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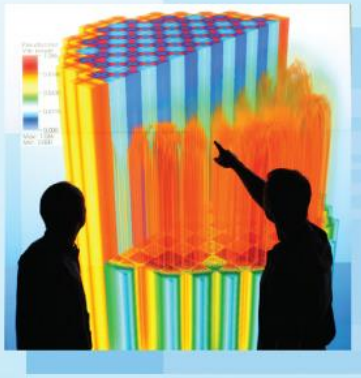

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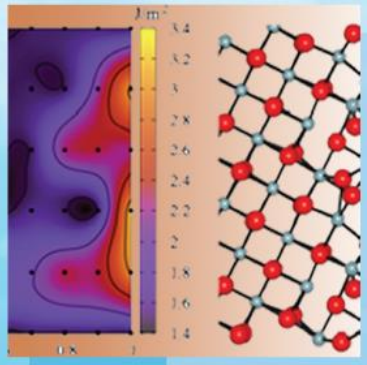

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L3:RTM.PRT.P6.03 Assessment of Improved Axial Scheme vs Baseline 2D/1D

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Assessment of Improved Axial Scheme vs Baseline 2D/1D

Milestone Number L3:RTM.PRT.P6.03

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This report assesses recent progress on the development of the new 2D/1D methodology, the implementation of the new "consistent" 2D/1D method in DeCART, comparisons of this method with the "baseline" 2D/1D method in DeCART, and projected future efforts.

I. BACKGROUND OF THE 2D/1D METHODOLOGY

The term "2D/1D" has been used to describe recently-developed computational methods for solving 3D whole-core neutronics problems in which the (1D) axial and (2D) radial derivative terms are approximated in different ways. These methods were proposed, implemented, and tested by two groups in Korea during 2002-2007 [1–11]. One group, located at KAIST (N.Z. Cho, G.S. Lee, C.J. Park, and colleagues), developed the "2D/1D Fusion" method for the CRX code [1, 3–5, 8, 9]. In this method, the 3D Boltzmann transport equation is solved by discretizing the radial derivative terms on a "fine" radial grid and the axial derivative term on a "coarse" radial grid. This method is an unconventional discretization of the 3D Boltzmann equation, which makes use of fine and coarse radial spatial grids. The other group, located at at KAERI (J.Y. Cho, H.G. Joo, K.S. Kim, and S.Q. Zee and colleagues), developed a different "planar MOC solution-based 3D heterogeneous core method" for the DeCART code [2, 6, 10, 11]. This method also discretizes the axial derivative term using a "coarse" radial grid – but most importantly, it alters this term in a way that (i) is accurate for problems in which the axial leakage can be represented by Fick's Law, and (ii) offers major computational advantages for parallel-architecture computers.

Early in the CASL project, the version of DeCART (Deterministic Core Analysis Based on Ray Tracing) at the University of Michigan (UM) was used for 3D neutronics simulations. DeCART had certain advantages: (i) it could run problems much faster than a 3D discrete ordinates or Method of Characteristics code, (ii) for many problems it was sufficiently accurate, (iii) it allowed for a fine non-Cartesian radial spatial grid to accurately resolve pin cells, and (iv) it permitted very coarse axial grids for problems in which the neutron flux was expected to vary slowly in the axial direction.

Unfortunately, DeCART also had disadvantages: (i) it was based on an unfamiliar "2D/1D" methodology whose theoretical basis was not understood, (ii) the iterative method in DeCART failed to converge for problems in which the axial grid (Δz) became sufficiently small, and (iii) the documentation and coding of DeCART were not conducive to locating and correcting the deficiencies. The users of DeCART were historically accustomed to running codes in which, as the underlying grid is refined, the numerical solution becomes increasingly accurate (the truncation errors reduce to zero). With the 2D/1D method in

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DeCART, approximations had been introduced that made it impossible to state theoretically what the numerical solution might converge to as the grid was refined. Moreover, it was not possible to test DeCART on small axial grids to see whether the solution converged or not; the *iteration* process in the code failed for these problems. These were (are) the technical issues with the original "baseline" 2D/1D method in DeCART.

Given these difficulties, the idea of developing a new 3D reactor physics code that would employ a more robust 2D/1D methodology – and would use modern software procedures to make the code easier to understand, maintain, and modify for CASL tasks – became increasingly attractive. This was the origin of the new MPACT (Michigan Parallel Characteristics Transport Code) code [12, 13]. To help accomplish the task of developing a robust 2D/1D method for MPACT, we decided to attempt to formulate a mathematical foundation for the 2D/1D methodology in DeCART – in order to better understand this methodology, and to suggest systematic ways to improve it. The remainder of this report briefly describes the resulting "consistent" 2D/1D theory, the progress made in implementing the new method in MPACT, and projected future efforts.

