International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
Saratoga Springs, New York, May 3-7, 2009, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2009)

TWO-DIMENSIONAL WHOLE CORE TRANSPORT CALCULATIONS USING PARAGON

Vefa N. Kucukboyaci, Mohamed Ouisloumen, and Fausto Franceschini
Westinghouse Electric Company LLC
P.O Box 355, Pittsburgh, Pa, 15230-0355, USA
kucukbvn@westinghouse.com

ABSTRACT

PARAGON is Westinghouse's state-of-the-art code for two-dimensional lattice calculations. It is based on collision probability with interface current method and written entirely in FORTRAN 90/95 with dynamic memory allocation. As such, PARAGON provides great flexibility in increasing the problem size, mesh structure, and number of energy groups, hence the solution accuracy with respect to standard lattice codes. The purpose of this paper is to demonstrate the applicability of PARAGON to whole core simulations and to validate its theoretical models. A two-dimensional PWR core model has been developed and studies have been performed, investigating the effects of the coupling order of the interface current method. Results have been compared to those from continuous energy MCNP calculations, showing excellent agreement in both core reactivity and pin- and assembly-power distributions.

Key Words: PARAGON, Lattice Code, Collision Probability, Monte Carlo

1. INTRODUCTION

PARAGON [1] is Westinghouse's state-of-the-art two-dimensional lattice transport code. It is being used as part of Westinghouse's core design package, providing lattice cell data for three-dimensional core simulator codes. These data include macroscopic cross sections, microscopic cross sections for feedback adjustments, pin factors for pin power reconstruction calculations, and discontinuity factors for three-dimensional nodal method solution of the diffusion equation.

The PARAGON code was designed and written from its inception with flexibility in mind. It is based on collision probability and interface current coupling methods and has the ability to solve problems with any size of spatial, angular, and energy discretization. By taking advantage of the ever more powerful computing environment, PARAGON retains the design flexibility to improve the prediction accuracy and to expand its modeling capabilities to future concepts of reactor lattices and cores with complicated geometry designs.

This paper gives an overview of the calculations performed for a two-dimensional whole-core PWR model using PARAGON. Flexibility of PARAGON will be emphasized with its ability to run large problems with increasing coupling-orders of the interface current method and to demonstrate high accuracy in comparison to Monte Carlo calculations using the MCNP code [2].

2. METHODOLOGY

In this section, the PARAGON features that enable performing large scale transport theory calculations are discussed.

2.1. Solution Method

The flux solution in PARAGON is based on the interface current formalism using Collision Probability method within the cells. The flux at the surfaces is first discretized into a set of cones where the flux is independent of angular variables:

$$\psi_{\pm,\alpha}^{\rho\upsilon}\left(\vec{\Omega}\right)=\frac{1}{\sqrt{A_{\alpha}^{\rho\upsilon}}}H\left(\vec{\Omega}\in\vec{\Omega}_{\rho\upsilon}\right) \tag{1}$$

and $H\left(\vec{\Omega}\in\vec{\Omega}_{\rho\upsilon}\right)$ is the Heaviside distribution defined by:

$$H\left(\vec{\Omega}\in\vec{\Omega}_{\rho\upsilon}\right)=\begin{cases}1\ if\ \vec{\Omega}\in\vec{\Omega}_{\rho\upsilon}\ i.e.[\varphi,\theta]\in\left[\varphi_{\rho},\varphi_{\rho+1}\right]\times[\theta_{\upsilon},\varphi_{\upsilon+1}]\\0\ elsewhere\end{cases} \tag{2}$$

