FORM TI-12
08/2007

B-T-3711

CALCULATION OF ACCURATE HEXAGONAL DISCONTINUITY FACTORS FOR PARCS

Justin Pounders[1], Bernard Bandini[2], and Yunlin Xu[3]

[1]Georgia Institute of Technology, Atlanta, GA
[2]Bettis Atomic Power Laboratory, West Mifflin, PA
[3]Purdue University, West LaFayette, IN

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Justin Pounders
Georgia Institute of Technology
Atlanta, GA

Bernard Bandini
Bettis Atomic Power Laboratory
West Mifflin, PA

Yunlin Xu, Thomas Downar
Purdue University
West Lafayette, IN

Abstract

In this study we derive a methodology for calculating discontinuity factors consistent with the Triangle-based Polynomial Expansion Nodal (TPEN) method implemented in PARCS for hexagonal reactor geometries. The accuracy of coarse-mesh nodal methods is greatly enhanced by permitting flux discontinuities at node boundaries, but the practice of calculating discontinuity factors from infinite-medium (zero-current) single bundle calculations may not be sufficiently accurate for more challenging problems in which there is a large amount of internodal neutron streaming. The authors therefore derive a TPEN-based method for calculating discontinuity factors that are exact with respect to generalized equivalence theory. The method is validated by reproducing the reference solution for a small hexagonal core.

1. Introduction

Solving the neutron diffusion equation with high spatial resolution can become very computationally intensive at the geometrically detailed full-core level. An alternative to this approach is to subdivide the reactor core into homogenized nodes where each node usually corresponds radially to a single fuel assembly. One gains the advantage of reducing the number of spatial meshes in the problem but is faced with the disadvantage of poor spatial resolution and high discretization errors associated with large meshes. To compensate for these disadvantages higher fidelity nodal updates are applied periodically during the coarse mesh iterations. The nodal updates improve upon the coarse mesh solution by generating spatial expansions of the neutron flux within each node. These local expansions are used to force a higher order of accuracy on the global solution through the use of corrective coupling coefficients.

The homogenized nodal cross sections are computed so that reaction rates are conserved, but it has been shown that there are insufficient degrees of freedom to simultaneously conserve reaction rates, leakages and the multiplication eigenvalue [1]. Generalized equivalence theory (GET) solves this problem by introducing additional degrees of freedom at node boundaries.

Specifically, the scalar neutron flux of the homogenous calculation is allowed to be discontinuous at node interfaces. The discontinuities are prescribed such that the heterogeneous neutron flux (i.e. the flux solution without homogenization) is made continuous at the boundaries. This condition can be written

$$\phi_{g,hom}^{m,s} f_g^{m,s} = \phi_{g,hom}^{n,s} f_g^{n,s}$$

where $\phi_{g,hom}^{n,s}$ is the group g homogenous scalar flux on bounding surface s of node n. The discontinuity factor can therefore be defined

$$f_g^{n,s} = \frac{\phi_{g,het}^{n,s}}{\phi_{g,hom}^{n,s}} . \tag{1}$$

In general, the heterogeneous flux will not be known. A common approximation is to perform an infinite medium (zero-current) calculation of a single node using an accurate transport method and use this result as an approximation to the heterogeneous solution [1]. In this case, the homogenous flux is spatially flat, and the discontinuity factor can be expressed as the ratio of the surface average heterogeneous flux to the node average heterogeneous flux. The zero current approximation may not produce accurate nodal parameters in some cases, such as in small reactor problems with significant internodal streaming. Also, in benchmarking applications it may be desirable to avoid the zero-current approximation solely to isolate errors arising from other aspects of the methodology.

To avoid the zero-current approximation one must compute reliable values of both the heterogeneous and homogenous surface fluxes for all nodal interfaces in the core. If we assume that the reference heterogeneous solution is known, one must only compute the homogenous solution and Equation (1) can be solved exactly. The methodology for computing the homogenous flux in the denominator of Equation (1) must be consistent with the methodology that will be used in the calculation of the global homogenous solution and will therefore be unique for different nodal methodologies. In the current study the authors derive such a methodology for the Triangle-based Polynomial Expansion Nodal (TPEN) [2] method, which is the hexagonal method employed by the Purdue Advanced Reactor Core Simulator (PARCS) [3]. A brief overview of important elements from the TPEN methodology is presented in the following section, followed by the derivation of a method capable of calculating discontinuity factors for TPEN-based nodal reactor calculations. Finally, we use the new methodology to compute discontinuity factors for a small example problem and compare our nodal results with the reference heterogeneous solution.

2. TPEN Methodology

The underlying theory of the TPEN methodology is documented [2-4], so this section will provide only a brief overview, emphasizing certain aspects that are important for the derivation presented in the next section.

