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ASYMPTOTIC FREEDOM IN THE DIFFUSIVE REGIME OF NEUTRON TRANSPORT

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Abstract. The accuracy of a numerical method for solving the neutron transport equation is limited by the smallest mean free path in the problem. Since problems in the asymptotic diffusive regimes have vanishingly small mean free paths, it seems hopeless, given a limited amount of computer memory, that an accurate solution can be obtained for these problems. However we found that the accuracy of a numerical method improves as the scattering ratio increases with the total cross section and the grid spacing held fixed for problems that are in the asymptotic diffusive regime. This phenonmenon is independent of the numerical method and can be explained on physical grounds. The numerical results by the Diamond Difference Method are given to show this phenomenon.

1. Introduction. In order to achieve a desired degree of accuracy in the numerical solution of the neutron transport equation, a zone's diameter is usually limited to a part of a mean free path. While this limitation on the zone's diameter is alleviated by higher order methods, it is however not eliminated. Since the mean free path is vanishingly small in the asymptotic diffusive regime, one is daunted by the computer memory needed to calculate an asymptotic diffusive neutron problem accurately. However, we found an interesting phenomenon in the asymptotic diffusive regime. With the mean free path and the grid spacing held fixed, we found that the accuracy improves as the scattering ratio approaches 1. The phenonmenon is physical and is independent of the discretization method. The purpose of this note is to report and to explain this phenomenon.

The phenomenon of improved accuracy in the asymptotic diffusive regime, is exhibited by the mono-energy transport equation in the 1-D spherical coordinate system [1] with an isotropic source $q_0(r)$,

$$\left(\frac{\mu}{r^2}\frac{\partial r^2}{\partial r} + \frac{1}{r}\frac{\partial(1-\mu^2)}{\partial \mu} + \sigma_t(r)\right)\psi(r,\mu) = \frac{\sigma_0(r)}{2}\int_{-1}^{1}\psi(r,\mu')\,d\mu'.$$
$$+\frac{q_0(r)}{2}\,,\quad 0<r<1,\quad \mu\in[-1,1]\;, \tag{1.1}$$

and Dirichlet boundary condition

$$\psi(r,\mu) = \psi_b(\mu),\quad r=1,\quad \mu\in[-1,0).$$

The integral on the right hand side (rhs) of (1.1) is called the scalar flux,

$$\phi(r) \equiv \int_{-1}^{1}\psi(r,\mu')\,d\mu',$$

and it plays a central role in asymptotic transport theory [2].

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In the asymptotic diffusive regime [2], the total cross section σ_t is enormously large $\sim 1/\epsilon$, and the scattering cross section σ_0, bounded by σ_t such that the difference of these two cross sections, the absorption cross section, $\sigma_a \equiv \sigma_t - \sigma_0$ is vanishingly small, $\sim \epsilon$. Since the mean free path λ is defined as the inverse of the total cross section, the asymptotic diffusive regime is the regime of small mean paths $O(\epsilon)$. Accurate numerical results for asymptotic diffusive problems appear hopelessly confined to grid spacings of order ϵ. However as we shall show, the angular flux ψ is a slowly varying function of its coordinates, r and μ and can be approximated accurately on grids with spacings much larger than the mean free path $1/\sigma_t$.

When transport is dominated by isotropic scattering, as in the asymptotic diffusive regime, the angular flux, ψ, varies slowly with μ, and thus is well approximated by an expansion in Legendre polynomials. In fact, a two term expansion is sufficient, i.e.

$$\psi(r,\mu) \approx \frac{1}{2}\,\phi(r) + \frac{3}{2}\,\mu\, J(r). \tag{1.2}$$

