Chapter 2

Higher- and Lower-order Nodal Diffusion Methods

2.1 Introduction

Modern nodal methods, as overviewed in Chapter 1, aim at calculating the 3D multi-group neutron flux distribution in large homogeneous volumes, or nodes. The main aim of this approach is to determine the power distribution in fuel elements and primarily to use this information for the calculation of material depletion.

In this chapter, we will sketch the history of these methods in more detail, focusing on the approaches which have stood the test of time and as such are implemented in modern nodal codes today. Special attention is paid to the well known Analytic Nodal Method (ANM) which, to some extent, forms the basis of the development in this work. Since the ANM (Smith, 1979) is based on the transverse integration technique, this description will highlight the formulation of the transverse leakage source and as such serve as a vehicle to introduce and describe the standard quadratic leakage approximation (SQLA) as originally incorporated into the Nodal Expansion Method (NEM) by Finnemann et al. (1977). In the ANM, the transverse leakage source approximation is the only approximation used. As overviewed in the opening chapter, the improvement of this leakage approximation is the primary focus of this work and thus the theoretical background needed for this proposed improvement, which is to be found in the class of higher-order nodal methods, is also given here.

Higher-order nodal methods are not as well known as the ANM and NEM approaches and hence a somewhat more comprehensive description of this class of nodal methods is provided. The higher-order formalism allows the transverse leakage term to be expressed exactly and in principle is capable of producing (fine-mesh) reference solutions for sufficiently high expansion orders, albeit at a significant computational

cost. The chapter is concluded with a reformulation of the proposed work in terms of the theoretical basis now provided and thus serves to formalize the aim of the thesis.

2.2 Progress in Nodal Methods

Most commonly, fine-mesh finite-difference methods have historically been used to solve reactor core diffusion problems. In early review papers (Froehlich, 1972), it was shown that sufficient accuracy is only obtained with these methods if the mesh size is of the order of a diffusion length, which leads to substantial numbers of meshpoints. In order to address the computational burden associated with these methods, a number of coarse-mesh approaches were investigated, amongst which the first application of Finite Element Methods (FEMs) (Kang and Hansen, 1973) to numerical reactor calculations. The class of FEMs provide a common framework according to which nodal, synthesis and finite-difference methods can be analyzed, especially in terms of convergence and error properties. Four steps are typically applied in the formulation of FEM based solutions and can be summarized as:

1. Reformulation of the given boundary value problem into a so-called "weak" (or variational) form;

2. Discretization of the domain into geometrically simple parts (or elements);

3. Replacement of the infinite dimensional representation resulting from (1) with finite dimensional functions defined over the elements in step (2); and

4. The formulation of a linear algebraic problem for the coefficients of the expansion in step (3).

An extensive analysis of how classical nodal methods (Dorning, 1979) may be related to FEMs within the context of these steps is presented in Grossman and Hennart (2007) and such a work is valuable in classifying nodal methods within the wider scope of methods in numerical analysis. Nevertheless, FEM based methods were, in this field, never accepted to the same level as the class of nodal methods, which first appeared during the 1960s. The reason for this is probably due to the process of homogenization, which largely simplifies the geometric complexity of the core models and hence does not require the natural geometric flexibility which FEMs provide.

In this section we aim to describe the class of nodal methods, its evolution and its current state of application. These methods have shown extreme longevity and as such still form the basis of industrial code systems today, as discussed in Section 1.3.2.

To begin this discussion, we introduce the primary problem under consideration and formulate it as a within-group (multi-group formulation is also possible) form of the 3D diffusion equation, written here in arbitrary Cartesian coordinates (u, v, w) as

$$- \bigtriangledown \cdot [D^g(u,v,w) \bigtriangledown \phi^g(u,v,w)] + \sigma^{g,\mathrm{rem}}(u,v,w)\phi^g(u,v,w) - Q^g(u,v,w) = 0. \quad (2.1)$$

In eq. (2.1) $D^g(u,v,w)$ denotes the diffusion coefficient, $\phi^g(u,v,w)$ the flux in energy group g, $\sigma^{g,rem}(u,v,w)$ the removal cross-section and $Q^g(u,v,w)$ the group source comprising both the scattering and fission sources within the node. Note that, throughout this text, $\sigma^{g,t}$(where t denotes the reaction type) represents the macroscopic cross-sections of the designated types. The 3D *nodal* diffusion equation, as presented in eq. (2.2), is obtained by dividing the system into $(N_u \cdot N_v \cdot N_w)$ nodes (with node n having node sizes $(h_{n,u}, h_{n,v}, h_{n,w})$) and assuming that the material properties are constant within each node. The nodal diffusion equation, written here for node n as subscript, is

$$-D_n^g \bigtriangledown^2 \phi_n^g(u,v,w) + \sigma_n^{g,\mathrm{rem}}\phi_n^g(u,v,w) - Q_n^g(u,v,w) = 0 \quad (2.2)$$

and is typically integrated over the volume V_n of node n and then divided by the node volume. After applying the divergence theorem, we obtain the nodal balance equation,

$$\sum_{m=1}^{6} a_n^{nm}\overline{J}_{mn}^g + \sigma_n^{g,\mathrm{rem}}\overline{\Phi}_n^g = \overline{Q}_n^g, \quad (2.3)$$

with

$$\overline{\Phi}_n^g = \frac{1}{V_n}\int_{V_n} \phi_n^g(u,v,w)dV_n,$$

$$\overline{J}_{mn}^g = -\frac{D_n^g}{S_{mn}}\frac{\partial}{\partial \overrightarrow{n}} \cdot \int_{S_{mn}} \phi_n^g(u,v,w)dS_{mn}$$

and the node-averaged source in energy group g defined as

$$\overline{Q}_n^g = \frac{1}{V_n}\int_{V_n} Q_n^g(u,v,w)dV_n.$$

In eq. (2.3) $\overline{J}_{mn}^g$ denotes the normal component of the side-averaged net current on the surface between node m and node n (with the normal pointing outward from node n), S_{mn} represents the surface between nodes m and n and a_n^{nm} the surface to volume ratio of that surface. $\overline{\Phi}_n^g$ represents the node-averaged flux in energy

