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Solving the Neutron Diffusion Equation on Combinatorial Geometry Computational Cells for Reactor Physics Calculations

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An approach is developed for solving the neutron diffusion equation on combinatorial geometry computational cells, that is computational cells composed by combinatorial operations involving simple-shaped component cells. The only constraint on the component cells from which the combinatorial cells are assembled is that they possess a legitimate discretization of the underlying diffusion equation. We use the Finite Difference (FD) approximation of the *x*,*y*-geometry diffusion equation in this work. Performing the same combinatorial operations involved in composing the combinatorial cell on these discrete-variable equations yields equations that employ new discrete variables defined only on the combinatorial cell's volume and faces. The only approximation involved in this process, beyond the truncation error committed in discretizing the diffusion equation over each component cell, is a consistent-order Legendre series expansion. Preliminary results for simple configurations establish the accuracy of the solution to the combinatorial geometry solution compared to straight FD as the system dimensions decrease. Furthermore numerical results validate the consistent Legendre-series expansion order by illustrating the second order accuracy of the combinatorial geometry solution, the same as standard FD. Nevertheless the magnitude of the error for the new approach is larger than FD's since it incorporates the additional truncated series approximation.

KEYWORDS: Neutron Diffusion Equation, combinatorial geometry, Finite Difference, core calculations, solution accuracy

1. Introduction

Steady state models of physical phenomena usually express a natural balance between particle sources and sinks, forces, etc. Numerical methods applied to such models result in a discretization of this balance to hold over finite volumes in phase space. In nuclear applications the discretized balance relations are usually exact. However, to obtain as many algebraic equations as discrete variables to be solved for, it is necessary to derive additional approximate relations, e.g. central differencing, nodal formalism, etc. The resulting stencil is valid locally, i.e. over an individual computational cell. In a typical computer code this stencil is replicated with specific parameter settings to cover the entire problem domain. In this work we apply stencils of the Finite Difference (FD) approximation of the neutron diffusion equation in two-dimensional Cartesian geometry to multiple computational cells, i.e. component cells (cc), comprising a composite cell (CC), then analytically eliminate all discrete variables internal to this cell via local series expansions.

The basic idea behind the new method is to express a computational cell geometrical shape as a

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combinatorial geometry object, or *composite cell*, whose *component objects* are simple geometric constructs. The only requirement on the components' shapes is that they possess a discretization of the underlying PDEs relating cell- and face-averaged values of the solution in a simple algebraic expression. A catalogue of familiar basic cc's, and commonly occurring CC's can be compiled for the neutron diffusion equation using the formalism developed in this paper. The relationship between the discrete variables of the cc's and the CC are based entirely on geometric considerations. Such mathematical formulas are combined with the discretized form of the underlying PDE over the cc's to eliminate discrete variables *internal* to the CC. The resulting expressions relating the cell- and face-averaged neutron flux over the CC are then obtained.

In this paper we will describe the new approach and illustrate its utility by applying it to the case of a unit cell comprised of a square fuel region concentric with a square moderator region. Using reflective symmetry along the vertical and horizontal midplanes we reduce the problem domain to a quarter-unit cell in which the fuel region is still a square, but the moderator region is an inverted *L*-shape. In Sec. 2 we will present the new formalism and demonstrate it for this geometric configuration using FD. Numerical tests of the resulting equations as implemented in a test code are summarized in Sec. 3, including comparisons to standard-method solutions converged with mesh refinement. These comparisons illustrate that the new approach yields discrete-variable equations that possess the same (second) order error as the standard FD diffusion method. We summarize the work and our conclusions in Sec. 4.

2. Combinatorial Method Formalism

We illustrate the combinatorial methodology via the difference operation between two rectangular cells for the steady state, one-speed neutron diffusion equation in two-dimensional Cartesian geometry. This amounts to a Cartesian approximation of one quarter of the typical unit cell configuration as depicted in Fig. 1 with reflective boundary conditions on all four faces.

The FD approximation of the monoenergetic diffusion equation in a rectangular computational cell of dimensions $2a \times 2b$ is comprised of the discretized balance equation[1]

$$\frac{\bar{J}_R^y - \bar{J}_L^y}{2a} + \frac{\bar{J}_T^x - \bar{J}_B^x}{2b} + \sigma_a \varphi = q \tag{1}$$

and discretized forms of Fick's law, e.g.

$$\bar{J}_R^y = -D\frac{\bar{\varphi}_R^y - \varphi}{a}, \quad \bar{J}_L^y = -D\frac{\varphi - \bar{\varphi}_L^y}{a} \tag{2}$$

In Eqs. (1) and (2) σ_a and D are the macroscopic removal cross section and diffusion coefficient, respectively; φ and q are the cell-averaged scalar flux and source, respectively; $\bar{\varphi}_R^y$ and $\bar{J}_R^y$ are the y-averaged flux and current evaluated on the right face of the rectangle, respectively, with analogous notation for the other three faces.