This leads to an arbitrary coupling order parameter that the user can control in the input. To enhance the accuracy of the solution, the user has also the ability to sub-divide the cylindrical regions into an arbitrary number of rings. The code also allows for a diagonal sub-division of regions. The resulting system of equations:

$$\begin{aligned}\phi_i &= \sum_{\alpha,\rho\upsilon} P_{is_\alpha}^{\rho\upsilon} J_{-,\alpha}^{\rho\upsilon} + \sum_j V_j P_{ij} F_j \\ J_{+,\alpha}^{\rho\upsilon} &= \sum_{\beta,\eta\mu} P_{s_\alpha s_\beta}^{\rho\upsilon\eta\mu} J_{-,\beta}^{\eta\mu} + \sum_i P_{s_\alpha i}^{\rho} F_i \\ J_{-,\alpha}^{\rho\upsilon} &= \sum_{\beta,\eta\mu} B_{\alpha\beta}^{\rho\upsilon\eta\mu} J_{+,\beta}^{\eta\mu}\end{aligned} \tag{3}$$

is solved by iterating on flux and currents using SOR (Successive Over Relaxation) method. Details of the methodology and the notation definitions can be found in Reference 3.

PARAGON library uses ENDF/B-VI as the source of the basic evaluated data. The standard library has 70 neutron energy groups (and 48 gamma energy groups), and explicit fission products. PARAGON is designed to accept any number of energy groups that is specified in the library. Recently, a cross-section library with an optimized energy group structure has been developed for PARAGON [4] to alleviate the prediction discrepancies due to self-shielding approximations in the standard multigroup libraries. This fine-energy group library has 6064 points with 5877 points spanning the resonance range. Albeit requiring large computational resources, PARAGON is able to perform calculations using this library for solving large problems, such as the whole core models.

2.2. Software Design Features of PARAGON

PARAGON provides modeling flexibility including exact cell geometry representation, with multiple regions (fuel pin, moderator, clad, etc.) and rings within each region, and variable cell pitch. The solution method permits flexibility in choosing the quality of the calculation by both

increasing the number of regions modeled within the cell and the number of angular current directions tracked at the cell interfaces.

PARAGON employs advanced numerical methods that reduce the computation time, such as taking advantage of the configuration symmetries to reduce the amount of calculations and data to store. A good example for that is the module of collision probability, where only necessary matrix elements are directly computed and others are obtained by symmetry, reciprocity relations and transformation laws. The code has a modern modular architecture and is written entirely in FORTRAN 90/95. The modularity of the code simplifies maintenance and implementation of new modules. By making full use of dynamic memory allocation, derived type structures, pointers, and data hiding, PARAGON can model large problems with many cells/regions, energy groups, and high angular coupling order without exhausting computational resources. The code is highly optimized for industrial applications that require accurate as well as fast lattice code calculations.

3. ANALYSIS

3.1. PARAGON and MCNP Two-Dimensional Whole Core Models

Figure 1 shows the 1/8 symmetry model of a representative PWR first core that was used for both PARAGON and MCNP calculations. The core consists of 17x17 fuel assemblies with enrichments ranging from 0.74 w/o to 4.8 w/o ^{235}U, varying intra-assembly enrichments, multiple types and arrangement of burnable absorbers. In particular, the Westinghouse Integral Fuel Burnable Absorber (IFBA) and the Wet Annular Burnable Absorber (WABA) were used. The core-and intra-assembly loading pattern used in the calculations present a challenging problem, beyond that is posed by a typical PWR core.

Beginning of Life (BOL) conditions were assumed for the core; therefore fresh fuel isotopics were prescribed in both PARAGON and MCNP models. The moderator was borated at a typical BOL value. Fuel, clad, and moderator temperatures were set at 900°K, 600°K, and 600°K, respectively. A cross-section library was generated at these temperatures for continuous energy MCNP to ensure consistency between the deterministic and Monte Carlo calculations.

Each fuel assembly was characterized in a detailed pin-by-pin definition, including IFBA/ WABA pins, and instrumentation and guide tubes, along with inter-assembly gaps. Note that for simplicity, the structural material outside the core region was ignored; the reflector region was modeled to include only the moderator.

