A Theoretical Study on A Convergence Problem of Nodal Methods

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Abstract

The effectiveness of modern nodal methods is largely due to its use of the information from the analytical flux solution inside a homogeneous node. As a result, the nodal coupling coefficients depend explicitly or implicitly on the evolving eigen-value of a problem during its solution iteration process. This poses an inherently non-linear matrix eigen-value iteration problem. This paper points out analytically that, whenever the half wave length of an evolving node interior analytic solution becomes smaller than the size of that node, this non-linear iteration problem can become inherently unstable and theoretically can always be non-convergent or converge to higher order harmonics. This phenomenon is confirmed, demonstrated and analyzed via the simplest 1-D problem solved by the simplest analytic nodal method, the Analytic Coarse Mesh Finite Difference (ACMFD, [1]) method.

KEYWORDS: Nodal methods, Convergence, ACMFD

1. Introduction

Modern nodal methods can use large nodes because it homogenizes the nodes so that the analytic solution inside a node is obtainable, and whereby information can be extracted to construct nodal coupling equations. The effectiveness of a modern nodal method relies to a large extent on its utilization, in various ways and to different degrees, of the available information from a node interior analytical flux solution. As a result, the nodal coupling coefficients depend explicitly or implicitly on the evolving eigen-value of a problem during its solution iteration process. This poses an inherently non-linear matrix eigen-value iteration problem. Strictly speaking, there is no proven mathematical theorem guaranteeing the convergence and stability of this non-linear iteration problem. Here well-established linear algebra results do not rigorously apply.

This paper points out that, whenever the half wave length of an evolving node interior analytic solution becomes smaller than the size of that node, this non-linear iteration problem can become inherently unstable and theoretically can always be non-convergent or converge to higher order harmonics. The reason for this is quite simple. The node interior analytic solution (for example a cosine function) typically has a "wave length", which depends on the evolving eigen-value. If during the eigen-value iteration, at some stage (most likely in the first few iterations), the half wave length happens to become smaller than the node size, then the node interior analytic function must have a negative value somewhere inside that node. However, when this happens, the parameters and variables in the nodal equations can not detect it, as nodal methods reduce unknown variables to a few node-wise quantities which do not reveal the node interior local

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information. Obviously when this happens, the flux solution is far from the fundamental mode. From then on, the subsequent iterations may not be able to alter the eigen-value sufficiently to enlarge the wave length to longer than the node size, and therefore iteration may not converge or may converge to the higher order harmonics. This phenomenon is confirmed, demonstrated and analyzed in this paper via the simplest 1-D problem solved by the simplest analytic nodal method, the Analytic Coarse Mesh Finite Difference (ACMFD, [1]) method.

2. ACMFD Review for the 1-D And 1-G Case

ACMFD is the simplest nodal method using the complete node interior analytic information. Details of the method are given in [Ref. 1, 2 and 3]. Here we will give a brief review of it for the simple 1-D and 1-G diffusion case, where the flux solution in any homogeneous node is analytically given by

$$\phi(x) = A\sin\kappa x + B\cos\kappa x \tag{1}$$

with κ defined as

$$\kappa = \left(k_\infty / k_{eff} - 1\right)^{1/2} / L \tag{2}$$

where L is the diffusion length. For each node, there are two unknown coefficients, A and B of Eq. (1). If we consider two adjacent nodes, there are then four unknowns to be determined. Given the average fluxes of the two nodes and the two interface boundary conditions of flux and current continuity, these four coefficients can be determined. Therefore the analytic flux solutions in both adjacent nodes, and consequently their interface flux and current as well, can be completely determined in terms of only two quantities: the average fluxes in the two adjacent nodes. This way the following relation is rigorously derived for the interface current of the two adjacent nodes, n and n+1,

$$J_{n,n+1} = -[D^L_{n+1}\bar{\phi}_{n+1} - D^R_n\bar{\phi}_n] \tag{3}$$

where the directional dependent effective diffusion coefficients are related to the physical diffusion coefficients and the values of k in the adjacent nodes.

Using Eq. (3) to express the leakage term in the neutron balance relation in a node, we obtain the complete nodal coupling equation,

$$-\frac{D^R_{n-1}}{a_n}\bar{\phi}_{n-1} - \frac{D^L_{n+1}}{a_n}\bar{\phi}_{n+1} + \frac{(D^L_n + D^R_n)}{a_n}\bar{\phi}_n + \Sigma_{an}\bar{\phi}_n = \frac{\Sigma_{fn}}{k_{eff}}\bar{\phi}_n \tag{4}$$

where a_n is the node size. This ACMFD nodal equation contains only one unknown per each node, i.e. the node average flux. This is the simplest and most analytic formulation of all the nodal methods. For the 1-D case, the ACMFD solution is exact regardless of node sizes, so long as each node is homogeneous.

