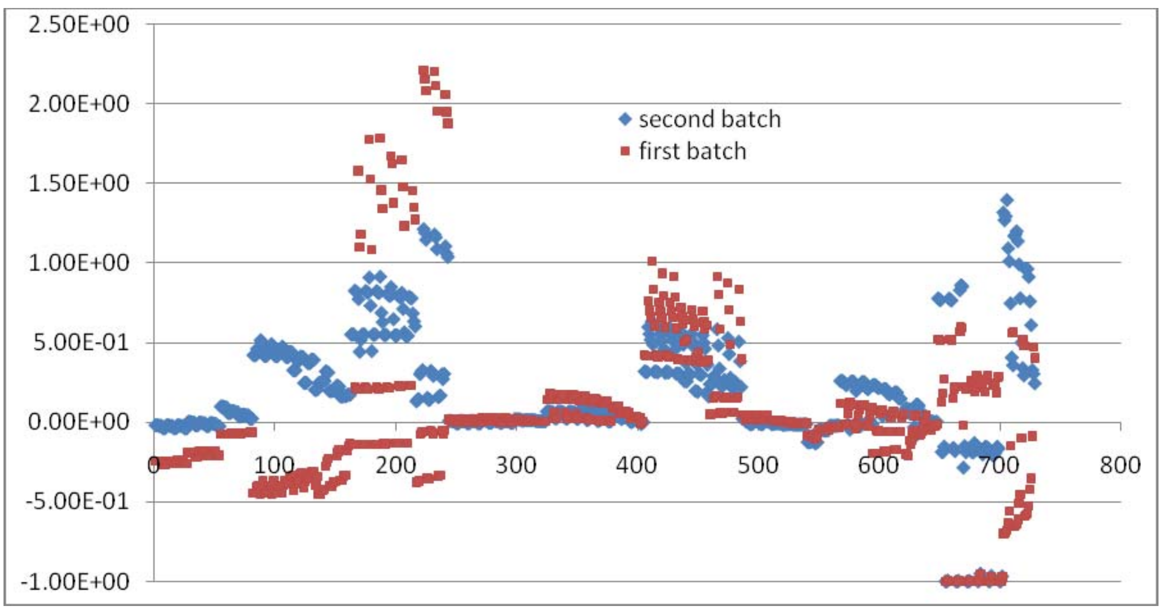

Figure. 5 Relative Difference between TITAN and MCNP for Quantity 3.i for all cases.

The largest differences occur for some cases in which the fluxes on the corners are ~7 orders of magnitude lower than in the source region. Table II compares the TITAN results (Second batch run) with the reference solution for Case 333333.

Table I. MCNP reference and TITAN comparison for Case 333333

Quantity	MCNP	MCNP Relative Error	TITAN	Relative Difference
1.a	6.90E-05	1.00E-04	6.92E-05	2.59E-03
1.b	1.08E-05	3.00E-04	1.12E-05	3.17E-02
2.a	-2.59E-04	1.00E-04	-2.58E-04	-2.43E-03
2.b	3.82E-06	3.00E-04	4.01E-06	4.93E-02
2.c	-1.00E-04	2.00E-04	-1.01E-04	5.91E-03
2.d	4.33E-12	4.00E-04	4.71E-12	8.84E-02
2.e	-7.72E-06	9.00E-04	-7.81E-06	1.07E-02
2.f	2.95E-06	6.00E-04	3.11E-06	5.37E-02
2.g	2.14E-05	6.00E-04	2.18E-05	2.17E-02
2.h	7.00E-12	8.00E-04	7.70E-12	9.98E-02
3.a	3.52E-02	2.57E-04	3.48E-02	-9.82E-03
3.b	5.33E-05	3.08E-04	5.44E-05	2.09E-02
3.c	9.69E-09	3.48E-04	1.01E-08	4.29E-02
3.d	6.67E-12	8.59E-04	8.25E-12	2.37E-01
3.e	4.44E-06	1.92E-03	4.37E-06	-1.51E-02
3.f	1.27E-06	1.04E-03	2.08E-06	6.37E-01
3.g	2.62E-12	1.07E-03	2.91E-12	1.09E-01
3.h	2.62E-12	1.08E-03	3.00E-12	1.48E-01
3.i	2.62E-12	1.08E-03	3.26E-12	2.44E-01
3.j	1.31E-05	3.16E-04	1.36E-05	4.07E-02
3.k	7.17E-06	3.05E-04	7.75E-06	8.03E-02
3.l	1.01E-08	3.52E-04	1.03E-08	2.62E-02
3.m	9.87E-09	3.50E-04	1.02E-08	3.56E-02

As shown in Table II, the fluxes for Quantities 3g, 3.h and 3.i are significantly lower. MCNP relative errors for these quantities are also larger than other quantities. The relative differences between TITAN and MCNP are worsened for these quantities as well.

5. CONCLUSIONS AND FUTURE WORK

We apply TITAN code to solve the OECD/NEA benchmark problem over a range of parameter space. Except for a small fraction of cases for certain quantities, the TITAN results in are in good agreement with the reference Monte Carlo predictions. Two batch runs are performed with the uniform quadrature order of S_{50} and S_{60}. High quadrature order is necessary for some cases to overcome the ray-effects and evaluate some quantities accurately. For some cases, accurate results may be acquired with much lower quadrature. We will continue to identify these cases. As we did for the spatial meshing, an adaptive quadrature order scheme could be applied on the case-by-case basis, instead of using the uniform high quadrature order for all cases. The large differences for some cases could be caused by ray-effects and numerical difficulties for certain quantities. We will further study these cases and investigate algorithms to improve the deterministic solution.

TITNA is written in FORTRAN 90 with some FORTRAN 2003 features. Object-oriented Programming paradigm (OOP) is applied in both S_N and characteristics solvers, and also in some transport calculation data structure, such as angular quadrature and spatial coarse meshes. With OOP, TITAN demonstrates an excellent scalability and high computational performance. The running time for the first batch is about ~30 hours on a single AMD Opteron processor 242 (1.6 GHz) for all 729 cases with a S_{50} quadrature. For the second run with higher quadrature order (S_{60}) and refined meshing, we used the new parallel version of TITAN with 20 CPUs. The wall clock time is ~ 5 hours. Currently, only source iteration scheme is used in TITAN. We also intend to implement efficient iteration acceleration techniques to further improve the code performance, especially for the pure scattering cases.

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