Chapter 1

Introduction

1.1 Background

The nuclear industry has emerged from a difficult era and clear signs of growth are visible over the past ten years. Earlier, partly due to international politics around issues such as nuclear safeguards and waste disposal and partly due to accidents such as Chernobyl and Three Mile Island, the nuclear landscape was relatively stagnant. Very few countries actively developed new technologies and even the building of new reactors based on the existing generation II and III class concepts was scarce. In the more recent past, given the hunger for energy and concerns over resource sustainability, the momentum has built in this industry resulting in new and existing technology development in various countries. Most significantly, applications for the construction of new nuclear power reactors in countries such as the USA, France, Finland, China, South Korea and the United Arab Emirates have also encouraged the potential development of nuclear power in a host of developing countries. The full effect of the recent natural disaster in Japan and subsequently the Fukushima reactor accident on this growth remains to be seen; significant nuclear cutbacks have already been made in Japan, and also in Germany.

South Africa has played a part in the resurgence, with the announcement in May 2011 of an extensive energy resourcing plan spanning the next 30 years (Department of Energy, 2011). In this projection, nuclear energy will contribute to approximately 13% of the electricity needs of South Africa by 2030, and thus 17% of new build over the next 20 years should be based on nuclear technology. Such a step, which implies 9.6 GW new nuclear capacity, operational by 2030, requires a strong growth in nuclear-related activities in the country from this moment onward. Given the fact that some nuclear capacity exists in South Africa, it is foreseen that this process is feasible in the suggested time scales. Nevertheless, it would be a blatant understatement to

say that the design, construction and operation of nuclear power plants are costly and complex, and many specialized disciplines have to merge and overlap synergistically in a field with carefully controlled margins and significant skills shortages.

Within this myriad of disciplines and stakeholders, and probably at its heart, lie the design and analysis of the nuclear reactor core. It would entail specialist areas such as, and amongst others, neutronic design, thermal hydraulic design, reactor kinetics and system dynamics. Within these fields the primary focus is on reactor safety and utilization to which computer simulations are an invaluable tool. The ability to predict accurately quantities such as neutron flux and temperature distribution during operation and accident conditions, dose levels during maintenance, and operational parameters such as criticality, cycle length and power levels are central to the design and operation of nuclear reactors. The accuracy of these calculations have a direct bearing on the engineering margins built into both the operation and construction of these plants, and hence are of the utmost importance. On the other hand, a large number of these calculations are needed within short turnaround times; an acceptable balance must thus be found between accuracy and speed in these reactor analysis packages and code systems. In selecting the appropriate tools for a given task, the landscape of available neutronic codes and methods has to be investigated. Broadly, two classes of solution are available.

Firstly, full core transport solutions, be it via deterministic or stochastic solution methods, should be mentioned. This class of solutions is highly accurate and allows for a very detailed solution in terms of energy and spatial detail of the neutron flux, but still suffers from exorbitant calculational running times. The advent of cheaper, massively parallel computing has started to make these approaches feasible for certain classes of calculations, but as yet cannot underpin the usage of such methods for day-to-day reactor operational support. In this regard, some of the most widely utilized code packages would include the Monte Carlo based MCNP (Brown et al., 2002) code system developed by the Los Alamos National Laboratory, the French APOLLO III code (Golfier et al., 2009) developed by the CEA, the DRAGON code (Marleau et al., 1994) developed at the Ecole Polytechnique de Montreal in Canada or more recently the SERPENT code (Leppanen, 2007) developed at the VTT technical research center in Finland. A further promising field of research is the class of hybrid transport methods which aim at combining various higher and lower-order formalisms (and often code systems) into integrated solution schemes.