group g. The averaged flux on the interface between node n and node m will be denoted by $\overline{\phi}^g_{mn}$. The node-averaged cross-sections and diffusion coefficients (as well as, potentially, discontinuity factors) are assumed known here. Typically these values would derive from a set of single- or multi-node transport calculations and aim to conserve equivalence between the heterogeneous transport and homogeneous diffusion solution. Although not the topic of this thesis, a good overview of these approaches may be found in Smith (1986). Thus, in eq. (2.3), we have formulated a set of equations for the primary unknowns of interest in nodal methods and established a system of simultaneous equations that couple all the nodes via the continuous side-average net currents. The system however, is underspecified and various approaches are utilized within the class of nodal methods to find the relationship between the node-averaged fluxes and the side-averaged net currents, so that eq. (2.3) may be solved. This distinction in how the expression for side-averaged current is obtained, is also the primary differentiating factor between the various classes of nodal methods.

The FLARE model, developed in 1964 and overviewed in (Gupta, 1981), probably represents the first significant step in nodal methods and falls into the class of nodal simulators. In the case of these methods, the expression for current on the surface between node m and node n were written as

$$\overline{J}_{mn} = C^*_{mn}\left(\overline{\Phi}_m - \overline{\Phi}_n\right) \tag{2.4}$$

where C^*_{mn} was determined to match experimental data or obtained by auxiliary fine-mesh calculations. These methods could not be described as "consistent", since they did not necessarily converge to the fine-mesh finite-difference solution for decreasing mesh size. Although successfully used for some time, these methods show the need for the so-called consistently defined (or modern) coarse-mesh methods, which may be described as true coarse-mesh approximations to the neutron diffusion equation.

We may classify the various nodal approaches from here onward into two major categories, namely those which utilize the so-called transverse integration procedure and those which proceed with a direct solution of the 3D diffusion equation. We discuss both these categories in the coming sections, but focus on the class of transversely-integrated methods, given their extensive usage in industrial code systems.

2.3 Transversely-integrated Nodal Methods

The most common approach employed in modern nodal methods is that of transverse integration, which essentially decomposes the 3D partial differential equation into 3 ordinary, inhomogeneous differential equations. In this technique, the diffusion equation is integrated over two directions, say v and w, to yield a one-dimensional equation in the u direction given in eq. (2.5) as

$$-D_n^g \frac{d^2}{du^2}\phi_n^g(u) + \sigma_n^{g,\text{rem}}\phi_n^g(u) = Q_n^g(u) - L_n^{g,vw}(u). \tag{2.5}$$

In eq. (2.5) $\phi_n^g(u)$ represents the transversely-integrated one-dimensional flux and is given by

$$\phi_n^g(u) = \frac{1}{h_{n,v}}\frac{1}{h_{n,w}}\int_{h_{n,v}h_{n,w}} \phi_n^g(u,v,w)dvdw, \tag{2.6}$$

and $L_n^{g,vw}(u)$ represents the transverse leakage term which appears due to the integration of the v- and w- components of the leakage term. We have

$$L_n^{g,vw}(u) = L_n^{g,v}(u) + L_n^{g,w}(u)$$

$$= -D_n^g \left[\frac{1}{h_{n,v}}\frac{1}{h_{n,w}}\int_{h_{n,v}h_{n,w}} \left(\frac{\partial^2}{\partial v^2} + \frac{\partial^2}{\partial w^2}\right)\phi^g(u,v,w)dvdw\right] \tag{2.7}$$

$$L_n^{g,vw}(u) = \frac{1}{h_{n,v}}\left(\overline{J}_{n,v}^g(u,\frac{h_v}{2}) + \overline{J}_{n,v}^g(u,-\frac{h_v}{2})\right) + \tag{2.8}$$

$$\frac{1}{h_{n,w}}\left(\overline{J}_{n,w}^g(u,\frac{h_w}{2}) + \overline{J}_{n,w}^g(u,-\frac{h_w}{2})\right).$$

Here $\overline{J}_{n,v}^g(u,\frac{h_v}{2})$ represents the $w-$integrated, one-dimensional current on the right hand side of the $v-$direction transverse surface. It is of interest to note that, although these expressions for the transverse leakages are quite complicated, the average value $\overline{L}_n^{g,vw}$ of the transverse leakage source can be quite simply expressed in terms of side-averaged currents as

$$\frac{1}{h_{n,u}}\int_{h_{n,u}} L_n^{g,vw}(u)du = \frac{1}{h_{n,v}}\left(\overline{J}_{n,v}^g(\frac{h_v}{2}) + \overline{J}_{n,v}^g(-\frac{h_v}{2})\right) + \frac{1}{h_{n,w}}\left(\overline{J}_{n,w}^g(\frac{h_w}{2}) + \overline{J}_{n,w}^g(-\frac{h_w}{2})\right). \tag{2.9}$$

Some of the earliest efforts to formulate more rigorous expressions of coupling coefficients were the so-called Nodal Synthesis Methods (NSM) (Wagner, 1974) and the analytical procedure (Antonopoulous, 1972). These approaches assumed a separable

flux within the node (as a product of one-dimensional solutions) to compute bucklings for the sake of the transverse leakages and hence utilized the shape of the flux as an approximation for the shape of the transverse leakage. The NSM, specifically, required off-line auxiliary one-dimensional finite-difference calculations for the definition of the coupling coefficients (which were then updated during the nodal calculation), whereas the analytic procedure made use of a truncated Taylor series expansions for formulating the side-averaged current to node-averaged flux relationship. These two developments proved paramount as they provided crucial building blocks for the nodal methods utilized today. The need to eliminate the auxiliary finite-difference calculations from the NSM method eventually led to the development of the well known Nodal Expansion Method (NEM) (Finnemann et al., 1977) and the analytic procedure preceded probably the most widely used nodal method today, namely the Analytic Nodal Method (ANM) (Smith, 1979). The primary difference between the polynomial and analytic approaches lies in whether information of the analytic solution of eq. (2.5) is incorporated into the numerical scheme (the ANM) or whether the flux is approximated as a polynomial expansion within the node (NEM). If the one-dimensional equations in the ANM formulation contains an explicit representation of the fission and scattering sources, the method is referred to as the Semi Analytic Nodal Method (SANM), since these sources should be additionally represented in terms of typically some flux moment expansion.