The diffusion approximation of (1.1) is derived by the substitution of (1.2) into (1.1) and taking moments of the result. Multiplying the result by $P_0(\mu) = 1$, and then by $P_1(\mu) = \mu$, followed by integration with respect to μ, give respectively

$$\frac{1}{r^2}\frac{\partial r^2 J}{\partial r} + \sigma_a \phi = q_0\ , \tag{1.3}$$

and

$$\frac{1}{3r^2}\frac{\partial r^2 \phi}{\partial r} - \frac{2\phi}{3r} + \sigma_t J = 0\ . \tag{1.4}$$

Solving (1.4) for J and substituting the result into (1.3) gives

$$-\frac{1}{3r^2}\frac{\partial}{\partial r}\left(\frac{r^2}{\sigma_t}\frac{\partial \phi}{\partial r}\right) + \sigma_a \phi = q_0. \tag{1.5}$$

Furthermore, at the boundary, $r = 1$, we append Marshak's boundary condition,

$$\frac{\phi}{4} - \frac{1}{6\sigma_t}\frac{\partial \phi}{\partial r} = -\int_{-1}^{0} \mu\,\psi_b(\mu)\, d\mu\ , \tag{1.6}$$

and at the origin we impose the Neumann condition,

$$\left.\frac{\partial \phi}{\partial r}\right|_{r=0} = 0. \tag{1.7}$$

Since the angular flux ψ, the solution of the the transport equation (1.1), is well approximated by solution of the diffusion equation (1.5) in the asymptotic diffusive regime [2], then we can deduce the spatial variation of ψ in this regime from the spatial variation of the solution of diffusion equation (1.5). For the sake of argument, let us assume that parameters of the diffusion equation (1.5) are the constants, i.e. $\sigma_t = 1/\epsilon$, $\sigma_a = \epsilon$, and $q_0 = \epsilon$. Except for a boundary layer at $r = 1$, the constant function $\phi \approx 1$ satisfies (1.5) in the region, $r < (1-\epsilon)$, for these parameters. *Thus the spatial variation of ψ is independent of the mean free path ($\sim 1/\sigma_t$) in the asymptotic diffusive regime.* Since the angular flux ψ is smooth in the asymptotic regime, then

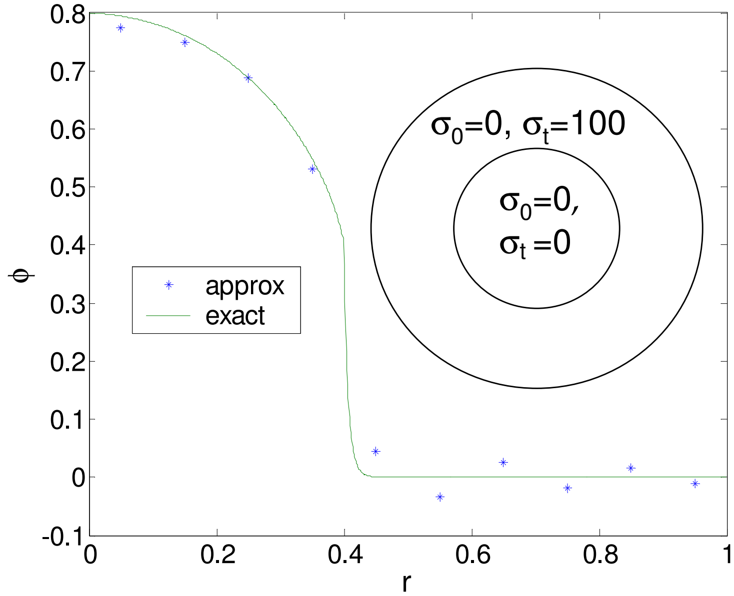

FIG. 2.1. *Results of the first test problem, the transport in a void that is surrounded by a strong absorber. The solid curve is the exact solution, and the points are the numerical solution.*

an accurate numerical solution should be attainable with a grid spacing that is much larger than the mean free path.

The accuracy of a numerical method depends on how well it captures the variations in the solution. A rapidly varying function is approximated poorly on the grid that a slowly varying function is approximated accurately. Now, if we hold the total cross section fixed and increase the scattering cross section, then ψ should become smoother as the scattering cross section increases. Therefore the error in the numerical solution should decrease as the scattering ratio increases for transport in the asymptotic diffusion regime.

