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Skin Effect in Neutron Transport Theory

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We identify a neutron-flux “skin effect” in the context of neutron-transport theory. The skin effect, which emerges as a boundary-layer at material interfaces, plays a critical role in a correct description of transport phenomena. A correct accounting of the boundary-layer structure helps bypass computational difficulties reported in the literature over the last several decades, and should lead to efficient numerical methods for neutron transport in 2D and 3D.

The physical character of the neutron fluxes within and around heterogeneous materials, for given sources, has been the subject of significant literature over the last seventy years [1–7]. Much of this literature has been devoted to unraveling the complex interactions that result from the combined effect of neutron collision and transport phenomena [2–5]. This paper describes and analyzes a previously unrecognized physical observable, namely, a neutron-flux “skin effect” near physical boundaries, wherein sizeable neutron fluxes exist for *incoming directions* nearly parallel to the boundary even in cases in which the exterior region is a source-free vacuum. The skin effect impacts in a significant way the simulation of nuclear reactors, and, as it concerns neutron fluxes that are nearly tangential to the boundary (which can eventually cross curved boundaries), it provides a useful system state indicator affecting reactor shielding and control as well as design and optimization [8, 9].

The boundary skin effect under consideration arises as neutrons may travel for relatively long distances near the material-vacuum boundary along paths approximately parallel to the boundary, and can thus create significant neutron fluxes for *incoming directions* at material points *arbitrarily close to the boundary*—even when, for the vacuum-enclosed systems considered, the incoming fluxes *at the material boundary* vanish exactly. The geometrical context can be easily visualized in Fig. 1 for the flat-boundary case considered in this paper, but such long neutron-paths exist near curved boundaries as well.

Mathematically the skin effect is encapsulated in sharp “boundary-layer” structures of the type described in [10, Ch. 9] and detailed below. Albeit present in *e.g.* eigenfunction solutions for neutron transport problems in one dimensional [2, Ch. 4] or separable configurations [6], these boundary-layer transitions, which lead to unbounded gradients arbitrarily close to interface boundaries, have not previously been correctly accounted for or even fully recognized. A mathematical reformulation of the neutron-transport problem via a combination of changes of variables for the spatial and angular variables

is presented in this paper, which facilitates the skin-effect analysis. In particular, this approach enables accurate modeling of neutron fluxes at arbitrarily small distances from the domain boundary, and, therefore, everywhere in the combined angular-spatial domain.

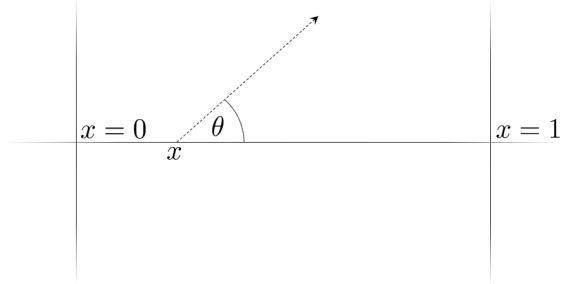


FIG. 1. One-dimensional finite “slab” geometry: $\xi = \cos(\theta)$.

The equation for time-independent neutron transport in a one-dimensional plane-parallel geometry (Fig. 1), with isotropic scattering and vacuum boundary conditions, is given by [9, 11]

$$\begin{aligned} \xi \frac{\partial}{\partial x} u(x, \xi) + \mu_t(x) u(x, \xi) = \\ \frac{\mu_s(x)}{2} \int_{-1}^1 u(x, \xi') d\xi' + q(x, \xi), \quad (1) \\ u(x=0, \xi) = 0 \quad \forall \xi > 0, \\ u(x=1, \xi) = 0 \quad \forall \xi < 0. \end{aligned}$$

Here, letting $\xi = \cos(\theta)$ (Fig. 1), and calling $\mu_s(x)$, $\mu_a(x)$ and $\mu_t(x) = \mu_a(x) + \mu_s(x)$ the macroscopic scattering, absorption, and total transport coefficients, respectively, $u(x, \xi)$ denotes the neutron flux at point x in the direction θ . The integral term accounts for the angular redistribution of neutrons due to scattering, $q(x, \xi)$ is a neutron source, and the vacuum boundary conditions model the absence of particles entering the spatial domain through its boundary. It is worthwhile noting that Eq. (1) also governs the transport of photons and other neutral particles, and it therefore impacts upon a wide range of important disciplines [2, 3, 6, 12–23].