II. A CONSISTENT 2D/1D METHODOLOGY

Our derivation of a "consistent" 2D/1D methodology rests on a new approximation to the linear 3D Boltzmann equation, which (not surprisingly) we call the "2D/1D equation. This new equation is intermediate in both accuracy and cost of solution between the 3D Boltzmann equation and the standard 3D diffusion equation. *The underlying premise of the 2D/1D equation is that it preserves transport physics in the radial (x and y) directions, and it uses approximate diffusion physics in the axial (z) direction.*

The derivation of the 2D/1D equation begins with the linear 3D Boltzmann transport equation formulated on a "cylindrical" system V, consisting of points $\boldsymbol{x} = (x, y, z)$ with the *radial* variables $(x, y) \in R$ (a convex but otherwise arbitrary 2D region), and the *axial* variable z in the interval $0 \leq z \leq Z$.

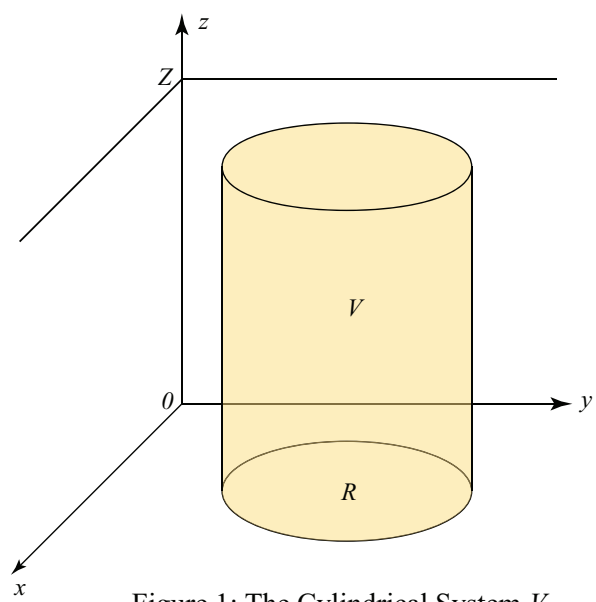

Figure 1: The Cylindrical System V

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For simplicity, we assume monoenergetic transport with isotropic scattering and vacuum boundaries. Using the standard notation:

$$\boldsymbol{\Omega} = (\Omega_x, \Omega_y, \Omega_z) = (\sqrt{1-\mu^2}\cos\omega, \sqrt{1-\mu^2}\sin\omega, \mu) \ , \tag{1}$$

we have the fixed-source transport equation:

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega}) + \Sigma_t(\boldsymbol{x})\psi(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{\Sigma_s(\boldsymbol{x})}{4\pi}\int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega' + \frac{Q(\boldsymbol{x})}{4\pi} \ , \quad \boldsymbol{x}\in V \ , \ \boldsymbol{\Omega}\in 4\pi \ , \tag{2a}$$

with the vacuum boundary condition:

$$\psi(\boldsymbol{x},\boldsymbol{\Omega}) = 0 \ , \quad \boldsymbol{x}\in\partial V \ , \ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0 \ . \tag{2b}$$

In typical light water reactors, the cross sections are highly complicated functions of the radial variables x and y, but are relatively simple (almost constant) functions of the axial variable z. *This suggests that the z-dependence of ψ is weak, and that the small axial leakage term $\mu\partial\psi/\partial z$ in Eq. (2a) can be approximated advantageously, with a minimal loss of accuracy.* To proceed, we write Eq. (2a) as:

$$\sqrt{1-\mu^2}\left(\cos\omega\frac{\partial\psi}{\partial x} + \sin\omega\frac{\partial\psi}{\partial y}\right) + \frac{\partial F}{\partial z} + \Sigma_t\psi = \frac{1}{4\pi}\big(\Sigma_s\phi + Q\big) \ , \tag{3}$$

where

$$F(\boldsymbol{x},\boldsymbol{\Omega}) = \mu\psi(\boldsymbol{x},\boldsymbol{\Omega}) \ , \tag{4a}$$

$$\phi(\boldsymbol{x}) = \int_{4\pi}\psi(\boldsymbol{x},\boldsymbol{\Omega}')d\Omega' \ , \tag{4b}$$

and we consider various approximations to F.

