Computer Code Abstract

The HEXAB-3D Three-Dimensional Few-Group Improved Coarse-Mesh Diffusion Code for Hexagonal-z Geometry

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1. Program Identification: HEXAB-3D is a three-dimensional few-group improved coarse-mesh diffusion code for hexagonal-z geometry useful for steady-state neutronics core analysis.[1]
2. Function: The HEXAB-3D computer code determines the effective multiplication factor, the group neutron flux and power distributions, the peaking factors, the control rod worth, etc., in a nuclear power reactor with a hexagonal core configuration and a heterogeneous structure in the axial direction. There are two options for the diffusion equation solution in the horizontal plane: a 30-deg sector of the reactor core (with reflective conditions on the internal reactor boundaries) or the full core.
3. Method of Solution: The three-dimensional multigroup neutron diffusion equations are solved using a nine-point, mesh-centered, finite difference approximation. The standard inner-outer iterative strategy is applied. Inner iterations are solved using incomplete factorization techniques: the AGA two-sweep iterative method[2,3] and the MAGA modified two-sweep iterative method[4] both accelerated by the double successive overrelaxation procedure. The power method, combined with two- or three-term Chebyshev polynomial acceleration for outer iterations, is applied in the code.

The specific merits of the algorithm applied in the HEXAB-3D code are as follows. An effective approach,[5,6] the so-called finite difference type nodal method, was developed to improve the accuracy of the calculated integral and local reactor parameters without significantly increasing the computer time and storage. Correcting the finite difference scheme coefficients results in a decrease in the errors due to the use of a coarse mesh. The advantages of the proposed nodal method are a more precise expression of the radial neutron leakage in the nine-point diffusion balance equations as well as the use of average flux values for reaction rate calculations. The modified finite difference equations in the usual notations are as follows:

$$\sum_{j=1}^{6}\left[-\frac{2D_{jr}^{g^*}D_{ir}^{g^*}S_{ir}}{h_r(D_{jr}^{g^*}+D_{ir}^{g^*})}(\phi_j^{g^*}-\phi_i^{g^*})\right]+\sum_{j=7}^{8}\left[-\frac{2D_{jz}^{g}D_{iz}^{g}S_{iz}}{h_{iz}D_{jz}^{g}+h_{jz}D_{iz}^{g}}(\phi_j^{g^*}\tau_j-\phi_i^{g^*}\tau_i)\right]+\Sigma_{ti}^{g^*}\phi_i^{g^*}V_i$$
$$=\frac{\chi_i^g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{fi}^{g'^*}\phi_i^{g'^*}V_i-\sum_{g'\neq g}^{G}\Sigma_{si}^{g'\to g^*}\phi_i^{g'^*}V_i\,, \qquad (1)$$

where

$$\Sigma_{xi}^{g^*}=\Sigma_{xi}^{g}\tau_i^g \quad (x=f,s,t)\,,$$
$$D_{ir}^{g^*}=D_{ir}^{g}\alpha_i^g\,,$$

and

$$D_{iz}^{g}=D_i^g\,.$$

The expressions obtained for the correction coefficients in two important cases[5,6] are as follows:

$$\tau_i^g=\left(1-\frac{a}{27}h_r^2\beta_{ig}^2\right)\left(1-\frac{4}{81}h_r^2\beta_{ig}^2\right)$$

and

$$\alpha_i^g=1-\frac{5}{16}h_r^2\beta_{ig}^2\,, \qquad (2)$$

where $a=2.4$ for the absorber part of the boron carbide control rods, $a=1.8$ for the rest of the core, and

$$\beta_{ig}^2=\frac{1}{D_i^g}\left(\frac{\chi_i^g}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{fi}^{g'}\frac{\phi_i^{g'}}{\phi_i^g}-\sum_{g'\neq g}^{G}\Sigma_{si}^{g'\to g}\frac{\phi_i^{g'}}{\phi_i^g}-\Sigma_{ti}^{g}\right)\,.$$

In addition, the code uses the theoretically well-founded MAGA effective inner iteration method[4] based on a modification of the AGA iterative scheme, which improves the convergence rate in comparison with the AGA method and with the conventional iterative methods and decreases the computing time, thus, increasing the effectiveness of the code.

The code also uses an optimized iterative solution strategy, which provides satisfactory accuracy within a short computation time. As a result, the increases in the computation time and computer memory requirements are no more than 23% of those of the conventional coarse-mesh finite difference method.

4. Related Material: Related programs include FREIFE and FELDE, which dynamically allocate the central computer storage, and DAFDEF, which serves for data array input-output operations with direct access files.
5. Restrictions: Flexible dimensioning is used, and the following restrictions, determined by IBM 370/145 and IBM 3031 resources, are imposed on individual problem parameters: maximum of 10 energy groups, 30 horizontal layers, and 100 material compositions. For users with access to greater computing resources, these limitations may be eased.
6. Computers: HEXAB-3D is designed to be applicable to IBM computers (IBM 370/145 and IBM 3031).
7. Running Time: The CPU time used in the k_{eff} calculations for three-dimensional reactor models with four energy groups and convergence criteria between successive iterations on group flux iterations ($\epsilon_\phi \leq 10^{-4}$) and on ($k_{eff} - \epsilon_{k_{eff}} \leq 10^{-6}$) on an IBM 3031 ($1 \times 10^6$ floating point operations per second) is ~240 s for the SNR-300 benchmark[7] B1 problem in 360 deg with 7940 mesh points and ~603 s for the BN-1600 benchmark[8] in 360 deg with 21 567 mesh points.
8. Machine Requirements: Virtual storage required is 1024 kilobytes. The IBM 3350 and IBM 3330 disk storage devices can be used for work files. The total disk space required is not larger than 40 cylinders on IBM 3350 storage devices.
9. Programming Languages: FORTRAN-IV and Assembler on IBM computers.
10. Operating System: OS/VS1 and MVS (IBM).
11. Additional Programming Information: The program has ~3400 lines of coding instructions.
12. Materials Available: Program abstract, user's guide,[9] and validation report; the source code HEXAB-3D; the source auxiliary assembler programs FELDE, FREIFE, and DAFDEF; simple problem solution.
13. References:

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