PHYSOR 2004 -The Physics of Fuel Cycles and Advanced Nuclear Systems: Global Developments
Chicago, Illinois, April 25-29, 2004, on CD-ROM, American Nuclear Society, Lagrange Park, IL. (2004)

PANDA Code Application to the OECD/NEA 2D/3D MOX Assembly Benchmark Calculations

Philippe Humbert*
Commissariat à l'Energie Atomique, 91680 Bruyères-le-Châtel, France

Panda is an all purpose dicrete ordinates transport code developed at CEA/Bruyères-le-Châtel. It is applied to stochastic neutronics applications like backward time dependent neutron number and count fluctuations or extinction probability calculations. The code can also be used for more conventional applications like the effective multiplication factor. It is based on a classic discrete ordinate (S_N) transport solver which can be used for 1D, 2D and 3D computations. In order to validate PANDA code in two and three spatial dimensions, benchmark computations are performed.

In this paper we present PANDA results on the international OECD/NEA C5G7 MOX benchmark. This test problem was designed by the expert group on 3D radiation transport benchmark of the OECD/Nuclear Agency in order to assess the ability of current deterministic transport codes to treat two and three dimensional core problems without homogenisation.

The obtained solutions seem to be not fully converged with regard to the MCNP reference solutions. Accurate solutions in 3D will require a high level of spatial and angular discretization leading to very expensive calculations in term of CPU time and memory usage

KEYWORDS : Deterministic Transport, Discrete Ordinates, Fuel Assembly Calculations, Benchmarks.

1. Introduction

In order to assess the ability of current deterministic transport codes to treat two and three dimensional reactor core problems without homogenisation, the expert group on 3D radiation transport benchmark of the OECD/Nuclear Energy Agency proposed the 2D/3D C5G7 MOX benchmark [5,6].

In this paper we present solutions of these benchmark problems obtained using PANDA code [1,2,3] which is a discrete ordinates transport code developped at CEA/Bruyères-Le-Châtel for stochastic neutronics and more conventional applications like eigenvalue problems.

After a brief description of the benchmark, PANDA code features and calculation conditions we will present the solutions obtained for the 2D and the 3D extension benchmark with the three rod insertion configurations.

2. Description of the C5G7 2D/3D MOX Fuel Assembly Benchmark

This benchmark was designed in order to test the ability of deterministic transport codes to treat reactor core problems without spatial homogenisation.

The problem is a quarter symmetric MOX/UO2 core surrounded by light water moderator. It consists of an array of 34x34 pins gathered in two MOX assemblies and two UO2 assemblies.

* Corresponding author, Tel.. 33(1)69-26-53-17, FAX 33(1)69-26-70-96, E-Mail: philippe-p.humbert@cea.fr

The benchmark was proposed in two-dimensional and three-dimensional versions (2-D/3-D C5G7 MOX). A new 3-D benchmark was proposed later with a reduced height and three levels of control rod insertion (3-D extension C5G7 MOX).

The benchmark specifications include the geometry and isotropic transport-corrected cross sections (7 energy groups).

The objectives of the benchmark are to calculate the effective multiplication factor and the normalized fission rates (pin power) distribution. A detailed description of the 2D/3D benchmark specifications and contributed solutions are presented in [5]. The 3D extension benchmark with control rods is specified in [6].

In the following we present solutions of the 2-D and 3-D extension C5G7 benchmarks using PANDA discrete ordinates neutron transport code.

3. Panda features

PANDA is a discrete ordinates general purpose code developed at CEA/Bruyères-le-Châtel. It is applied to standard deterministic calculations like k_{eff} and α eigenvalues, reactivity perturbations [3], static and time dependent source problems. Moreover it was also adapted to stochastic neutronics applications, the extinction/survival probabilities and the variance of the neutron number probability distribution [2] and stochastic neutron counting problems [3].

PANDA makes use of conventional deterministic neutron transport numerical methods. It is based on the multigroup S_N discrete ordinates method. One, two and three dimensional transport equations in cartesian and curvilinear coordinate systems are solved using orthogonal structured (regular) spatial meshes. The angular discretization uses S_N equi-weight quadratures and the anisotropic scattering is handled by Legendre expansion for neutron flux scattering cross sections.

Two methods can be used for effective multiplication factor calculations, the classic power iteration method and iterative eigenvalue extrapolation in an automatically adjusted interval. The eigenvalue computation can be accelerated using initial convergence on a coarse spatial mesh.

An integrated cartesian mesh generator is used for simple geometry modelling, for more complex problems we use the GIBI CAD [4] and the resulting mesh is projected on a regular grid with mixed cells produced at material boundaries.

