

# Chapter 3

## The development of a consistent transverse leakage approximation

### 3.1 Introduction

Thus far nodal methods, their history and their main line developments have been overviewed and the problem at hand described. Chapter 2 is concluded with a derivation of the class of so-called higher-order nodal diffusion methods with a brief overview of their strengths and weaknesses. It is echoed in this work, as suggested by the original authors, that this class of higher-order nodal methods represents the natural extension of standard nodal methods to higher-orders and thus should provide a strong theoretical base from which an appropriate simplification, for the purpose of improving the transverse leakage approximation, could be derived. This chapter is thus focused on the development of such a simplification and represents an important part of the contribution put forward in this work.

The higher-order methods have been demonstrated to significantly improve upon the accuracy of the quadratic transverse leakage approximation, but thus far with a large and unacceptable associated computational cost. Typically, standard nodal methods provide performance improvement factors of between 100 and 1000 in 3D relative to finite-difference methods. The current status of higher-order nodal methods decreases this advantage by between 10 and 20 times and hence makes the coarse-mesh methods less attractive. The performance advantage of nodal methods is not without penalty and issues such as homogenization, coarse-mesh burnup, intra-nodal cross-section shape approximations and flux reconstruction are considered manageable drawbacks. Nevertheless, this balance between benefit and disadvantage limits the willingness of industrial code developers to significantly compromise the efficiency of the current state of the art nodal methods.

In this work, a method is suggested which would aim to maintain the accuracy benefits of the higher-order approaches, but limit the computational cost penalty to approximately 50% as compared to the standard ANM, utilizing the quadratic leakage approximation. It should be stated that the class of higher-order nodal diffusion methods provides not only significant accuracy improvements, but inherently provides information regarding the detailed intra-nodal flux shape, which is needed for features such as homogeneous flux reconstruction. This work therefore also aims to make these additional benefits of this powerful class of solution methods practical for use in production codes.

## 3.2 Overview of the Approach

The method we propose in this work and the associated development we suggest as novel is divided into two parts, described in Chapters 3 and 4. In this current chapter the proposed simplification to the standard higher-order nodal method is developed, which aims to reduce the number of unknowns as compared to full higher-order methods. The basic premise for this reduction, is the decision that one is only interested in improving the representation of the transverse leakage expression as it appears in the standard one-dimensional equations (or zero-order nodal methods) and not, as is typical in higher-order methods, in the full intra-nodal flux shape. We will however explore a like-minded simplification for the sake of homogeneous flux reconstruction in Chapter 4.

Nevertheless, the current chapter aims at defining what we term a “consistent” leakage approximation and establishes the base accuracy of the proposed approach. The reduction in the number of unknowns does not, however, yet provide sufficient calculational efficiency and Chapter 4 focuses on the development of a number of iteration and solution schemes to accelerate and make the proposed approach practical.

## 3.3 A Consistent Leakage Approximation

### 3.3.1 Adaptation of standard (zero-order) nodal method

The underlying idea of the contribution in this work, as touched upon in the previous section, is the effort to represent the transverse leakage expression without solving the full set of higher-order nodal equations. The first step in this process, is to investigate the form of the transverse leakage term, as it appears in the zero-order

one-dimensional nodal equations. Here we reconnect with the notation in the previous chapter and restate, for clarity, eq. (2.7), which is the exact expression of the transverse leakage term in terms of flux as

$$\begin{aligned}
L_n^{g,vw}(u) &= L_n^{g,v}(u) + L_n^{g,w}(u) \tag{3.1} \\
&= -D_n^g \left[ \frac{1}{h_{n,v}} \frac{1}{h_{n,w}} \int_{h_{n,v}h_{n,w}} \frac{\partial^2}{\partial v^2} \phi^g(u, v, w) dv dw \right] \\
&\quad - D_n^g \left[ \frac{1}{h_{n,v}} \frac{1}{h_{n,w}} \int_{h_{n,v}h_{n,w}} \frac{\partial^2}{\partial w^2} \phi^g(u, v, w) dv dw \right]
\end{aligned}$$

where we have separated the contribution from the  $v$  and  $w$  directions to  $u$ . The value of this expression is largely academic since typically, in standard nodal methods, no information is available regarding the intra-nodal flux shape  $\phi^g(u, v, w)$ . On the other hand, higher-order methods, through the establishment of the appropriate intra-nodal trial function in Altiparmakov and Tomašević (1990), give us this information (originally given in eq. (2.23) as discussed in Section 2.5), with all directions expanded to order  $M$  as

$$\phi(u, v, w) = \sum_{l=0}^M \sum_{k=0}^M f_{lk}(u) P_l\left(\frac{2v}{h_v}\right) P_k\left(\frac{2w}{h_w}\right) + \sum_{m=0}^M \sum_{k=0}^M g_{km}(v) P_k\left(\frac{2w}{h_w}\right) P_m\left(\frac{2u}{h_u}\right) + \tag{3.2}$$

$$\sum_{m=0}^M \sum_{l=0}^M h_{ml}(w) P_m\left(\frac{2u}{h_u}\right) P_l\left(\frac{2v}{h_v}\right) - 2 \sum_{m=0}^M \sum_{l=0}^M \sum_{k=0}^M c_{mlk} P_m\left(\frac{2u}{h_u}\right) P_l\left(\frac{2v}{h_v}\right) P_k\left(\frac{2w}{h_w}\right).$$

All the terms have the same meaning as discussed for eq. (2.23). Note again, as in Section 2.5, we have dropped the node index  $n$  and the group index  $g$ , with the order of integration and directions determined in a cyclic manner ordered as  $uvw$ , carrying indices  $mlk$ . Thus, quantities in direction  $v$ , would have indices ordered as  $km$ . To clarify this further, consider Figure 3.1 which illustrates the cyclic nature of the directions.

