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E. E. Lewis

Department of Mechanical Engineering
Northwestern University
Evanston, IL 60208, USA

and

G. Palmiotti, H. S. Khalil, K. Laurin-Kovitz, T. Fanning, U. R. Hanebutte

Reactor Analysis Division
Argonne National Laboratory
Argonne, IL 60439

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THREE-DIMENSIONAL TRANSPORT
WITH VARIATIONAL NODAL METHODS

E. E. Lewis,[a] G. Palmiotti,[b] H. Khalil,[b] K. Laurin-Kovitz,[b]
T. Fanning[b] & U. R. Hanebutte[b]

[a] Department of Mechanical Engineering
Northwestern University
Evanstion, IL 60208, USA

[b] Reactor Analysis Division
Argonne National Laboratory
Argonne, IL 60439, USA

Abstract

The development of the variational nodal method contained in the three-dimensional transport code VARIANT is reviewed. This Argonne National Laboratory code treats two- and three- dimensional multigroup problems with anisotropic scattering in hexagonal and Cartesian geometries. The methodology couples hybrid finite elements in space, which enforce nodal balance, with spherical harmonics expansions in angle. The resulting response matrix equations are solved by red-black or four-color iterations. Several enhancements to VARIANT are discussed: The simplified spherical harmonics option provides near spherical harmonic accuracy for many problems at a fraction of the cost.. Adjoint and perturbation calculations are performed without the physical- and mathematical adjoint dichotomy appearing in other nodal methods. Heterogeneous node methods extend the problem classes to which the method may be applied. . Computational strategies and trade-offs are discussed and possible future research directions are outlined.

Introduction

The Ansatz of the Variational Nodal Method is a variational formulation of the even-parity form of the transport equation in which odd-parity Lagrange multipliers at the interfaces enforce nodal balance.[1] Classic Ritz procedures, with spherical harmonics in angle and complete spatial polynomials within the nodes and along the interfaces, are employed to obtain discretized within-group equations in the form of hybrid finite elements. The physical properties of these equations are then utilized to recast them as the response matrices upon which the solution algorithms are based. Thus the method may be considered a synthesis of finite element, nodal and response matrix methods.[2] The within-group equations are combined in a conventional multigroup formalism from which both eigenvalue and fixed-source calculations can be performed.[3] In what follows we trace the evolution of the method, summarize current capabilities, and discuss possible future directions.

1

Physics Capabilities

Following formulation in a number of stand-alone test codes, the method was first implemented in a production environment to perform multigroup P_1 and P_3 calculations in two- and three-dimensional Cartesian and hexagonal geometries.[3] Since that time the variational nodal method has been generalized and features added to increase the utility of the method over wider classes of problems. The first major addition was the inclusion of within-group and group-to-group anisotropic scattering.[4] A second was the formulation of Rumyantsev interface conditions. These allow rigorous treatment of arbitrary odd-order spherical harmonic approximations in the angular variables.[5]

The Argonne National Laboratory code, VARIANT[6] (VARIational Anisotropic Neutron Transport) is presently available with anisotropic scattering in the P_1, P_3 and P_5 approximations. In VARIANT the spatial neutron distribution within the nodes may be treated by complete quadratic through fourth-order (Cartesian) or sixth order (hexagonal) polynomials with, flat, linear or quadratic interface conditions, with the ratio of the two constrained by matrix rank conditions. VARIANT thus offers the unique feature amongst nodal transport codes in that the approximations can be refined systematically both with p and h refinement in space (by proceeding to higher order polynomials or to smaller mesh spacing, respectively) and in angle by employing successively higher-order spherical harmonic expansions.

Simplified Spherical Harmonics

The versatility of the variational nodal method has been increased substantially with the realization that the Simplified Spherical Harmonics equations can be cast in variational nodal form.[7] This has lead to the implementation of SP3 and SP5 approximations in VARIANT, utilizing the same spatial approximations as are available for the standard spherical harmonics approximation. Moreover the inclusion of anisotropic scattering in the simplified spherical harmonics approximation has been straight forward.