Secondly, and more traditionally, we consider the full-core diffusion solutions utilizing transport-based lattice codes for multi-group cross-section generation (Duder-

stadt and Hamilton, 1976). Detailed neutron transport calculations are performed in fine energy groups with heterogeneous spatial detail on an assembly level to produce multi-group (orderly 2 - 10 groups) equivalence parameters for each component in the core. These lattice calculations are independently performed for each material region with representative boundary conditions; cross-sections are typically tabulated against relevant state parameters. This is a once-off process and results in a library of tabulated assembly-homogenized cross-sections. The cross-sections obtained in this step are used as input data for the global core diffusion calculation, which is utilized to calculate 3D core wide-flux and power profiles. Diffusion methods are derived as an approximation to neutron transport and are therefore less accurate, but provide a substantial performance increase. Nevertheless, these calculations are very often run, both within the realm of steady-state and time-dependent solutions, and require even further performance improvements to be feasible. Typically, the class of nodal diffusion methods (Lawrence, 1986) are utilized to solve the global diffusion problem, which allows for a coarse calculational mesh, hence less mesh elements and consequently a much faster solution. This class of nodal diffusion core solvers still represents the industry standard in power reactor analysis today (Smith, 2003). These nodal methods will be described in detail in this work.

The success of nodal methods is evident from their longevity in the industry and their primary benefit is surely found in the performance advantage over traditional finite-difference approaches, which ranges between two and three orders of magnitude. Nevertheless, the following drawbacks exist in this approach:

1. The need for assembly homogenization (spectrally and spatially) which requires prior knowledge of the assembly environment and thus incorrectly "freezes" certain environmental effects into the produced multi-group equivalence parameters. Various approaches for retaining equivalence between the transport and diffusion solution methods have been developed, particularly by Koebke, and are well described by Smith (1986).

2. The need for a transverse leakage approximation, which is required within the sub-class of transversely-integrated nodal methods. The most often used approach in this regard is termed the Standard Quadratic Leakage Approximation (Bennewitz et al., 1975; Smith, 1979). Although it works well for most applications, it can introduce nodal power errors of a couple of percent and in some cases can cause instabilities in the convergence of nodal codes. In extreme cases this approximations can cause complete non-convergence of the solution

scheme. It should be pointed out that this approximation has no theoretical justification, but has remained the approach of choice over about 30 years due to its simplicity and reasonable accuracy when applied to LWR problems.

3. The need for flux and power reconstruction methods in order to regain heterogeneous detail on the pin or plate level within an assembly, after the global nodal diffusion calculation has been completed. The reconstruction calculation is typically factored into a homogeneous flux reconstruction step performed in the diffusion solver and a heterogeneous step in which the homogeneous pin-wise flux is multiplied by pin form factors which were tabulated in the lattice code. A wide range of reconstruction techniques are available with a good overview presented by Zhang et al. (1997).

These three points are intimately related, since it has been found that accuracy in reconstructing local information from a converged coarse-mesh solution depends in a large measure on an effective method of spatially averaging group reaction cross-sections and diffusion constants for a ''node''. All three these points will be discussed on an overview level later on in this chapter.

1.2 Aim of the Thesis

During this work, the impact and implications of these shortcomings to modern nodal methods will be highlighted, discussed and numerically illustrated, with specific reference to points 2 and 3 of the previous section. Point 1, although outside the scope of this work, is an active area of research in the industry, but will probably only truly be resolved once the full-core transport solutions become a viable alternative to coarse mesh diffusion solutions.

The aim of this thesis is to provide an integrated approach to solving the difficulties presented by the transverse leakage approximation and the homogeneous flux reconstruction in nodal methods. Although it might not be immediately apparent how these two goals are connected, suffice at this point to say that the developed method is aimed to be scalable in accuracy such that the shape of the neutron current on the node surfaces (needed for improved transverse leakages) or the full intra-nodal flux shape (needed for flux reconstruction) may be generated from the same approach as a matter of selection. As a matter of fact, the development in this work supports order refinement and will allow for a nodal code to become fully scalable in accuracy to the point where user selection can approximately determine the maximum nodal flux

error in the solution, thus even producing reference 3D fine mesh solutions if needed. Nevertheless, the work is primarily focused on finding an acceptable balance between improved accuracy in node-averaged power and a practically acceptable calculational cost penalty.