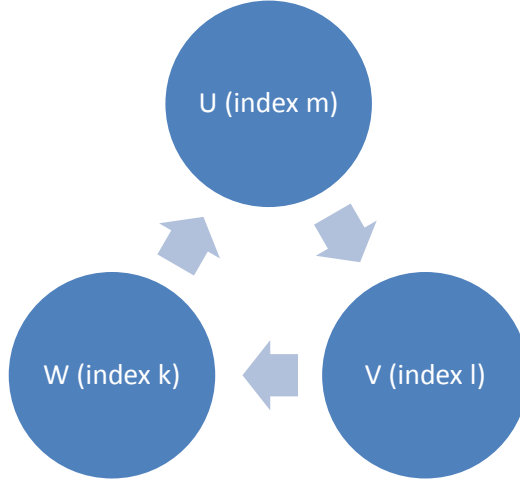


Figure 3.1: A graphical depiction of the indexing and directional cycling notation employed in the higher-order derivations.

In this text we would typically consider direction  $u$  as the primary direction under consideration and perform transverse integration firstly over direction  $w$  and then direction  $v$  in order to produce the one-dimensional  $u$ -equations. We insert expansion (3.2) into eq. (3.1) to obtain the exact (up to the order of the expansion) expression for the transverse leakage terms. We treat each term in the trial function separately and illustrate here the four resulting terms specifically for the contribution from the  $v$ -direction. We utilize the orthogonality of Legendre polynomials and obtain:

$$\begin{aligned}
\text{Term 1: } & -\frac{2D}{h_v^2} \sum_{l=0}^M f_{l0}(u) \left( P'_l(1) - P'_l(-1) \right), \\
\text{Term 2: } & \frac{1}{h_v} \sum_{m=0}^M \left( J_{0m}^v \left( \frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right), \\
\text{Term 3: } & -\frac{2D}{h_v^2} \sum_{l=0}^M \sum_{m=0}^M \left( \int_{h_{n,w}} h_{ml}(w) P_0 \left( \frac{2w}{h_w} \right) dw \right) P_m \left( \frac{2u}{h_u} \right) \left( P'_l(1) - P'_l(-1) \right), \\
\text{Term 4: } & +\frac{4D}{h_v^2} \sum_{l=0}^M \sum_{m=0}^M c_{ml0} P_m \left( \frac{2u}{h_u} \right) \left( P'_l(1) - P'_l(-1) \right)
\end{aligned} \tag{3.3}$$

where  $J_{0m,v}(\pm \frac{h_v}{2})$  denotes the net side-current moment of order  $m$  on the  $(\pm)$  surface in the  $v$ -direction, or more precisely

$$J_{0m}^v \left( \pm \frac{h_v}{2} \right) = \mp D \frac{\partial}{\partial v} g_{0m}(v) \Big|_{v=\pm \frac{h_v}{2}}. \quad (3.4)$$

We notice that  $\int_{h_n,w} h_{ml}(w) P_0 \left( \frac{2w}{h_w} \right) dw$  and  $c_{ml0}$  both represent full flux moments of the same order and may be combined to yield:

$$\begin{aligned} L^v(u) = & -\frac{2D}{h_v^2} \sum_{l=0}^M f_{l0}(u) \left( P_l'(1) - P_l'(-1) \right) + \\ & \frac{1}{h_v} \sum_{m=0}^M \left( J_{0m}^v \left( \frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) \\ & + \frac{2D}{h_v^2} \sum_{l=0}^M \sum_{m=0}^M c_{ml0} P_m \left( \frac{2u}{h_u} \right) \left( P_l'(1) - P_l'(-1) \right) \end{aligned} \quad (3.5)$$

again given here only for contribution from  $v$  to  $u$  (contribution from  $w$  to  $u$  has similar form). Now we exchange the index of the second sum in the third term from  $m$  to  $i$ , group first and third term together and exchange the index of the first sum from  $l$  to  $m$ , to obtain

$$\begin{aligned} L^v(u) = & \frac{1}{h_v} \sum_{m=0}^M \left( J_{0m}^v \left( \frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) - \\ & \frac{2D}{h_v^2} \sum_{m=0}^M \left[ \left( P_m'(1) - P_m'(-1) \right) \left( f_{m0}(u) - \sum_{i=0}^M c_{im0} P_i \left( \frac{2u}{h_u} \right) \right) \right]. \end{aligned} \quad (3.6)$$

In eq. (3.6)  $M$  denotes the maximum order of the intra-nodal expansion, which is not necessarily equal to the order of the leakage expansion  $M_l$ , as in point 2 above. We thus choose  $M_l$  independently as the leakage expansion order and analyze the full expression of transverse leakage (3.6) for various values of  $M_l$  :

- If  $M_l = 0$ , we obtain the standard zero-order flat leakage approximation, in terms of the side-averaged net currents in the  $v$ -direction:

$$L^v(u) = \frac{1}{h_v} \left( J_{00}^v \left( +\frac{h_v}{2} \right) + J_{00}^v \left( -\frac{h_v}{2} \right) \right). \quad (3.7)$$

The average (flat) leakages in three adjacent nodes are typically utilized in the standard zero-order nodal methods to approximate the leakage polynomial via a quadratic fit.