3. Demonstration and Analysis of the Convergence Problem

3.1 The Simple 1-D and 1-G Problem

The simple problem that we use is a homogeneous slab core with vacuum boundary condition on the two sides. We will assume only one energy group so that the rigorous solution is a simple cosine function. The problem parameters are given in Tab. 1, where the rigorous eigen-value (k_{eff}) is also provided.

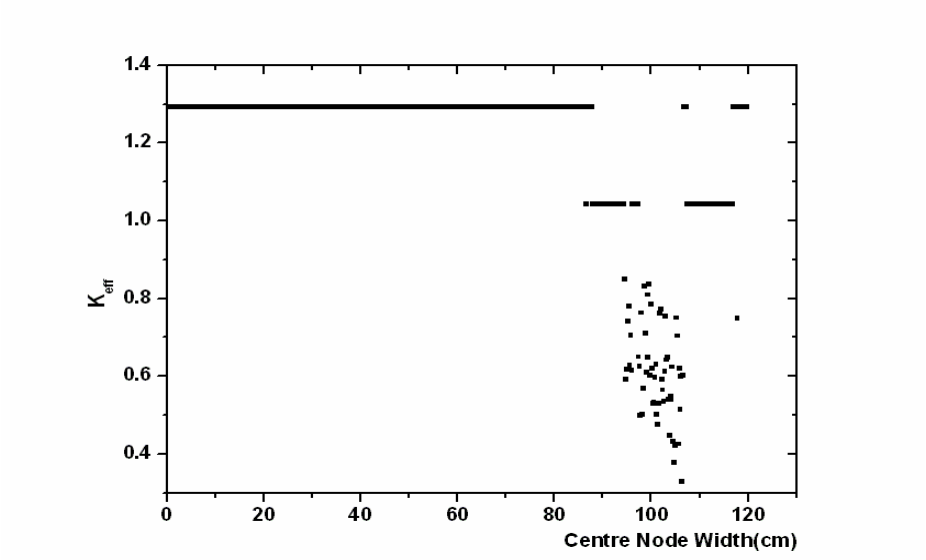
Table 1: The 1-D Slab Problem.

Width	D	Σ_a	$\upsilon\Sigma_f$
120cm	1.5cm	0.03/cm	0.04/cm
Diffusion Length (L)		k_∞	k_{eff}
7.071068cm		1.333333	1.293131

3.2 Solving the Problem with ACMFD

The simple 1-D problem is solved with ACMFD using varying number of nodes and node sizes. It is confirmed that iterations always converge nicely to the rigorous solution except for cases with some very large nodes, where non-convergence or convergence to higher harmonics does occur. For the clarity of discussion, all the cases presented in this paper contain three nodes in the slab core with two end nodes of the same size and the center node of a different size. The node sizes are varied by increasing the center node size from a small node to a very large node. Fig. 1 shows how convergence problems occur when the center node becomes too large.

Figure 1: Convergence Versus Node Size



When the center node size increases to greater than about 80cm, the solution becomes unstable

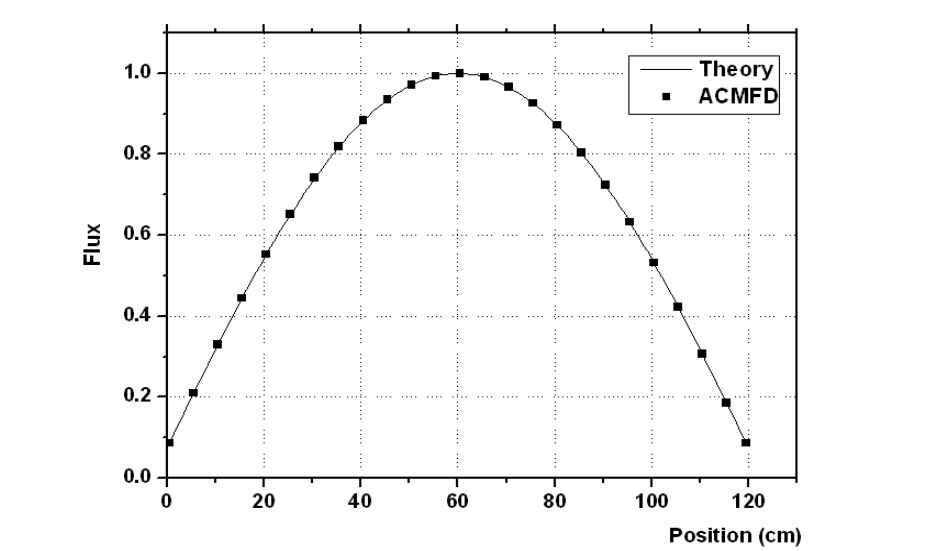
such that it may not converge (scattered points in the figure indicating non-convergence up to 100 iterations) or may converge to the first harmonic mode. It should be noted that the largest size of the two (equal) end nodes is 60cm, so that in this demonstration problem only the center node can become large enough to cause the convergence problem.