Each fuel cell in the PARAGON model was refined using multiple equal-volume concentric rings to maximize accuracy in flux and pin-power predictions. Various coupling-orders, ranging from 3 to 9, were employed. Coupling-order signifies the number of interface currents on each PARAGON cell surface, coupling the cell to its neighbors. Overall, the PARAGON model is represented by a 143 x143 computational mesh super-lattice, resulting in a total of 10224 computational cells in two-dimensional geometry with diagonal symmetry. This is a significantly large model, as the total number of currents that PARAGON calculates reaches ~25.8 million, considering 10224 cells, coupling-order of 9, and 70 energy groups.

The MCNP model represents identical geometry and sub-structures. Simulations used sufficiently large number of cycles, particles per cycle, and discarded initial cycles. A point source in each fuel pin was provided as a detailed initial source distribution. The combination of these parameters maximized the precision of the Monte Carlo results, both in eigenvalue predictions and pin-power distributions. As a result, the effective multiplication factor (k_{eff}) was predicted within ±0.00006 (6 per cent mille [pcm]) uncertainty and the maximum Monte Carlo error on the pin-power tallies was less than 1%, which was adequate to enable consistent comparisons with the PARAGON results.

3.2. Results

The reference continuous energy Monte Carlo calculation resulted in an effective multiplication factor (k_{eff}) of 1.00027 (±0.00006). Results from PARAGON with the standard 70-group library deviated from the reference solution by at most 149 pcm. Table I shows k_{eff} values calculated by PARAGON using different coupling-orders. It was determined that for this large problem, coupling-order 3 did not produce a reactivity prediction at the desired accuracy level. Coupling orders 5 and above, however performed well. This is an expected outcome because of the large reflector region [3].

Another parameter of interest in core calculations is the *peaking factor*, referred to here as the pin with the highest relative power. As seen in Table I, PARAGON prediction with coupling-order of 5 is already very good, and higher orders produce excellent results, within <1% of the reference solution. Not only the magnitude but also the location of the peaking factor is of great importance in core calculations, and PARAGON performed remarkably well also in that regard.

Figure 2 shows the pin-power distribution calculated by PARAGON using the standard 70-group library and a coupling-order of 9. In this problem, pins with high powers are clustered around the assembly center and pins close to the inter-assembly gaps had relatively low powers. Pin-power tended to taper off towards the periphery of the core due to leakage. As expected, assemblies with highly-enriched fuel pins had the highest relative pin-powers. A very similar pin-power distribution was observed from the Monte Carlo calculations.

Figure 3 shows the percent difference between MCNP and PARAGON pin power distributions. Note that the percent difference was determined using the following expression:

$$\left(\frac{PinPower_{MCNP} - PinPower_{PARAGON}}{PinPower_{MCNP}} \right) \bullet 100 \qquad (4)$$

As seen in Figure 3, the differences are evenly distributed throughout the core, with the exception of the core (low-power) peripheral assemblies. For the remaining assemblies, the differences are evenly distributed around zero, indicating no bias in the PARAGON prediction. The discrepancy in power-distribution is generally less than 2%, with the larger discrepancies occurring in the low-enriched, typically low-power pins. Moreover, PARAGON predicts the magnitude and the location of the peak power quite accurately.

Fuel pins at the south-periphery facing the reflector region shows the largest discrepancy (up to -4.7%). We believe that this is due to limitations of the self-shielding treatment of the fuel pin cross-sections for these peripheral cells. The large moderator cells in the nearby reflector region may have contributed to incorrect prediction of the resonance absorption, when self-shielded cross-sections were generated for these cells. This would lead to over-prediction of the PARAGON pin-powers relative to continuous energy MCNP, as observed. Another potential contributor to this discrepancy might be an inadequate Monte Carlo convergence in these peripheral cells. Further investigation towards the resolution of these discrepancies is underway.