If ψ on the right side of Eq. (4a) is approximated by its classic diffusion approximation, the axial leakage term becomes:

$$\frac{\partial F}{\partial z} \approx \frac{\partial}{\partial z}\frac{\mu}{4\pi}\left[\phi - \frac{1}{\Sigma_t}\left(\Omega_x\frac{\partial\phi}{\partial x} + \Omega_y\frac{\partial\phi}{\partial y} + \mu\frac{\partial\phi}{\partial z}\right)\right] \ . \tag{5a}$$

In a simpler approximation, the radial derivative terms in Eq. (5a) are discarded, yielding:

$$\frac{\partial F}{\partial z} \approx \frac{\partial}{\partial z}\frac{\mu}{4\pi}\left(\phi - \frac{\mu}{\Sigma_t}\frac{\partial\phi}{\partial z}\right) \ . \tag{5b}$$

In an even simpler approximation, the right side of Eq. (5b) is replaced by its zero-th angular moment, giving:

$$\frac{\partial F}{\partial z} \approx -\frac{\partial}{\partial z}\frac{D}{4\pi}\frac{\partial\phi}{\partial z} \ , \tag{5c}$$

where $D = 1/3\Sigma_t$. The progression from Eq. (5a) to Eq. (5b) to Eq. (5c) becomes increasingly simple and (presumably) less accurate. In this paper we consider the simplest of these approximations, Eq. (5c). Using this in Eq. (3), we obtain the following "simplest" 2D/1D equation:

$$\boxed{\sqrt{1-\mu^2}\left(\cos\omega\frac{\partial\psi}{\partial x} + \sin\omega\frac{\partial\psi}{\partial y}\right) - \frac{\partial}{\partial z}\frac{D}{4\pi}\frac{\partial\phi}{\partial z} + \Sigma_t\psi = \frac{1}{4\pi}\Big(\Sigma_s\phi + Q\Big)} \ . \tag{6a}$$

The vacuum boundary conditions for Eq. (6a) remain the standard transport vacuum boundary condition on the "sides" of ∂V:

$$\psi(\boldsymbol{x}, \boldsymbol{\Omega}) = 0 \ , \quad (x, y) \in \partial R \ , \ 0 < z < Z \ , \ \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0 \ , \tag{6b}$$

but become "diffusion" boundary conditions on the "top" and "bottom" of V:

$$\phi(x, y, 0) - 2D \frac{\partial \phi}{\partial z}(x, y, 0) = 0 \ , \quad (x, y) \in R \ , \tag{6c}$$

$$\phi(x, y, Z) + 2D \frac{\partial \phi}{\partial z}(x, y, Z) = 0 \ , \quad (x, y) \in R \ . \tag{6d}$$

The second-order integrodifferential 2D/1D Eq. (6a) approximates the linear Boltzmann equation only in its axial derivative term; here this is done using the standard diffusion approximation. The radial derivative terms in Eq. (6a) are not approximated, and – unlike the standard diffusion equation – the angular variable is not eliminated from the 2D/1D equation. More complicated, but presumably more accurate 2D/1D equations can be obtained using the approximations (5b) or (5a) instead of Eq. (5c).

The underlying premise of the new "consistent" 2D/1D methodology is that it should be based on a consistent discretization of Eqs. (6). In other words, Eqs. (6) should be systematically discretized, and then an iteration scheme should be developed to solve the resulting discrete equations. The discrete solution will then approximate the exact solution of Eqs. (6). Also, as the space-angle grid is refined, the numerical solution of the discrete 2D/1D equations should converge to the exact solution of the 2D/1D Eqs. (6).

Thus, to proceed, Eqs. (6) must first be systematically discretized. An axial discretization for the 2D/1D Eq. (6a) can be derived by integrating the equation over axial "slices" $z_{k-1/2} < z < z_{k+1/2}$ of width $\Delta_k = z_{k+1/2} - z_{k-1/2}$, and using a standard finite difference approximation for the axial leakage term. Assuming that the cross sections are independent of z on each slice and defining:

$$\frac{1}{\Delta_k} \int_{z_{k-1/2}}^{z_{k+1/2}} \psi(\boldsymbol{x}, \boldsymbol{\Omega}) dz = \psi_k(x, y, \boldsymbol{\Omega}) \ , \tag{7a}$$