Tab. 2 shows how the ACMFD iteration solution converges to the fundamental mode for the case of 40cm center node. Using Eqs. (1) and (2), the fine mesh node interior flux can be reconstructed via the ACMFD coarse mesh nodal solution. This is compared in Fig. 2 against the analytical solution, showing a perfect agreement that confirms the ACMFD theory.

Table 2: Convergence to the Fundamental Mode for the Case of 40cm Center Node.

Iteration	Node-1 flux	Node-2 flux	Node-3 flux	k_{eff}
1	1.150871	1.307181	1.150871	1.00000
2	1.194382	1.429075	1.194382	1.20297
3	1.187009	1.476666	1.187009	1.27261
4	1.172987	1.510507	1.172987	1.28356
5	1.159230	1.540387	1.159230	1.28549
6	1.146494	1.567683	1.146494	1.28628
Converged	1.009364	1.860665	1.009364	1.29313
Analytical	1.009362	1.860670	1.009362	1.29313

Figure 2: Comparison of the Reconstructed ACMFD Solution to the Analytical Solution for the Fundamental Mode



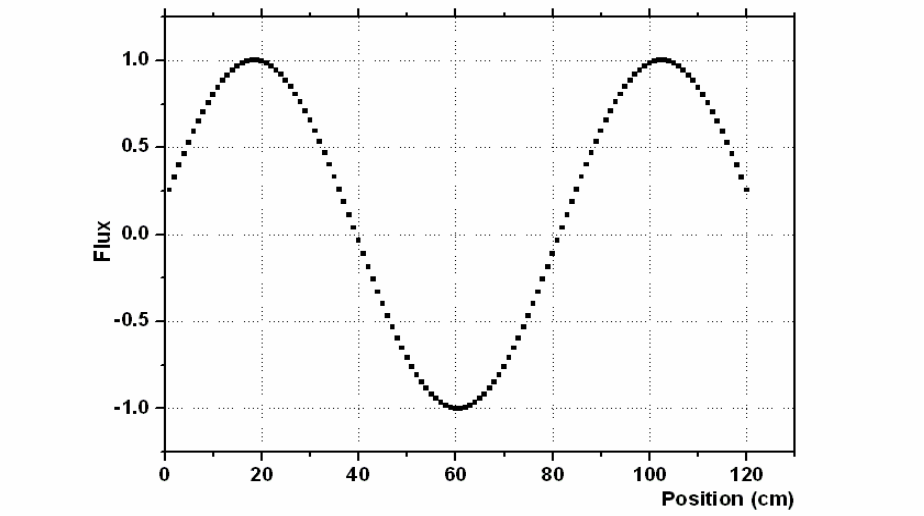
Tab. 3 shows how the iteration solution converges to the first harmonic mode for the case of 90cm center node. The nodes interior fine mesh flux reconstructed via the ACMFD coarse mesh nodal solution reproduces the analytical solution for the first harmonic mode, which is shown in Fig. 3. As one can see in Tab. 3, throughout the iteration the average fluxes in the three nodes remain positive without any direct information indicating the appearance of negative flux

anywhere in the core. Numerically this is an entirely acceptable coarse mesh solution.

Table 3: Convergence to the First Harmonic Mode for the Case of 90cm Center Node.

Iteration	Node-1 flux	Node-2 flux	Node-3 flux	k_{eff}
1	1.821679	0.943443	1.821679	1.00000
2	3.230873	0.333691	3.230873	1.16300
3	3.480037	0.199462	3.480037	1.05799
4	3.183782	0.324661	3.183782	1.01961
5	3.175597	0.333238	3.175597	1.03944
6	3.222479	0.312963	3.222479	1.04383
Converged to the 1st Harmonic	3.205042	0.320340	3.205042	1.04152
Fundamental Mode Reference	1.009362	1.860670	1.009362	1.29313

Figure 3: Reconstructed ACMFD Solution for the First Harmonic Mode



3.3 Analysis of the Convergence Dependency on Node Size

To better understand the above results, we consider the wave length in Eq. (1),

$$\lambda = 2\pi / \kappa \tag{5}$$

where κ via Eq. (2) depends on the eigen-value of the numerical solution. As the eigen-value evolves with iteration, the wavelength varies as well. As pointed out in the above, the convergence stability of the iteration depends crucially on how the half wavelength compares to the node size. Given in Tab. 4 is the comparison of the evolving half wavelength to the node size for the three different cases of node size 60cm, 90cm and 104cm, which represent respectively the cases of converging to the fundamental mode, converging to the first harmonic mode, and no convergence.