- If  $M_l \rightarrow \infty$  and using the definition of  $f_{m0}(u) = \sum_{i=0}^{\infty} c_{im0} P_i \left( \frac{2u}{h_u} \right)$ , the second term falls away and we obtain:

$$L^v(u) = \frac{1}{h_v} \sum_{m=0}^{M_l} \left( J_{0m}^v \left( +\frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right). \quad (3.8)$$

- For any practical application, we may differentiate between  $0 < M_l \leq M < \infty$  in which case we rewrite

$$L^v(u) = \frac{1}{h_v} \sum_{m=0}^{M_l} \left( J_{0m}^v \left( \frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) \quad (3.9)$$

and  $0 < M < M_l < \infty$ , which yields, after exchanging indices  $m$  and  $i$  in the second term,

$$L^v(u) = \frac{1}{h_v} \sum_{m=0}^{M_l} \left( J_{m0}^v \left( \frac{h_v}{2} \right) + J_{m0}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) - \quad (3.10)$$

$$\frac{2D}{h_v^2} \sum_{m=M+1}^{M_l} \left[ \sum_{i=0}^M \left( P_i'(1) - P_i'(-1) \right) c_{mi0} P_m \left( \frac{2u}{h_u} \right) \right].$$

It can be seen that if we limit the leakage to a polynomial expansion order  $M_l$ , the second term in eq. (3.6), written after expansion as eq. (3.10), contributes only if  $M > 1$  (properties of Legendre polynomial derivatives) and only for cases where we choose  $M_l > M$  (index  $i$  starts at  $M + 1$ ). In the latter case, some terms above the order of the leakage approximation may be included in the expansion. The inclusion of these terms is a matter of interpretation, since the choice of  $M_l$  implies that we are not interested in polynomials of a higher-order than  $M_l$  in the expansion and thus we proceed by selecting  $M_l = M$ , in which case the second term disappears and we remain with eq. (3.9). For example, if we limit  $L^v(u)$  to a second order expansion with  $M_l = M = 2$ , we obtain expression (3.11) and have formulated what may be termed the consistent quadratic leakage approximation (CQLA), written here with contributions from both  $v$  and  $w$  as

$$L^{vw}(u) = \frac{1}{h_v} \sum_{m=0}^2 \left( J_{0m}^v \left( +\frac{h_v}{2} \right) + J_{0m}^v \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) + \quad (3.11)$$

$$\frac{1}{h_w} \sum_{m=0}^2 \left( J_{m0}^w \left( +\frac{h_w}{2} \right) + J_{m0}^w \left( -\frac{h_w}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right).$$

This expression for  $L^{wv}(u)$  describes the shape of the transverse leakage in direction  $u$  from direction  $v$  and  $w$  out of the node in terms of side-current moments. The generalized form of expression (3.6) was alternatively obtained in Section 2.5.1 via weighted transverse integration and eq. (3.6) could be recovered from eq. (2.27) by

1. substituting  $k = l = 0$ ; and
2. projecting the  $u$ -dependent leakage source onto a set of Legendre polynomials up to order  $M_l$ .

We note that in this consistent, higher-order leakage approximation, the transverse leakage terms may be expressed as a function of one-dimensional current moments ( $J_{0m}^v$  and  $J_{m0}^w$ ). Our task therefore is reduced to finding a method of generating these higher-order moments and to use them in the construction of the zero-order transverse leakage shape. Prior to considering how to obtain these current moment expressions, it is insightful to evaluate graphically how this consistent transverse leakage approximation differs from that which is obtained from the standard quadratic leakage approximation (SQLA).

To illustrate this difference more clearly, consider Figures 3.2 and 3.3, which depict the information utilized in constructing the SQLA vs the proposed CQLA.