PANDA is also a parallel code with energy group decomposition using the Message Passing Interface (MPI) library.

4. Calculation Conditions

The effective multiplication coefficient is computed using the power iteration method. The first outer iteration is composed of twenty inner iterations, then a maximum number of two inner iterations by outer is imposed. The eigenvalue and pin power calculation is converged when for two successive outer iterations, the global fission rate relative variation is less than 10^{-6}.

A simple multigrid eigenvalue acceleration method is used. The computation is performed on three successive embedded meshes. Each successive mesh is twofold refined in each direction using the previous eigenvalue and eigenvector as initial values. Typically this method reduces the number of outer iterations on the finest mesh by a factor ranging from 2 to 5. The number of outer iterations was 39 for the 2D problem and 113, 127, 145 for the three 3D problems.

The problems were run on CEA Tera system (HP alphaserver SC with DEC alpha EV68

1Ghz processors). Because energy decomposition is used, the number of processors is equal to the number of energy groups. For instance, a speed-up factor of 5.5 was obtained with the 2D problem with 306x306, S_{16} discretization.

5. Two-Dimensional Benchmark Results

A computer model of the benchmark was obtained using the PANDA integrated mesh generator which produces an XY orthogonal grid. For simplification the same spatial discretization was utilized on the whole reactor (square cells).

The benchmark is composed of seven materials : Moderator, UO2, three enrichments of MOX, guide tube and fission chamber. A colored map presenting these different materials is presented in figure 1. The lower and left boundaries are reflective. The core is a 34x34 fuel pin cell array.

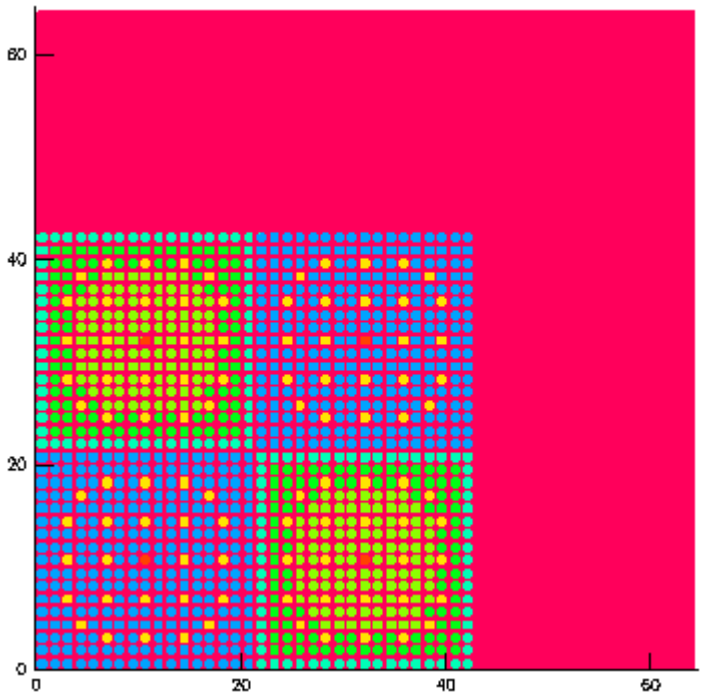

Fig.1 Material map for the 2-D C5G7 benchmark. Moderator (red), UO2 (dark-blue), MOX (light blue, light green, green), Guide Tube (Yellow), Fission Chamber(orange).

Each pin cell is composed of a centered circular fuel rod surrounded by light water moderator. The mesh generator does not represent the pin cell with a stair-stepped grid, mixed cells (homogenized cells) are produced at material boundaries. As can be seen on figure 2, the fraction of mixed cells decreases with mesh refinement.

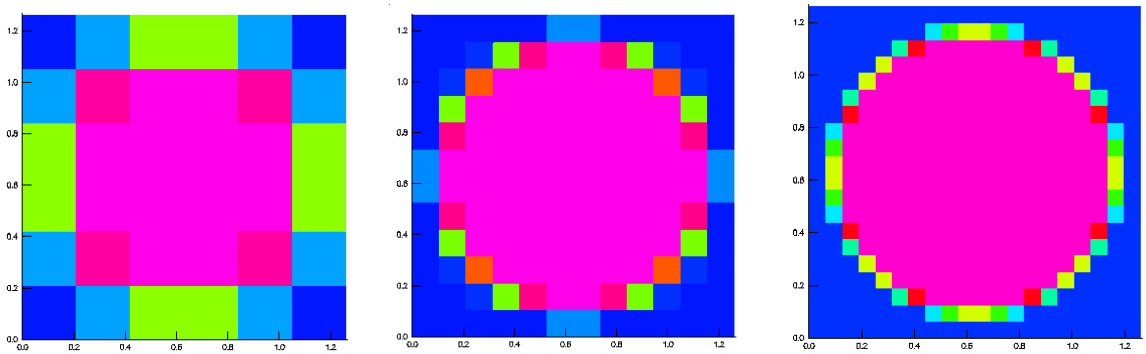

Fig.2 6x6, 12x12 and 20x20 lattice meshes. Pure fuel (Magenta), pure moderator (dark blue), other meshes are mixed material cells.