Application of the Eqs. (1) and (2) stencil to the fuel region shown in Fig. 1 is straightforward. Its application to the moderator region, however, has traditionally involved breakup of the inverted *L*-shape into three, or more, rectangular regions then applying the stencil to each of them. The variables in the various rectangles are coupled via interface conditions that preserve neutron flux and current. The combinatorial methodology seeks treatment of the moderator region as a single CC equal to the

difference of two rectangular regions as depicted in Fig. 1. The discrete variable equations for this CC are derived from those of the 2 cc's as described below.

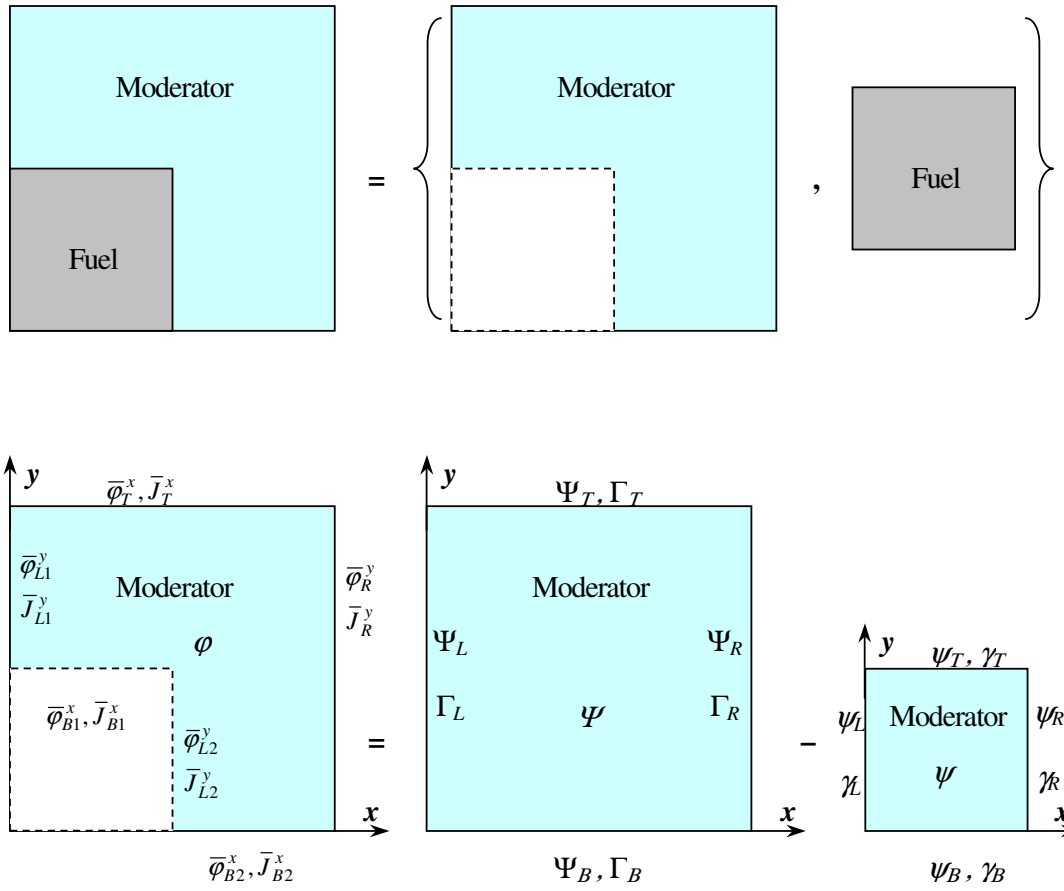

Fig.1 Cartesian-geometry approximation of the unit cell configuration (top), and representation of the moderator CC as the difference between two cc's (bottom).