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Noting that the coefficient ξ of the highest order derivative in (1) tends to zero as $\theta \rightarrow \pi/2$, the existence of unbounded spatial gradients at points (x, ξ) near $(0, 0)$ and $(1, 0)$ in the solution $u(x, \xi)$ may be expected [10, Ch. 9]. Such “boundary-layer” structures, which are caused by the existence of a spatial boundary condition in conjunction with a vanishingly small coefficient for the highest order differential operator, only take place for the incoming directions $\xi > 0$ (resp. $\xi < 0$) for points close to $x = 0$ (resp. $x = 1$)—since it is for such directions that boundary conditions are imposed in Eq. (1).

Following [10, Ch. 9], in order to characterize the boundary layer structure around *e.g.* $x = 0$ we consider the function $U(X, \xi) = u(\xi X, \xi)$ and, more precisely, its lowest-order asymptotics $U_0(X, \xi)$ as $\xi \rightarrow 0^+$ in a small neighborhood of the boundary (the boundary layer around $x = 1$ can be treated analogously). The function $U_0(X, \xi)$ (the *inner solution* in the nomenclature of [10, Ch. 9]) satisfies the *constant coefficient* equation

$$\frac{\partial U_0(X, \xi)}{\partial X} + \mu_t(0)U_0(X, \xi) = \frac{\mu_s(0)}{2} \int_{-1}^1 U_0\left(\frac{\xi X}{\xi'}, \xi'\right) d\xi' + q(0, \xi), \quad (2)$$

and boundary conditions induced by (1). Eq. (2) tells us that the derivative $\frac{\partial U_0(X, \xi)}{\partial X}$ remains bounded as $\xi \rightarrow 0^+$, and, therefore, that the function $U_0(X, \xi)$ characterizes the boundary layer structure in the solution $u(x, \xi)$ via the relation

$$u(x, \xi) \sim u_0(x, \xi) = U_0(x/\xi, \xi) \text{ as } (x, \xi) \rightarrow (0^+, 0^+). \quad (3)$$

Utilizing an integrating factor in (2) and letting

$$I(x, \xi) = \int_0^x e^{\frac{\mu_t(0)y}{\xi}} \left[\frac{\mu_s(0)}{2} \int_{-1}^1 u_0(y, \xi') d\xi' + q(0, \xi) \right] dy$$

the lowest-order boundary-layer approximation

$$u(x, \xi) \sim u_0(x, \xi) = \frac{e^{-\mu_t(0)x/\xi}}{\xi} I(x, \xi) \quad (4)$$

is obtained. This equation explicitly exhibits the exponential boundary-layer character of the solution. The argument can be extended to two and three-dimensional problems, and to include time-dependence and curved boundaries. In such cases, a boundary layer occurs, with unbounded normal derivatives near the boundary, for incoming directions nearly parallel to the domain interface.