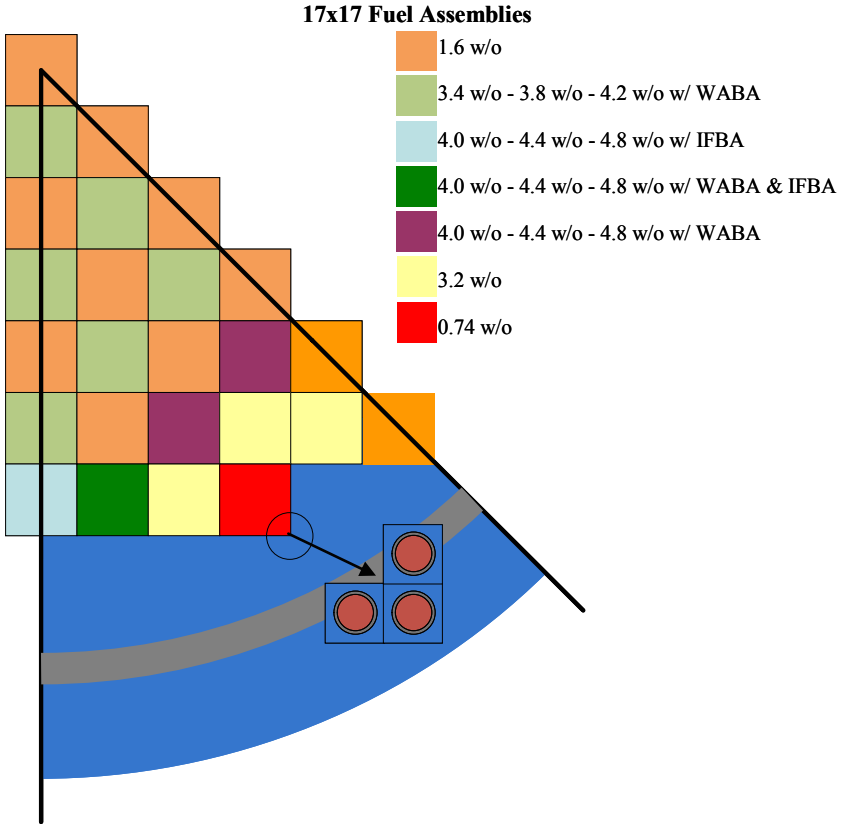

Figure 1. PWR Core Model Used in the Calculations

Table I. Summary of Core Reactivity and Peak Power Comparison between MCNP and PARAGON

	Coupling Order	k_{eff}	Δk_{eff} (pcm)	Peak Power	Peak Power Discrepancy (%)
MCNP	**-**	1.00027± 0.00006	-	1.800	-
PARAGON	**3**	1.00176	-149	1.913	6.28
	5	0.99990	37	1.828	1.56
	7	0.99895	132	1.783	0.944
	9	0.99891	136	1.785	0.833

Table II. Summary of Pin-Power Differences between MCNP and PARAGON

Coupling Order	Max. / Min. Discrepancy (%)	RMS Discrepancy (%)
3	6.2/-4.1	1.086
5	2.3/-4.5	0.668
7	2.2/+-4.7	0.666
9	2.2/-4.7	0.672

Table II presents a summary of the pin-power comparison. As mentioned above, the more negative percent discrepancy occurs in the peripheral region facing the south reflector. Looking at the core average values for the pin-power discrepancy, the RMS (Root Mean Square) value indicates that PARAGON and MCNP results are within less than 1%. Note that the MCNP results include ~±1% calculational uncertainty. We can then conclude that MCNP and PARAGON pin powers are within ~2% with a 99% confidence level.

Finally, in Table III, we present a comparison of the assembly average power distributions. As expected from the pin-power prediction, PARAGON results are quite favorable. The discrepancy in assembly power, MCNP vs. PARAGON, is between +0.9/-1.2%. It is important to note that PARAGON predicts the magnitude and the location of the 'hot-assembly' (i.e., the assembly with the highest power) in virtually perfect agreement with MCNP, establishing further confidence in the deterministic predictions from an operational and safety point-of view.