Referring to the discrete variables in the CC and two cc's as denoted in Fig. 1 and using the definition of the cell- and face-averaging operators we can express the CC discrete variables in terms of their cc counterparts. For example, the scalar flux averaged over the large rectangular cc is defined by

$$\Psi \equiv \frac{1}{(2A)(2B)} \int_{-A}^{A} dx \int_{-B}^{B} dy \varphi(x, y)$$

where $\varphi(x, y)$ is the space dependent scalar flux over that cc-region, and the dimensions of the small (large) cc are denoted by $2a \times 2b$ ($2A \times 2B$), respectively. The integral operators can be rewritten as

$$\Psi \equiv \frac{1}{(2A)(2B)} \left[\int_{-A}^{-A+2a} dx \int_{-B}^{-B+2b} dy \varphi(x, y) + \int_{-A+2a}^{A} dx \int_{-B}^{B} dy \varphi(x, y) + \int_{-A}^{-A+2a} dx \int_{-B+2b}^{B} dy \varphi(x, y) \right]$$

The first term on the right hand side is the definition of the small cc-averaged flux, ψ, multiplied by the cc's area, i.e. $(2a)(2b)\psi$, and the last two terms add up to the definition of the CC-averaged flux, φ, multiplied by the CC's area, i.e. $\left[(2A)(2B)-(2a)(2b)\right]\varphi$. It immediately follows that

$$\left(1-\alpha\beta\right)\varphi=\Psi-\alpha\beta\psi\,, \tag{3.a}$$

where $\alpha\equiv a/A,\ \beta\equiv b/B$.

The face-averaged variables on the right and top faces are identical in the CC and the large cc, hence

$$\bar{\varphi}_R^y=\Psi_R,\quad \bar{J}_R^y=\Gamma_R,\quad \bar{\varphi}_T^x=\Psi_T,\quad \bar{J}_T^x=\Gamma_T\,. \tag{3.b}$$

On the bottom there are two faces for the CC: the first is identical to that on the top face of the small cc so that

$$\bar{\varphi}_{B1}^x=\psi_T,\quad \bar{J}_{B1}^x=\gamma_T\,, \tag{3.c}$$

while the second requires splitting the averaging process on the left face in analogy to the derivation of Eq. (3.a) to produce,

$$(1-\alpha)\bar{\varphi}_{B2}^x=\Psi_B-\alpha\psi_B,\quad (1-\alpha)\bar{J}_{B2}^x=\Gamma_B-\alpha\gamma_B\,, \tag{3.d}$$

Analogous expressions apply on the two left faces of the CC.

Writing Eqs. (1) and (2) for each of the two cc's, then subtracting the equations for the small cc from those of the large cc, and using the relations summarized in Eqs. (3) we obtain the balance equation over the moderator CC

$$\frac{\bar{J}_R^y-\beta\bar{J}_{L2}^y-\left(1-\beta\right)\bar{J}_{L1}^y}{2A}+\frac{\bar{J}_T^x-\alpha\bar{J}_{B1}^x-\left(1-\alpha\right)\bar{J}_{B2}^x}{2B}+\left(1-\alpha\beta\right)\sigma_a\varphi=\left(1-\alpha\beta\right)q\,. \tag{4}$$

Equation (4) is an ***exact*** expression of neutron balance between the source, *q*, and ***only*** the CC discrete variables. The discrete versions of Fick's law also are exact within the FD approximation, nevertheless they involve both the cc and CC variables, e.g.

$$\bar{J}_R^y=-D\frac{\bar{\varphi}_R^y-\Psi}{A},\quad \bar{J}_{B1}^x=-D\frac{\bar{\varphi}_{B1}^x-\psi}{b}. \tag{5}$$

Eliminating the cc variables in favor of the CC variables requires the only approximation (beyond FD) mandated by the new method: expanding the flux in the large cc in a linear Legendre series

$$\varphi(x,y)\simeq\chi_0+\frac{x}{A}\chi_x+\frac{y}{B}\chi_y\,. \tag{6}$$

Since the FD error is second order in cell size,[2] this additional approximation should not adversely affect the order of the error in the solution to the new method as verified numerically in the test

configuration described in Sec. 3. The expansion coefficients are determined in terms of the large cc variables using the series representation in the cell- and face-averaged flux definitions

$$\Psi \equiv \frac{1}{4AB}\int_{-A}^{A} dx \int_{-B}^{B} dy \left(\chi_0 + \frac{x}{A}\chi_x + \frac{y}{B}\chi_y \right) = \chi_0 \Rightarrow \chi_0 = \Psi . \tag{7.a}$$

Similarly

$$\chi_x = \frac{\Psi_R - \Psi_L}{2}, \quad \chi_y = \frac{\Psi_T - \Psi_B}{2} . \tag{7.b}$$