The boundary layer structure can be visualized by considering the exact solution of Eq. (1) that is obtained for the scattering-free case ($\mu_s(x) = 0$) with constant-coefficients. The resulting solution

$$u(x, \xi) = \begin{cases} \frac{q}{\mu_a} \left[1 - e^{-\mu_a x/\xi} \right] & \forall \xi > 0, \\ \frac{q}{\mu_a} \left[1 - e^{-\mu_a (x-1)/\xi} \right] & \forall \xi < 0, \end{cases} \quad (5)$$

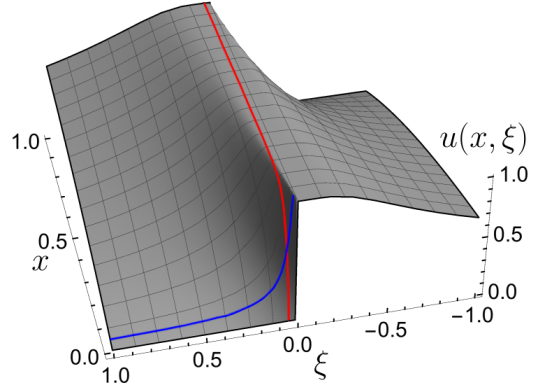


FIG. 2. Scattering-free solution (Eq. (5)). The boundary layers in the ξ and x directions are clearly emphasized by the superimposed blue (along the ξ direction) and red (along the x direction) coordinate curves.

presented in Fig. 2, clearly displays a boundary layer structure as $(x, \xi) \rightarrow (0^+, 0^+)$.

The skin effect significantly impacts the mathematical modeling of neutron transport processes. The foremost two numerical methods used in the area, namely, the Spherical Harmonics Method [2, Ch. 8] and the Discrete Ordinates Method [3, Ch. 3, 4], do not properly resolve the conflicting manifestations of the skin effect in the angular and spatial variables [5, pp. 65, 66.], leading to significant degradations in accuracy, [24–26], [27, p. 51]. Most conspicuously, [4, p. 40] shows that different numerical differentiation schemes may lead to different numerical solutions. It has been demonstrated that, for separable geometries, a degree of accuracy can be obtained for certain spatial “region averages” of the “angular average” of the neutron flux [6, 7, 12]; naturally, however, general domains are not separable, and, in addition, the full neutron flux (not just such multiply averaged quantities) is generally required for detector response calculations [3, 1-13, p. 60], [28, Sec. 6.4.3].

A combination of spatial and angular changes of variables can be used to eliminate the difficulties posed by the dual spatial/angular boundary layers. To introduce the angular change of variables we rely on the Gauss-Legendre method as an underlying quadrature rule, but other quadrature methods could alternatively be used. In view of the expression [29, p. 77], the ℓ -point Gauss-Legendre quadrature error decreases like $32V/15\pi j(2\ell + 1 - j)^j$ provided the $j \leq 2\ell$ derivative of the integrated function is bounded by the constant $V > 0$. Introducing the change of variables $\xi' = r^p$ in the integral in (1) we thus seek a bound V on the j -th derivative of the resulting integrand. Using an integrated version of (1), similar to (4), combining two exponential terms and using the fact that for each non-negative integer k the integral $\int_0^\infty t^k e^{-t} dt$ is finite, we find that

$$\left| \frac{\partial^j}{\partial r^j} [u(x, r^p) r^{p-1}] \right| \leq W r^{p-j-1} \quad (6)$$

for some constant W (even as $(x, r) \rightarrow (0^+, 0^+)$); setting $V = Wr^{p-j-1}$ yields the desired bound, which, importantly, is uniform for all relevant values of x and r (as long as $p \geq j+1$).

Splitting the integral on the right hand side of Eq. (1) at the boundary-layer point $\xi = 0$ and using the proposed change of variables yields

$$\int_0^1 u(x, \xi) d\xi \sim \sum_{i=1}^{M/2} w_i u(x, \xi_i), \quad (7)$$

with a similar expression for the integral between -1 and 0 . Here, letting r_i and w_i^{GL} denote the Gauss-Legendre quadrature abscissas and weights in the interval $[0, 1]$, we have set $\xi_i = r_i^p$ and $w_i = p \times r_i^{p-1} \times w_i^{GL}/2$. A