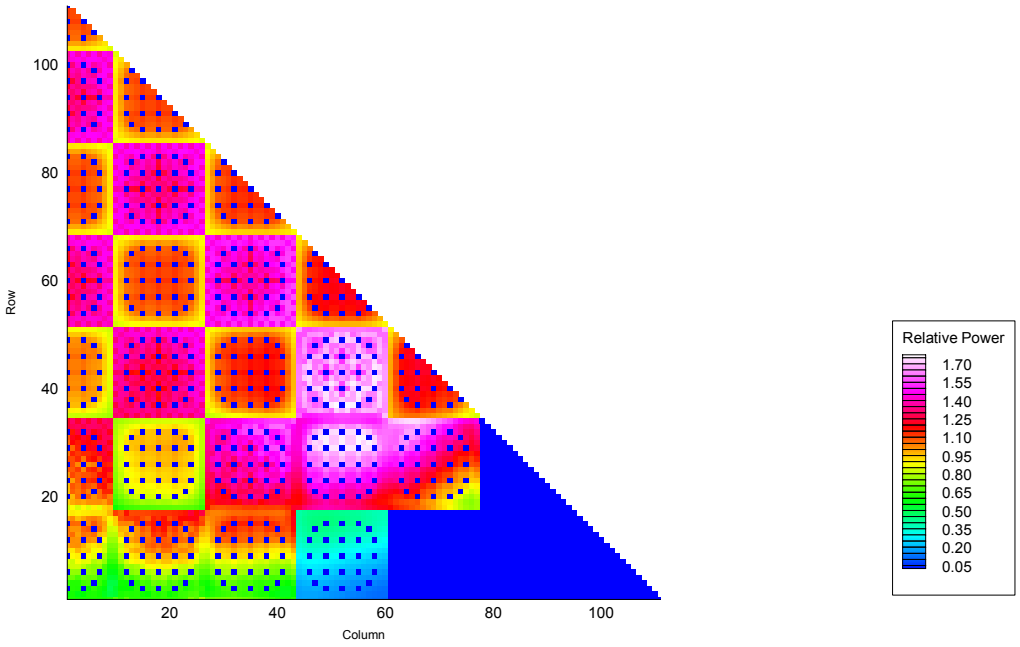

Figure 2. Whole Core Relative Pin-Power Distribution as Calculated by PARAGON

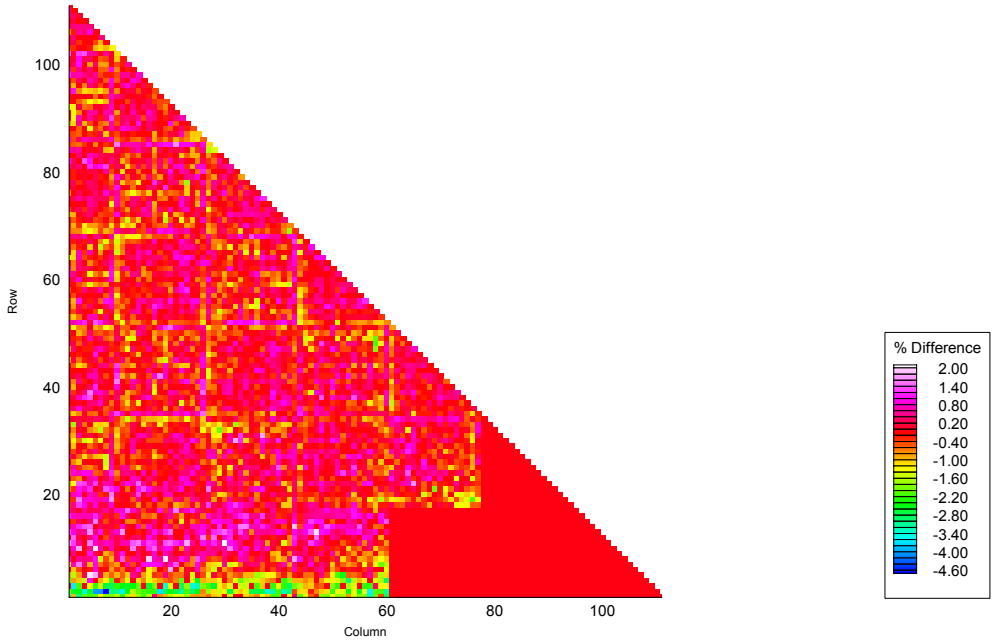

Figure 3. Percent Difference in Relative Pin Power between MCNP and PARAGON Calculations

Table III. Summary of Assembly-Power Differences between MCNP and PARAGON

PARAGON Power MCNP Power [Discrepancy (%)]				
1.026 1.032 [0.59]				
1.398 1.387 [-0.82]	1.027 1.029 [0.15]			
1.026 1.025 [-0.07]	1.412 1.400 [-0.88]	1.049 1.053 [0.39]		
1.377 1.361 [-1.20]	1.025 1.026 [0.10]	1.459 1.451 [-0.57]	1.102 1.109 [0.63]	
0.961 0.961 [0.09]	1.349 1.339 [-0.78]	1.061 1.068 [0.64]	1.648 1.648 [-0.02]	1.111 1.122 [0.93]
1.135 1.131 [-0.36]	0.872 0.877 [0.54]	1.379 1.381 [0.16]	1.523 1.536 [0.80]	1.281 1.283 [0.19]
0.824 0.823 [-0.06]	0.890 0.890 [0.04]	0.885 0.887 [0.33]	0.292 0.295 [0.91]	

Overall, for this large and complex problem, PARAGON was able to produce both global (k_{eff}) and local (pin-power) results with excellent accuracy. Further improvements should be expected in the future by using a fine-energy group cross-section library or better self-shielding treatment.

4. SUMMARY and CONCLUSIONS

We have performed two-dimensional whole-core calculations using the PARAGON code with 70 energy groups and benchmarked the results against continuous energy Monte Carlo calculations. The two major outcomes of this study are: 1) the PARAGON code, developed for standard assembly/lattice calculations, is capable of performing large-scale and complex