Now the approximation Eq. (6) with the expansion coefficients of Eq. (7) is integrated over the area and edges of the small cc to obtain expressions for $\psi, \psi_L, \psi_B,$ in terms of $\Psi, \Psi_f, f = R, L, T, B.$ Substituting these in Eqs. (3) provides a set of relations

$$\Psi_R = \varphi_R, \Psi_T = \varphi_T, \psi_R = \varphi_{L2}, \psi_T = \varphi_{B1} \tag{8.a}$$

in addition to three coupled equations for Ψ, Ψ_L, Ψ_B in terms of the CC variables. Solving these 3 equations simultaneously finally yields expressions for all discrete variables defined on both cc's in terms of the CC discrete variables, namely $\varphi, \varphi_f, f = R, L1, L2, T, B1, B2$. As a result the CC equations, i.e. Eq. (4) and subsequent relations derived from Eq. (5) and its analogues, will involve only CC variables as desired by the combinatorial methodology. One modification that we found necessary to preserve the physical sense of leakage from the fuel region to the moderator region is to replace the expression for $\bar{J}^x_{B1}$ in Eq. (5), and the analogous expression for $\bar{J}^y_{L2}$, by backward differencing formulas in the moderator region. The Legendre series, Eq. (6), is used to determine a flux value in the moderator from which the flux on the fuel-moderator interface is subtracted, and the difference divided by the distance between these two points to produce an estimate of the derivative on the interface.

There are two reasons to motivate the combinatorial geometry approach. First, by treating the moderator region as a single cell the number of discrete variables solved for is reduced amounting to savings in computational resources. Second, and more importantly, in future applications of the method one can avoid approximating the shape of the fuel-moderator interface by straight lines, and avoid homogenizing the clad region with the fuel. The reason this was not done in the present preliminary study is two-fold: (1) the FD equations for the cc's are readily available and easy to manipulate and implement in Cartesian geometry; (2) the approximation on Cartesian geometry permits the mesh refinement experiments necessary to justify the new method as detailed in Sec. 3.

3. Numerical Results

To test the combinatorial geometry method we applied the equations derived as described above to the unit cell problem depicted in Fig. 1.

As a rudimentary test we applied the new method to the homogeneous unit cell, i.e. both rectangular regions have the same material even though the scalar fluxes averaged over them are labeled φ_{Fuel} and $\varphi_{Moderator}$, with reflective boundary conditions on all four faces and a uniformly distributed source. The

exact solution to this problem is the constant solution $\varphi(x,y) = q/\sigma_a$. Indeed the exact solution, $\varphi_{Fuel} = \varphi_{Moderator} = q/\sigma_a$ is computed with the new method for all unit cell sizes and nuclear properties.

The second test configuration is the two-region unit cell shown in Fig. 1, again with reflective boundary conditions on all four faces, and with variable, square unit cell size and fixed $\alpha = \beta = 1/2$. Nuclear properties representative of the thermal group in light water and uranium are employed. The new method's equations are solved for the fuel- and moderator-averaged fluxes for varying unit-cell sizes. The FD solution is obtained via a simple code for each resulting unit-cell configuration on a sequence of diminishing uniform grids. For each case the mesh is refined until the FD-computed values of φ_{Fuel} and $\varphi_{Moderator}$ converge to their infinitesimal mesh values representative of the exact solution. These two sets of solutions, as well as the FD values computed on a 2×2 mesh are plotted against unit cell size in Fig. 2. Clearly all solutions converge to the same value as the unit-cell size approaches zero.

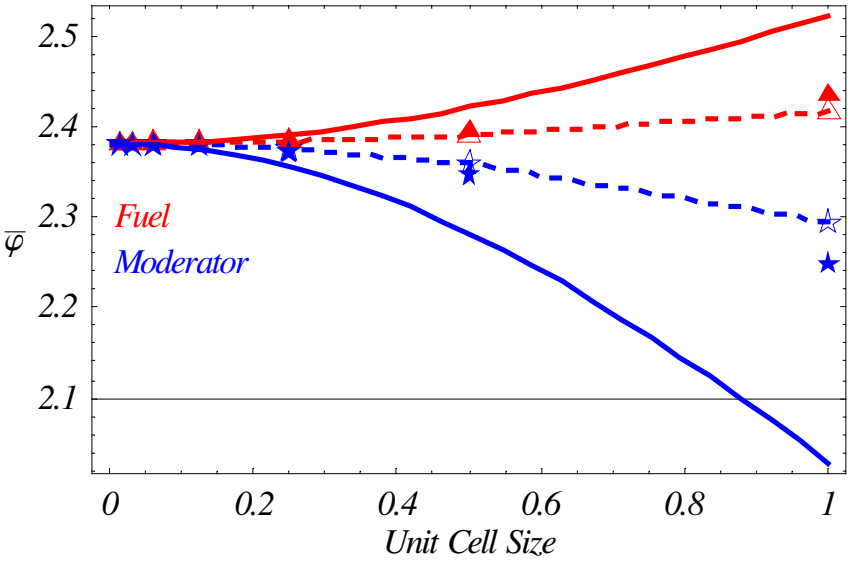

Fig. 2 Fuel- and moderator-averaged scalar fluxes *vs* unit-cell size as computed by the new method (solid lines), the FD method converged with mesh refinement (dashed lines), and the FD method on a 2×2 mesh (solid symbols).