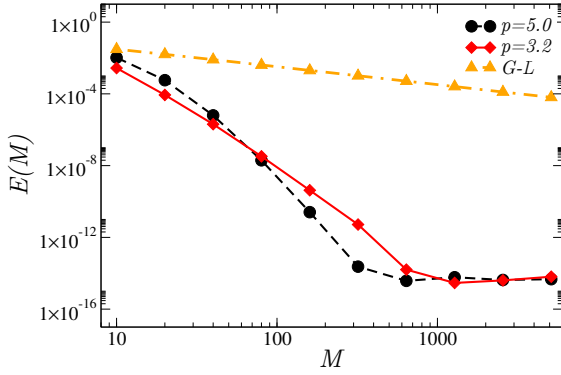


FIG. 3. Error of numerical against analytic integral, $E(M) = \max_{0 \leq x \leq 1} |\sum_{i=1}^M w_i u(x, \xi_i) - I^{\text{an}}(x)|$ for u given by Eq. (5). The errors are presented for the quadrature rule (7) (circles and diamonds) and the plain Gauss-Legendre (G-L) quadrature (triangles).

suitable power $p = 3.2$ was used, which provides excellent convergence (Fig. 3) for the integral in the ξ variable while limiting the sharpness of the numerical boundary layer in the x variable.

The logarithmic spatial change of variables $v = \log(\frac{x}{1-x})$, in turn, is used to resolve the spatial boundary layer, which gives rise to points x extremely close to the boundary (without detriment to the integration process, in view of the *uniform* r -derivative bounds (6)), leading to high order precision in both the ξ and x variables. If the change of variables $\xi' = r^p$ were not introduced, then finer and finer angular discretizations, without bound on the number of angular discretization points used, would be necessary to yield a fixed prescribed accuracy as the spatial point x approaches a boundary point. Similarly, the logarithmic change of variables allows for the resolution of the rapid changes in the angular flux arising from the spatial boundary layer near the boundaries.

The transport equation is solved in a computational spatial domain $[v_{\min}, v_{\max}]$, with $[x'_{\min}, x'_{\max}] = [\frac{e^{v_{\min}}}{e^{v_{\min}}+1}, \frac{e^{v_{\max}}}{e^{v_{\max}}+1}]$, and with boundary conditions at $x'_{\min}$ and $x'_{\max}$ obtained by enforcing the asymptotic relation (4) with $u_0(y, \xi')$ replaced by $u_0(x'_{\min}, \xi')$ and

$u_0(x'_{\max}, \xi')$, respectively. Using the new variables the time dependent transport problem

$$\begin{aligned} \frac{\partial}{\partial t} u(v, \xi, t) + \xi(2 + 2 \cosh(v)) \frac{\partial}{\partial v} u(v, \xi, t) + \\ \mu_t u(v, \xi, t) = \frac{\mu_s}{2} \int_{-1}^1 u(v, \xi', t) d\xi' + q, \end{aligned} \quad (8)$$

$$\begin{aligned} u(v, \xi, t_{\min}) &= 0, \\ u(v_{\min}, \xi, t) &= u_0(x'_{\min}, \xi, t) \quad \forall \xi > 0, \\ u(v_{\max}, \xi, t) &= u_0(x'_{\max}, \xi, t) \quad \forall \xi < 0 \end{aligned}$$

results. The time propagation is performed implicitly by means of a third order backward differentiation formula (BDF). The collisional term is obtained by means of the third-order polynomial extrapolation $\tilde{u}_j^{n+1} = \sum_{\kappa=0}^2 (-1)^\kappa \binom{3}{\kappa+1} u_j^{n-\kappa}$ [30, Eq. (12)], to avoid the inversion of large matrices at each time step. Using the identity operator $\hat{\mathbf{I}}$ and the **Fourier Continuation (FC)** spectral differentiation operator $\hat{\mathbf{D}}$ [31–33], the resulting discrete version of Eq. (8), which amounts to an implicit version of the FC-DOM method [33], thus reads