2. Numerical Results. We verify these qualitative arguments with two test problems. The test problems consist of a void in the region $r \in [0, .4)$, and a dense material with $\sigma_t = 100$ in the region $r \in [.4, 1]$. The isotropic external source q is 1 in the void region, and is 0 in the absorbing region. In the first test problem, the dense material is a pure absorber with a scattering ratio $\sigma_0/\sigma_t = 0$, and in the second test problem, the dense material is a pure scatterer with a scattering ratio of 1. The transport equation (1.1) was solved by the Diamond Difference Method (DD) [1]. The μ integral of (1.1) is approximated by a Gauss-Legendre quadrature in the DD method. The two test problems, calculated with $\Delta r = .1$ and a 10 point quadrature set, are compared to the 'exact' solutions in Figs. 2.1 and 2.2 respectively.

For these parameters, we found the DD scheme converges when Δr, the grid spacing, is .001 and the quadrature is a 10 point set. These converged results are taken to be the 'exact' solutions.

The results of the first test problem, shown in Fig. 2.1, illustrate the magnitude of discretization error for the transport in a void that is surrounded by a strong aborber. The exact solution, depicted as the solid line in Fig. 2.1, varies rapidly in

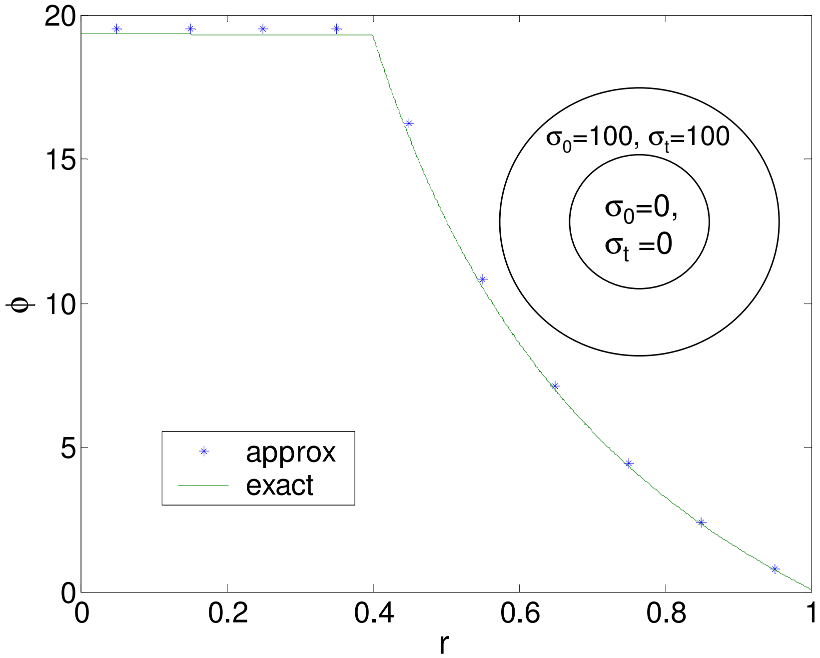

FIG. 2.2. *Results of the second test problem, the transport in a void that is surrounded by a pure scatterer. The solid curve is the exact solution, and the points are the numerical solution. Note that the numerical solution is positive and is non-oscillatory.*

the absorbing region. As expected, the scalar flux ϕ is poorly approximated on such a coarse grid, $\sigma_t \Delta r = 10$, with errors manifesting as oscillations in the absorbing region. The negative values of ϕ in the absorbing region are unphysical. On the other hand, the results of the second test problem, shown in Fig. 2.2, illustrate the magnitude of the discretization error for the transport in a void that is surrounded by a pure scatterer. The exact solution, as we have argued in the preceeding section, varies slowly in the diffusive region. Thus it is approximated reasonably well by the numerical solution for a grid spacing of 10 mean free paths. Furthermore, we note that the computed scalar flux ϕ is positive everywhere, in contrast to the situation which is depicted Fig. 2.1.