Several calculations were performed in order to investigate the effects of spatial and angular refinement. The spatial refinement level is the number of zones per dimension for a lattice cell. The angular refinement is given by the order N of the S_N quadrature (N(N+2)/2 angles). The effect on the effective multiplication factor of the assembly is given in figure 3. The spatial refinement increases from 4 to 16 for a fixed S_8 quadrature (red curve), the angular quadrature varies from 4 to 24 for a given level 6 spatial refinement (blue curve). These curves show that the eigenvalue is both sensitive to spatial and angular approximation with an opposite behavior. A convergent calculation requires a high level of angular and spatial refinement.

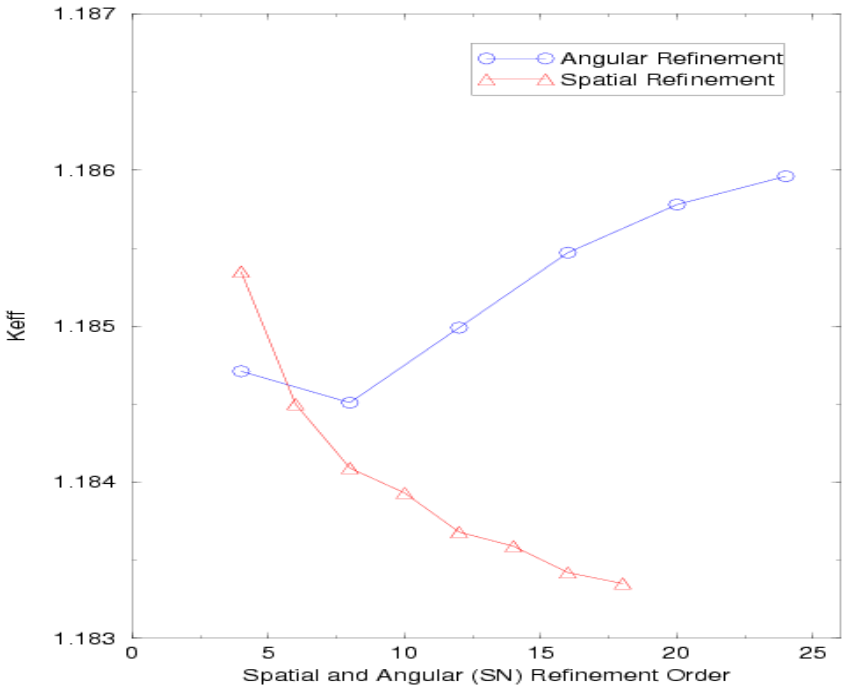

Fig.3 Keff eigenvalue versus angular and spatial discretization level.

The benchmark was calculated with PANDA using a 612x612 cartesian square mesh with a lattice cell size 12x12 and a S_{20} angular discretization (N(N+2)/2=220 angles). The eigenvalue and pin power results are summarized in table 1 and the pin power distribution is presented in figure 4.

Table 1 Eigenvalue and pin power reference and PANDA results for the 2-D C5G7-MOX benchmark.

C5G7 2-D	Reference **MCNP**	**PANDA** (612x612, S_{20})
CPU time		26mn 49s
K_{eff}	1.186550	1.185400
Maximum Pin Power	2.498	2.515
Minimum Pin Power	0.232	0.235
Inner UO2 Assembly Power	492.8	494.6
MOX Assembly Power	211.7	210.7
Outer UO2 Assembly Power	139.8	139.9

