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An Innovative Reactor Analysis Methodology Based on a Quasidiffusion Nodal Core Model

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Task 1

Research efforts in Task 1 are focused on the problem in one-dimensional geometry and development of basic ideas of functionalization and homogenization procedures. The spatial homogenization procedure must preserve the averaged reaction rates, surface-averaged group currents, and eigenvalue [1]. The homogenization fits naturally into the framework of the quasidiffusion (QD) method [2, 3] that is based on the idea of successive averaging of the transport equation over angular and energy variable. The averaging over spatial variable is the next logical step [3].

We formulated an approach for spatial assembly homegenezation which is based on the idea of consistent discretization of spatially averaged QD low-order equations and their fine-mesh discretization. Below is the description of the proposed method of the consistent coarse-mesh discretization of the QD low-order equations. This is a basis for the proposed homegenezation procedure. These results were submitted for the ANS 2000 International Winter Meeting.

1. The Quasi-Diffusion Method

We consider the k-eigenvalue transport problem for 1D slab geometry ($a \le x \le b$, $-1 \le \mu \le 1$)

$$\mu\frac{\partial}{\partial x}\psi(x,\mu)+\Sigma_t\psi(x,\mu) = \frac{1}{2}\left(\Sigma_s + \frac{1}{k}\nu\Sigma_f\right)\phi(x)\,, \quad \psi(a,\mu)|_{\mu>0} = 0\,, \quad \psi(b,\mu)|_{\mu<0} = 0\,, \quad (1)$$

The low-order QD equations [2] for the scalar flux ϕ and the current J are

$$\frac{d}{dx}J(x) + \left(\Sigma_a - \frac{1}{k}\nu\Sigma_f\right)\phi(x) = 0\,, \quad (2)$$

$$\frac{d}{dx}\left(D(x)\phi(x)\right) + \Sigma_t J(x) = 0\,, \quad (3)$$

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$$J(a) = C_a\phi(a)\ , \quad J(b) = C_b\phi(b)\ , \tag{4}$$

where the functionals

$$D(x) = \int_{-1}^{1} \mu^2\psi(x,\mu)d\mu \Big/ \int_{-1}^{1} \psi(x,\mu)d\mu\ , \tag{5}$$

$$C_a = \int_{-1}^{0} \mu\psi(a,\mu)d\mu \Big/ \int_{-1}^{0} \psi(a,\mu)d\mu\ , \quad C_b = \int_{0}^{1} \mu\psi(b,\mu)d\mu \Big/ \int_{0}^{1} \psi(b,\mu)d\mu \tag{6}$$

are calculated by the transport solution.

2. Fine-Mesh Discretization

We discretize spatially the low-order QD equations using a second-order difference scheme [4]. A spatial mesh is defined so that $x_{i+1/2}$ $(1 \le i \le N)$ correspond to the mesh edges, where $x_{1/2} = a$ and $x_{N+1/2} = b$. The mesh widths are given by $h_i = x_{i+1/2} - x_{i-1/2}$. Integer $\pm\frac{1}{2}$ subscripts refer to cell-edge quantities, and integer subscripts refer to cell-average quantities. The difference scheme for the low-order equations of the QD method is defined by $(i = 1, ..., N)$

$$J_{i+1/2} - J_{i-1/2} + \left(\Sigma_{a,i} - \frac{1}{k}\nu\Sigma_{f,i}\right) h_i\phi_i = 0\ , \tag{7}$$

$$D_i\phi_i - D_{i-1/2}\phi_{i-1/2} + \frac{1}{2}\Sigma_{t,i}h_iJ_{i-1/2} = 0\ , \tag{8}$$

$$D_{i+1/2}\phi_{i+1/2} - D_i\phi_i + \frac{1}{2}\Sigma_{t,i}h_iJ_{i+1/2} = 0\ , \tag{9}$$

$$J_{1/2} = C_a\phi_{1/2}\ , \quad J_{N+1/2} = C_b\phi_{N+1/2}\ . \tag{10}$$

Hereafter we assume that the transport solution is found by means of some method, and, thus, we can calculate all necessary functionals.