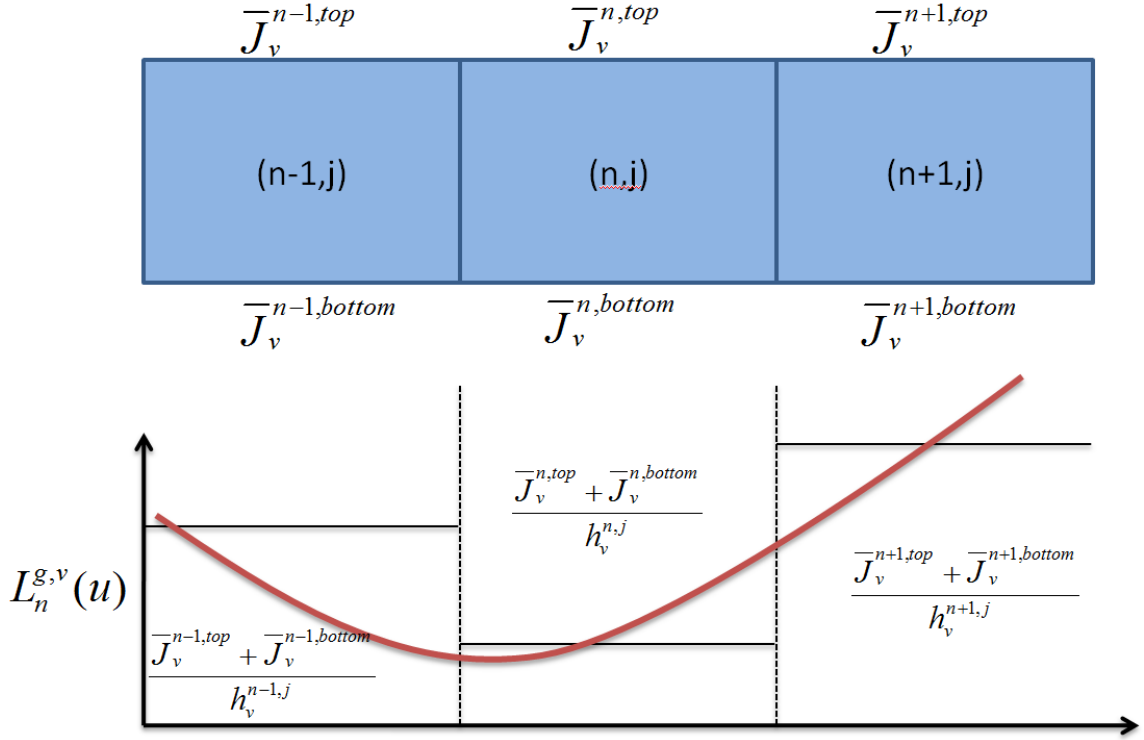


Figure 3.2: A graphical depiction of the information utilized in constructing the standard quadratic transverse leakage approximation.

We are interested to find the shape of the transverse leakage from the  $v$ - to the  $u$ -direction. In Figure 3.2 the SQLA approach is depicted and it can be seen that the average leakages on the  $v$ -surfaces are taken from three adjacent nodes in the  $u$ -direction. The three average leakages are then fitted with a quadratic polynomial over the three adjacent nodes to produce an  $u$ -dependent transverse leakage shape. This in itself is somewhat inconsistent, since only information from neighbours in the  $u$ -direction is used to estimate the leakage from the  $v$ -direction.



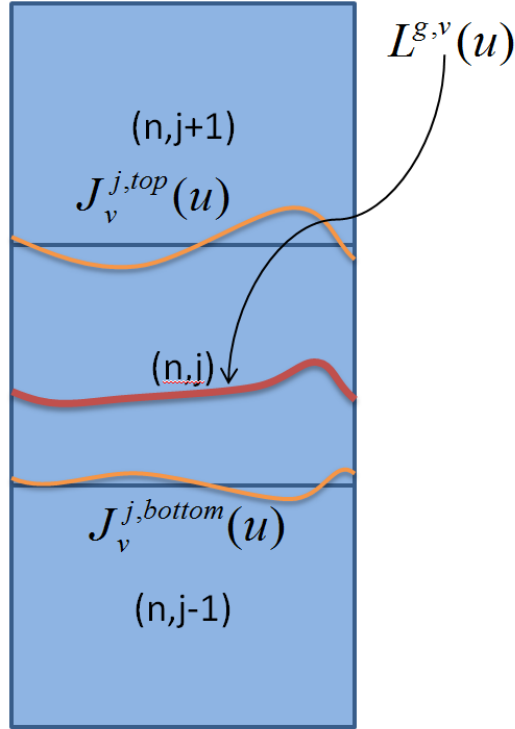


Figure 3.3: A graphical depiction of the information utilized in constructing the consistent quadratic transverse leakage approximation.

In Figure 3.3, the CQLA approach to the leakage shape is depicted. Here we see that the shape of the currents on the surfaces between the neighbours in the  $v$ -direction is used to determine the transverse leakage from the  $v$ -neighbours. It indeed seems more appropriate to use information from the neighbours in the  $v$ -direction to estimate the leakage shape from that direction. According to eq. (3.11) the leakage term is expressed in terms of the one-dimensional current moments on the top and bottom surfaces. The  $u$ -dependent information in the  $v$ -neighbours originates from the global solution.

Although these arguments are somewhat heuristic, they provide some intuitive reasoning behind why higher-order nodal methods are often classified as consistent and why utilizing the higher-order nodal formalism may prove to be the correct approach when approximating the transverse leakage terms specifically, as they appear in standard transversely-integrated nodal methods.

### 3.3.2 Higher-order calculation of current moments

We have identified, in eq. (3.11), that moments of the net current on the transverse surfaces are required in order to express the transverse leakage term, as it appears in the zero-order one-dimensional equations. We resort to techniques from standard higher-order methods once more and apply the weighted transverse integration procedure to generate a set of one-dimensional equations which may be solved to generate the current moments needed.

After this process, as discussed in Section 2.5.1, we obtain one-dimensional higher-order equations as given in eq. (2.25) and repeat it here for clarity

$$-D \frac{d^2}{du^2} \phi_{lk}^{vw}(u) + \sigma^{\text{rem}} \phi_{lk}^{vw}(u) = \chi^g \frac{\nu}{k_{\text{eff}}} \sum_{h=1}^G \phi_{lk}^{vw,h}(u) \sigma_{\text{fis}}^h + \sum_{h=1}^G \phi_{lk}^{vw,h}(u) \sigma_{\text{scat}}^h(h \rightarrow g) - L_{lk}^{vw,w}(u) - L_{lk}^{vw,v}(u) \quad (3.12)$$

with  $L_{lk}^{vw,w}(u)$  and  $L_{lk}^{vw,v}(u)$  representing the higher-order transverse leakage contributions from  $w$  and  $v$ , respectively. Their explicit form is provided in eqs. (2.26) and (2.27). If we connect with the notation utilized in the 3D trial function given in eq. (3.2), we can equate the moments in the trial function with the transversely-integrated flux moments in the following way:

$$f_{lk}(u) = \phi_{lk}^{vw}(u),$$

$$g_{km}(v) = \phi_{km}^{wu}(v),$$

$$h_{ml}(w) = \phi_{ml}^{vw}(w) \text{ and}$$

$$c_{mlk} = \phi_{mlk}^{uvw}.$$

As a reminder of this notation, the subscripts and superscripts denote the orders and directions over which a quantity has been integrated, respectively.