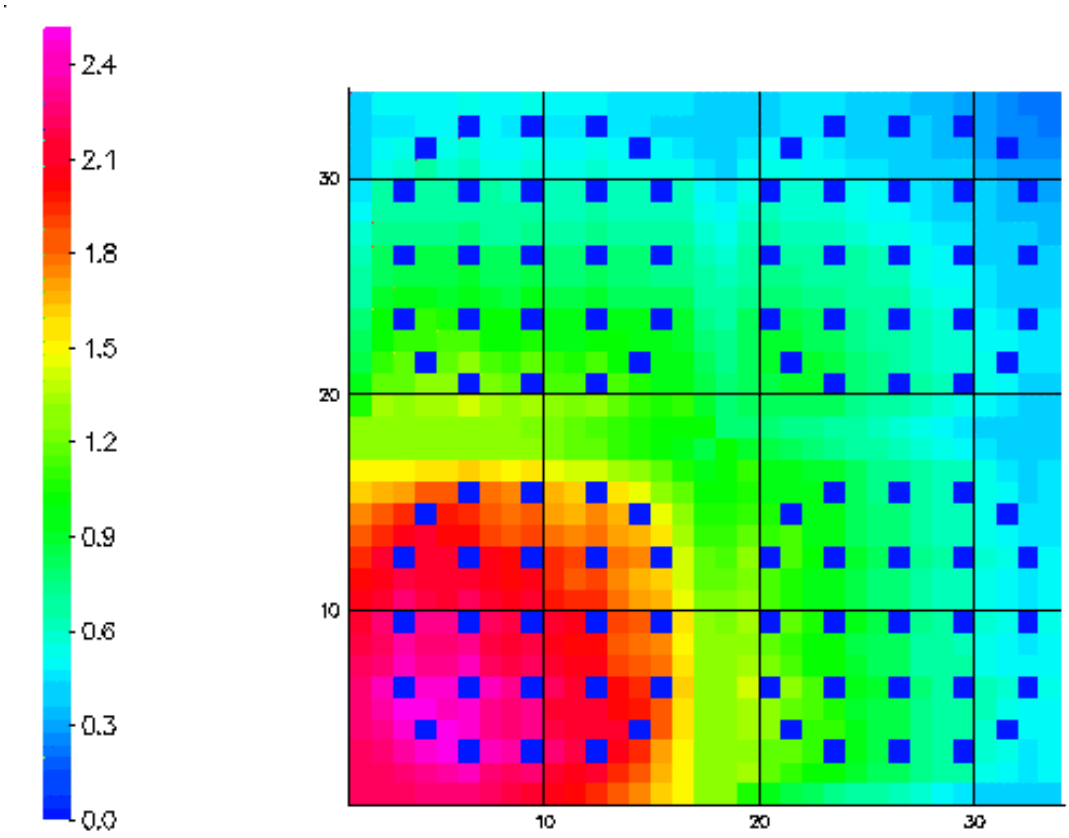

Fig. 4 Pin power map for the 2-D C5G7-MOX benchmark.

6. Three-dimensional Extension Benchmark Results

A computer model of the benchmark was obtained using the PANDA integrated mesh generator which produces an XYZ orthogonal grid. For simplification the same spatial discretization was utilized on the whole reactor.

Regarding the 3-D extension of the C5G7 benchmark it was difficult to investigate the sensitivities to spatial and angular approximations due to the computing time and memory requirements. For the presented solutions we used a 306x306x27 = 2 528 172 cells global mesh size with a 6x6x27 = 2187 cells lattice mesh size wit a S_{14} angular approximation (N(N+2)=224 angles).

The 3D geometry for the unrodded case is given in figure 5. The eigenvalue and pin power results corresponding to the three control rod insertion cases are summarized in table 2,3,4.