It is not immediately clear what such an acceptable cost penalty would be, especially given the rate of growth of computing power, but it is important to place the proposed target efficiency within context. If we aim at achieving an error reduction of about one order of magnitude, as compared to nodal methods employing the quadratic leakage approximation (which has a typical nodal power error of between 1% and 3%), the following options are currently available:

- Employ a fine mesh finite-difference solution, which incurs a time (calculational cost) penalty of between 50 and 100 times;
- Use twice subdivided nodal meshes, which incurs a cost penalty of between 8 to 10 times; or
- Employ full higher-order methods (up to the second order), which incurs a cost penalty of around one order of magnitude.

In this work we will aim at achieving approximately such an error reduction as compared to standard nodal methods, but with a targeted cost penalty of a 40% to 50% increase in calculational time (thus well below a factor 2). Based on various sources of literature, code user perspectives and code developer opinions, it is foreseen that an additional cost in such a range would be acceptable in the industry given the proposed potential advantages proposed. These then include:

- A consistent leakage approximation (not limited in order) free of issues such as false convergence, unexpected divergence as well as unbounded and unreported error levels;
- A nodal solution which does not place restrictions on user-defined meshing or nodal aspect ratios;
- Improvement of the maximum nodal power error to below 0.5% for "difficult" problems;
- Dual use of the method as a consistent, accurate homogeneous flux reconstruction tool.

In order to accomplish this, the specific class of nodal methods known as higher-order nodal methods will be investigated. We will endeavour to make this promising past development, which has not generally been utilized due to its computational cost, practical for the purpose of addressing the issues of transverse leakage and homogeneous flux reconstruction.

It is envisaged and shown in this work, that such a simplified higher-order nodal method could be developed and packaged into a stand-alone computer code module which is easily pluggable into most of the existing nodal diffusion codes. Although, within the scope of the work, the developed module is connected to various nodal solvers (two of which are described in this document), the primary target platform for this development is the Necsa developed OSCAR-4 code system (Stander et al., 2008). Furthermore, Necsa operates the SAFARI-1 reactor at Pelindaba, hence the primary area of application of this work is on research reactors, and specifically the class of Material Testing Reactors (MTRs). For this purpose, the set of numerical examples utilized for illustration of the method accuracy and performance includes a number of standard LWR benchmark problems, but also a realistic SAFARI-1 reactor benchmark problem.

1.3 Nodal Diffusion Methods

1.3.1 Development history

The class of nodal diffusion methods, as applied to global reactor calculations (Duderstadt and Hamilton, 1976; Greenspan et al., 1968; Stamm'ler and Abbate, 1983), has grown into a mature and trusted technique in recent times. Nodal methods first appeared in reactor literature in the 1960s. This class of methods was originally developed in order to obtain, in a less rigorous but more computationally efficient way, information about flux averages over fairly large spatially homogeneous regions or ''nodes'', from which came the name ''nodal methods''. An important step in the development was when these methods became "consistent", in the sense that they limited to the fine-mesh finite-difference solution for decreasing mesh size, as described by Lawrence (1986). The motivation for these earlier nodal methods was to reduce the computational expense of traditional finite-difference methods for multi-group diffusion calculations over large cores requiring many mesh points. As discussed in the previous section, this motivation for the use of nodal methods continues up to the present, as do fundamental questions of homogenization techniques and flux reconstruction (dehomogenization) (Grossman and Hennart, 2007). In Dorning (1979) a

subtle distinction is made between nodal and coarse mesh methods, in claiming that true nodal methods, in contrast with many forms of coarse mesh methods, do not yield the full intra-nodal flux shape as part of the solution, since only node-averaged quantities are available from the solution. This is an important distinction within the context of this work and we will adopt this differentiation in later chapters.