The time savings achieved in replacing P_N with SP_N approximations is dramatic. This is apparent if one considers that in a three dimensional calculation there are $N(N+1)/2$ angular trial functions per interface in a P_N response matrix, but only $(N+1)/2$ in a SP_N approximation. Comparisons of CPU times and eigenvalues for the Hex-Z Takeda Benchmark #4[8] are given in Table I, where linear interface conditions are employed. In addition, while P_N approximations require that linear or quadratic interface conditions be employed to obtain reasonable truncation errors, the SP_N method may employ flat interface conditions, which results in a reduction in the response matrix dimension by a factor of two.

For most of the problems which we have encountered, eigenvalue and flux approximations for companion P_N and SP_N approximations are in close agreement. For example, as shown in Fig. 1 for a deep penetration problem, the SP_N results closely mimic the P_N results, again at a small fraction of the cost. Some exceptions do occur in the flux distributions, particularly near voided channels where very skewed angular distribution may appear.

The inclusion of SP_N along with P_N approximations in VARIANT utilizing the same hierarchical spatial approximations allows close comparisons of the effects of spatial and angular

truncation. Eigenvalue errors are plotted in Fig. 2 for the "rods in" Takeda Benchmark #2.[8] Very similar characteristics also have been observed in two- and three-dimensional problems and in both Cartesian and hexagonal geometries. In all cases the net eigenvalue error is the difference between a positive contribution from spatial truncation and a negative contribution from the finite angular expansion. The eigenvalue decreases in going from flat to linear to quadric spatial interface approximation while holding the angular approximation constant. Likewise, in all cases the eigenvalue increases as the order of the P_N or SP_N approximation is increased while retaining the same spatial approximation.

The SP_N approximations do not converge to the reference eigenvalue with increased order. Rather, a residual remains as a result of the incomplete set of angular trial functions that constitutes the simplified spherical harmonics. As a result of the partial cancellation that occurs between spatial and angular truncation errors, however, it is sometimes possible to obtain eigenvalues which decrease in accuracy even though the spatial or the angular approximations has been improved. This phenomena was first observed by Wagner in interface current nodal transport approximations.[9] Note also the large spatial truncation errors for the flat interface P_N calculations that grow with the order N. In contrast, the spatial truncation error for the SP_N calculation is roughly independent of the order N.

Perturbation Theory

A second recent development is the formulation of the adjoint variational nodal method coupled with the capability for performing both first order and exact perturbation calculations in all geometries and with all angular approximations.[10] Forward and adjoint capabilities are incorporated into VARIANT such that the outputs can be electronically transferred to a perturbation post-processor where the perturbation calculations are performed.

Perturbation calculations utilizing the variational nodal method offer a distinct advantage over other nodal methods, where adjoint formulations exist only in the diffusion approximation. In conventional nodal methods, the physical adjoint, obtained by discretizing the adjoint equation, is not the same as the mathematical adjoint, obtained by transposing the coefficient matrix that results from discretizing the forward equation. Since these methods employ computational algorithms that are based on the physical adjoint, but the perturbation calculations require the mathematical adjoint, similarity transforms or related techniques are required to relate the two. With the variational nodal method this complication is obviated, since the physical and the mathematical adjoints are identical.

The VARIANT post-processor is being modified to treat SP_N as well as P_N approximations, thus allowing comparisons to be made. In Figs. 3 and 4 are shown results for perturbations applied to the Takeda Benchmarks #1 and #4.[8] For the Takeda Benchmark #1, the standard rods-in problem is used as a base state. The applied perturbation consists of increasing the thermal capture cross section of the control rod material. A more severe test is the Takeda Benchmark #4, in which the base state is the standard rods-out problem. Initially the control rod channel contains sodium. The perturbation consists of sodium voiding of the channel.