3. Consistent Coarse-Mesh Discretization

Let us consider a two-zone problem: $a \le x \le g$ (α-zone) , $g \le x \le b$ (β-zone). We introduce $x_{M+1/2} = g$, two sets of indices $I_\alpha = \{i : 1 \le i \le M\}$ and $I_\beta = \{i : M+1 \le i \le N\}$, and a coarse mesh consisting of just one cell per zone. The coarse-mesh solution is defined by $\overline{\Phi}_\xi$, Φ^R_ξ, Φ^L_ξ, J^R_ξ, and J^L_ξ, where ξ is the index of a zone and the corresponding coarse cell $(\xi = \alpha, \beta)$, $\overline{\Phi}_\xi$ is the cell-average scalar flux, and the superscripts L and R indicate respectively the left and right cell-edge values in the ξ-th coarse cell. The coarse-mesh discretization of the QD low-order equations consistent with the difference scheme (7)-(10) is given by the following set of equations:

$$J^R_\xi - J^L_\xi + \left(\overline{\Sigma}_{a,\xi} - \frac{1}{k}\overline{\nu\Sigma}_{f,\xi}\right) H_\xi\overline{\Phi}_\xi = 0\ , \quad \xi = \alpha, \beta\ , \tag{11}$$

$$\widetilde{D}^L_\xi\overline{\Phi}_\xi - D^L_\xi\Phi^L_\xi + \frac{1}{2}\Sigma^L_{t,\xi}h^L_\xi J^L_\xi = 0\ , \tag{12}$$

$$D_\xi^R \Phi_\xi^R - \widetilde{D}_\xi^R \overline{\Phi}_\xi + \frac{1}{2}\Sigma_{t,\xi}^R h_\xi^R J_\xi^R = 0 \,, \tag{13}$$

$$J_\alpha^R = J_\beta^L \,, \quad \Phi_\alpha^R = \Phi_\beta^L \,, \tag{14}$$

$$J_\alpha^L = C_a \Phi_\alpha^L \,, \quad J_\beta^R = C_b \Phi_\beta^R \,, \tag{15}$$

where

$$D_\alpha^L = D_{1/2} \,, \quad D_\alpha^R = D_\beta^L = D_{M+1/2} \,, \quad D_\beta^R = D_{N+1/2} \,, \tag{16}$$

$$\Sigma_{t,\alpha}^L = \Sigma_{t,1} \,, \quad \Sigma_{t,\alpha}^R = \Sigma_{t,M} \,, \quad \Sigma_{t,\beta}^L = \Sigma_{t,M+1} \,, \quad \Sigma_{t,\beta}^R = \Sigma_{t,N} \,, \tag{17}$$

$$H_\alpha = g - a \,, \quad H_\beta = b - g \,, \quad h_\alpha^L = h_1 \,, \quad h_\alpha^R = h_M \,, \quad h_\beta^L = h_{M+1} \,, \quad h_\beta^R = h_N \,, \tag{18}$$

$$\overline{\Sigma}_{a,\xi} = \sum_{i \in I_\xi} \Sigma_{a,i} \phi_i h_i \Big/ \sum_{i \in I_\xi} \phi_i h_i \,, \quad \overline{\nu\Sigma}_{f,\xi} = \sum_{i \in I_\xi} \nu\Sigma_{f,i} \phi_i h_i \Big/ \sum_{i \in I_\xi} \phi_i h_i \,, \quad \xi = \alpha, \beta \,, \tag{19}$$

$$\widetilde{D}_\alpha^L = F_\alpha^L D_1 \,, \quad \widetilde{D}_\alpha^R = F_\alpha^R D_M \,, \quad \widetilde{D}_\beta^L = F_\beta^L D_{M+1} \,, \quad \widetilde{D}_\beta^R = F_\beta^R D_N \,, \tag{20}$$

$$F_\alpha^L = \phi_1 H_\alpha \Big/ \sum_{i \in I_\alpha} \phi_i h_i \,, \quad F_\alpha^R = \phi_M H_\alpha \Big/ \sum_{i \in I_\alpha} \phi_i h_i \,, \tag{21}$$

$$F_\beta^L = \phi_{M+1} H_\beta \Big/ \sum_{i \in I_\beta} \phi_i h_i \,, \quad F_\beta^R = \phi_N H_\beta \Big/ \sum_{i \in I_\beta} \phi_i h_i \,. \tag{22}$$