The error in the new method's region-averaged fluxes is then computed with respect to the FD reference value and plotted *versus* unit-cell size in Fig. 3. Also shown in Fig. 3 is the error in the FD region-averaged fluxes computed on a 2×2 mesh.

The second order behavior of the new method's error evident from the plots in Fig. 3 verifies our conjecture in deriving the equations, namely that the local linear expansion of the flux does not alter the order of the FD method's error. It is also clear that the error in the combinatorial method's solution is larger than the 2×2 mesh FD solution for a given unit-cell size. This is not surprising since (1) the effective mesh size in the moderator in the combinatorial method is larger than in the standard FD method; and (2) the combinatorial method equations have the additional approximation embodied in the truncated local series.

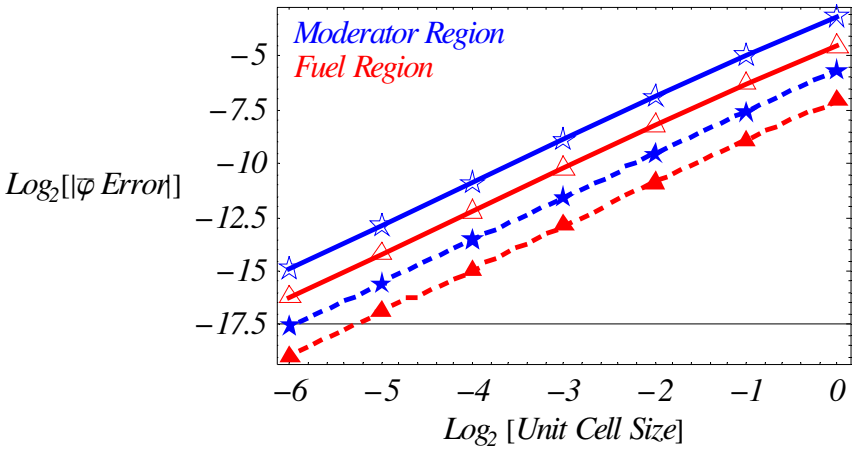

Fig. 3 Error in the fuel- and moderator-averaged scalar fluxes *vs* unit-cell size as computed by the new method (solid lines) and the FD method on a 2×2 mesh (dashed lines).

4. Conclusion

We established the framework for a new approach to develop discretized Diffusion Theory equations on combinatorial computational cells. In this preliminary study we used the Finite Difference (FD) approximation of the neutron diffusion equation in Cartesian geometry as the underlying numerical methodology but extension to advanced nodal methods should not be too difficult. The basic requirement for applying the new approach is that each component cell involved in the combinatorial operation possess a valid discretization of the diffusion equation. Then, by proper application of the same combinatorial operations that define the combinatorial computational cell to the discrete variable equations of the component cells we derive new discrete variable equations defined over the combinatorial cell alone. However, this requires an additional approximation beyond the FD approximation, namely a truncated local Legendre series of the scalar flux. Proper selection of the truncation order allows the solution to the resulting combinatorial method equations to have the same error order with mesh refinement as the straight FD method.

To demonstrate the new approach we applied it to a combinatorial cell composed from the difference of two square cells as a geometric approximation of the moderator region in a square unit cell in which the fuel region is approximated also with a square. We solved this problem using our new method, and using FD on the corresponding 2×2 mesh, as well as on successively refined meshes to obtain a reference-quality solution against which the error in the average flux in the fuel and moderator regions is computed. By varying the dimensions of the unit cell we are able to determine that the asymptotic behavior of the errors is second order in the unit cell's size, similar to the straight FD solution error. However, due to the additional truncated Legendre series approximation the magnitude of the error for each unit cell size is larger for the combinatorial method solution than the FD solution error.

We conclude that the combinatorial method will be most valuable in situations where it is desirable to eliminate geometric and homogenization approximations. The combinatorial method delivers a slightly larger error than standard methods, but at the same second order dependence on mesh size. A higher order local series representation of the flux, and/or high order methods might help bridge this error gap.

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