In both problems the SP_3 approximation produces improved eigenvalues compared to diffusion theory. However, the corresponding improvement in the change in reactivity estimated by the SP_3 perturbation theory is highly problem dependent. In the Takeda Benchmark #1, SP_3

estimates are nearly identical to the P_3 approximation. For the Takeda Benchmark #4, SP_3 theory fails to greatly improve the estimated change in reactivity because full P_3 expansions are required to accurately model the flux distribution about the small nearly-voided control rod channel. In contrast, it is found in some problems that the diffusion theory perturbation results give reasonable eigenvalue changes even though the accurate prediction of k requires a higher-order angular approximation.

Heterogeneous Nodes

Presently, VARIANT does not explicitly accommodate heterogeneous nodes. Rather node-averaged cross sections must be employed to obtain homogeneous nodes. For control rod channels and other strong heterogeneous structures, however, this is a weakness. It is being removed through the explicit formulation of heterogeneous nodes.[11] Through the use of numerical integration techniques, cross sections are represented explicitly, allowing both circular and rectangular intranode heterogeneities to be treated. In these two geometries heterogeneous methods are applied respectively to the estimation of fast reactor control rod worths and to the pin power distributions in light water reactor assemblies fueled with mixed uranium/plutonium oxides.

Computational Considerations

Throughout much of its development, the primary motivation for the variational nodal method has been in expanding the classes of physical problems that could be treated, rather than in minimizing the computing time required to perform a particular calculation. Thus far, algorithmic improvements has been a secondary consideration. However, they may be a particularly fruitful area for future investigation. Moreover, since VARIANT utilizes a general matrix formulation for all geometries and levels of approximations, it may be advantageous to develop modified versions of the code which are tuned to treat narrower problem classes more effectively. For example, if only diffusion solutions are of interest, a great deal of the code overhead required for the manipulation of the larger transport response matrices could be eliminated.

The variational nodal method was first developed on scalar, main-frame computers. At that time the primary algorithmic innovations was the partitioning of the response matrix into diffusion and transport-like contributions in order to accelerate the red-black or four-color iterations.[3] With the availability of the Cray - XMP at Argonne National Laboratory the algorithms were vectorized to take advantage of substantial speed-ups obtainable with the large transport arrays. In recent years, however, work stations with rapidly improving capability have become the predominant platform upon which VARIANT is employed. The vector coding, however, has not been eliminated. As a result, workstations of similar capability run VARIANT at speeds which vary by as much as a factor of two, depending on how well their architecture is able to take advantage of vectorization.

With larger problems, particularly for highly heterogeneous cores where many distinct node types are required, memory to store the response matrices may become a significant limitation. The response matrices, however are quite sparse, and include a substantial number of symmetries. Thus in VARIANT a packing algorithm is available to conserve memory by storing only the unique response matrix elements. In its present form, each matrix must be unpacked at the time of use, thus causing a memory - CPU time tradeoff to occur. Recoding in a scalar form to allow the matrix multiplications to be performed directly with the packed elements should substantially improve this tradeoff.

Parallel computation seems attractive for response matrix algorithms for at least two reasons. First, the spatial domains corresponding to one or more red-black node pairs can be assigned to each processor, thus allowing a high degree of parallelism to be exercised in the iterative solution. Second, memory limitations can be alleviated by distributing the response matrix construction and storage amongst the processors and their associated memories. The potential for parallelization of response matrix algorithms, such as those employed in VARIANT, is discussed in detail in a companion paper.[12]

Discussion

Future directions in the development of variational nodal methods naturally divide into expanding the capabilities to handle a wider range of physical problems, and to decreasing the computational effort required to obtain solutions. One may look toward present finite element capabilities in other engineering fields to identify attractive areas for development. These would include extension to r-z or other curvilinear coordinate systems, the development of arbitrary triangular node capabilities, and the formulation of space-angle adaptive grid methods. In improving the computational algorithms, methods are needed which reduce computational effort on engineering workstations as well as those that take advantage of the advancing capabilities of parallel computing.