The coarse-cell balance equations (11) were obtained by spatial averaging of fine-mesh equations (7) over each zone and introducing average cross sections (19). To get Eqs. (12) and (13), in each of coarse cells we approximated the first-moment QD equation (3) relating cell-edge and cell-average values of the coarse-mesh solution in a way that is similar to one used to obtain the difference equations (8) and (9). To accomplish this, we derived the definition of cell-average QD functional D [Eqs. (20)] which is based on special factors F_ξ^L and F_ξ^R [Eqs. (21) and (22)]. We note that these quantities are similar to discontinuity factors [1]. However, the proposed consistent coarse-mesh discretization preserves the continuity of the scalar flux and the current on cell interfaces [Eqs. (14)].homegenezation

The coarse-mesh discrete QD low-order equations (11)-(22) are consistent with the fine-mesh discrete QD low-order equstions (7)-(10) and the coarse-mesh solution has the following form in terms of the fine-mesh transport solution of Eqs. (7)-(10):

$$\overline{\Phi}_\xi = \sum_{i \in I_\xi} \phi_i h_i \Big/ \sum_{i \in I_\xi} h_i \,, \quad \xi = \alpha, \beta \,, \tag{23}$$

$$J_\alpha^L = J_{1/2} \,, \quad J_\alpha^R = J_\beta^L = J_{M+1/2} \,, \quad J_\beta^R = J_{N+1/2} \,, \tag{24}$$

$$\Phi_\alpha^L = \phi_{1/2} \,, \quad \Phi_\alpha^R = \Phi_\beta^L = \phi_{M+1/2} \,, \quad \Phi_\beta^R = \phi_{N+1/2} \,, \tag{25}$$

and k-eigenvalue is the same.

The coarse-mesh equations (11)-(22) were derived by means of equivalent manipulations. No approximations were made. If one substitutes the solution (23)-(25) into (11)-(22), then it easy to see that it meets these coarse-mesh discretized equations.

To develop a coarse-mesh solution that contains more details about the solution inside a zone, one can define in each zone a mesh consisted of three cells: (a) two original fine-mesh

boundary cells in the given zone, (b) one central cell that covers the rest area in the zone. Then, the described procedure of coarse-mesh discretization is applied to the central cell.

4. Spatial Decomposion

It is possible to reformulate equivalently the derived above two-cell problem (11)-(15) in the form of two one-cell problems each of which will reproduce the corresponding part of the original solution. To perform such decomposition, we replace two interface equations (14) by special boundary conditions. These conditions can be presented in different forms. We consider the albedo form:

$$J_\alpha^R = \frac{1-\lambda_1^\alpha}{1+\lambda_0^\alpha} C_g^\alpha \Phi_\alpha^R \,, \quad J_\beta^L = \frac{1-\lambda_1^\beta}{1+\lambda_0^\beta} C_g^\beta \Phi_\beta^L \,, \tag{26}$$

$$\lambda_n^\xi = \int_0^{\mu_\xi^*} \mu^n \gamma(-\mu)\psi(g,\mu)d\mu \Big/ \int_0^{\mu_\xi^*} \mu^n \psi(g,\mu)d\mu \,, \quad C_g^\xi = \int_0^{\mu_\xi^*} \mu\psi(g,\mu)d\mu \Big/ \int_0^{\mu_\xi^*} \psi(g,\mu)d\mu \,, \tag{27}$$

where $n = 0, 1$, $\xi = \alpha, \beta$, $\mu_\alpha^* = 1$, $\mu_\beta^* = -1$, and $\gamma(\mu)$ is the albedo. The albedo and any of these functionals [Eqs. (27)] can be calculated by the known fine-mesh transport solution.

5. Conclusion

We have developed an approach for spatial averaging the discretized QD low-order equations and generating a coarse-mesh discretization which is consistent with the given fine-mesh discretization. The proposed procedure was demonstrated on a two-zone problem. The developed method also implements the idea of discontinuity factors, however does it rather naturally and in theoretically sound manner. The resulting solution preserves continuity both of the scalar flux and the current. The procedure of spatial decomposition based on albedo boundary conditions was formulated. The presented approaches to coarse-mesh consistent discretization and spatial decomposition can be extended to multidimensional problems and nodal discretization methods. The proposed methodology creates a theoretical beackground for homogenization of spatial regions and parametrization of group constants using assembly transport solution.