$$\begin{aligned} \left[\hat{\mathbf{I}} + \beta \Delta t \xi_j (2 + 2 \cosh(v)) \hat{\mathbf{D}} + \beta \Delta t \mu_t \hat{\mathbf{I}} \right] u_j^{n+1} = \\ \sum_{k=0}^2 \alpha_k u_j^{n-k} + \beta \Delta t \frac{\mu_s}{2} \sum_{i=1}^M w_i \tilde{u}_i^{n+1} + \beta \Delta t q^{n+1}, \end{aligned} \quad (9)$$

where $u_j^{n+1} \sim u(v, \xi_j, t^{n+1})$, $t^{n+1} = n \Delta t$, and where α_k and β are the coefficients for the third order BDF formula. (The FC method enables representation of general smooth non-periodic functions by Fourier-series while avoiding the well-known Gibbs ringing phenomenon, with applicability to solution of partial differential equations in general multi-dimensional spatial domains with high accuracy and negligible numerical dispersion [31–33].)

Fig. 4 demonstrates the excellent convergence properties of the algorithm, for $\mu_s = \mu_a = q = 1$. The error was computed via comparison with the solution obtained on a finer grid. This high order of convergence clearly suggests that the changes of variables used in the x and ξ variables lead to adequate simultaneous grid resolution of the two boundary layers involved.

In what follows the numerical algorithm is utilized to explore and demonstrate the skin effect. For definiteness, in the rest of this paper we restrict attention to time-independent solutions, obtained by means of the time-dependent solver, relaxed for long time (as described in [33]). The resulting steady-state solutions are depicted in various forms in Figs. 5 through 7; similar boundary layer structures are of course present for all times in the time-dependent solutions.

Fig. 5 displays the skin-effect boundary-layer structures in the x and ξ variables with $\mu_s = \mu_a = q = 1$ (numerical parameter values $N = 250$ and $M = 40$ were used in these figures, with $-v_{\min} = v_{\max} = 25$). As can be seen in Fig. 5, as ξ decreases towards zero, steeper and steeper boundary layers result, over shrinking spatial regions, as expected from the proposed boundary