2.3.1 Polynomial methods and the nodal expansion method

Amongst the class of polynomial methods, the Nodal Expansion Method (NEM) is one of the most widely used. In the NEM formulation, along with the node average fluxes, side-average partial currents are typically utilized as primary unknowns. In obtaining the solution of eq. (2.5), the one-dimensional flux is typically approximated as

$$\phi_n^g(u) = \phi_{n,0}^g f_0(u) + \sum_{l=1}^{L} a_{n,l}^g f_l(u) \tag{2.10}$$

where various choices of basis functions $f_n(u)$ and conditions for solving the expansion coefficients $a_{n,l}^g$ would characterize the specific version of the methods (Lawrence, 1986). For example, if we define

$$\vartheta = \left(\frac{u}{h_{n,u}}\right), \quad -\frac{h_{n,u}}{2} \leq u \leq \frac{h_{n,u}}{2}$$

as in Finnemann et al. (1977), the chosen set of basis functions can be written as

$$\begin{aligned} f_0(\vartheta) &= 1 \\ f_1(\vartheta) &= \vartheta \\ f_3(\vartheta) &= 3\vartheta^2 - \frac{1}{4} \\ f_4(\vartheta) &= \vartheta(\vartheta - \frac{1}{2})(\vartheta + \frac{1}{2}) \\ f_5(\vartheta)(\vartheta^2 - \frac{1}{20})(\vartheta - \frac{1}{2})(\vartheta + \frac{1}{2}). \end{aligned} \tag{2.11}$$

The zeroth moment of the flux is the node-averaged flux obtained from the solution of the balance equation, while the first and second moments are normally obtained from enforcing flux and (normal component of the net) current continuity on the node interfaces. This is ensured via choosing

$$a^g_{n,1} = \overline{\phi}^{g,u}_{n,+} - \overline{\phi}^{g,u}_{n,-} \tag{2.12}$$

and

$$a^g_{n,2} = \overline{\phi}^{g,u}_{n,+} + \overline{\phi}^{g,u}_{n,-} - 2\phi^g_{n,0}$$

where $\overline{\phi}^{g,u}_{n,\pm}$ represents the side-averaged fluxes on the right and left hand sides in direction u of the node n. A number of variants exist for formulating expressions for the higher-order moments ($L > 2$). The most common approaches relate to the class of weighted residual methods, where either moment weighting (using $f_1(u)$ and $f_2(u)$) or Galerkin weighting (using $f_3(u)$ and $f_4(u)$) is applied, of which the former has been shown to be more accurate (Finnemann et al., 1977).

Expressions for the outgoing partial currents are obtained by substituting (2.10) into Fick's Law (Duderstadt and Hamilton, 1976). The expansion coefficients may be eliminated in favour of the node-averaged flux (via (2.12)) to yield a set of coupled equations where the outgoing partial currents are expressed in terms of incoming partial currents, node-averaged fluxes and higher-order expansion coefficients per direction. Finally the higher-order expansion coefficients may be eliminated via the weighted residual approach and hence, in 3D, a set of seven unknowns and seven equations (node-averaged flux and six outgoing partial currents) are obtained as a well posed problem.

The outstanding issue here is the treatment of the transverse leakage source in eq. (2.5). We defer this discussion to a little later (Section 2.3.3) given its common treatment across the different nodal methods and its central importance to this work.

2.3.2 Analytic methods and the (semi) analytic nodal method

This class of methods utilizes an analytical solution to the one-dimensional, transversely-integrated equations and a number of variants exist, with the Nodal Green's Function Method (Lawrence and Dorning, 1980) and the Analytic Nodal Method (Smith, 1979) probably the most well known. Considering its wide spread use, the ANM will be discussed in some detail. It was originally devised for two groups, later extended to four groups (Parsons D. K. and Nigg D. W., 1985) and has thereafter been extended to full multi-group (Vogel and Weiss, 1992). For the sake of consistency with the work in coming chapters, the derivation followed here is slightly different and is more accurately described as a semi-analytic solution, since the formulation is written as a group-by-group solution with the within-group scattering and fission sources expanded up to some predefined source order, in this case with Legendre polynomials as basis functions. Although this does not detract from the essence of the method, the truncation of the group source represents a second approximation (above and beyond the transverse leakage approximation) and hence the term *semi*-analytic.

In the case of the ANM, an auxiliary set of transversely-integrated one-dimensional equations is utilized to determine the node-averaged flux to side-averaged current relationship as needed in eq. (2.3). The one-dimensional equations obtained after transverse integration, take the form as given in eq. (2.5).

The distinguishing factor in the ANM is the rigorous analytic solution of this equation employed to solve eq. (2.5) for each direction $\{u, v, w\}$. We return to the form of the transverse leakage term in the next section and focus on the solution of the one-dimensional equation with a given source. For clarity, we present the form of the inhomogeneous source as it appears in eq. (2.5),

$$s_n^g(u) = Q_n^g(u) - L_n^{g,vw}(u)$$

$$= \chi_n^g \frac{1}{k_{\text{eff}}} \sum_{h=1}^{G} \nu^h \phi_n^h(u) \sigma_{n,\text{fis}}^h + \sum_{h=1, h\neq g}^{G} \phi_n^h(u) \sigma_{n,\text{scat}}^h(h \to g) - L_n^{g,vw}(u) \tag{2.13}$$

where χ^g refers to the fission spectrum, ν^h to the average number of neutrons released per fission in group h and k_{eff} to the multiplication factor of the system. The terms σ_{fis}^h and $\sigma_{\text{scat}}^h(h \to g)$ refer to the fission and scattering cross-sections, respectively. In practical implementations of the (Semi)ANM, $s_n(u)$ is typically expressed as an expansion around moments of the one-dimensional flux, for example on a Legendre

polynomial base, up to the fourth order. This implies a non-linear iteration, hence utilizing flux moments from the previous iteration to construct the source for the current iteration. The moments of the one-dimensional flux are, in the ANM, generally determined from the one-dimensional analytic solution.