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Table 1: PN and SPN CPU Time and Accuracy Comparisons

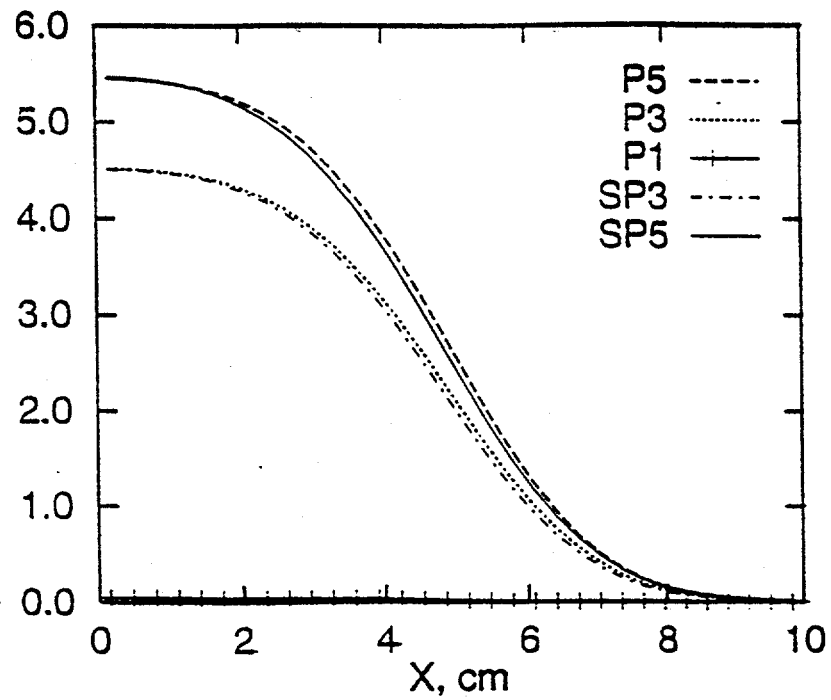| method	k	CPU
P 1 (l)	1.1727	1.23 min.
P 3 (l)	1.2035	25.8 min.
P 5 (l)	1.2052	217 min.
S P 3 (f)	1.2029	0.78 min.
S P 3 (l)	1.1991	2.98 min.
S P 5 (f)	1.2038	1.96 min.
S P 5 (l)	1.2000	5.87 min.
Monte Carlo	1.2041+0.0005	3 days

Fig. 1: Comparison of P_N and SP_N Flux Distributions
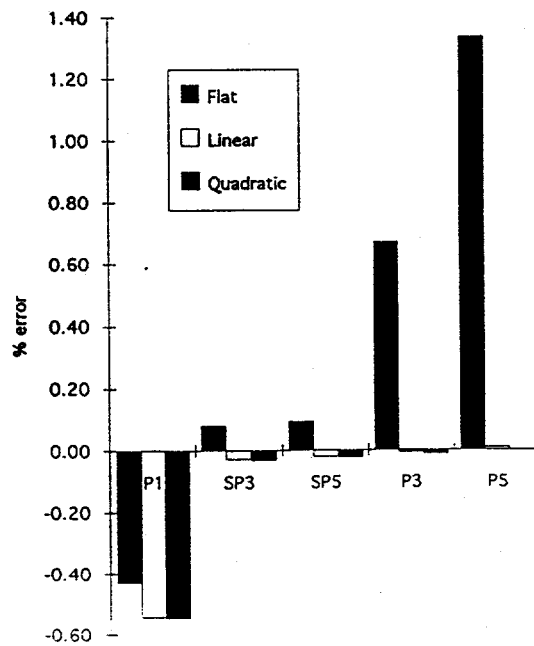for a Deep Penetration Problem