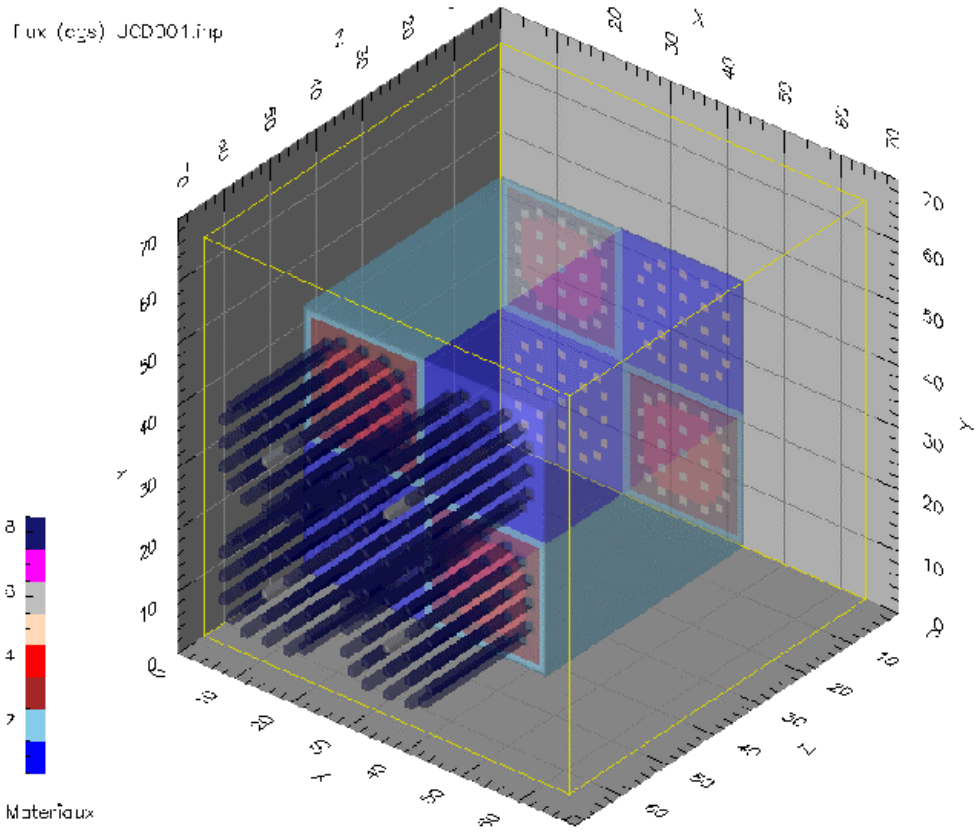

Fig.5 Unrodded 3D-EXT C5G7 geometry and materials.

Table 2 Eigenvalue and pin power reference and PANDA results for the 3-D extension C5G7-MOX unrodded benchmark.

C5G7 3-D Ext **Unrodded**	Reference **MCNP**	**PANDA** (306x306x27, S_{14})
CPU time		9h 51mn 25s
K_{eff}	1.143080	1.142040
Maximum Pin Power	2.481	2.517
Inner UO2 Assembly Power	491.21	494.76
MOX Assembly Power	212.70	211.70
Outer Assembly Power	139.39	139.05

Table 3 Eigenvalue and pin power reference and PANDA results for the 3-D extension C5G7-MOX rodded A benchmark.

C5G7 3-D Ext **Rodded A**	Reference **MCNP**	**PANDA** (306x306, S_{14})
CPU time		8h 51mn 34s
K_{eff}	1.128060	1.126720
Maximum Pin Power	2.253	2.282
Inner UO2 Assembly Power	461.18	464.11
MOX Assembly Power	221.71	220.27
Outer Assembly Power	151.39	151.36

Table 4 Eigenvalue and pin power reference and PANDA results for the 3-D extension C5G7-MOX rodded B benchmark.

C5G7 3-D Ext **Rodded B**	Reference **MCNP**	**PANDA** (306x306, S_{14})
CPU time		8h 43mn 31s
K_{eff}	1.077770	1.074970
Maximum Pin Power	1.835	1.846
Inner UO2 Assembly Power	395.43	395.57
MOX Assembly Power	236.62	235.63
Outer Assembly Power	187.34	189.17

7. Conclusion

In this paper we have presented the solutions of the 2D and 3D extensions C5G7-MOX OECD/NEA benchmarks obtained using PANDA discrete ordinates neutron transport code. The obtained solutions seem to be not fully converged with regard to the MCNP reference solutions. Accurate solutions will require a high level of spatial and angular discretization leading to very expensive calculations in term of CPU time and memory usage. Specifically, detailed 3D reactor deterministic calculations without spatial homogenisation will need massive parallel computation with phase space decomposition (spatial, angular and energy groups).

References

1) P. Humbert, “Stochastic Neutronics with PANDA Deterministic Code”, M&C 2003, Gatlinburg, TN, USA, April 6-10 (2003).
2) P. Humbert, “Neutron Noise Computation using PANDA Deterministic Code”, SNA 2003, Paris, France, September 22-24 (2003).
3) P. Humbert, B. Méchitoua, “Numerical Simulation of Caliban Reactivity Perturbation Experiments Using Neptunium-237 Samples”, Part I, M&C 2003, Gatlinburg, TN, USA, April 6-10 (2003), Part II, ICNC 2003, Tokai, Ibaraki, Japan October 20-24 (2003).
4) F. Axisa, “CASTEM 2000 – Opérateurs Généraux de Maillage (GIBI)”, Report CEA/DMT 96/498 (1996).
5) OECD/Nuclear Energy Agency, “Benchmark on Deterministic Transport Calculations Without Homogenisation”, NEA/NSC/DOC(2003)16.
6) M.A. Smith, G. Palmiotti, T.A. Taiwo, E.E. Lewis, N. Tsoulfanidis, “Benchmark Specification for Deterministic MOX fuel assembly Transport Calculations Without Spatial Homogenisation (3-D extension C5G7 MOX)” NEA/NSC/DOC(2003)6.