Table 4: Variation of Half Wavelength During Iteration for Cases of Different Node Size.

Iteration	60cm Center Node		90cm Center Node		104cm Center Node	
	keff	$\lambda/2$ (cm)	*keff*	$\lambda/2$ (cm)	*keff*	$\lambda/2$ (cm)
1	1.00000	38.476	1.00000	38.476	1.00000	38.476
2	1.29956	137.80	1.16300	58.046	1.10291	48.600
3	1.31196	174.02	1.05799	43.544	0.88023	30.962
4	1.31066	168.90	1.01961	40.047	0.72092	24.102
5	1.30776	158.85	1.03944	41.777	0.75923	25.546
6	1.30650	155.02	1.04383	42.181	0.66695	22.223
Converged	1.29313	125.99	1.04152	41.967	?	?

In all three cases, the initialization of the eigen-value gives a half wave length less than the center node size. This means that the initial analytic function assumed for the center node, (which can not be seen from the average flux of the center node), must have a negative value in the center node and is therefore in the first harmonic mode. After the first iteration, for the 60cm center node case, the estimated eigen-value increase to 1.29956 which gives a half wave length of 137.8cm, much greater than 60cm. The analytic flux function inside the center node now goes to the fundamental mode, and from then on maintains the fundamental mode for the subsequent iterations. On the other hand, for the 90cm center node case, after the first iteration, the estimated eigen-value increases only to 1.163 which gives a half wave length of 58.046cm, still smaller than 90cm. From there on, the half wave length continues to stay smaller than 90cm and the solution converges to the first harmonic mode. For the 104cm center node case, the half wavelength continues to decrease and oscillate with iteration such that harmonics higher than the first harmonic mode began to appear and the iteration failed to converge even with one hundred iterations. From Fig. 1 one can see that although most cases with very large center node do not converge, there are few cases that do converge to the first harmonic mode or even the fundamental mode. But it is obvious that the iteration becomes chaotic and unreliable, and convergence happens with very large node cases only by rare chance.

4. Discussion

Although this convergence problem due to large nodes is theoretically unavoidable, in practice it rarely occurs as practical node sizes are seldom so large. For practical applications, the problem can also be controlled. Since its root cause is the half wave length of the implicit analytic flux function inside a node becoming smaller than the node size, the problem can be avoided in practice by not allowing a node size to become too large. It could also be avoided by not allowing the evolving eigen-value to become too small. If the eigen-value is always approached in iterations from above instead of from below, this convergence problem would not happen. By the same token, in the examples presented in this paper, had the initialization of the eigen-value been properly tailored for each case, convergence to fundamental mode could be realized for all the cases regardless the node size.

However, the existence of this convergence problem does show that one has to be careful in concluding or proving the convergence of a nodal method. So long as the matrix equation in a nodal method is derived from an implicit node interior solution and it evolves with the iteration process, this problem is inherently behind the nodal method formulation. This includes as well various kinds of method for accelerating a higher level formulation via using a lower level coarse mesh finite difference (CMFD) formulation, where the CMFD coupling coefficients are iteratively calculated from the higher level method which in turn makes use of node interior flux function information. In this regards, it is worth of pointing out that there have been studies on the convergence of non-linear CMFD methods, where non-conditional convergence for any node size was concluded for certain cases (for example, Ref. 4 and references cited therein.) However those studies were limited to the asymptotic behavior of fixed source inner iterations when the iterative solution gets close to the true solution so that Fourier analysis can be applied to the approximate linearization around the true solution of the fixed source problem. The assumption for that Fourier analysis method is not valid for the current study, and an attempt to apply it to the current study lead to physically meaningless results. The study in this paper raises a caution to the proper understanding and interpretation of the findings of the asymptotic Fourier analysis application to non-linear CMFD iterations.

It is worth pointing out another interesting result of this study using the ACMFD formulation. Table 3 shows the rigorous nodal solution for the first harmonic mode. The node average flux distribution in the three nodes is all positive, although the analytic function for the first harmonic mode must necessarily have negative flux values as shown in Fig. 3. Therefore the first harmonic mode nodal solution is not orthogonal to the fundamental mode nodal solution as one might naively expect. However, this is not contradictory to the fact the one group diffusion equation is self-adjoint and therefore its harmonic modes are all orthogonal to each other. This paradox is due to the difference between the continuous flux distribution function versus a coarse mesh nodal average flux distribution function. This problem is not only related to the relation between physical adjoint function versus mathematical adjoint function, or nodal formulation versus finite difference formulation, but related to the intrinsic nonlinearity of the iteration process as well. These topics will be for future study.

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