Fig. 2 P_N and SP_N Eigenvalue Errors for Different Spatial Interface Approximations
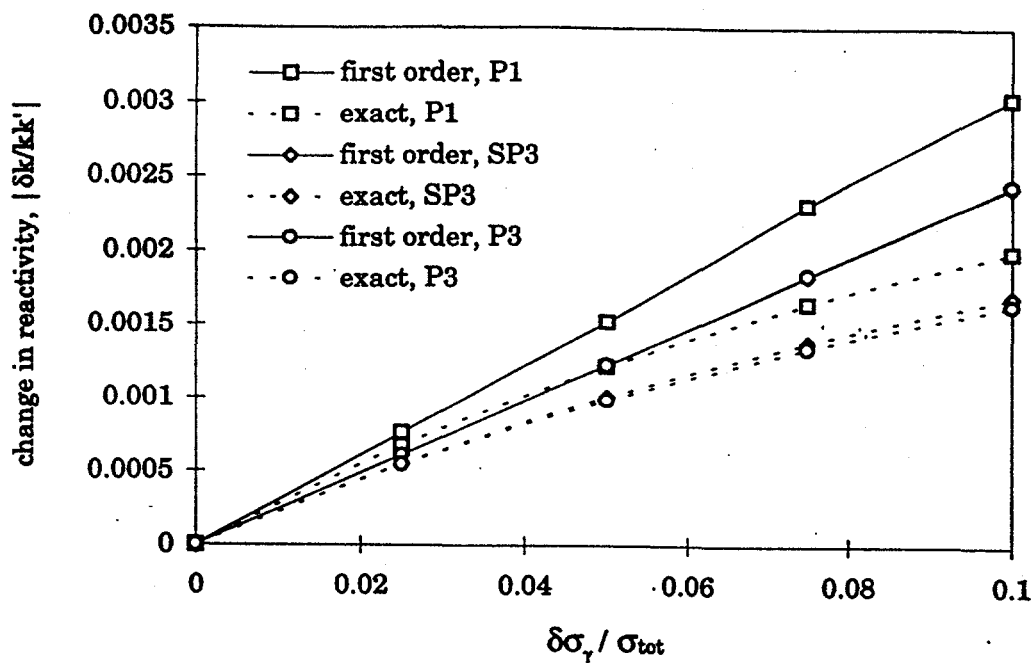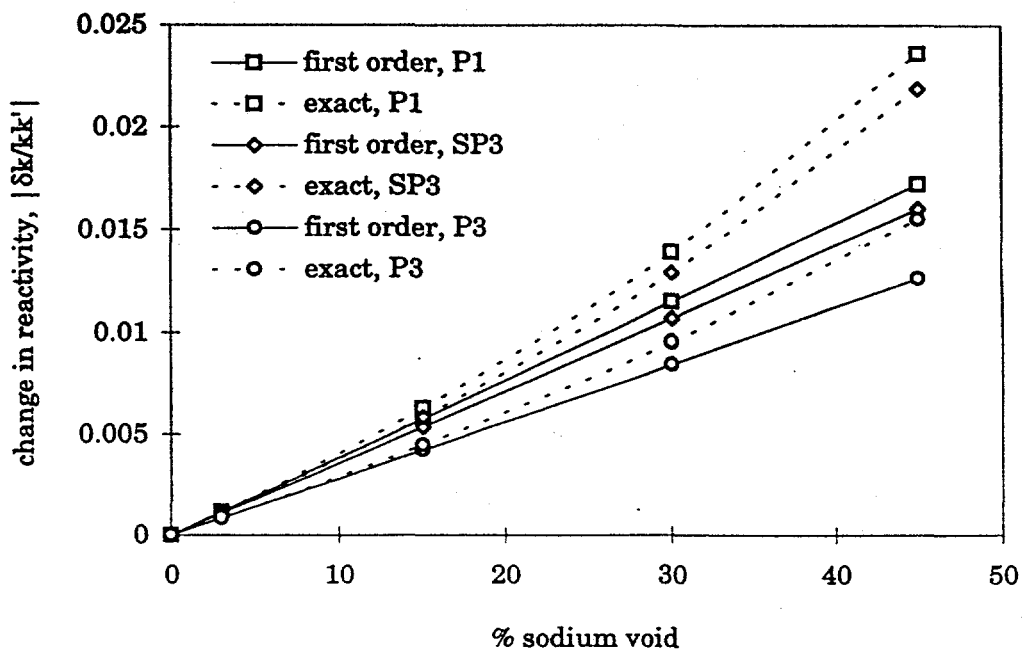
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Fig. 3 Takeda Benchmark #1 Perturbations

Fig. 4 Takeda Benchmark #4 Perturbations

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