In the 1970s the class of transversely-integrated nodal methods was developed in the form of the Nodal Expansion Method (NEM) (Finnemann et al., 1977), the use of integral nodal equations (Nodal Greens Function Method) (Lawrence and Dorning, 1980) and the Analytic Nodal Method (Smith (1979)). A mix of the NEM and ANM approaches was further developed some time later in the form of the AFEN code by Noh and Cho (1993). During the late 1980s a further development in nodal methods included the emergence of higher-order nodal methods (Ougouag and Rajić, 1988; Altiparmakov and Tomašević, 1990; Guessous and Akhmouch, 2002) which in principle could reproduce the full intra-nodal flux solution and steered away from the concept of simply requiring averages as primary unknowns. This development, although promising, incurred significant calculational cost and did not enter the mainstream of nodal codes. During the 1990s a number of developments enhanced the maturity of nodal methods and extended their shelf-life well into the present era. These include, amongst others, the generalization of the ANM to a full multi-group (Vogel and Weiss, 1992), the inclusion of non-linear extensions such as nodal rehomogenization (Smith, 1994) and intra-nodal cross-sections shape feedback (Wagner et al., 1981), and more recently axial homogenization (Smith, 1992; Reitsma and Muller, 2002) techniques to eradicate the well known cusping effect. In 1989, as part of the NODEX code (Sutton, 1989), the Coarse Mesh Finite-Difference (CMFD) iteration scheme, described in Sutton and Aviles (1996), was developed. It has proven to be a successful acceleration approach and as such has been implemented in many modern nodal diffusion methods or codes. In this approach, the nodal equations are cast into a finite-difference form and nodal calculations are utilized to generate corrections to standard finite-difference node coupling coefficients in an iterative sense.

Although the work in this thesis is particularly focused on Cartesian geometry, the code systems overviewed are typically capable of modelling reactor designs with Cartesian, hexagonal and cylindrical geometries. Contributions in this regard would include the extension of the Analytic Nodal Method to hexagonal geometry (Chao, 1995), as well as to cylindrical geometry (Prinsloo and Tomašević, 2008). Both of these developments applied approaches of conformal mapping in order to preserve, as far as possible, the structure of equations from Cartesian geometry solvers.

A significant number of refinements in the application of nodal methods continue to be visible in literature, with the most attention being paid to improved intra-nodal depletion and flux reconstruction issues. Nevertheless, these methods have reached a level of maturity and it can be expected that developments in nodal diffusion methods will continue in an evolutionary manner until full core transport approaches become practical. An important bridging step in this regard is the so-called semi-heterogeneous methods which aim at limiting the impact of homogenization by subdividing assemblies into various spectral zones. In these schemes traditional coarse mesh nodal methods, combined with some form of global rehomogenization, become accelerators for submesh solutions. An example of such a development in modern nodal codes may be seen in Bahadir and Lindahl (2009).

1.3.2 Modern nodal codes

Given the theoretical background of nodal diffusion methods, it is of interest to survey the landscape of modern-day reactor core simulation code systems. Some of the most prevalent systems utilized in industry today for core-follow and reload analysis, be it for PWRs, BWRs, MTRs or even fast reactors, are nodal diffusion-based solvers. In particular, we briefly highlight some of the more significant code systems in this regard.

SIMULATE-4 and SIMULATE-5, developed by Studsvik Scandpower, Inc.

SIMULATE is Studsvik's nodal code which has been developed along with CASMO, Studsvik's lattice physics code. The SIMULATE code has grown over 25 years and has been primarily utilized for LWR analyses. It should be noted that the development of SIMULATE-3 was followed by SIMULATE-4, as described below. During the development of the code, it was decided to extend the scope and upon completion the project was named SIMULATE-5.

In SIMULATE-4 (Bahadir et al., 2005) the model for solving the three-dimensional multi-group diffusion equation with node-wise constant cross-sections, is the standard Analytic Nodal Method (ANM). The transverse leakage is approximated by a quadratic fit of the known average out-leakages of three adjoining nodes. The one-dimensional multi-group equation is converted into G 'one-group' equations by a transformation employing the eigenvectors of the buckling matrix. Should the node be materially heterogeneous in the axial direction, a heterogeneous axial model is used to compute homogenized cross-sections and axial discontinuity factors. A hybrid macroscopic/microscopic cross-section model is employed.

In SIMULATE-5 (Bahadir and Lindahl, 2009) burnup and nuclide data are stored subnode-wise. In the x-y direction, assemblies are further refined in $n \times n$ submeshes (typically $n = 5$). The standard concept of a "node" is utilized in the 3D calculation to couple the submesh 2D calculation with the subnode 1D axial calculations. Radial leakage in the 1D subnode axial calculation, as well as the axial leakage for a 2D radial submesh calculation are both obtained from the global 3D nodal calculation. These leakages are represented as equivalent absorption cross-sections. In this case, the global 3D nodal calculation does not obtain the value of the transverse leakage from the traditional 3-node quadratic fit, but from information present in the 2D submesh solution.