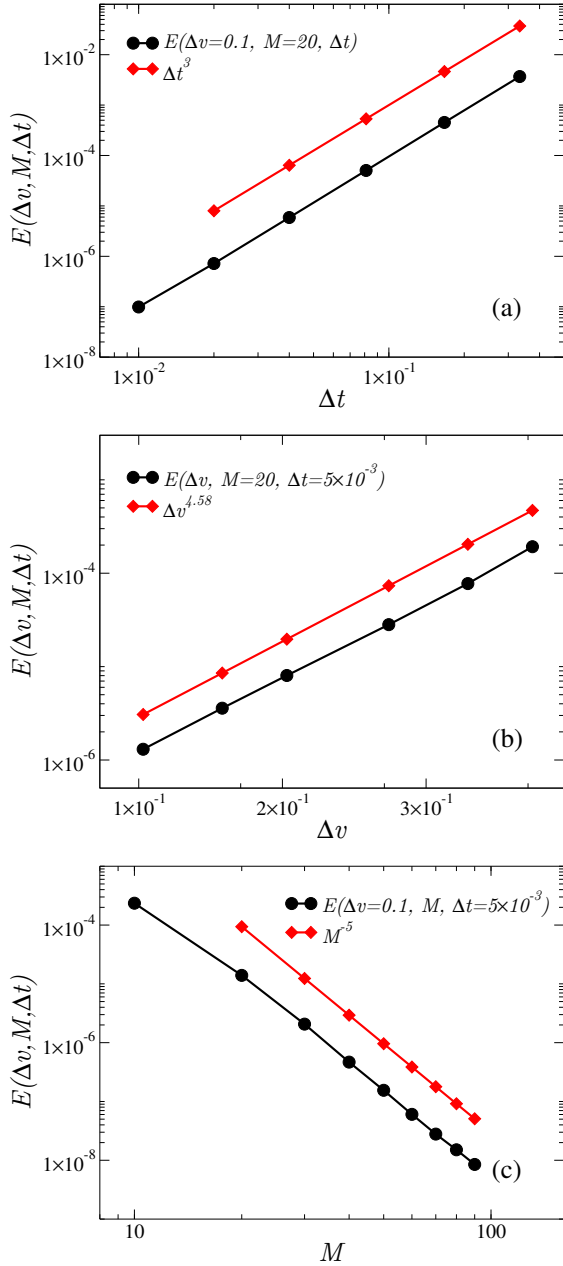


FIG. 4. Convergence properties of the proposed algorithm for (a) the time discretization, (b) the spatial discretization and (c) the number of discrete ordinates employed. In circles, the error $E(\Delta v, M, \Delta t) = \max_{x, \xi} |u(x, \xi) - u^c(x, \xi)|$ is displayed for various grids, where $u^c(x, \xi)$ denotes the converged solution.

layer analysis—thus giving rise to large nearly boundary-parallel incoming neutron fluxes in close proximity to boundaries.

Fig. 6 demonstrates the persistence of the boundary layer in presence of high scattering coefficients (with $\mu_a = q = 1$ fixed). The case $\xi = \xi_{\min} \simeq 10^{-6}$ is considered in the figure, with parameter values $N = 200$, $M = 20$ and $-v_{\min} = v_{\max} = 20$. Clearly, even though diffusive problems (large μ_s) tend to be more regular

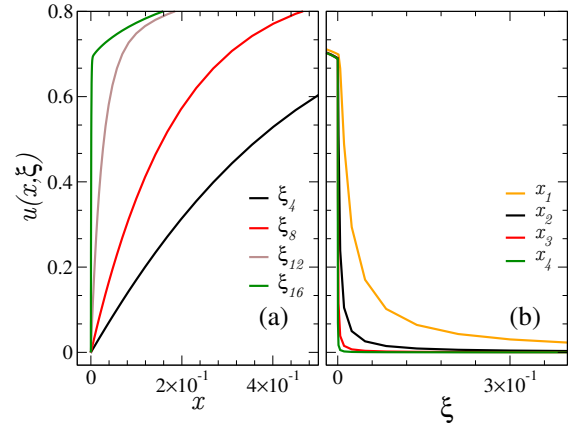


FIG. 5. Boundary layers near $x = 0$, obtained by solving Eq. (8) with $\mu_a = \mu_s = q = 1$ for various values of ξ and x , with $0.84 > \xi_i > \xi_{i+1} > 10^{-7}$ and $10^{-2} > x_i > x_{i+1} > 10^{-6}$. Panel (a) shows the boundary layer along the x variable for various values of ξ , and panel (b) shows the boundary layers along the ξ variable for various values of x . The neutron flux $u(x, \xi)$ does not vanish on the boundary for the outgoing directions $-1 \leq \xi < 0$, and, therefore, no boundary layer exists at $x = 0$ for such directions (not shown).

over the ξ variable—owing to the strong averaging and smoothing induced by the large scattering coefficient—the boundary layers that arise in the spatial variable with increasing μ_s lead to even larger slopes as $x \rightarrow 0^+$.