$$\frac{1}{\Delta_k} \int_{z_{k-1/2}}^{z_{k+1/2}} \phi(\boldsymbol{x}) dz = \phi_k(x, y) = \int \psi_k(x, y, \boldsymbol{\Omega}) d\Omega \ , \tag{7b}$$

$$\begin{aligned} \frac{1}{\Delta_k} \int_{z_{k-1/2}}^{z_{k+1/2}} \frac{\partial}{\partial z} D(\boldsymbol{x}) \frac{\partial \phi(\boldsymbol{x})}{\partial z} dz &= \frac{1}{\Delta_k} \left[D_{k+1/2}(x, y) \frac{\partial \phi_{k+1/2}(x, y)}{\partial z} - D_{k-1/2}(x, y) \frac{\partial \phi_{k-1/2}(x, y)}{\partial z} \right] \\ &\approx \frac{1}{\Delta_k} \left[\frac{D_{k+1/2}(x, y)}{\Delta_{k+1/2}} \Big(\phi_{k+1}(x, y) - \phi_k(x, y) \Big) - \frac{D_{k-1/2}(x, y)}{\Delta_{k-1/2}} \Big(\phi_k(x, y) - \phi_{k-1}(x, y) \Big) \right] \ , \end{aligned} \tag{7c}$$

where:

$$D_{k+1/2} = \frac{\Delta_k + \Delta_{k+1}}{\frac{\Delta_k}{D_k} + \frac{\Delta_{k+1}}{D_{k+1}}} \quad , \quad \Delta_{k+1/2} = \frac{1}{2}(\Delta_k + \Delta_{k+1}) \ , \tag{8}$$

the axially-discretized 2D/1D equation becomes:

$$\left(\Omega_x \frac{\partial}{\partial x} + \Omega_y \frac{\partial}{\partial y} + \Sigma_{t,k}\right) \psi_k(x, y, \mathbf{\Omega}) = \frac{1}{4\pi} \Bigg\{ \Sigma_{s,k} \phi_k(x, y) + Q_k(x, y)$$
$$+ \frac{1}{\Delta_k} \left[\frac{D_{k+1/2}(x, y)}{\Delta_{k+1/2}} \Big(\phi_{k+1}(x, y) - \phi_k(x, y) \Big) - \frac{D_{k-1/2}(x, y)}{\Delta_{k-1/2}} \Big(\phi_k(x, y) - \phi_{k-1}(x, y) \Big) \right] \Bigg\} . \tag{9}$$

For each $1 \leq k \leq K$, this is a 2-D transport equation, which is coupled in a simple way (requiring minimal storage and passage of information) to the neighboring slices $k-1$ and $k+1$. The special cases $k = 1$ and K are handled using the boundary conditions (6c), (6d) in the standard manner.

In our numerical simulations, we employed the 2D Method-of-Characteristics (MOC) [13] to discretize the radial and angular variables in Eq. (9). The only feature of these discretizations requiring comment is that in DeCART, the axial leakage terms [the second line of Eq. (9)] are discretized on a *coarse* radial grid, while the remaining terms are discretized on a *fine* radial grid. Typically, a coarse spatial cell consists of a pin cell (which is about one mean free path in width), and the fine spatial cells resolve the inner structure of a pin cell (and are small fractions of a mean free path in width). In practice, the radially discretized ϕ's in the axial leakage terms in Eq. (9) are volume-averaged over a coarse cell, and the axial diffusion coefficients $D_{k\pm1/2}$ are homogenized over a coarse cell.

The restriction of the axial leakage terms to coarse mesh scalar fluxes implies that the resulting 2D/1D equation can be parallelized, in such a way that each processor performs sweeps on one slice, and *only minimal information (coarse grid scalar fluxes) needs to be passed between processors.* (If spatially fine-grid or angularly fine-grid information had to be transmitted between processors, the method would have significantly less parallel efficiency.)

Next, we consider the likely simplest iteration scheme for solving Eq. (9) that can be made stable for all $\Delta_z > 0$. Noting that the right side of Eq. (9) depends only on the scalar flux ϕ, we consider a standard 2D sweep on each slice to update the scalar flux:

$$\left(\Omega_x \frac{\partial}{\partial x} + \Omega_y \frac{\partial}{\partial y} + \Sigma_{t,k}\right) \psi_k^{(\ell+1/2)}(\boldsymbol{x}, \mathbf{\Omega}) = \frac{1}{4\pi} \Bigg\{ \Sigma_{s,k} \phi_k^{(\ell)}(\boldsymbol{x}) + Q_k(\boldsymbol{x})$$
$$+ \frac{1}{\Delta_k} \left[\frac{D_{k+1/2}}{\Delta_{k+1/2}} \Big(\phi_{k+1}^{(\ell)}(\boldsymbol{x}) - \phi_k^{(\ell)}(\boldsymbol{x}) \Big) - \frac{D_{k-1/2}}{\Delta_{k-1/2}} \Big(\phi_k^{(\ell)}(\boldsymbol{x}) - \phi_{k-1}^{(\ell)}(\boldsymbol{x}) \Big) \right] \Bigg\} , \tag{10a}$$

$$\phi_k^{(\ell+1/2)}(\boldsymbol{x}) = \int \psi_k^{(\ell+1/2)}(\boldsymbol{x}, \mathbf{\Omega}') d\Omega' , \tag{10b}$$

followed by a (nonstandard) relaxation step to define the end-of-iteration scalar flux:

$$\phi_k^{(\ell+1)}(\boldsymbol{x}) = \theta \phi_k^{(\ell+1/2)}(\boldsymbol{x}) + (1-\theta) \phi_k^{(\ell)}(\boldsymbol{x}) . \tag{10c}$$

The relaxation parameter θ in Eq. (10c) is to be determined; if $\theta = 1$, the method defined by Eqs. (10) is basically Source Iteration (and is very similar, if not identical, to the original iteration method encoded in DeCART). In each iteration, the numerical solutions in slice k are directly coupled only to the numerical solutions in the neighboring slices $k+1$ and $k-1$. Therefore, many iterations may be required for the numerical fluxes in all the axial slices $1 \leq k \leq K$ to sufficiently "communicate."

We have Fourier-analyzed this method and have found it to be unconditionally stable if the relaxation parameter θ is chosen optimally ($\theta = \theta_{opt}$). If $\theta = 1$ (the "DeCART" value), then the method is stable for coarse Δz but unstable for fine Δz. The iterative instability for $\theta = 1$ and small Δz reflects the iterative behavior of DeCART. The following figure depicts the stability ($\rho < 1$) of the iterative method with $\theta = \theta_{opt}$, and the instability for small Δz ($\rho > 1$) of the "DeCART" method with $\theta = 1$.

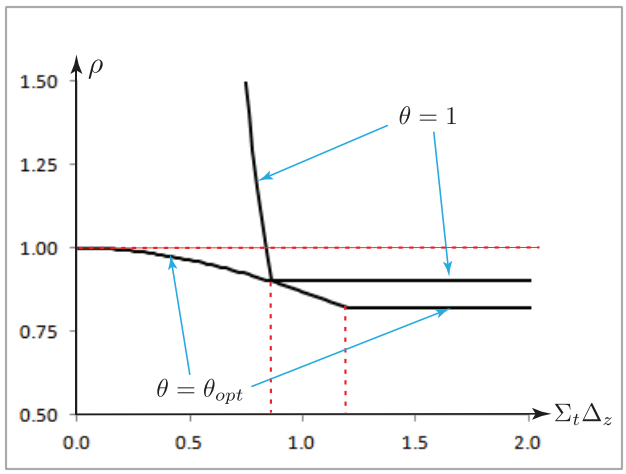

Figure 2 : Spectral Radius ρ vs Axial Optical Cell Width $\Sigma_t \Delta z$

To summarize: we have proposed a new "2D/1D" equation, which is intermediate in both cost of execution and accuracy between the 3D Boltzmann equation and the standard 3D diffusion equation. The 2D/1D equation preserves transport physics in the radial variables, and uses approximate diffusion physics in the axial variable. The 2D/1D equation has been systematically discretized using familiar discretization methods, and a simple iteration scheme for solving the resulting discrete equations has been Fourier-analyzed to optimize its stability and efficiency. The "consistent" discretized 2D/1D equation closely resembles the discretized 2D/1D method in DeCART. However, the consistent discretized equations unambiguously limit to the continuous 2D/1D equation as the space-angle grid is refined, but it is not known whether the discrete "baseline" 2D/1D equations in DeCART have a limit as the space-angle grid is refined.

III. IMPLEMENTATION IN MPACT

The consistent 2D/1D method described above has been implemented in MPACT and has recently been tested on several problems. To date, *all the results that we have observed from these simulations are consistent with the underlying predictive theories.* The iteration method presented above is observed to be stable, its performance is consistent with the Fourier analysis, and the new 2D/1D solution can be obtained for extremely small values of Δz. Also, the converged 2D/1D solution itself has the expected properties. For classically diffusive problems, the Boltzmann, 2D/1D, and standard diffusion solutions all closely agree. However, for problems in which the solution varies slowly in z but not in x and y, the new 2D/1D solution is a much closer approximates the Boltzmann solution than the standard diffusion solution.