ANDES, developed by the Universidad Politécnica de Madrid

The ANDES code (Lozano, 2007) applies the Multi-group Analytic Nodal Method, implemented in a near similar manner to what was originally proposed by Vogel and Weiss (1992) to solve the 3D multi-group diffusion equation. On top of this scheme, the Course Mesh Finite-Difference (CMFD) formulation (Sutton and Aviles, 1996) is applied to accelerate the nodal solution. Three transverse leakage approximations are implemented, namely flat, parabolic and cubic. The parabolic option resembles the standard transverse leakage approximation and the cubic option (not fully described in related references) does not, by the developers' own admission, add any significant accuracy.

OSCAR-4, developed by Necsa, South Africa

The OSCAR-4 calculational system (Stander et al., 2008), developed by Necsa over approximately 20 years, has been primarily applied to MTR-type research reactors. MGRAC is the core diffusion solver and employs the multi-group Analytic Nodal Method (Vogel and Weiss, 1992), along with a microscopic depletion model for isotopic tracking. Axial heterogeneities are treated with an axial homogenization procedure on axial subnodes, and the standard quadratic transverse leakage approximation is utilized in the one-dimensional equations. This code is described in significantly more detail in a later chapter, since it forms part of the work in this thesis.

AFEN, developed by KAERI, South Korea

The AFEN code (Noh and Cho, 1993), developed by KAERI, South Korea, makes use of a direct, non-separable analytic function expansion of the 3D intra-nodal flux. As such, this code does not employ the transverse integration principle and hence

does not require a transverse leakage approximation. The intra-nodal flux is typically expanded in a combination of trigonometric and hyperbolic basis functions. Combinations of fluxes and currents are utilized to generate the necessary conditions for determining the expansion coefficients. An increased number of unknowns incurs a significant performance penalty as compared to the transversely-integrated methods, but improves upon the typical nodal flux error. It is further claimed that the method would ensure superior accuracy when supplying information to homogeneous flux reconstruction methods.

CRONOS, developed by CEA, France

The CRONOS code system, developed by the French CEA and discussed in Lautard et al. (1991), is based on a Finite Element Method (FEM) solver and hence does not make use of the traditional transverse integration procedure. The code is capable of modeling fine-mesh detail and is typically utilized to model variable levels of heterogeneous detail, depending on the overall calculational scheme within which it is applied.

NEM, developed by Penn. State University

The NEM code (Beam et al., 1999), developed at the Penn. State University (PSU) in the U.S. is a widely utilized research test platform and forms the bases of a number of industry related projects at PSU. The nodal diffusion equation is solved utilizing the Nodal Expansion Method (discussed in some detail in the next chapter) and thus makes use of the transverse integration procedure. The code supports a wide range of geometries including Cartesian, cylindrical and hexagonal and is extensively utilized in the developed and evaluation of various spatial kinetic coupling schemes with thermal-hydraulic solvers.

Other notable code systems

A large number of further nodal codes exist, amongst which should be mentioned the POLCA-7 / POLCA-T codes developed by Westinghouse (Panayotov, 2004) which utilize both the ANM and the so-called "plane wave solution" (which may be classified as a form of Fourier expansion); the PARCS code developed at Purdue University in the U.S. (Downar et al., 2004) which utilizes the ANM solution and the NESTLE code (Turinsky, 1994) which applies the NEM as primary solution algorithm.

1.3.3 Transversely-integrated nodal methods

As can be clearly seen, the class of transversely-integrated nodal methods, at which the work in this thesis is directed, is still quite prevalent in the industry today and addressing the issues pertaining to these code systems will still add value for a number of years to come. The class of transversely-integrated nodal methods provide substantial performance increases, while simultaneously maintaining high levels of accuracy. These methods mostly share three characteristics (Tomašević, 1996).

