Congreso Internacional Conjunto Cancún 2004 LAS/ANS-SNM-SMSR/International Joint Meeting Cancun 2004 LAS/ANS-SNM-SMSR
XV Congreso Anual de la SNM y XXII Reunión Anual de la SMSR/XV SNM Annual Meeting and XXII SMSR Annual Meeting
Cancún, Q.R., México, 11-14 de Julio, 2004/Cancún, Q.R., Mexico, July 11-14, 2004

Nodal Methods in Numerical Reactor Calculations

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Abstract

The present work describes the antecedents, developments and applications started in 1972 with Prof. Hennart who was invited to be part of the staff of the Nuclear Engineering Department at the School of Physics and Mathematics of the National Polytechnic Institute. Since that time and up to 1981, several master theses based on classical finite element methods were developed with applications in point kinetics and in the steady state as well as the time-dependent multigroup diffusion equations . After this period the emphasis moved to nodal finite elements in 1, 2 and 3D cartesian geometries. All the thesis were devoted to the numerical solution of the neutron multigroup diffusion and transport equations, few of them including the time dependence, most of them related with steady state diffusion equations. The main contributions were as follows: high order nodal schemes for the primal and mixed forms of the diffusion equations, block-centered finite-differences methods, post-processing, composite nodal finite elements for hexagons, and weakly and strongly discontinuous schemes for the transport equation. Some of these are now being used by several researchers involved in nuclear fuel management.

1. INTRODUCTION

In 1972, the head of the Nuclear Engineering Department at the School of Physics and Mathematics of the National Polytechnic Institute, invited Prof. Jean Pierre Hennart, who by that time had recently got his PhD degree. Prof. Hennart worked by 5 years in this Department starting the applied mathematics research field in nuclear reactor calculations. The first topic was devoted to the numerical solution of the steady state multigroup diffusion equations using Lagrange finite elements [1]. The code DELFIN (Diffusion by Finite Elements) was developed as

a partial result in this research A second one was on point kinetics where classical finite elements were applied [2]. Afterwards the topic was extended to a wide variety of classical and non-classical finite elements where special quadratures were applied to simplify the structure of matrices involved in the discretization in the code WHALE (We Have A Lot of Elements) [3]. Finally, in 1981, the time-dependent diffusion problem was solved using backward Euler, Crank-Nicolson and the more generalized θ scheme to discretize the time-dependence. This application was for 1 and 2D cartesian geometries [4]. After a period of maturity the researches were re-oriented to nodal finite elements and their corresponding applications. One of the first theses in this new area tackled the slab neutron transport equation that was solved with a unified formalism developed in 1985. Two nodal methods were introduced here, namely the quadratic and cubic continuous schemes [5]. Using these two nodal schemes, the diffusion synthetic acceleration (DSA) scheme was applied and tested in 1986 [6]. In the same field, another thesis developed exponential nodal finite elements that were applied to solve again the slab neutron transport equations using also the DSA iterative scheme [7]. The non-linear problem corresponding to the burnup problem was also considered and solved in 1990 [8]. After experience was gained for 1D problems a master thesis was devoted to the numerical solution of the steady-state neutron transport equations in XY geometry [9]. Then the DSA iterative scheme was introduced in the numerical solution of the neutron transport equation in XY geometry [10]. 3D diffusion problems were solved using physical and mathematical nodal methods [11]. After reconsidering the way we discretized the spatial-dependence in the discretization of the neutron transport equation new nodal schemes arose, namely the weakly and strongly discontinuous schemes [12], and finally, block-centered finite-differences were obtained from nodal methods using appropriate quadrature rules and a composite nodal scheme was developed to solve the diffusion equations in hexagonal geometry [13].

