Chapter 7

Conclusions

Nodal diffusion methods represent a standard in full-core global-diffusion solutions and have done so for over 30 years. Although these methods have evolved over this time, the basis for their development was laid in the late seventies and early eighties and adaptations since then may be considered as relatively minor. The transversely-integrated nodal methods may be regarded as the solution methods of choice amongst the various development lines, with the ANM and NEM formulations being the most widely utilized. Common to the transversely-integrated nodal methods, is the need for a transverse leakage approximation. Over the years a number of efforts have been made to suggest a remedy to this problem, with the primary efforts (as discussed in Chapter 2) notably being the buckling approximation by Shober and Henry (1976a), the flat leakage approximation by (Shober and Henry, 1976b; Shober et al., 1977), the quadratic leakage approximation by Bennewitz et al. (1975) and the method of successive smoothing as discussed in Beam et al. (1999) and Finnemann et al. (1992). Of these the quadratic leakage approximation has by some margin been the most successful and although it has little theoretical basis, does exhibit reasonable accuracy for a large proportion of problems.

Alternative nodal formulations were developed to entirely circumvent the need for a leakage approximation and here we may consider higher-order nodal methods (Ougouag and Rajić, 1988; Altiparmakov and Tomašević, 1990) and direct expansion methods such as those proposed by Noh and Cho (1994). The latter grouping is essentially Fourier expansion approaches as discussed by Makai (1984). These alternative formulations significantly expanded the amount of intra-nodal information available from the solution, but generally at an unacceptable computational cost as compared to standard nodal methods. We may, as discussed in the conclusion of Chapter 2, refer to these methods as coarse-mesh methods (since they provide the full intra-nodal solution) as compared to that which we are interested in, namely nodal methods (formulated with only node-averaged quantities as primary unknowns). It is the opinion of the author that the class of higher-order nodal methods provides a strong theoretical basis for potentially formulating an improved transverse leakage approximation, given its equivalent formulation from either a variational or weighted transverse integration perspective. An effort in this regard was made by Tomašević (1997) to reformulate the higher-order solution in terms of a single node problem, but this approach proved inaccurate on some of the problems considered.

In this thesis then, an effort is made to provide a next evolutionary step in the development of nodal methods, by the introduction of a consistent transverse leakage approximation. The foundation for this development is rooted in the higher-order nodal methods and the major challenge faced in the scope of this work is the construction of a solution scheme which exhibits both superior accuracy as well as acceptable efficiency as compared to the standardly utilized transverse leakage approximation, namely the standard quadratic leakage approximation (SQLA).

From the overview of industrial codes presented in Chapter 1 it is clear that nodal codes, utilizing the SQLA, still exist as the method of choice in most modern and industrial full core solvers today and thus the difficulties associated with SQLA still remain relevant. In short we may summarize that the SQLA approximation is highly efficient in terms of calculational time, but largely ad-hoc in respect to theoretical basis and associated nodal flux and power error distribution. In fact, in some variants of nodal methods the SQLA is the only approximation and thus represents the major stumbling block regarding the generation of reference quality solutions via nodal methods. Errors associated with SQLA are typically between one and three percent in nodal powers and significantly higher in terms of flux distribution, while the ad-hoc nature of the approximation can lead to various convergence related difficulties for some problems.

Of course the question should be posed whether these problematic issues surrounding the use of the SQLA approximation are of concern today, as well as in the medium term future, specifically given its longevity in the industry. This issue is relevant and the primary question concerns the error of SQLA as compared to other errors introduced within the scope of full the deterministic calculational path. Here we refer to the impact on nodal power errors due to cross-section and engineering uncertainties (order of couple of hundred pcm in k_{inf}), homogenization and the use of diffusion theory (5% - 10%), the use of nodal methods and the SQLA (about 1% - 3%) and eventually the accuracy of flux reconstruction methods (about 3% - 5% in pin powers), with listed error estimates taken from Rearden et al. (2011), Smith (1986) and Smith (2003). We argue that although the SQLA approximation constitutes one of the smaller contributors in this list, it represents a non-negligible component of the overall error, given the state-of-the-art capabilities and accuracy requirements of industrial codes today. The issue thus still warrants attention, although only within the framework of an acceptable computation cost. Furthermore, although this work is primarily focused on steady state analysis, transverse leakage is a concern in nodal spatial kinetic analysis also and future work shall aim at investigating this further within the context of the developments in this work.