1. Unknowns are defined in terms of volume-averaged fluxes and surface-averaged net or partial currents.

2. The volume (node) averaged fluxes and surface-averaged currents are related through auxiliary relationships. Such relationships, in the case of modern nodal methods, are often obtained via a transverse integration procedure.

3. Transverse leakage terms appear due to the transverse integration procedure and these are approximated in some way. Typical approaches would include the "flat leakage" approximation and the "quadratic leakage" approximation. The latter introduces a three node quadratic fit for the transverse leakage term in the transversely-integrated equations and has become the industry standard in Cartesian geometry.

Beyond these similarities, methods differ largely in the form of the intra-node solution. As mentioned in Section 1.3.1 two classes of methods, which are most often utilized, are the Analytic Nodal Method (ANM) and the Nodal Expansion Method (NEM). In the case of the analytic method, the intra-node flux shape is the analytic solution of the one-dimensional transversely-integrated diffusion equation. This approach requires no approximations other than the transverse leakage approximation mentioned in point three above. In one dimension, therefore, the analytic method is formally exact.

In the case of polynomial methods, the intra-node one-dimensional flux is approximated to the n^{th} order on some set of polynomial basis functions. Expansion coefficients may be determined in various ways and the transverse leakage approximation is, of course, still required.

The pros and cons of these methods do not lead to any clear preference in selection, but some arguments (Tomašević, 1996) suggest that the ANM exhibits both slight performance and accuracy advantages over its polynomial counterpart.

In both the ANM and NEM approaches, which constitute the most widely used nodal approaches, the quadratic transverse leakage approximation (QLA) is the major source of inaccuracy, but also of convergence problems. The standard method for generating the three leakage coefficients in a given direction is to apply a three-node quadratic fit of average transverse leakages in adjacent nodes. This approach uses information from the direction under consideration to construct the leakage shape from the transverse directions. This implies a certain level of long-range coupling between nodes and a statement regarding the quadratic transverse leakage approximation is often made that it works well in checkerboard-type material arrangements. Typically, the simple three-node fit breaks down in the following cases:

- Near the core/reflector interface of the reactor and typically in reflector nodes near the boundary where the flux gradient due to thermalization is sharper than that which the quadratic approximation can match. In such cases the numerical scheme can lead to negative fluxes, which in turn may destabilize the entire calculation and lead to non-convergence (Smith, 1979). In these reflector areas, node-averaged errors in excess of 10% in the nodal flux are not unusual for the quadratic leakage approximation and may be substantially larger if convergence problems occur. There is no natural extension of the three-node fit to higher leakage orders;

- At boundary nodes, where a three node fit will suffer, since no average leakage may be consistently defined outside of the system. In this case some approximate leakage, dependent on the boundary conditions of the system, is typically utilized in a fictitious outer node. Alternatively, a two node linear fit could be utilized in order to avoid the boundary problem;

- At interfaces with sharp material changes, as would be the case near control rod positions (Ougouag and Rajić, 1988). In turn, such errors may lead to the misprediction of important safety parameters such as control rod worth. At such interfaces, errors in node-averaged power distribution in excess of 2% could be found for difficult problems. Errors in node average flux distribution may be substantially higher; and

- In adjacent nodes which have very different sizes, or within nodes with large aspect ratios. This deficiency places a restriction on the code user with respect to the choice of meshing scheme and in extreme cases, leads to non-convergence of the solution.

These situations occur regularly in power reactors and especially in research reactor cores with compact, heterogeneous designs.