If the source terms in eq. (3.12) are resolved, it can be solved analytically as per the standard ANM procedure, only here for higher-order flux moments as unknowns. Fission and scattering sources are treated as known by utilizing the higher-order flux moments from the previous iteration and we are left to investigate the higher-order transverse leakage sources. However, before proceeding to investigate these sources,

we first aim at determining which  $(l, k)$  pairs are needed and thus how many one-dimensional equations have to be assembled.

If we revisit eq. (3.11), in an effort to determine which current moments are needed for the case of a second order expansion (rewritten here in full higher-order notation) as

$$L_{00}^{vw}(u) = \frac{1}{h_v} \sum_{m=0}^2 \left( J_{0m}^{wu,v} \left( +\frac{h_v}{2} \right) + J_{0m}^{wu,v} \left( -\frac{h_v}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right) + \quad (3.13)$$

$$\frac{1}{h_w} \sum_{m=0}^2 \left( J_{m0}^{uv,w} \left( +\frac{h_w}{2} \right) + J_{m0}^{uv,w} \left( -\frac{h_w}{2} \right) \right) P_m \left( \frac{2u}{h_u} \right)$$

in direction  $u$  with contributions from both  $v$  and  $w$ , we see that we are only interested in current moment pairs of orders  $(0, 0)$ ,  $(0, 1)$ ,  $(0, 2)$ ,  $(1, 0)$  and  $(2, 0)$ . Thus only these five equations per direction need to be generated via weighted transverse integration and solved analytically.

This implies that limiting the leakage expansion to order 2 and only solving the higher-order equations needed for the representation of the transverse leakage term reduce the number of one-dimensional higher-order equations from 27 in full second order solutions to 15 in 3D (if we include the zero-order 1D equations in this count). This is an important simplification as compared to full higher-order approaches.

### 3.3.3 Treatment of higher-order leakage terms

After we perform the weighted transverse integration and obtain one-dimensional equations, we proceed to solve these equations analytically, as is typically done in the ANM zero-order methods. From the analytic solution, we obtain the needed side-current moments by solving two-node problems in each direction (as is also typically done in zero-order methods). The major difference in these higher-order equations (as compared to the zero-order equations), is the structure of the higher-order transverse leakage terms. These terms are still quite complicated and contain various current, side-flux and full flux moments, which are not standardly available in nodal codes and require us to add additional one-dimensional equations (see eqs. (2.26) and (2.27)). Here, however, we make an important observation. The average value of the leakage terms in the higher-order equations for direction  $u$  and contribution from  $w$ , for arbitrary  $k$ , is

$$\bar{L}_{lk}^{vw,w} = \frac{2k+1}{h_w} \left( J_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + (-1)^k J_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) + \quad (3.14)$$

$$\frac{D(2k+1)k(k+1)}{h_w^2} \left( \phi_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + (-1)^k \phi_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) - D \sum_{t=0}^{k-2} \frac{2k+1}{2t+1} \lambda_{tk}^w \phi_{0l,t}^{uv,w}(u).$$

where  $J_{0l}^{uv,w}(\pm \frac{h_w}{2})$  refers to the side-current moment and  $\phi_{0l}^{uv,w}(\pm \frac{h_w}{2})$  to the side-flux moment on the  $\pm w$ -sides and  $\phi_{0l,t}^{uv,w}$  to the  $(0, l, t)$  full flux moment, calculated from the one-dimensional equation in direction  $w$ . Thus explicitly, written up to the second order (since these are the terms we need to consider for a second order leakage expansion), we have:

$$\begin{aligned} \bar{L}_{l0}^{vw,w} &= \frac{1}{h_w} \left( J_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + J_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) \\ \bar{L}_{l1}^{vw,w} &= \frac{3}{h_w} \left( J_{0l}^{uv,w} \left( \frac{h_w}{2} \right) - J_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) + \frac{6D}{h_w^2} \left( \phi_{0l}^{uv,w} \left( \frac{h_w}{2} \right) - \phi_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) \\ \bar{L}_{l2}^{vw,w} &= \frac{5}{h_w} \left( J_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + J_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) + \\ &\quad + \frac{30D}{h_w^2} \left( \phi_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + \phi_{0l}^{uv,w} \left( -\frac{h_w}{2} \right) \right) - \frac{60D}{h_w^2} \phi_{0l,0}^{uv,w} \end{aligned} \quad (3.15)$$

Using only the average value of the higher order leakage terms (or in other words a “flat” leakage approximation) in the higher order equations, the expressions above may be constructed from quantities which are already available within the solution. To clarify this, it is instructive to list which data is typically available from zero-order nodal methods and thus clarify which data, needed in the proposed development, would require additional calculations. Table 3.1 describes the set of nodal quantities typically calculated as routine within transversely-integrated nodal methods. Note that, once again, the node index  $n$  and the group index  $g$  are dropped in the table and quantities are given in higher-order notation.

Table 3.1: Notational description of nodal quantities available in standard nodal codes, with  $I$  referring to the maximum source order (typically 4).