If we consider the future trends in nodal code development, as also discussed in Chapter 1, we may further notice that the medium term evolution of modern codes are directed toward solution schemes which are less dependent on coarse homogenization (as in the case of the SIMULATE-5 code described by Bahadir and Lindahl (2009)) and even more slowly toward schemes which are less dependent on diffusion theory. It is not yet fully clear what role transverse integrated nodal methods will play in this so-called semi-heterogeneous setting, be it as global accelerators or sub-mesh solver, but clearly some form of transverse leakage approximation shall remain for some time to come. We thus once more state that the development in this work is aimed not at revolutionizing the standard calculational procedure, but rather at providing an evolutionary step in the development of nodal methods.

7.1 Summative Conclusions

As such we briefly summarize the primary technical aims of this thesis and then formulate a set of conclusions to support the argument that these aims have indeed been met. This work is aimed at:

- The development of 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 all problems considered, aiming at an additional computational cost of around 50% as compared to standard nodal solutions employing SQLA; and

- Investigation into further applications of the approach, such as use of the method as a consistent, accurate homogeneous flux reconstruction tool. This point appears since the class of higher-order nodal methods utilized in this work essentially provides additional information on the intra-nodal flux distribution.

To achieve these goals, higher-order nodal methods were investigated as a basis for formulating a suitable simplification. Essentially these methods project the intra-nodal flux shape on a multi-dimensional polynomial expansion, with Legendre polynomials as basis functions. It is reasonable to assume that such intra-nodal flux distributions are smooth functions and as such we postulate that a reduced 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 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. These formulations support the arguments that a lower-order subset of the full expansion may retain much of the intra-nodal shape information. In our case though, a subset of the expansion is naturally found by inspecting the transverse leakage expression, as it appears in the standard nodal methods, and then retaining only those bases functions from the full higher-order expansion needed to express the quantities which appear in the leakage terms. This motivation leads to a reduction in unknowns dependent on the method (or expansion) order. For example, for method order 2, the number of full flux moments reduces from 27 to 15, whilst for method order 3 the reduction would be from 64 to 21. It is fair to expect that this reduction, although still adhering to the requirement of producing a consistent leakage approximation, would not prove sufficient to meet the aim in calculational time as set out above and as such a number of iteration schemes are considered for providing additional improvement in calculational efficiency. Upon formulation of these schemes, a detailed numerical analysis is performed, both for fixed cross-section problems in a test code environment and for realistic reactor core calculations within the framework of an industrial nodal diffusion code.

In particular, given the work performed in this thesis, we may formulate the following summative conclusions:

1. From the discussion and history of nodal methods in Chapter 1, it may be concluded that modern nodal codes, utilized in industry today, still largely

depend on the SQLA, since transversely-integrated nodal methods are the most widely used variant of coarse-mesh methods. These codes generally make use of either the Analytic Nodal Method (ANM) or the Nodal Expansion Method (NEM) as primary solution scheme, both of which are discussed in detail in Chapter 2. Various sources of literature place the accuracy of these methods at between 1% and 3% in nodal power error depending on the problem under investigation, with the primary contribution to this error resulting from the SQLA.

2. Higher-order nodal methods, overviewed in Chapter 2, mostly developed in the late 1980's, provide the necessary information to improve upon the SQLA, but were never absorbed into industry codes due to their unacceptable computational cost. These methods may be generated either via a weighted transverse integration procedure or via a variational approach, utilizing the appropriate trial function. Full second order solutions, for example, although highly accurate, would increase the computational time by around one order of magnitude (for 3D problems).

3. A number of alternatives to SQLA were proposed during the years, but improvements achieved, pertaining to accuracy, were marginal and mostly problem dependent. As such SQLA has remained the option of choice. Methods free of transverse leakage, or direct expansion methods, have been proposed as alternatives, but have similarly not been absorbed in the mainstream of global solvers given their computation cost. As an example we may cite the AFEN code (Noh and Cho, 1994), which requires up to 49 unknowns per node for a 3D calculation.

4. In this work a so-called Consistent Quadratic Leakage Approximation (CQLA) is proposed in Chapter 3. The term consistent results from the fact that only information from the nodal diffusion solution is utilized to construct the leakage expression and no additional approximation is necessary. The CQLA is constructed as a simplification of a full higher-order solution, with the primary aim to retain only the information needed in order to represent the transverse leakage source as it appears in the standard nodal equations and not, as in the case of typical full higher-order methods, in order to represent the full intra-nodal flux shape. The full expression for the transverse leakage term, as it appears in the standard nodal equations, is obtained by inserting the trial function (extended to 3D as compared to the 2D form developed by Altiparmakov

and Tomašević (1990)) into the rigorous expression for transverse leakage. We notice that the resulting expression requires a combination of side-current moments of various orders in each contributing direction and furthermore that these quantities are derivable from the one-dimensional flux moments typically calculated in standard nodal codes. We obtain these side-current moments by formulating a higher-order version of the standard ANM solution method and solving two-node problems on every surface of the node under consideration.