2.3.2.1 One-dimensional analytic solution

In the standard (S)ANM, eq. (2.5) is solved analytically to yield the one-dimensional flux profile. To facilitate this, eq. (2.5) is manipulated by introducing a buckling coefficient and transforming to dimensionless coordinates to yield

$$\frac{d^2}{d\xi^2}\phi_n(\xi) + (\beta_n^{nm})^2\phi_n(\xi) = -\frac{1}{D_n^g}\left(\frac{h_{n,u}}{2}\right)^2 s_n(\xi) \tag{2.14}$$

with

$$(\beta_n^{nm})^2 = \left[\frac{\sigma_n^{g,\mathrm{rem}}\left(\frac{h_{n,u}}{2}\right)^2}{-D_n^g}\right]$$

and

$$\xi = \frac{2u}{h_{n,u}},\ -\frac{h_{n,u}}{2} \leq u \leq \frac{h_{n,u}}{2}.$$

Note that the currents then scale as $\overline{J}_{mn}^g(u) = \frac{2}{h_{n,u}}\overline{J}_{mn}^g(\xi)$. The rigorous analytic solution to the inhomogeneous eq. (2.14) is given by the sum of a complementary solution (a linear combination of two linearly-independent solutions to the homogeneous Helmholtz equation) and a particular solution. This yields

$$\phi_n(\xi) = A \cdot \cosh(|\beta_n^{nm}|\,\xi) + B \cdot \sinh(|\beta_n^{nm}|\,w) + Z_n(\xi) \tag{2.15}$$

where A and B are constants to be determined from current and flux continuity conditions and $Z_n(\xi)$ represents the particular solution. Specifically

$$A = \frac{(\phi_n(+1) - Z(+1)) + (\phi_n(-1) - Z(-1))}{2\cosh\left(|\beta_n^{nm}|\right)},$$

$$B = \frac{(\phi_n(+1) - Z(+1)) - (\phi_n(-1) - Z(-1))}{2\sinh\left(|\beta_n^{nm}|\right)}$$

where $Z_n(\xi)$ is determined as the analytic source integral

$$Z_n(\xi) = \frac{1}{|\beta_n^{nm}|}\int^{\xi} \sinh(|\beta_n^{nm}|\ (\xi - u))\, s_n(u)du$$

of which the notation implies that the integration is performed over u, after which u is replaced by ξ. In practice the particular solution is determined from a recurrence

relationship which expresses the Legendre moments of the particular solution in terms of the Legendre moments of the source.

2.3.2.2 Net current relationship

In principle, the analytic solution obtained in the adjacent nodes is used, along with flux and current continuity, to eliminate side-fluxes from the equations and hence to express the side-averaged current in terms of the two adjacent node-averaged fluxes. A full derivation of these expressions may be found in Smith (1979), but the basic relations are provided here.

Using the one-dimensional analytic solution which we have obtained in eq. (2.15) over multiple nodes, and after some algebraic manipulation, two expressions result. The first for surface-averaged current and the second an expression for side-averaged flux, respectively as

$$\overline{J}^g_{mn} = \widetilde{d}^{mn}_n p^{mn}_n [\overline{\Phi}^g_n - Z_{mn}] - \widetilde{d}^{mn}_n \overline{\Phi}^g_{mn} \tag{2.16}$$

and

$$\overline{\Phi}^g_{mn} = p^{mn}_n [\overline{\Phi}^g_n - Z_{mn}] - \frac{\overline{J}^g_{mn}}{\widetilde{d}^{mn}_n} \tag{2.17}$$

with the boundary value of the so-called tensorial source calculated as

$$Z_{mn} = -\frac{\left(\frac{h_{n,u}}{2}\right)^2}{2\left(|\beta^{nm}_n|\right)^2} \int_{-1}^{1} (1 - \cosh(|\beta^{nm}_n| \pm |\beta^{nm}_n| \, u)) s_n(u) du. \tag{2.18}$$

This source is so named due to the fact that it has a value on the left $(-)$ and right $(+)$ hand sides of the node which has contributions from the directions under consideration, as well as contributions from the transverse directions. The analytic coefficients are given by

$$t^{mn}_n = \frac{|\beta^{nm}_n|}{\tanh(|\beta^{nm}_n|)},$$

$$\widetilde{d}^{mn}_n = (\frac{2}{h_{n,u}}) D^g_n t^{mn}_n$$

and the node size correction factor as

$$p^{mn}_n = \frac{2\,|\beta^{nm}_n|}{\sinh(2\,|\beta^{nm}_n|)}.$$

Note that eq. (2.16) expresses the side-current in terms of the node-averaged flux in the same node and similarly (2.17) expresses the side-averaged flux in terms of the node-averaged flux in the same node. At this point any of these may be chosen as primary unknowns and we proceed here with node-averaged flux as the chosen primary unknown. In order to determine the node-averaged flux to the side-averaged current relationship required in eq. (2.3), a two node problem is constructed. Together with continuity conditions for both the side-averaged flux and side-averaged current at the interface between adjacent nodes, expressions (2.16) and (2.17) are utilized to express the side-averaged current as

$$\overline{J}^g_{mn} = C^g_{mn}(\overline{\Phi}^g_n - Z_{mn}) - C^g_{nm}(\overline{\Phi}^g_m - Z_{nm}) \tag{2.19}$$

with

$$C_{mn} = d_{nm} p^{mn}_n$$

$$C_{nm} = d_{nm} p^{mn}_m$$

where the harmonic averaged surface diffusion coefficient is given by

$$d_{nm} = [(\widetilde{d}^{mn}_n)^{-1} + (\widetilde{d}^{mn}_m)^{-1}]^{-1}.$$

After inserting eq. (2.19) into eq. (2.3) we obtain a system of N equations with node-averaged fluxes as primary unknowns. This system can be solved with an appropriate iteration scheme. In the limit of infinitesimally small node sizes (as $h_{n,u} \to 0$), it can be shown that expression (2.19) limits to the traditional fine-mesh finite-difference expression for the side-averaged current, which is an important property of nodal methods.