2. NODAL SCHEMES

With nodal methods, in more than one dimension problems, Legendre moments at edges and cells are used to approximate the dependent variable. Several nodal schemes were developed that climbing consistently in order of accuracy. One of these nodal schemes are the family of the Raviart-Thomas that was originally developed for the mixed diffusion equation, where both the scalar flux and the current are simultaneously and independently approximated. For the primal form of the diffusion equation, the scalar flux is the dependent variable and it is approximated by a polynomial space S_h of dimension $(k+1)(k+5)$ where k is an integer greater or equal 0. The approximation must interpolate $(k+1)(k+5)$ parameters in a given set D. Some other nodal schemes were also developed, namely the BDM*k* (Brezzi-Douglas-Marini), the BDFM*k* (Brezzi-Douglas-Fortin-Marini), and HdV (Hennart-del Valle). Extensions to 3D problems were also developed in 1993. For the neutron transport equations, discontinuous schemes were also developed with very attractive features, mainly to damp the oscillations arising when optically thick media are considered.

3. THE DIFFUSION EQUATIONS

In reactor physics diffusion equations are written mainly in two different but equivalent forms. The first one is the primal form where the independent variable is the neutron flux for each

energy group *g*. These equations are the following

$$-\nabla \cdot D\nabla \phi_g + \Sigma \phi_g = S_g, \forall g = 1,...,G, (x,y) \in \Omega \tag{1}$$

On the other hand the second form is known as the mixed form or P1 form given by

$$\begin{aligned} \nabla \cdot \vec{J}_g + \Sigma \phi_g &= S_g \\ \vec{J}_g + D_g \nabla \phi_g &= \vec{0} \end{aligned} \tag{2}$$

and this time the neutron current is the second independent variable. First attempts to solve numerically these set of equations using nodal methods were described in [14]. With the years these methods were matured and a long paper with full details regarding this method, both theoretically and numerically for 2D problems in [15]. Although the description of the nodal methods was given for monoenergetic diffusion equations the methods were extended and applied successfully to the solution of the steady state multigroup diffusion equations [16]. More recently the method was extended to hexagonal geometry where a composite nodal finite element was introduced in conjunction with a Gordon Hall transfinite transformation obtaining excellent results for typical test problems [17]. A Richardson acceleration technique was devised to solve the discretized problem in an efficient way. Besides, unconventional nodal methods were introduced to solve also this problem in Madrid obtaining similar results to those obtained in [17]. Another technique consisting in the decomposition of the hexagon in three parallelograms was developed and applied by Schneider practically in parallel [18].

4. PRIMAL, MIXED, AND MIXED-HYBRID FORMULATIONS

In [14] primal, mixed and mixed-hybrid formulations are fully described. The first one is related to the numerical solution of the primal form of the diffusion equation (1) and the second and third formulations are linked to the mixed form of the diffusion equations (2). In the primal formulation there is only one dependent variable, in this case the scalar flux, that is approximated by a polynomial or a quasi-polynomial approximation, a space (*S*), where the interpolation parameters are edge/cell Legendre moments belonging to a set of degrees of freedom (*D*).

The weak form of the primal diffusion equation is obtained following the classical finite element procedure à la Galerkin where the weighting functions are taken as the basis functions of the interpolant here above mentioned. The use of these approximations leads in a natural way to well structured algebraic systems that may be solved iteratively in an efficient way.

In the mixed form, not only the scalar flux but also the components of the neutron current $\vec{J}$ are approximated using polynomial approximations that must satisfy the following condition:

$$\nabla \cdot \vec{K} \in V \tag{3}$$

where $\vec{K}$ are the basis functions for $\vec{J}_h$ and V is the polynomial space for basis functions of ϕ_h.

The idea behind this is to avoid that the neutron current loses one order of accuracy if it is

obtained by differentiating the scalar flux.

The last formulation, the mixed-hybrid one, has the advantage that the scalar flux can be post-processed at no extra cost using the Lagrange multiplier, formerly edge Legendre moments, and the cell Legendre moments of the flux.

Third order nodal finite element methods with transverse and reduced integration were systematically applied to solve elliptic problems [19].