5. In Chapter 3 four adaptations are made to full higher-order methods to formulate the CQLA: generate only the subset of higher-order one-dimensional equations needed to represent the zero-order leakage source; limit the expansion order of that source 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; hierarchically construct the higher-order node-averaged flux moments as opposed to solving an explicit linear system to solve for them. 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, yielding an expected relative calculational cost, as compared to SQLA, of between 3 and 4.

6. In order to reach the target efficiency of around a 50% increase in calculational time, further acceleration is provided via three proposed iteration schemes developed in Chapter 4. These schemes are combined into an integrated strategy referred to as the Reduced Leakage Correction Scheme (RLCS). The RLCS comprises three components: partial convergence of the higher-order coefficients; model reduction via ANOVA decomposition and higher-order correction of the SQLA leakage coefficients. When combined, these strategies significantly reduce the number of outer iterations requiring higher-order calculations and as such are expected to improve upon the efficiency of the solution, without detracting from the accuracy. Chapter 4 further describes how the CQLA solution, combined with RLCS scheme, is packaged into a standalone Fortran module which may be coupled to any transversely-integrated nodal code. Interfaces are defined to be straightforward in order to facilitate such a coupling effort; the driver nodal code should supply nodal fluxes and side-currents (as a minimum) and the developed module (termed HOTR) returns leakage coefficients. This

interaction occurs whenever the driver code requires an update of the transverse leakage source and may be performed either per energy group or for all energy groups simultaneously. A full higher-order solution, up to the order set by the user, is also included in the functionality of the module. A nodal test code (3D ANM, utilizing a group-by-group solution) is developed in order to test the functionality of HOTR and is termed SANS. SANS is coupled to HOTR and the coupling is described in Chapter 4.

7. Numerical results on fixed cross-section problems, as discussed in Chapter 5, provide a baseline for the accuracy and efficiency of the CQLA solution. Generally, considering all problems evaluated, the proposed method improves the accuracy of SQLA by about a factor of 4, requiring a computational cost of, on average, 3 times that of SQLA. This accuracy improvement indeed confirms that CQLA represents a significant improvement over SQLA, the root of which may be found in its consistent formulation and non-penalizing approximations. For the particular problem for which SQLA does not converge at all due to skewed aspect ratios (the ZION benchmark problem), the CQLA solution converges without any difficulty.

8. The further application of the developed iteration schemes for acceleration to the CQLA solution, in particular for the case of the integrated RLCS, indeed improves upon the efficiency of the CQLA solution without affecting the accuracy to any noticeable degree. Performance figures, relative to those of SQLA, range from between 1.04 and 1.7 for the various 3D problems analyzed and thus generally meet the original aim of a relative performance, as compared to SQLA, of around 1.5.

9. An effort is made to couple HOTR to the OSCAR-4 reactor calculational system, which may be deemed an industrial nodal diffusion code. This work is described in Chapter 6 and investigates the efficiency of the method in the context of multiple calculational cases, control rod searches, varying nodal iteration schemes, core burnup and typical non-linear nodal extensions. It is noted that the performance of the HOTR deteriorates somewhat in the OSCAR-4 environment with efficiency factors nearer to a factor of 2 for similar cases as considered with the coupling to SANS. This may be understood given the need for better integration between the topology and iteration schemes between OSCAR-4 and HOTR.

10. A realistic SAFARI-1 reload and core-follow scenario is analyzed and performance is maintained for burnup, multi-cycle cases, as well as control rod searches, with a slight deterioration when utilizing non-linear extensions such as the use of intra-nodal cross-section shape feedback and axial homogenization. Performance does however degrade in conjunction with both the Wielandt eigenvalue acceleration scheme and the Transverse Leakage Source Iterative Method (TL-SIM). These acceleration techniques significantly decrease the number of outer iterations needed for convergence and thus the higher-order iterations needed to converge the SQLA correction factors represent a higher fraction of the total calculational time. CQLA (without RLCS) performs as expected for the cases considered, i.e. at an efficiency of about 3 times that of SQLA.

11. It is illustrated that homogeneous flux reconstruction is a natural extension of the method, since the intra-nodal trial function implicit in the higher-order method is directly applicable for intra-nodal flux tabulation. Although detailed error and reconstruction time analyses is not performed, homogeneous flux reconstruction is implemented in HOTR and applied for illustration purposes to a number of problems in Chapter 5. Depending on the selected method order during reconstruction, scalable accuracy is achievable.