Task 2

Our efforts are currently focused on continued development of the 2D nodal QD code with "extra" leakage terms lagged at the previous iteration step (similar to the standard transverse leakages), Fourier analyses of this iterative technique, investigation of another solution strategy which treats all the terms in the QD equations implicitly, and adaptation of a traditional "marching" method to the solution of nodal QD equations.

The results from the Fourier analysis of our "lagged QD leakage" approach will be pivotal in determining the strategy used to solve the QD equations. The general idea is to try to make the QD nodal equations look as much like standard nodal diffusion as possible. In the QD method, we find that the current in a direction u, where $u = x, y$, can be written as

$$J_u = -\frac{1}{\sigma_t}\left[\frac{\partial\left(D_{u,u}\phi\right)}{\partial u} + \frac{\partial\left(D_{v,u}\phi\right)}{\partial v}\right], \tag{28}$$

where the fractional functionals, D, are computed from the solution of a transport equation. To make our QD equations look like standard diffusion equations, we move the second term in the brackets in the above equation to the right hand side of our iterative system (calculate it from previously obtained solutions). After discretization, we now have a slightly modified transverse integrated leakage term. The overall iterative system has the form:

$$\phi^{(l+1)} = A^{-1}F\phi^{(l)}, \tag{29}$$

where A is a 2×2 block matrix, each block containing a $20N_{u,v} \times 20N_{u,v}$ system, $N_{u,v}$ being the number of nodes in either the u or v direction. F is a matrix operator which computes transverse-integrated leakages from flux moments, and ϕ is a vector containing $20N_u + 20N_v$ flux moment unknowns. A Fourier analysis of this iterative scheme involves approximating the system as an infinite homogeneous medium, performing a Fourier series expansion of the unknowns in the spatial variable, and solving the resulting eigensystem for the iteration eigenvalues. If the technique is stable, all the eigenvalues will be less than 1 in magnitude. We have constructed the eigensystem, and are currently implementing a Fortran code to solve it.

In our new implicit strategy, the complete QD leakage operator is treated with a nodal discretization, which means that we keep all of the terms in Eq. (28) on the left-hand side of the matrix equation. This means that the right-hand side of the matrix equation contains terms which are completely analogous to standard diffusion. We expect that this technique will converge much more quickly than our first technique; however, it may not be as seamlessly incorporated into existing nodal diffusion codes.

We have also digressed briefly to gain an understanding of the marching technique used to solve the finite volume discretization of the QD equations developed by [9]. Ultimately, we intend to implement this method for the QD low-order equations; however, at this time, we are applying it just to the finite volume differenced diffusion equation described in [10]. In essence, this method is very similar to an alternating direction implicit technique, with the interesting twist that the unknowns which exist in the problem (ϕ, J) are replace by quantities $(\mu, \tau$ and $\sigma)$ which are less sensitive to iteration errors. In this way, μ and τ can

be converged very quickly (independent of σ), and then the iteration on σ can be completed with these converged values of μ and τ. This iteration procedure has been shown to converge very rapidly for a wide variety of physical situations. At this time, we are coding the solution technique for the finite volume diffusion equation, but we will be evaluating the suitability of this marching method for the solution of more sophisticated differencing schemes applied to both the diffusion and QD equations.

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Status Summary of NERI Tasks - Phase 1

Task 1

The development of the following methods in 1D slab geometry:

1. Homogenization and definition of discontinuity factors,
2. Group constants functionalization using assembly transport solution of multigroup eigenvalue problem with albedo boundary conditions,
3. Solving coarse-mesh effective few-group 1D QD moment equations using tables of data parametrized with respect to the ratio $\vec{n} \cdot \tilde{J}^G / \tilde{\phi}^G$ on boundaries.

Planned completion date: August 14, 2000

Task 2

Development of a numerical method for solving the 2D few-group moment QD equations:

1. Development of a nodal discretization method for 2D moment QD equations,
2. Development of an efficient iteration method for solving the system of equations of the nodal discretization method for 2D moment QD equations.

Planned completion date: August 14, 2000