Quantity	Description
$\bar{\Phi}_{000}$	Node-averaged flux
$J_{00}^{vw,u} \left( \pm \frac{h_u}{2} \right), J_{00}^{wu,v} \left( \pm \frac{h_w}{2} \right), J_{00}^{uv,w} \left( \pm \frac{h_w}{2} \right)$	Side-averaged current
$\phi_{00}^{vw,u} \left( \pm \frac{h_u}{2} \right), \phi_{00}^{wu,v} \left( \pm \frac{h_w}{2} \right), \phi_{00}^{uv,w} \left( \pm \frac{h_w}{2} \right)$	Side-averaged flux
$\phi_{00,m}^{vw,u}, \phi_{00,l}^{wu,v}, \phi_{00,k}^{uv,w}$	Flux moments $k, l$ or $m$ ( $\{k, l, m\} \in \{0 \dots I\}$ )

In Table 3.1  $\bar{\Phi}_{000}$  refers to the node-averaged flux,  $J_{00}^{vw,u}(\pm \frac{h_u}{2})$  to the side-averaged current on the  $\pm$  surface in the  $u$  direction and  $\phi_{00,m}^{vw,u}$  refers to the  $m^{th}$  order Legendre moment of the one-dimensional flux in the  $u$  direction. With this table in hand, consider eq. (3.14) again and note:

- when  $l = 0$  all quantities are from the standard zero-order nodal solution - namely surface-averaged net currents ( $J_{00}^{uv,w}$ ), surface-averaged fluxes ( $\phi_{00}^{uv,w}$ ) and node-averaged flux ( $\bar{\Phi}_{000}$ ); and
- when  $l > 0$ , then  $k = 0$  since we need only (0,0), (0,1),(0,2),(1,0),(2,0) pairs and eq. (3.14) reduces to

$$\bar{L}_0^{vw,w} = \frac{1}{h_w} \left( J_{0l}^{uv,w} \left( \frac{h_w}{2} \right) + J_{0l}^{vu,w} \left( -\frac{h_w}{2} \right) \right). \quad (3.16)$$

However, these surface-current moments will be available since the equation pairs were already identified as necessary to be solved for expressing the zero-order transverse leakage term in expression (3.11).

This implies that a "flat leakage" approximation in the higher-order equations allows us to resolve the higher-order leakage terms without the need for solving any further equations. This is an important assumption which differentiates this method from the typical higher-order approach. In justification of such an assumption, it is important to note that we are in actual fact discarding only cross-term flux moments from the intra-nodal expansion, or terms which have more than one index different from zero. It is reasonable to assume that our intra-nodal flux distributions are smooth functions and as such we postulate that a reduced lower-order subset of the full expansion may yield a representation sufficiently accurate to express the shape of the nodal side-currents, as are needed in the resolution of the one-dimensional transverse leakage terms. Various alternative approaches for reduction of the expansion could be adopted, such as ANOVA analysis which allows the rejection of bases functions based on their contribution to the total function variance (An and Owen, 2001) or sparse grid based integration (Griebel and Grestner, 1998) which assumes a limited summative order for the multi-dimensional expansion. Although not directly applied here, these formulations support the arguments that a lower-order subset of the full expansion may retain much of the intra-nodal shape information and specifically that the discarded cross-terms may be regarded as smaller higher-order contributions.

At this point we make a final important observation. In order to solve the higher-order one-dimensional equations and thus to obtain the surface-current moments

which we require in the zero-order transverse leakage expression, we construct a two-node problem utilizing current and flux moment continuity conditions at shared interface surfaces and solve for the interface current moments. This approach is analogous to the standard zero-order ANM and requires the average value of the flux moment under consideration (see description in Section 2.3.2.2). We reproduce the side-current expression here, based on eq. (2.19), but rewritten for the higher-order case. Note that the neighbouring node numbers  $s$  and  $p$  are reintroduced to indicate from which node a quantity is taken and yields

$$J_{s,kl}^{vw,u} \left( +\frac{2u}{h_{s,u}} \right) = C_s^u \left( +\frac{2u}{h_{s,u}} \right) \left( \bar{\Phi}_{s,0lk}^{uvw} - Z_{s,kl}^{vw,u} \left( +\frac{2u}{h_{s,u}} \right) \right) - \quad (3.17)$$

$$C_p^u \left( -\frac{2u}{h_{p,u}} \right) \left( \bar{\Phi}_{p,0lk}^{uvw} - Z_{p,kl}^{vw,u} \left( -\frac{2u}{h_{p,u}} \right) \right).$$

In eq. (3.17),  $C_s^u \left( +\frac{2u}{h_{s,u}} \right)$  refers to the nodal coupling coefficient on the outer surface in the  $u$  direction of node  $s$  and  $Z_{s,kl}^{vw,u} \left( +\frac{2u}{h_{s,u}} \right)$  to the value of the tensorial source on the outer  $u$ -boundary of node  $s$ . From this equation it can be seen that the average value of the higher-order flux moments,  $\bar{\Phi}_{s,0lk}^{vwu}$  and  $\bar{\Phi}_{p,0lk}^{vwu}$ , from neighbouring nodes  $s$  and  $p$  are needed in order to solve the higher-order interface current moment at the surface which these nodes share. In full higher-order methods, the average value of the flux moments are obtained from a full spatial sweep of the system for each moment. If we, once again, inspect the set of equation pairs needed to represent only the zero-order transverse leakage term, we identify that, for the  $u$  direction, we require node-averaged flux moments with indices (000,001,002,010,020). Moreover, if we consider all three directions, we require node-averaged flux moments with indices (000,001,002,010,020,100,200). Since only one index is different from 0, these flux moments are actually the moments of the one-dimensional flux, written in full higher-order notation, for moments in the  $u$  direction, as

$$\phi_{00,m}^{vw,u} = \frac{2m+1}{h_u} \int_{h_u} \phi_{00}^{vw}(u) P_m \left( \frac{2u}{h_u} \right) du. \quad (3.18)$$

All of these one-dimensional flux moments are typically calculated by nodal codes by projecting the one-dimensional solutions onto a set of Legendre polynomials and hence are already available (see Table 3.1). It is thus not needed to sweep the system to obtain these flux moments and the subsequent current moments from the solution of the constructed two-node problems.