In this work node-averaged fluxes are selected as primary unknowns and hence eliminating side-averaged currents in equation (2.3) via relation (2.19) yields the final form of the nodal balance equation

$$\left[\sum_{m=1}^{6} a^{nm}_n C_{mn} + \sigma^{g,\mathrm{rem}}_n\right] \overline{\Phi}^g_n - \sum_{m=1}^{6} a^{nm}_n C_{nm} \overline{\Phi}^g_m = \sum_{m=1}^{6} a^{nm}_n \left[C_{mn} Z_{mn} - C_{nm} Z_{nm}\right] + \tag{2.20}$$

$$\frac{1}{k_{\mathrm{eff}}} \chi^g \sum_{h=1}^{G} v^h \sigma^h_{n,\mathrm{fis}} \overline{\Phi}^h_n + \sum_{h=1, h\neq g}^{G} \sigma^{h\to g}_{n,\mathrm{scat}} \overline{\Phi}^h_n.$$

If, for instance, we preferred to eliminate the node-averaged flux in favour of the side-averaged current, we would obtain a set of coupled three-point equations (in each direction) for interface currents. In this case we obtained a set of 7-point balance equations for the node-averaged flux.

Importantly, we may note that the ANM utilizes only four unknowns per node, namely the node-averaged flux and three directional average leakages (which are carried within the tensorial sources). As described in Section 2.3.1, the NEM approach solves for seven unknowns per node and hence, the ANM may exhibit slight performance advantages over the NEM.

2.3.3 Transverse leakage approximations

The so-called ''transverse leakage'' terms play an important role. Physically, they represent particle exchange between neighbouring cells in the transverse direction; mathematically they ensure the coupling between the one-dimensional equations. These terms appear due to the transverse integration procedure and if treated exactly, would allow the nodal methods to essentially recover the reference node-averaged fluxes, especially in the case of the ANM which does not contain any further approximations. Given the importance of this treatment to the accuracy of the solution, a number of approaches has been implemented over the years; some of the most prominent efforts are summarized in this section. These approximations all share the common characteristic (with the exception of the "flat leakage approximation") that they are external to the nodal diffusion solution, do not have clear error bounds and have been generally and probably aptly, described in Dilbert and Lewis (1985) as *ad hoc*, yet effective.

2.3.3.1 Buckling approximation

One of the first attempts to resolve the transverse leakage term was proposed in (Shober and Henry, 1976a,b) and entailed the assumption that the transverse leakage shape was the same as that of the one-dimensional flux, hence

$$L_n^{g,vw}(u) = B_{nm}^g \phi_n^g(u)$$

where the value of B_{nm}^g is determined by requiring that the average transverse leakage from the two transverse directions is conserved. This approximation would prove accurate as long as the three-dimensional flux in the node is spatially separable, which is often not the case in reactor problems.

2.3.3.2 Flat leakage approximation

Given the relatively large errors that could occur due to the "Buckling approximation", Shober and Henry (1976a), Shober and Henry (1976b) and Shober et al. (1977) further proposed a "flat leakage approximation", which probably is conceptually the simplest solution. Here we assume that the leakage is simply equal to its average value, as given in eq. (2.9). Although this approach improved upon the large errors for highly non-separable problems, it significantly constrained the accuracy in general problems. As a further suggestion, a flat two step solution was proposed in Shober (1978), which improved upon the accuracy of the flat leakage approximation.

2.3.3.3 Quadratic leakage approximation

Probably the most successful transverse leakage approximation to date was proposed in Bennewitz et al. (1975). Its simplicity and relatively good accuracy, very quickly attracted attention and this "Standard Quadratic Leakage Approximation" (SQLA) became a near industry standard in nodal codes, up to the present day. The approach suggested a three-node quadratic fit (in the direction of interest) of average transverse leakage, with the constraint that the average leakage in each node be maintained by the fit. The obtained shape was then only applied in the central node. Thus,

$$L_n^{g,vw}(u) = q_{n,0}^g + q_{n,1}^g u + q_{n,2}^g u^2 \tag{2.21}$$

and the coefficients determined from

$$\begin{aligned} \frac{1}{h_{n-1,u}} \int_{h_{n-1,u}} L_n^{g,vw}(u) du &= \overline{L}_{n-1}^{g,vw}, \\ \frac{1}{h_{n,u}} \int_{h_{n,u}} L_n^{g,vw}(u) du &= \overline{L}_n^{g,vw} \end{aligned} \tag{2.22}$$

and

$$\frac{1}{h_{n+1,u}} \int_{h_{n+1,u}} L_n^{g,vw}(u) du = \overline{L}_{n+1}^{g,vw}.$$

It is with this quadratic leakage approximation and its potential improvement that this thesis is primarily concerned. Although implemented in most modern nodal codes today, some specific difficulties, as outlined in Section 1.3.3, exist with this approach, which lead in some cases to node-averaged power errors in excess of 2%. While these errors were quite acceptable at the time of the QLA development, modern accuracy requirements could benefit from both a more consistent and a less error prone

approach, but only if such an proposal did not incur an excessive calculational time penalty.

Some of the earliest efforts to address the issue of the transverse leakage approximation in a fully consistent way, culminated in a class of nodal methods referred to as higher-order methods. We will investigate these methods in Section 2.5 as a basis for a practical, yet improved solution scheme, for the issue of resolving the transverse leakage terms in transversely-integrated nodal methods.