simulations, including whole core geometry; and 2) PARAGON can accurately predict the core reactivity and pin-power distribution. The design features of PARAGON, written entirely in FORTRAN 90/95 with dynamic memory allocation, provide great modeling flexibility in setting up models of any size, dimension, and energy groups, and result in excellent accuracy when compared to Monte Carlo calculations.

Also, the recently developed ultra-fine energy group cross-section library, with 6064 energy groups, is being utilized to predict the core reactivity and pin-power. It is expected that this fine-group library, which altogether by-passes the self-shielding methodology will lead to even more accurate PARAGON predictions.

REFERENCES

1. Ouisloumen M., et al., "PARAGON: The New Westinghouse Assembly Lattice Code," *Proceedings of the ANS International Meeting on Mathematical Methods for Nuclear Applications*, Salt Lake City, Utah, USA (2001).
2. X-5 MONTE CARLO TEAM, "MCNP — A General Monte Carlo Particle Transport Code, Version 5," LA-UR-03-1987, Los Alamos National Laboratory (April 2003).
3. Ouisloumen M., et al., "The Two-Dimensional Collision Probability Calculation in Westinghouse Lattice Code: Methodology and Benchmarking", *International Conference on the Physics of Reactors,* Mito, Japan, (1996).
4. Huria, H. and M. Ouisloumen, "An optimized ultra-fine energy group structure for neutron transport calculations*," International Conference on the Physics of Reactors,* Interlaken, Switzerland, (2008).