In TPEN, 2D hexagonal nodes are subdivided into six triangular domains. The scalar flux is expanded within each triangular domain by a nine-term, third order polynomial:

$$\phi_g^m(x, y) = c_{g0}^m + a_{gx}^m x + a_{gy}^m y + b_{gx}^m x^2 + b_{gu}^m u^2 + b_{gp}^m p^2 + c_{gx}^m x^3 + c_{gu}^m u^3 + c_{gp}^m p^3$$

where x, u, and p are the local coordinates normal to the three triangle surfaces. The x direction is normal to the surface corresponding to the outer surface of the hexagon, while u and p are normal to the inner surfaces:

$$u = -\frac{1}{2}x - \frac{\sqrt{3}}{2}y$$

$$p = -\frac{1}{2}x + \frac{\sqrt{3}}{2}y$$

The flux expansions for each of the six triangles can be coupled and written as a sparse linear system for which there is an efficient algebraic solution. The boundary conditions for this system are the incoming partial currents along each of the exterior hexagonal surfaces and the point fluxes at each of the hexagon's six corners. The incoming partial currents can be computed by

$$j_g^{inc,m,k} = \frac{1}{4}\phi_{g,hom}^{m,k} - \frac{1}{2}J_g^{m,k} \tag{2}$$

where the surface averaged flux and current are written, respectively,

$$J_g^{m,k} = -\tilde{D}_g^{mn}(\bar{\phi}_g^n - \bar{\phi}_g^m) - \hat{D}_g^{mn}(\bar{\phi}_g^n + \bar{\phi}_g^m) \tag{3}$$

$$\phi_{g,het}^{m,k} = \left(\frac{D_g^n}{D_g^m + D_g^n}\right)\bar{\phi}_g^n + \left(\frac{D_g^m}{D_g^m + D_g^n}\right)\bar{\phi}_g^m + \hat{\alpha}(\bar{\phi}_g^n + \bar{\phi}_g^m) \tag{4}$$

where surface k is the coincident surface between nodes m and n, and $\bar{\phi}_g^m$ is the group g node-averaged flux in node m. The factors $\hat{D}$ and $\hat{\alpha}$ are corrective coupling coefficients updated after each TPEN nodal iteration, calculated by solving Equations (3) and (4) using updated values of the surface current and flux. Note that the surface flux given by Equation (4) has been denoted the heterogeneous flux. This is because this value of the flux is identical for both nodes m and n, implying a continuity of flux at this surface which, in turn, means that this value should converge to the heterogeneous value of the flux. Equation (2) can be rewritten in these terms by

$$j_g^{inc,m,k} = \frac{1}{4}\phi_{g,hom}^{m,k}\left(\frac{\phi_{g,het}^{m,k}}{\phi_{g,het}^{m,k}}\right) - \frac{1}{2}J_g^{m,k}$$

$$= \frac{1}{4}\phi_{g,het}^{m,k}\left(f_g^{m,k}\right)^{-1} - \frac{1}{2}J_g^{m,k}. \tag{5}$$

In addition to the incoming current, the corner point fluxes are needed to compute the TPEN solution. There is not a straight forward way of computing these values using corrective coefficients like in Equations (3) and (4), so another approach must be taken. In PARCS, the corner points of all nodes in a given plane are coupled using a corner point balance. The corner point flux for each node is computed by expanding the intra-hexagonal flux in a 13-term polynomial whose coefficients are expressed in terms of the node averaged flux, 6 surface averaged fluxes and 6 corner point fluxes. The node averaged fluxes are assumed to be known from the coarse mesh calculation, and the surface averaged fluxes are computed by Equation (4), which should again be multiplied by the inverse of the discontinuity factor to yield the homogenous surface flux. This leaves only the 6 corner point fluxes as unknowns. The resulting corner point system of linear equations is strongly diagonally dominant and efficiently solved by a Gauss-Seidel method.

3. Calculation Of Discontinuity Factors

Our goal is to compute exact discontinuity factors defined by Equation (1). If we assume that the heterogeneous reference solution is known, then the numerator of the right hand side of Equation (1) should also be known. The remaining task is therefore to compute the homogenous solution. This can be done by solving the TPEN system of equations for each node in the core given boundary conditions from the reference solution. As was shown in the previous section, however, the boundary conditions to the TPEN problem, both the incoming partial current and the corner point fluxes, depend on the homogenous surface flux and therefore require *a priori* knowledge of the discontinuity factors.