To clarify this, consider once more the node averaged higher moments needed in eq. (3.17) and investigate the distinction between  $\phi_{lk,0}^{vw,u}$  and  $\bar{\Phi}_{s,0lk}^{uvw}$ . The former refers to the one-dimensional flux moment in the direction  $u$ , of order 0, as projected from the solution of the higher-order one-dimensional equation weighted with the Legendre polynomial of order  $l$  in direction  $v$  and order  $k$  in direction  $w$ . The latter, with the same indices, refers to the **node-averaged** higher-order flux moment of order  $0lk$ . In actual fact there are three different higher-order one-dimensional moments with indices  $0lk$ , one in each direction and  $\bar{\Phi}_{s,0lk}^{uvw}$  is actually computed as the average of these three. It should of course be so that, since the order of integration is arbitrary, all four these moments (average and three one-dimensional counterparts) are equal, but this is only true at convergence of the solution and thus the averaging process is needed in order to stabilize the iteration sequence. Thus, in this case, node-averaged flux moment  $\bar{\Phi}_{s,0lk}^{uvw}$  is calculated from

$$\bar{\Phi}_{s,0lk}^{uvw} = \frac{(\phi_{lk,0}^{vw,u} + \phi_{k0,l}^{wu,v} + \phi_{0l,k}^{uv,w})}{3} \quad (3.19)$$

as an alternative to generating the set of higher-order balance equations and solving the resulting linear system for each moment.

This observation of using the one-dimensional flux moments obtained from any typical nodal code instead of sweeping the system for their average values, is the final differentiating factor between the described method and the full higher-order methods and supports the claim that this formulation could prove to be the basis for a local, or hierarchically constructed, higher-order transverse leakage approximation. This step further allows the decoupling of the higher- and lower-order components of the solution, as discussed in more detail in Chapter 4.

In summary, the proposed method, for a second order expansion, adapts the typical higher-order nodal diffusion method in the following ways:

- generate only the higher-order equations, or  $(l, k)$  pairs per direction, needed for the representation of the standard one-dimensional transverse leakage expression - thus retain only  $(l, k)$  pairs with one index different from zero. The resulting expression requires only one-dimensional current moments on each surface;
- limit the order of the transverse leakage expansion in the zero-order equations to 2;

- apply a "flat" leakage approximation in the higher-order one-dimensional equations, which “decouples” the remaining unknowns in full higher-order methods and closes the system. This approximation effectively neglects cross-terms from the solution of the higher-order equations and constitutes the major approximation in the proposed method;
- instead of sweeping the system, obtain the node-averaged values for the higher-order flux moments from the zero-order nodal solution. This is possible since only a subset of surface-current moments (as compared to full higher-order) are needed to express the zero-order transverse leakage term and specifically only higher-order moments with a single non-zero index;
- solve a two-node problem on each surface to obtain the surface-current moments from the analytic solution of the one-dimensional higher-order equations. This implies 15 two-node problems to be solved per node in 3D; and
- The proposed CQLA method, in 3D, would require the calculation of 7 node-averaged flux moments, as compared to 27 for a full second order, higher-order solution. The expected gain then, in terms of computational cost, taking into account the additional burden of solving the two-node problems, is around a factor of 3. Numerical analysis in Chapter 5 aims to quantify this estimate on practical problems.

This description concludes the definition of the consistent transverse leakage approximation (CLA) and in particular the definition of the consistent quadratic transverse leakage approximation (CQLA). The proposed method is not limited to the second order and may be extended to an arbitrary order if the required higher-order one-dimensional equations are added to the solution set. However, further performance improvements to the CQLA approach are needed to make this approach practical and these are introduced and discussed in Chapter 4. Numerical examples to quantify the performance and accuracy of the CQLA approach are analyzed in Chapter 5.

### 3.4 Extension of the Method to a Full Higher-order Solution

As discussed in Section 3.3, the solution method proposed for the subset of higher-order equations differs from previously published work, primarily in the calculation of



higher-order node-averaged flux moments. In past higher-order solution schemes (Altiparmakov and Tomašević, 1990; Ougouag and Rajić, 1988; Guessous and Akhmouch, 2002) higher-order flux (or in some cases side-current) moments are obtained iteratively via spatial sweeps over the system for each moment.

In this work the aim is to solve the higher-order equations, so far possible, locally, using the zero-order nodal solution as a driver. Such a scheme would facilitate the development of a standalone higher-order module and in doing so simplify the connection to existing nodal codes. The discussion in Section 3.3.3 achieves this requirement, since the needed higher-order node-averaged flux moments are constructed from one-dimensional flux moments available in zero-order nodal codes.

Due to the flat leakage approximation in the higher-order equations, the set of equations was restricted, but if the full expressions for higher-order transverse leakage are kept (as in eqs. (2.26 and 2.27)) all 27 moments (in the case of 3D second order) are required. The question arises whether such a hierarchical construction could be utilized to perform a full higher-order solution and thus avoid spatial sweeps for all the higher-order flux moments.

To illustrate this hierarchical principle, Table 3.2 extends Table 3.1 in that all the additional quantities, available from the CQLA method, are listed. For brevity, only the quantities obtained from the one-dimensional  $u$ -equation are shown.