5. TRANSPORT EQUATION

The neutron transport equation in its discrete-ordinates S_N approximation in x-y geometry reads:

$$L\psi_k \equiv \mu_k \frac{\partial \psi_k}{\partial x} + \nu_k \frac{\partial \psi_k}{\partial y} + \Sigma_t \psi_k = \Sigma_s \sum_{\ell=1}^{M} \omega_\ell \psi_\ell + S_k, \equiv Q_k, k = 1,..., M \qquad (4)$$

where the unknown is ψ_k, the angular neutron flux corresponding to the k-th ray of the S_N approximation, M being the total number of rays considered which is given in this case by $N(N+2)/2$. The domain to be considered is of the union of rectangles type and boundary conditions must also be imposed.

Classically, with nodal methods, the domain of interest is decomposed in relatively large homogeneous regions or "nodes", over which each angular flux ψ is approximated by a generalized interpolant with interpolation parameters which are cell and/or edge Legendre moments. This unique interpolant is piecewise continuous using in most cases polynomial shape functions. For a ray in the first quadrant, the possible left and bottom edge parameters are known from the boundary conditions or from the neighboring left and bottom cells. The unknowns are thus the right and top edge parameters as well as the cell ones.

In this paper, we present two classes of polynomial nodal methods. In essence, both classes of methods lead to discontinuous approximations as they at most conserve some edge moments between adjacent nodes, as in the case of the first class of methods which we call *weakly discontinuous*. In this case one or several moments of the angular flux are conserved between a given cell and its upstream neighbors. The second class of methods, called *strongly discontinuous*, is fully discontinuous and only has outgoing (at top and right) edge moments as parameters, in addition to possible cell moments.

Before dealing with these methods in detail, we present in the next section some notation and the basic formalism.

5.1 Notation and Basic Formalism

Assuming that the domain Ω of the union of rectangles type has been discretised in N_e nodes or rather *cells* or *elements*, i.e., each cell Ω_e is mapped onto a reference cell $\hat{\Omega} \equiv [-1,+1]\times[-1,+1]$, as it is traditional with finite element methods. A particular finite element is then defined by a set of degrees of freedom D and a space of functions S with *card(D)=dim(S)*. With degrees of freedom which are cell and/or edge moments as in this paper, we shall speak of *nodal finite*

elements. For practical purposes, these moments will be taken as Legendre moments.

To describe D and S in a compact way in the *nodal* case, some notation will be helpful. Let P_i be the normalized Legendre polynomial of degree i over [-1,+1] which satisfies

$$P_i(+1) = 1\ ,\ P_i(-1) = (-1)^i\ ,\ \text{and}\ \int_{-1}^{+1} P_i(x)P_j(x)dx = N_i\delta_{ij}\ .$$

with $N_i = 2/(2i+1)$. Define moreover $P_{ij}(x,y)$ as $P_i(x)\ P_j(y)$. Assuming that $L\psi = Q$ is the given equation, ψ is approximated by ψ_h and over Ω, cell moments of ψ_h (x,y) $\in S$ are defined as follows

$$\psi_C^{ij} = \int_{-1}^{+1} P_{ij}(x,y)\psi_h(x,y)dxdy / N_i \cdot N_j\ .$$

Edge moments are moreover given by

$$\psi_E^{i} = \int_{-1}^{+1} P_i(s_E)\psi_h(x_E,y)dx / N_i$$

where E is a generic symbol corresponding to *L, R, B*, and T for the left, right, bottom, and top edges respectively, x_E or y_E is +1 depending on the particular edge considered, the other coordinate being s_E, the coordinate along that edge.