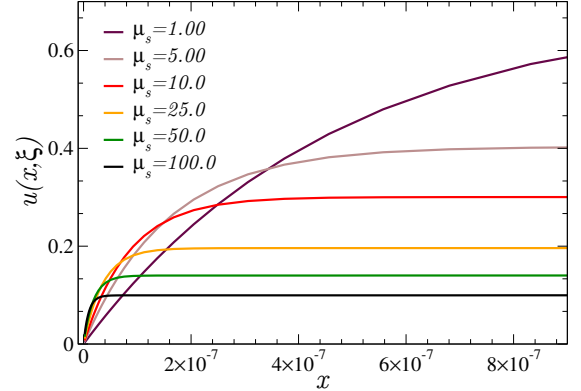


FIG. 6. Boundary layers obtained by solving Eq. (8), with $\mu_a = q = 1$ and different values of μ_s . Solutions for the direction $\xi = \xi_{\min} \simeq 10^{-6}$ are shown. Note the large μ_t -dependent slopes of the transport solution as $x \rightarrow 0^+$ (cf. Eq. (4), where $\mu_t = \mu_s + \mu_a$).

There have been many attempts to understand unphysical oscillations associated with the widely used Diamond Difference scheme (DD) for the transport equation [4, 34, 35]. The recent paper [24] avoids this problem by using only directions ξ away from $\xi = 0$. References [4, 34] attribute this type of oscillations to anisotropic boundary conditions, non diffusive boundary layers and/or high absorption; the present paper, which demonstrates existence of boundary layers even in the

isotropic case and for all values of the scattering and absorption coefficients, presents a starkly contrasting interpretation: exponential boundary layers are triggered by the boundary condition and vanishing ξ values.

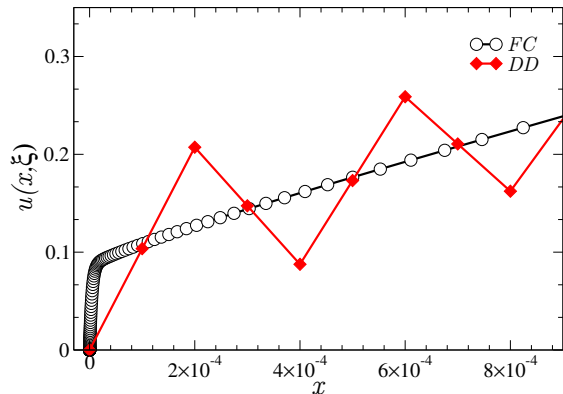


FIG. 7. DD and FC-DOM approximations of $u(x, \xi_{15})$ for $\mu_t = \mu_s = 1000$, $q = 0.1$ and $\xi_{15} \simeq 10^{-3}$. The boundary-layer oscillations resulting from the DD scheme are clearly visible. $N = 400$ and $N = 10000$ discrete points were used in the spatial variable for the FC and DD methods, respectively. Note the high near-boundary resolution that results, in view of the exponential spatial change of variables used, from the $N = 400$ FC-DOM discretization.

For example, reference [34] treats a diffusive transport problem (Problem 1 in that reference) which, under rescaling, can be reformulated as in Eq. (1) with $\mu_s = \mu_t = 1000$, and $q = 0.1$. This is an extremely diffusive problem with isotropic boundary conditions for which [34, pp. 317] states: “...since the leading order term in the asymptotic expansion of the analytic transport equation is itself isotropic, this term in these prob-

lems does not contain a boundary layer.” In contrast, Fig. 7 shows that boundary layers are present in this problem. The FC-DOM solution displayed in this figure was obtained by means of $M = 40$ discrete directions and $N = 400$ points in the spatial variable. In contrast, $N = 10000$ were used in the DD-scheme solution presented in Fig. 7—which clearly displays the spurious oscillations produced by the DD scheme in this context.

The skin-effect boundary-layer structure described in this paper, which was not previously reported in the literature, constitutes a physical effect which was overlooked for nearly seventy years [1, p. 360], [34, pp. 317], and which, as demonstrated in Fig. 7 and throughout this paper, has a significant impact on the physics and the numerical simulation of transport phenomena. In particular, this work provides a sound theoretical basis for the development of new, accurate and efficient methods for the numerical solution of neutron-transport and other neutral particle-transport problems in general 2D and 3D domains and it leads to valuable state indicators concerning reactor dynamics.

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