2.3.3.4 Method of successive smoothing

A less widely utilized approach, but one which is found as alternatives in both the NEM (Beam et al., 1999) and AFEN (Noh and Cho, 1994) codes, is the so-called "method of successive smoothing". This approach applies a two-dimensional Taylor series approximation of within-node quantities to approximate the shape of the currents on the node surfaces, up to the second order, for the purpose of constructing the leakage polynomial. Corner point fluxes are needed in the expansion and are obtained during the nodal solution via a smoothing procedure as described by Finnemann et al. (1992). According to published results in these listed papers, this approach does improve upon the accuracy of the SQLA, but only marginally so.

2.4 Transverse Leakage Free (Direct) Nodal Methods

A number of coarse-mesh methods have been developed during the life cycle of nodal methods, which aim at solving the intra-nodal flux distribution directly (Sutton and Aviles, 1996). Most of these may be classified as flux expansion methods, with the QUABOX (Langenbuch et al., 1977a) and CUBBOX codes (Langenbuch et al., 1977b) as some of the earliest efforts, although in these cases they were aimed at space-time application. In QUABOX quadratic polynomials are used and basis functions are expressed as sums and products of Taylor polynomials, with support points chosen as box and surface centered fluxes. Flux values at the support points are obtained by generating matrix equations via a weighted residual approach. In the CUBBOX code, the set of basis functions are extended to cubic and include one-dimensional polynomials, splines and three-dimensional polynomials. The flux support points no longer provide sufficient conditions and typically Galerkin weighting is used in this case.

Although many such variants exist, most of these "direct" coarse-mesh solvers have not been accepted in the industrial code systems to nearly the same degree as the class of transversely-integrated nodal methods, with a small number of exceptions. Here we can mention the more traditional FEM option implemented in the CRONOS code system (Lautard et al., 1991) and the Analytic Function Expansion Nodal (AFEN) method (Noh and Cho, 1993). We discuss the latter here as an illustrative example of how such methods are constructed.

2.4.1 The analytic function expansion method

The AFEN solution method makes use of a direct, non-separable analytic function expansion of the 3D intra-nodal flux and hence aims to solve eq. (2.2) directly. The intra-nodal flux is expanded in a combination of trigonometric and hyperbolic basis functions, each of which satisfies the diffusion equation at any point in the node. In the original 2D development, as discussed in Noh and Cho (1993) and Noh and Cho (1994), nine basis functions are used and coefficients are expressed in terms of the node-averaged flux, four side-averaged fluxes and four corner point fluxes.

Coupling conditions for node-averaged fluxes are determined by the set of nodal balance equations. Conditions for the side-averaged fluxes are obtained from current continuity conditions and conditions for corner fluxes are determined by considering neutron balance in a small box around the corner point. This original development proved quite accurate, but at a computation cost orderly 30% - 40% more expensive than standard transversely-integrated nodal methods (in 2D). The authors further indicated that the method would naturally lend itself to supply more accurate information to existing homogeneous flux reconstruction methods.

In subsequent developments of AFEN (Cho et al., 1997; Woo and Cho, 2000) the method was extended to support hexagonal geometry and the need for corner fluxes as support points was identified as a weakness. It was proposed to extend the set of basis functions in the intra-nodal expansion to include products of trigonometric functions and combinations of linear functions from the transverse directions (thus adding basis functions such as $y\sin(kx)$ or $yz\sin(kx)$). Given the additional coefficients in the expansion, further conditions were required to close the system of equations. Continuity of flux and current moments at node interfaces were utilized for this purpose, yielding excellent accuracy. In Noh and Cho (1994) and Woo and Cho (2000), the intra-nodal flux expansion is given in full detail, for 2D and 3D respectively; given the algebraic complexity of the expressions they are not repeated here. The method has

been further expanded to include cylindrical geometry (Cho, 2006) with the intention to support the class of pebble bed high temperature gas cooled reactor designs.

This method provides a good example of how "transverse leakage free" methods could be assembled and what benefit they aim to provide, be it in a non-rigorous fashion where the reasoning for the selection of required basis functions in the expansion is somewhat arbitrary. Although not clearly stated in associated publications for 3D problems, it may be deduced from the number of unknowns per node that the computational cost of this approach is probably comparable to full higher-order methods. In fact, in Noh and Cho (1994) it is indicated that 49 nodal unknowns are utilized, which would place the computational effort required to resolve the set of equations, to somewhere between a full second order and full third order higher-order solution. The meaning of this will be clarified in the following section, but suffice to say that this implies a calculational efficiency of around 10 times slower than the standard ANM with the quadratic leakage approximation in 3D (recall that the standard ANM carries 4 unknowns per node in 3D).

In the opinion of the author of this thesis, the AFEN method represents an ad-hoc simplification to the full higher-order methods, as they are described in Section 2.5, but in essence echoes the underlying aim of this work - how to justifiably enhance the accuracy of nodal methods for the purpose of improving the primary shortcomings of the leakage approximation and the intra-nodal flux reconstruction, at an acceptable cost.

2.5 Higher-order Nodal Methods

A short historical overview of higher-order nodal methods was provided in Section 1.4. This class of methods aim to describe (to an arbitrary order), the intra-node flux solution exactly. Since these methods are also generally based on the transverse integration principle, they provide, as a natural addition, the correct expression for the transverse leakage terms. Work in this regard was first suggested by Dorning (1979) and Dilbert and Lewis (1985), and later furthered by Ougouag and Rajić (1988), Altiparmakov and Tomašević (1990) and Guessous and Akhmouch (2002). This class of nodal methods will form the basis of the development of this thesis and hence, a more comprehensive overview is provided (in conjunction with Appendix A).