Table 3.2: Nodal quantities available in the CQLA solution.

Symbol	Description
$\overline{\Phi}_{m00}^{uvw}, \overline{\Phi}_{0m0}^{uvw}, \overline{\Phi}_{00m}^{uvw}$	Higher-order node-averaged flux moments
$J_{0m}^{vw,u}(\pm \frac{h_u}{2}), J_{m0}^{vw,u}(\pm \frac{h_u}{2})$	Side-averaged current moments
$\phi_{0m}^{vw,u}(\pm \frac{h_u}{2}), \phi_{m0}^{vw,u}(\pm \frac{h_u}{2})$	Side-averaged flux moments
$\phi_{m0,i}^{vw,u}, \phi_{0m,i}^{vw,u}$	One-dimensional flux moments of order $i$

The critical observation from Table 3.2 is the availability of  $\phi_{m0,i}^{vw,u}$  and  $\phi_{0m,i}^{vw,u}$ , which represent the one-dimensional moments of the analytic solution of eq. (3.12). Details regarding the calculation of these higher-order moments are available in Appendix A Section A.1.3. We thus note that solving the one-dimensional higher-order equations for  $(l, k)$  pairs with a single index different from zero, allows the generation of one-dimensional flux moments with **two** indices different from zero (as moments of the analytic solution). This is analogous to the principle utilized in Section 3.3.3 where higher-order flux moments with a single index different from zero are obtained from

the solution of the standard one-dimensional nodal equations. This process may continue in a hierarchical fashion to produce the full set of higher-order flux moments.

For instance, the availability of moment  $\phi_{m0,i}^{vw,u}$  for the CQLA method, allows the construction of  $(l, k)$  pair  $(i, m)$  in direction  $w$ . Utilizing the value of  $\phi_{m0,i}^{vw,u}$  in neighbouring nodes, a two-node problem may be solved for the interface current moment  $J_{im}^{uv,w}(\pm \frac{h_u}{2})$  and side-flux moment  $\phi_{im}^{uv,w}(\pm \frac{h_u}{2})$ , after which the analytic solution for  $\phi_{im}^{uv}(w)$  could be expressed in terms of Legendre moments up to the chosen source order (say index  $j$ ) and hence generate flux moments  $\phi_{im,j}^{uv,w}$ .

As in Section 3.3.3, it is important to note the distinction between  $\phi_{im,j}^{uv,w}$  and  $\bar{\Phi}_{im,j}^{uvw}$ . The former refers to the one-dimensional flux moment in direction  $w$ , of order  $j$ , as projected from the solution of the higher-order one-dimensional equation weighted with a Legendre polynomial of order  $m$  in direction  $v$  and order  $i$  in direction  $u$ . The latter, with the same indices, refers to the **node-averaged** higher-order flux moment of order  $imj$ . In actual fact there are three different higher-order one-dimensional moments with indices  $imj$ , one in each direction and  $\bar{\Phi}_{im,j}^{uvw}$  is actually computed as the average of these three. Thus, in general, node-averaged flux moments are calculated from

$$\bar{\Phi}_{mlk}^{uvw} = \frac{(\phi_{kl,m}^{vw,u} + \phi_{lm,k}^{wu,v} + \phi_{mk,l}^{uv,w})}{3} \quad (3.20)$$

as an alternative to generating the set of higher-order balance equations and solving the resulting linear system for each moment.

We thus hierarchically proceed to construct  $(l, k)$  pairs and then solve the associated one-dimensional equations to eventually construct the full set of higher-order moments as needed in expansion (3.2). The approach produces all quantities needed to express the higher-order transverse leakage terms fully (without the ‘‘flat leakage’’ approximation of Section 3.3.3), as required in eqs. (2.26 and 2.27) and constitutes a full higher-order solution. Naturally, this solution retains the 27 unknowns per node (in 3D second-order) and is not the primary intention of this work, but the associated capability to selectively extend the accuracy of the higher-order module to a full higher-order when needed, for applications such as homogeneous flux reconstruction or reference solution generation, is attractive.

## 3.5 Conclusion

In this chapter the derivation for a consistent (as opposed to ad-hoc) transverse leakage approximation is presented. Although the development is largely described

up to the second order, the method is of a general-order and may be expanded to higher orders if needed, although additional higher-order equations would have to be solved.

The development makes use of elements of full higher-order methods, by utilizing the higher-order intra-nodal trial function to express the transverse leakage term, as it appears in the standard nodal methods. Further, the process of weighted transverse integration is utilized to determine the side-averaged current moments needed in the final form of the transverse leakage term. The minimum subset of higher-order equations needed are determined and the system is closed by applying a “flat” leakage approximation in the higher-order equations.

The need for explicit spatial sweeps to determine higher-order node-averaged flux moments is also eradicated due to the proposed local hierarchical approach, although some coupling of the higher order quantities exist through the feedback from the driver code. This hierarchical approach is seen as a crucial step in decoupling the higher and lower-order solutions and thus facilitates the development of a standalone higher-order code module which can be easily coupled to existing nodal codes.

The proposed development reduces the number of higher-order unknowns from 27 to 15 in 3D (for a second order expansion) and thus it is estimated that the calculational cost of this so-called CQLA method would be between 3 and 5 times greater than standard nodal methods applying the SQLA (full second order requires 10 times more calculational time than the SQLA). Thus, the calculational cost is still significantly greater than the target set for this work of around 50% increase calculational time. Chapter 4 investigates a number of iteration and solution schemes in order to facilitate the additional reduction needed and describes the higher-order code module developed during this work.