In conclusion, we may consider that, for the first time, higher-order nodal methods have been reformulated as a practical and complimentary contribution to standard nodal methods. This contribution is formulated primarily in terms of the improvement of the representation of transverse leakages, but it is clear that further benefits could be derived regarding other problematic areas in nodal methods, such as flux reconstruction. Timing and accuracy comparisons show that significant benefit can be achieved if the proposed approach is applied within the framework of existing transversely-integrated nodal codes and that the typical problems associated with the quadratic transverse leakage approximation are largely, if not fully, eradicated.

It should however be stated that, even though the interfaces between a standard nodal code and a module such as HOTR are relatively straight-forward, the solution scheme inside HOTR exhibits significantly higher levels of complexity than those presented by the standard quadratic leakage approximation. This should be taken into account when implementation decisions are taken and it is suggested that the effort in coupling HOTR is justified only within the context of fully exploiting the additional benefits it represents, as compared to simply the CQLA solution option. These then include CQLA itself, full higher-order solutions up to a user selectable order for reference solution generation and homogeneous flux reconstruction. Further benefits derivable from the additional intra-nodal information will be discussed in the section on future work.

7.2 Future Work

Future work on this topic can be classified into two distinct focus areas. The first being the migration of the HOTR module into an industrial quality pluggable module and the second the further investigation into areas of benefit for nodal methods based on the information available from a module such as HOTR (and higher-order methods in general).

With respect to the first activity, a number of implementation improvements to HOTR are envisaged. The module should be stripped of research related solution options which are not deemed optimal and the integration strategy with the driver code should be reconsidered. Optimal performance will only be obtained if the topology module of the driver code can be more directly accessed and if code sharing between the driver code and HOTR is optimized. The OSCAR-4 code platform will be used for these investigations.

Regarding the solution options in HOTR, it is shown that the CQLA method performance is consistent across all driver code solution options, but the RLCS iteration scheme performs poorly for acceleration schemes such as the Wielandt eigenvalue shift method. This issue is thus far only briefly investigated and indications are that the convergence measures for the SQLA correction factors are potentially to blame. This matter deserves further attention.

It is further of crucial importance to extend the list of driver codes to which HOTR is coupled, in order to grow the maturity level of the module. Work has begun on coupling HOTR both to an ANM test code which utilizes side-averaged currents as primary unknowns (as compared to node-averaged flux in SANS and OSCAR-4), as well as coupling to the Penn. State University NEM code (discussed in Beam et al. (1999)), which applies the nodal expansion method. In this latter coupling it is envisaged that the issue of transverse leakage during a time dependent solution (as is available in NEM) will be investigated.

Regarding the second focus area, namely the investigation into additional areas of benefit for nodal methods,the following is considered:

- Finalize the implementation of homogeneous flux reconstruction in HOTR and evaluate the accuracy of the scheme against a range of flux reconstruction benchmark problems. It is expected (based on current experience) that accuracy could be much improved when compared to the existing approaches, but that once again the calculational cost of the full system reconstruction would require optimization. HOTR flux reconstruction shall be connected to OSCAR-4 and as such realistic heterogeneous flux reconstruction problems may be investigated. Outstanding development issues in this regard includes the usage of spatially dependent cross-sections within the heterogeneous reconstruction path; and

- Investigation into the usage of the additional intra-nodal shape information for the typical non-linear nodal extensions. These include intra-nodal cross-section shape, nodal rehomogenization and axial-homogenization. The common thread in these areas pertains to the usage of 2D and 3D spatial information as compared to the 1D information currently utilized. In the case of intra-nodal cross-section feedback and rehomogenization, this might include the extraction of additional information from related lattice codes and as such the practicality of such improvements may be in question. Nevertheless, developments in this regard could extend the usage of nodal methods with regard to coarse-mesh homogenization and coarse-mesh burn-up and as such could provide a bridge to the so-called semi-heterogeneous approaches.

These activities are planned during the following year and are accepted as ongoing development activities within Necsa.

7.3 Final Remarks

The reactor modelling and simulation arena presents an unusual research challenge. The industry moves slowly with current state-of-the-art methods rooted in 30-year old developments. Even more disconcerting is the fact that the next generation methods, such as full core transport and heterogeneous pin-by-pin core solvers (be it deterministic or stochastic), are also long since established, awaiting the computing capability required to make such solutions practical. Nevertheless, the industrialization of these next generation methods seems to continually shift their horizon and the focus in this current development cycle is more closely tied to small evolutionary steps than revolutionary developments. As such, historical code systems are adapted to modern reactor physics problems and a significant amount of research is devoted to integrating dedicated systems, which model various physical phenomena, into large multi-physics packages, all within an ever stricter regulatory environment. As such, the incremental development of these existing systems remains of paramount importance, particularly in the context of new requirements resulting from such system integration and regulatory compliance. It is within this broad framework that the work in this thesis was motivated and within which the proposed incremental improvements to standard nodal methods may find a place.