1.4 Higher-order Nodal Methods

Higher-order nodal methods were first developed from the perspective of creating consistent nodal diffusion methods. In this sense the property of consistency is defined such that all numerical approximations result from the basic discretization method. Thus, the numerical solution converges when either the mesh size is decreased or the approximation order is increased. The application of the quadratic leakage approximation clearly violates this principle and some of the earliest efforts to address this were by Dorning (1979) and Dilbert and Lewis (1985). The first significant step in formulating a consistent, transversely integrated, higher-order nodal method was achieved by Ougouag and Rajić (1988). In this work, a coupled set of higher-order balance equations and auxiliary one-dimensional higher-order nodal diffusion equations were generated via the process of weighted transverse integration. This formalism, which is akin to the class of weighted residual methods (Nakamura, 1977), represents a natural extension to the standard ANM in the sense that it reduces to the standard ANM for order zero. This approach provides a detailed intra-nodal flux shape up to the order of the method and hence contains sufficient information to represent the detailed transverse leakage shape. In actual fact, the method obviates the need for an additional homogeneous flux reconstruction step. This development was specifically focused on performing detailed intra-nodal burnup (Rajić and Ougouag (1987)). The method showed significant promise and the possibility was explored to vectorize the scheme (Rajić and Ougouag, 1989) to alleviate the computational cost it incurred.

Following this development, the theoretical placement and understanding of this approach was strengthened via an equivalent variational formulation (Nakamura, 1977) of the scheme (Altiparmakov and Tomašević, 1990). In this work the proper interpretation of the intra-nodal trial function was formulated and it is shown that a higher-order solution with a method order of one provides similar accuracy to standard (or zero-order) nodal methods with the quadratic leakage approximation. Second order higher-order solutions already improve the accuracy by one order of magnitude. Some additional work in this regard followed in 2002 and involved the casting of the higher-order solution into a response matrix form (Guessous and Akhmouch, 2002).

Although the class of higher-order nodal methods has significant advantages, further work in this class was quite limited, due to the high associated computational

cost.

1.5 Homogeneous Flux Reconstruction Methods

The concept of flux reconstruction is well known in nodal methods and appears directly from the coarse mesh approximation. The decision to define coarse mesh node-averaged fluxes as primary unknowns is typically sufficient for performing reactor core reload and core-follow analyses, but it should be clear that safety parameters such as maximum pin power requires much finer detail in the solution. To facilitate this, the flux reconstruction problem is defined and typically factorized as a product of a homogeneous and heterogeneous reconstruction step. Homogeneous reconstruction entails the recovery of the fine-mesh diffusion solution in the node of interest and can be performed with information only available from the diffusion solution. Heterogeneous reconstruction aims to recover the detailed flux solution within the heterogeneous assembly (prior to homogenization) and typically entails the tabulation of so called form factors during the transport calculations, which are defined as the ratio of the heterogeneous transport to the homogeneous diffusion solution within the subcells of the node. The synthesis of the form factors with the homogeneous reconstructed flux then provides an estimate of a detailed heterogeneous reconstructed flux. Given that the transport calculation is performed in 2D, the homogeneous reconstruction step is typically only performed in 2D. Originally, two-dimensional polynomials (Koebke and Wagner, 1977) were used in the representation of the intra-nodal flux distribution and later exponential functions were introduced to augment the thermal flux variation (Koebke and Hetzelt, 1985). More recently, analytic functions were used in both energy groups (Boer and Finnemann, 1992). Apart from those mentioned, a large number of techniques and methods exist in this area, with almost all of these homogeneous reconstruction techniques suffering from the following shortcomings:

- Reconstruction methods are often limited to two energy groups, as compared to modern nodal solutions in group structures of 4 - 10 energy groups; and
- Reconstruction methods are often external fit-based schemes and more often than not require nodal corner fluxes as interpolation support points. Corner fluxes are singular points in the nodal diffusion solution and hence some external approximation is utilized to recover these quantities, which degrades the quality of the solution.

Recently, Bahadir and Lindahl (2006) introduced a multi-group pin power reconstruction method in the SIMULATE-4 code, but this solution strategy is somewhat dependent on the nodal submesh scheme inherent to the SIMULATE-4 code and may not work sufficiently well for traditional nodal methods. Another promising multi-group reconstruction method was suggested by Joo et al. (2009). Although this method still requires the external estimation of corner fluxes, the solution is based on an analytic 2D diffusion solution for the node and hence shows good accuracy.

Nevertheless, it would be fair to say that the class of multi-group reconstruction methods is still very much an area of development. In this work, as a secondary outcome, it will be shown how the class of higher-order methods almost seamlessly takes care of both the multi-group and corner flux approximation difficulties.