3.1. Reformulation of TPEN boundary condition

In order to solve the TPEN "1-node" problem for the homogenous surface flux, the boundary condition must be changed to a quantity that will be preserved between the heterogeneous and homogenous problems and can therefore be taken directly from the reference solution. In the current study this is accomplished by replacing the incoming partial current with the surface net current by making the substitution

$$j_g^{inc,m,k} = j_g^{out,m,k} - J_g^{m,k} \;. \tag{6}$$

The outgoing partial current is already an unknown in the TPEN system, and the net current is taken from the reference solution. This substitution has the advantage of not changing the structure of the TPEN linear system, so the same efficient algebraic solver can be used with only slight modification to the matrix coefficients.

3.2. Corner point solution methodology

In the original TPEN methodology, the corner point fluxes were determined from a linear system expressed in terms of node average fluxes and (homogenous) surface fluxes. A new approach must now be taken since the homogenous surface fluxes are not known from the reference solution. One possible solution is to derive the polynomial expansion coefficients in terms of net surface currents instead of surface fluxes. This new formulation, however, results in a linear

system which is no longer diagonally dominant and is also unstable. Since the same methodology must be used when generating discontinuity factors as when generating the final nodal solution, the PARCS implementation of the corner point solver would also need modification. Replacing the efficient solver currently in PARCS with a less stable one is undesirable.

An alternative approach is to determine the discontinuity factors by iterating between the TPEN and corner point solvers. This approach has the advantage of maintaining the numerical benefits of the original formulation and avoiding modification of PARCS. An algorithmic description of the iterative process follows, where $f^{(n)}$ is the set of discontinuity factors at the nth iterate and $\phi_{hom}^{(n)}$ is the set homogeneous surface fluxes at the nth iterate:

1. $f^{(0)} = 0, f^{(1)} = 1,$

2. $n = 1, \rho = 1$

3. While $(\rho > \varepsilon)$

   a) Solve corner point system for current plane with $f^{(n)}$

   b) For each node in the plane,

      solve TPEN with net current BCs $\rightarrow \phi_{hom}^{(n)}$

   c) $f^{(n+1)} = \dfrac{\phi_{g,het}}{\phi_{g,hom}^{(n)}}$ for all surfaces

   d) $n = n+1$

   e) $\rho = \max_i \left[\dfrac{f_i^{(n)} - f_i^{(n-1)}}{f_i^{(n-1)}} \right]$

The convergence properties of this method have not been rigorously demonstrated. In the following example problem, it was observed that the iterations produced negative corner point and surface fluxes in some areas of the core with steep flux gradients. In order to aid convergence and ensure a physical solution, limits were placed on the possible values of discontinuity factors. For the problem that follows, the maximum allowable discontinuity factor was set to 4. This prevented the non-converged homogenous surface fluxes from becoming too small. It was observed that the solution changed very little when the maximum discontinuity factor was limited between 3 and 8. When this limit was greater than or equal to 9 the PARCS solution would not converge. When the limit was less than 2 the discontinuity factors did not allow enough freedom in the homogenous solution to produce accurate solutions. The convergence tolerance, ε, was set to 10^{-8}.

4. Results

The above methodology was tested in two dimensions and two groups on a small problem with 19 fissile nodes and a water reflector. A fine-mesh diffusion solution was generated with the PDQ diffusion theory code to provide the heterogeneous reference solution ($k_{eff} = 0.989403$). PARCS was used to generate the nodal diffusion solution both with and without discontinuity

factors developed by the above method. A nodal solution was also generated for comparison using the hexagonal nodal expansion method (NEM) from NESTLE [5]. Table I gives the effective multiplication errors in pcm [10^{-5}] and summarizes the nodal power errors in terms of the root-mean-square error (RMS), mean-relative error (MRE), maximum error (MAX) and error at the node of highest power. Note that the NESTLE solution was generated without discontinuity factors, since a methodology for computing discontinuity factors consistent with NEM in hexagonal geometry has not been derived.

TABLE I. Solution Comparison

	NESTLE (NEM)	PARCS (TPEN) w/o DF	PARCS (TPEN) w/ DF
$\Delta keff$	-3016 pcm	865.4 pcm	0.208 pcm
Power, RMS	3.30%	2.91%	0.02%
Power, MRE	2.85%	1.75%	0.01%
Power, MAX	7.23%	8.59%	0.05%
Max Power	2.02%	0.85%	0.003%

As shown in the table, adding discontinuity factors to the PARCS nodal calculation reproduced the reference solution almost exactly.

5. Conclusions

We have described a methodology for generating assembly discontinuity factors for hexagonal reactor calculations that is capable of reproducing the reference solution. This methodology is certainly useful for benchmark calculations. It would be insightful for future studies to investigate the sensitivity of these discontinuity factors to their core environment and better establish the accuracy of this method. This study applied limits on the discontinuity factors by trial and error to ensure stable convergence to a physical solution. It would be desirable to make the method more robust by better understanding the convergence properties of the iterations.

Acknowledgements

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