In the work by Ougouag and Rajić (1988) a weighted transverse integration approach, akin to weighted residual methods (particularly closer to Galerkin methods), is followed to generate the set of equations for higher-order flux moments. This

approach will also form the basis of the development in this thesis and as such, is described in detail in Section A.1. The method was later variationally derived by Altiparmakov and Tomašević (1990) which yielded useful insight regarding the actual intra-nodal flux expansion used in this class of higher-order nodal methods. It was made clear that the weighted residual method is equivalent to the variational formulation with the following intra-nodal trial function:

$$\phi_n^g(u,v,w) = \sum_{l=0}^{L}\sum_{k=0}^{K} f_{lk}(u)P_l(\frac{2v}{h_{n,v}})P_k(\frac{2w}{h_{n,w}}) + \sum_{m=0}^{M}\sum_{k=0}^{K} g_{km}(v)P_k(\frac{2w}{h_{n,w}})P_m(\frac{2u}{h_{n,u}})+ \tag{2.23}$$

$$\sum_{m=0}^{M}\sum_{l=0}^{L} h_{ml}(w)P_m(\frac{2u}{h_{n,u}})P_l(\frac{2v}{h_{n,v}}) - 2\sum_{k=0}^{K}\sum_{l=0}^{L}\sum_{m=0}^{M} c_{mlk}P_m(\frac{2u}{h_{n,u}})P_l(\frac{2v}{h_{n,v}})P_k(\frac{2w}{h_{n,w}})$$

with $f_{lk}(u)$, $g_{km}(v)$ and $h_{ml}(w)$ representing one-dimensional semi-moments in each direction and c_{lkm} denoting the full flux moments. All of the semi-moments may be related to the full flux moments (c_{lkm}) quite simply via

$$\begin{aligned} c_{mlk} &= \frac{2m+1}{h_{n,u}}\int_{h_u} f_{lk}(u)P_m(\frac{2u}{h_{n,u}})du \\ &= \frac{2l+1}{h_{n,v}}\int_{h_v} g_{km}(v)P_l(\frac{2v}{h_{n,v}})dv \\ &= \frac{2k+1}{h_{n,w}}\int_{h_w} h_{ml}(w)P_k(\frac{2w}{h_{n,w}})dw. \end{aligned} \tag{2.24}$$

Here K, L and M represent the order of the method in each direction and the same order is typically assumed in each direction (M). These higher-order methods clearly contain significantly more unknowns per node than the traditional nodal methods and hence incur a substantial calculational cost penalty. In subsequent work by Guessous and Akhmouch (2002) the solution was developed with partial currents as primary unknowns and recast in a response matrix formalism.

Independent of approach utilized, it is insightful to note that in 3D:

- Selecting the expansion order in (2.23) equal to 1, roughly matches the accuracy of the standard nodal method when employing the quadratic transverse leakage approximation, but at about three times the calculational cost; and

- Selecting the expansion order equal to 2 improves the error of the quadratic leakage approximation by about one order of magnitude, but at a cost penalty of about 10 times.

It can thus be understood why these methods have not found their way into the main stream of nodal diffusion methods, even though they provide a very elegant solution to the issues of both transverse leakage and homogeneous flux reconstruction.

Some initial efforts to amend these methods for the purpose of improving the transverse leakage approximation were made in Tomašević (1997), wherein an effort was made to perform local single node higher-order calculations and thus avoid spatial coupling. Although effective in significantly reducing calculational time, the governing assumption that higher-order side-flux moments were zero on node surfaces was too limiting and obtained accuracy was only marginally better than the ANM using the standard quadratic leakage approximation.

2.5.1 Description of weighted transverse integration in Cartesian geometry

As the weighted transverse integration approach is adopted in this work in order to develop a practical transverse leakage approximation, the derivation, as in principle described in Ougouag and Rajić (1988) is given in quite some detail. The full derivation is described in Appendix A and the important steps are repeated in this section to illuminate the characteristics of the approach and introduce notation needed in subsequent chapters.

The development produced here does differ somewhat from that which is proposed by Ougouag, since the method was originally formulated with side-averaged current moments as primary unknowns, whereas here the solution is built around the traditional ANM structure in which node-averaged fluxes, or in this case, node-averaged flux moments, are the primary unknowns.

As stated before, transverse integration requires that eq. (2.2) is integrated over the two transverse directions, in order to produce a one-dimensional equation in the third direction. This process is repeated for all three directions. To achieve this for a weighted transverse integration approach, it is again convenient to adopt the notation of three arbitrary directions (u, v, w), with u representing the direction of choice and v and w the transverse directions. To produce the set of transversely-integrated, one-dimensional, higher-order nodal equations, eq. (2.2) is multiplied by Legendre polynomials in both transverse directions, of order l and k, respectively. We let l

and k range from 0 to M for all the combinations of (l,k), where M denotes the order of the method. Note that $M=0$ denotes the standard lower-order equations. Furthermore, I will denote the maximum source expansion order used to formulate the source terms in the one-dimensional equations. Hence, a specific higher-order solution is classified by both indices (M,I). Note that we drop both the group index g and the node index n, in this section, for simplicity.

After completion of the weighted transverse integration process, the following equation for the higher-order one-dimensional moments is obtained:

$$-D\frac{d}{du^2}\phi_{lk}^{vw}(u)+\sigma_{\text{rem}}\phi_{lk}^{vw}(u)=\chi^g\frac{\nu}{k_{\text{eff}}}\sum_{h=1}^{G}\phi_{lk}^{vw,h}(u)\sigma_{\text{fis}}^{h}+ \tag{2.25}$$

$$\sum_{h=1}^{G}\phi_{lk}^{vw,h}(u)\sigma_{\text{scat}}^{h}(h\rightarrow g)-L_{lk}^{vw,w}(u)-L_{lk}^{vw,v}(u).$$