1.6 Thesis Layout

In this work the class of higher-order nodal methods is utilized as a basis for formulating a consistent, ***practical*** general-order leakage and flux reconstruction module, capable of being connected to most existing nodal diffusion codes. To facilitate the description of the work, the thesis is set out in the list below.

1. Chapter 2 introduces both lower and higher-order nodal methods as well as the choice of mathematical notation in this work. In this chapter higher-order nodal methods are derived and described by way of the weighted transverse integration approach. It will be shown how these methods represent a natural extension to the standard ANM and the quadratic leakage approximation is placed in the context of these methods.

2. Chapter 3 primarily focuses on the issue of developing a practical simplification to the full higher-order nodal formalism, for the sake of addressing the shortcomings of the quadratic transverse leakage approximation. The chapter defines and derives what we term the consistent leakage approximation. Further, the chapter focuses on the extension of the solution scheme towards a full higher-order solution. The proposed full higher-order solution is novel in the sense that it employs a hierarchical approach to the construction of the higher-order flux moments and as such does not require a full system sweep of higher-order balance equations (as in Altiparmakov and Tomašević (1990); Guessous and Akhmouch (2002); Ougouag and Rajić (1988)). The full higher-order functionality of the eventual test code is to be utilized to produce reference solutions

for all the numerical problems in this work and forms the code base for the proposed practical higher-order transverse leakage and flux reconstruction module developed in later chapters.

3. Chapter 4 describes the developed test code and stand-alone module and then focuses on a series of proposed numerical iteration schemes needed to make the consistent leakage approximation practical. Both the nodal test code and developed higher-order module are algorithmically described and interfaces are defined. This chapter further illustrates how this same computational module, with minor modifications, could be utilized as an accurate homogeneous flux reconstruction tool.

4. Chapter 5 illustrates both the accuracy and efficiency of the developed method on a set of fixed cross-section benchmarks, utilizing the developed higher-order module as coupled to the nodal test code. This chapter aims to quantify the potential benefit of combining higher-order methods to existing lower-order code systems. The problems range from idealized test scenarios to the 3D 6-group models of currently operating reactors and span both LWR and MTR type.

5. Chapter 6 signifies an important achievement in coupling the developed module to the OSCAR-4 code system and investigating the additional complexities which arise from interfacing with an "industrial" nodal code. The coupling, although not entirely straight forward, is shown to be generally independent of the solution scheme of the underlying lower-order code. The coupled code is applied to a set of SAFARI-1 reload and core-follow calculations, as is regularly performed by the OSCAR-4 code.

6. Finally, Chapter 7 summarizes the major conclusions of the work and looks ahead toward the identified issues to be resolved during final integration of the developed module into existing state of the art core calculational systems.

1.7 Development of the Work

The inspiration and motivation of this work has resulted from extensive usage (over a number of years) of nodal diffusion codes for reactor analyses and the resulting difficulties which often arise due to the application of the standard quadratic leakage approximation. In particular, past work by the author has included an MSc thesis (Prinsloo, 2006) and resulting publication (Prinsloo and Tomašević, 2008) on the topic

of extending the ANM to cylindrical geometry for PBMR application, in which case the quadratic leakage approximation posed an even greater problem due to cylindrical meshing.

The work described in this thesis has been developed over the past three years and was detailed in two peer-reviewed international conference publications, namely Prinsloo and Tomašević (2011) and Prinsloo and Tomašević (2012). These papers generally summarize the developments as described in Chapters 3 and 4, respectively. It is foreseen that a summary journal publication would follow the submission of this thesis.

1.8 Conclusion

This introductory chapter discussed the history, background and current status of nodal diffusion methods at an overview level and described some of the major shortcomings as they currently exist in industrial nodal diffusion based core calculational systems. The aim of the thesis was formulated and specific attention was placed on the shortcomings of both the so called transverse leakage approximation and homogeneous flux reconstruction methods as currently implemented in many modern nodal codes. The class of higher-order nodal methods was identified as a possible candidate for addressing these issues, but only on the condition that their accuracy advantage could be maintained at a much reduced calculational cost than has been previously achieved. Such a development could become a valuable addition to all existing industrial nodal diffusion-based code systems.