S is a space of functions, which are *polynomials* in this paper. To describe them in a systematic way, let us introduce the spaces of polynomials of degree i in x and j in y, $Q_{ij}(x,y) = \{x^a y^b \mid 0 \le a \le i, 0 \le b \le j\}$, with in particular $Q_i \equiv Q_{ii}(x,y)$ and also the spaces of polynomials of degree i in x and y, where a and b are integers. For each nodal finite element, we shall call $N_p=dim(D)$ the total number of parameters and N_u the number of unknowns which is less than N_p in the weakly discontinuous case, as the interpolation parameters on the left and bottom edges are taken from the neighboring cells or given by the boundary conditions. In the strongly discontinuous case, there are no left and bottom parameters and we have $N_p=N_u$. In the following, each particular method will be assigned a symbol consisting of two capital letters, *WD* in the weakly discontinuous case and *SD* in the strongly discontinuous one, indexed by the two numbers N_p and N_u in the first case, and by N_p or N_u indifferently in the second case. In the weakly discontinuous case, $(N_p - N_u)/2$ is the number of edge moments conserved between adjacent cells. In most practical cases, this number is one or two.

In both cases, we have programmed all the methods from two to eight unknowns per cell and applied them to multiplicative and nonmultiplicative benchmark problems of the nuclear literature. In the weakly discontinuous case, we have given in Hennart *et al.* [14] a constructive algorithm to deduce the space of functions S if the set of degrees of freedom D is known. We always assumed that we had the same number of edge moments on each pair of opposite edges. This is clearly not true in the strongly discontinuous case and we had to adapt the earlier algorithm to that situation for applications in neutron transport problems.

Let us give a concrete example, namely the element WD_{53}. In this case, $D \equiv \{\psi_L^0, \psi_R^0, \psi_B^0, \psi_T^0, \psi_C^{00}\}$

and correspondingly $S \equiv \{P_{00}, P_{01}, P_{10}, P_{02}, P_{20}\}$. On each cell, ψ is approximated by

$$\psi_h = \sum_E \psi_E^0 u_E^0 + \psi_C^{00} u_C^{00}$$

where the basis functions have very compact expressions in terms of the P_{ij}'s. For instance, $u_L^0 = -\frac{1}{2}(P_{10} - P_{20})$ and $u_C^{00} = P_{00} - P_{20} - P_{02}$, the other edge basis functions being obtained by changing the sign of x and/or y or by permuting them.

Replacing ψ by ψ_h in each cell, a local residual $L\psi_h - Q_h$ arises where Q_h is evaluated from a previous iterate in the standard source iteration procedure which can be accelerated or not. If the ray (μ_k, ν_k) is in the first quadrant, one proceeds cell by cell by a standard *diagonal sweeping* beginning with the first cell in Ω_h seen by the particular ray considered. Consequently, we know from the boundary conditions at the left or bottom of the domain or from the left or bottom neighbors which have been processed previously the edge moments on the left and bottom edges. If as it is the case with the weakly discontinuous methods, some of these moments are conserved between neighbors, they are directly known in either cell. The moment equations we shall now mention make actually appear edge moments which are not interpolation parameters and it is indispensable to know precisely if we must evaluate them in the current cell or in the previous ones. Locally, Legendre moments of the residual $L\psi_h - Q_h$ are taken to obtain as many equation as unknowns. Since L is a first order partial differential operator, its application to a *discontinuous* approximation ψ_h generates delta distributions and the correct way to take them into account is to derive the moment equations over a cell Ω_e which is shifted upstream by ε, in the limit of a vanishing ε. For a ray in the first quadrant that means that the cell considered is moved slightly downward and to the left. As $\varepsilon \to 0$, boundary terms arise at the left and the bottom of the cell, connecting it to its upstream neighbors or boundaries. This *upwinding* procedure is classical when discontinuous approximations are used for first order ordinary or partial differential equations. See for example Hennart and del Valle [20] for the derivation of various discontinuous schemes in the slab geometry transport case.

Going back to the *WD53* example, the zeroth order moment of the residual should be taken, which ensures balance, i.e. *particles conservation*. Let p_{ij} be P_{ij} scaled to the particular cell considered $[x_L, x_R] \times [y_B, y_T]$. The balance equation corresponds to taking the moment of the residual with respect to p_{00}. The missing equations correspond for instance to taking that moment with respect to p_{10} and p_{01} by symmetry, in other words the three moments are taken with respect to P_1.

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