Here we identify $\phi_{lk}^{vw}(u)$ as the one-dimensional (lk) moment of the three-dimensional flux, integrated over directions v and w. As a convention, we shall denote the directions over which a quantity has been integrated via superscripts (vw) and the order of the Legendre Polynomials (in those directions) with which the quantity has been folded in the integral, by the corresponding subscripts (lk). The order of integration and indexing is determined in a cyclic manner ordered as uvw. Equation (2.25) looks very much like the standard zero-order one-dimensional equations, with the exception of the form of the leakage source contribution from the $w-$direction $L_{lk}^{vw,w}(u)$ and from the $v-$direction $L_{lk}^{vw,v}(u)$. These quantities may be expressed as:

$$L_{lk}^{vw,w}(u)=\frac{2k+1}{h_w}\left(J_l^{v,w}(u,\frac{h_w}{2})+(-1)^kJ_l^{v,w}(u,-\frac{h_w}{2})\right)+ \tag{2.26}$$

$$\frac{D(2k+1)k(k+1)}{h_w^2}\left(\phi_l^{v,w}(u,\frac{h_w}{2})+(-1)^k\phi_l^{v,w}(u,-\frac{h_w}{2})\right)-D\sum_{t=0}^{k-2}\frac{2k+1}{2t+1}\lambda_{tk}^{w}\phi_{lt}^{vw}(u)$$

and

$$L_{lk}^{vw,v}(u)=\frac{2l+1}{h_v}\left(J_k^{w,v}(u,\frac{h_v}{2})+(-1)^lJ_k^{w,v}(u,-\frac{h_v}{2})\right)+ \tag{2.27}$$

$$\frac{D(2l+1)l(l+1)}{h_v^2}\left(\phi_k^{w,v}(u,\frac{h_v}{2})+(-1)^l\phi_k^{w,v}(u,-\frac{h_v}{2})\right)-D\sum_{t=0}^{l-2}\frac{2l+1}{2t+1}\lambda_{lt}^{v}\phi_{tk}^{vw}(u).$$

.These expressions are quite complicated and as indicated, the full derivation of how these terms are obtained may be found in Appendix A. Here we simply identify terms and define $\phi_k^{w,v}(u, \pm\frac{h_v}{2})$ as the $u-$dependent k^{th} moments in w of the side-flux on the top and bottom $v-$surfaces; $J_k^{w,v}(u, \pm\frac{h_v}{2})$ as the $u-$dependent k^{th} moments in w of the net current on the top and bottom $v-$surfaces. In other words, these quantities define the u-dependent shape of moments in the transverse directions and on the transverse surfaces. Additionally

$$\lambda_{tk}^w = \frac{2t+1}{h_w} \int_{h_w} P_k''(\frac{2w}{h_w}) P_t(\frac{2w}{h_w}) dw \tag{2.28}$$

represents double Legendre integrals which may be expressed in terms of recurrence relationships (given in Appendix A) as

$$\lambda_{tk}^w = \left(\frac{2}{h_w}\right)^2 \left(\frac{2t+1}{2}\right) \left(\frac{k(k+1) - t(t+1)}{2}\right) \left(1 + (-1)^{k+t}\right).$$

The difficulties presented in solving eq. (2.25) is primarily in resolving the expressions for the higher-order transverse leakage terms. These higher-order one-dimensional equations may be solved via the same approach described in Section 2.3.2.1 and hence can make use of significant parts of existing nodal solvers to determine the side-flux and side-current moments, if the full flux moments are known (analogous to zero-order expressions (2.16) and (2.17)). The node-averaged higher-order flux moments are typically determined via the solution of the set of coupled higher-order balance equations, once again analogous to their zero-order counter parts via eq. (2.20). The set of higher-order balance equations, with triple index flux moments as primary unknowns, are generated by multiplying eq. (A.23) with $P_i(u)$ and integrating it over u. In this work, we will apply a somewhat different approach to solve for the higher-order full flux moments, as described in Chapter 3. The approach will yield a set of $(M+1)^3$ balance equations and $3(M+1)^2$ one-dimensional equations in 3D.

2.6 Formulation of the Proposed Solution

This overview of the most important classes of nodal methods, as applied in modern nodal codes, highlights the fact that the transverse leakage approximation is currently, and has been for some time, the primary source of error in code systems which utilize the ANM and NEM solution methods. Numerical support for this statement will be forthcoming in future chapters. In terms of the notation in this chapter, a solution is thus sought, which allows a more rigorous and accurate method of resolving the

expression for the transverse leakage term as it appears in eqs. (2.7) or (2.8). We notice from the overview of higher-order nodal methods and specifically expressions (2.26) and (2.27) for the case $k = l = 0$, that these methods provide us with this rigorous expansion in terms of moments of the flux, side-current and side-flux. The unacceptable penalty we then face is the cost of having to calculate all moments needed for reproducing the full intra-nodal flux shape as in expression (2.23) to close the system. Herein lies the primary challenge and the central question of this work:

Which set of justifiable simplifications may be introduced within the class of higher-order nodal methods to improve the representation of the zero-order transverse leakage term?

We may further compact this question in terms of the distinction introduced by Dorning (1979) between nodal (unknowns as node-averaged quantities) and coarse-mesh methods (unknowns as intra-nodal distribution) as:

How can one reformulate the class of higher-order "coarse-mesh" methods as true "nodal" methods?

Independent of which phrasing we select, these statements of the problem are dealt with in the upcoming chapters with the following requirements:

- The proposed development should be packaged into a standalone software module, pluggable into existing nodal codes as a leakage module with a simple interface;
- Full higher-order capability should be available in the module for the purpose of reference solution generation and homogeneous flux reconstruction; and
- The module should be capable of supplying leakage coefficients to a wide variety of nodal codes, independent of whether they utilize ANM or NEM (or other) solution schemes, and be compatible with a variety of acceleration and iteration schemes.

2.7 Conclusion

In this chapter a detailed overview of modern nodal methods was provided, with specific focus on the Analytic Nodal Method, the Nodal Expansion Method and the Analytic Function Expansion Nodal method. The origin and typical solution methods regarding the treatment of the so-called transverse leakage term was discussed and as such, the primary area of investigation of this thesis was defined. The class of higher-order nodal methods, from which a solution strategy is to be derived, was

presented. Finally, the problem statement and proposed solution were defined in terms of these existing schemes and the next chapters will focus on the development of such a solution and the quantification of its accuracy and performance.