The most important deviation between the theory presented above and the methodology encoded in MPACT rests in the use of a nonlinear iterative acceleration technique in MPACT, based on the standard CMFD (Coarse Mesh Finite Difference) methodology. Student Blake Kelley is currently developing a linearized Fourier analysis of this method, to theoretically validate its observed rapid convergence, and to ensure that this method is as robust as possible. At the time of the writing of this report, it seemed that without relaxation, there was the possibility of an instability, but with relaxation, this possibility could be made to vanish.

IV. PROJECTED FUTURE WORK

The theory sketched here applies only to the simplest 2D/1D equation, using a standard finite-difference approximation for the 1D axial diffusion discretization, and a relatively simple "Source Iteration" method with under-relaxation. For the new 2D/1D method to become applicable to realistic reactor core problems, it must be generalized in several ways:

1. It must include multigroup energy dependence with anisotropic scattering. UM graduate student Blake Kelley has this task on his agenda.

2. Eq. (9) can be directly applied to problems with radial spatial variation of the type found in reactor cores. This basic procedure is followed in DeCART, and useful numerical results are obtained. However, in these problems classic diffusion theory is not valid, and the logic that leads to Eq. (5c) with $D = 1/3\Sigma_t$ is also not valid. Therefore, although the 2D/1D Eq. (9) with $D = 1/3\Sigma_t$ *can* be solved, there is no theoretical reason why the classic diffusion coefficient $D = 1/3\Sigma_t$ should yield the most accurate solution. Fortunately, an asymptotic theory has been developed that provides the logic needed to specify D [14, 15]. This approach is also on Blake's agenda.

3. A related item on Blake's agenda is that not only does the baseline 2D/1D method only communicate coarse-grid scalar fluxes between processors to represent axial leakages, but also, *the axial leakages that are used in the 2D transport equations on each slice have no fine spatial or angular dependence*. Clearly, this is erroneous. Fortunately, the asymptotic theory makes it possible to describe the fine spatial and angular-dependence of the axial leakage terms using *form functions*, which can be precomputed and stored. We anticipate that the inclusion of this new feature should significantly enhance the accuracy of the new 2D/1D method.

4. Currently, DeCART uses a nodal (not a finite difference) axial diffusion discretization in z. The option of a nodal discretization in z is now being implemented in MPACT.

5. As stated above, Blake is now Fourier-analyzing the CMFD acceleration method encoded in MPACT, to provide as complete a theory as possible on its efficiency and range of stability.

6. Blake will also make comparisons to determine how much more accurate Eq. (5a) is than Eq. (5b), and how much more accurate Eq. (5b) is than Eq. (5c). Other angular

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approximations to the axial leakage term, more accurate than the P_1 representation in Eq. (5a), will also be considered. The following issues will be kept in mind:

(a) If the angular discretizations of F and ψ satisfy Eq. (4a), then the angularly-discretized 2D/1D Eq. (3) becomes identical to the angularly-discretized linear Boltzmann equation. Thus, by systematically increasing the accuracy of the angular dependence of the axial leakage term, the solution of the *continuous* 2D/1D equation should systematically limit to the solution of the *continuous* Boltzmann equation. In this sense, there are many possible 2D/1D equations, corresponding to different approximations to F.

(b) However, as the angular complexity of the transverse leakage term increases, the amount of computational work will increase, and the amount of information that must be passed between processors will increase – causing the parallel efficiency of the resulting method to decrease. Thus, there is a tradeoff between accuracy and parallelizability.

(c) An extra degree of complexity occurs because of the fine and coarse radial spatial grids: no amount of angular refinement will cause the discrete 2D/1D solution to limit to the discrete Boltzmann solution unless all the spatial grids are refined.

For further details on the new consistent 2D/1D method, we refer the reader to two conference papers that will appear on the topics discussed above [16, 17]. In the near future, we plan to aggressively continue the systematic development and implementation of consistent 2D/1D methods in MPACT, along the lines described above. Specifically, the tasks listed above will form the remainder of Blake Kelley's PhD project. Hopefully, when these tasks are complete, the resulting new 2D/1D method will be just about as optimized as possible for realistic problems.

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