Let us now show that the accuracy of a numerical scheme improves as the scattering ratio increases with the grid spacing and the quadrature set held fixed. Since the quadrature set is converged, the error in numerical solution, $\psi^h_{i,d}$, is due to spatial zoning, and can be taken as the spatial discretization error in its zeroth moment, $\phi^h_i \equiv \sum_{d=1}^{n_r} \psi^h_{i,d}\, w_d$. In the figures below, we plot the L_2 error of $\phi^h - \phi$, where the L_2 norm of u is defined as

$$\|u\|_2^2 \equiv \left(\frac{\sum_{i=1}^{n_r} u_i^2 \, V_i}{\sum_{i=1}^{n_r} V_i} \right)^{\frac{1}{2}} \quad ,$$

with, $V_i = (4/3)\pi\Big(r^3_{i+\frac{1}{2}} - r^3_{i-\frac{1}{2}}\Big)$, being the volume of zone i. The graph in Fig. 2.3 shows that the accuracy of unconverged results (calculated with $\Delta r = .1$) improves

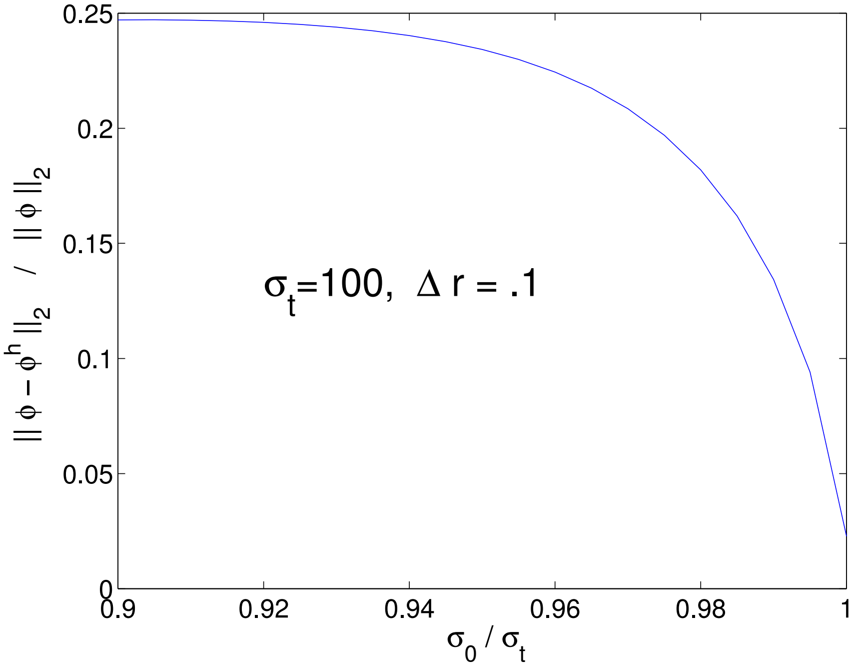

FIG. 2.3. *The relative error decreases as the scattering ratio increases.*

as the scattering ratio increases in the asymptotic diffusive regime. This phenomenon persists as Δr decreases. When we decrease Δr to .01, we see that the relative error in Fig. 2.4 also decreases as the scattering ratio increases. The relative error in Fig. 2.4 is smaller than the relative error in Fig. 2.3 because the results of Fig. 2.4 were calculated with a smaller Δr than the results of Fig. 2.3.

3. Conclusions. We have shown that the accuracy of a numerical scheme for solving the neutron transport equation in the asymptotic diffusive regime improves as the scattering ratio increases for a fixed total cross section. For problems with hopelessly small mean free paths, this work offers a glimmer of hope that the calculations may not be as inaccurate as one might think if the scattering ratio is very close to 1.

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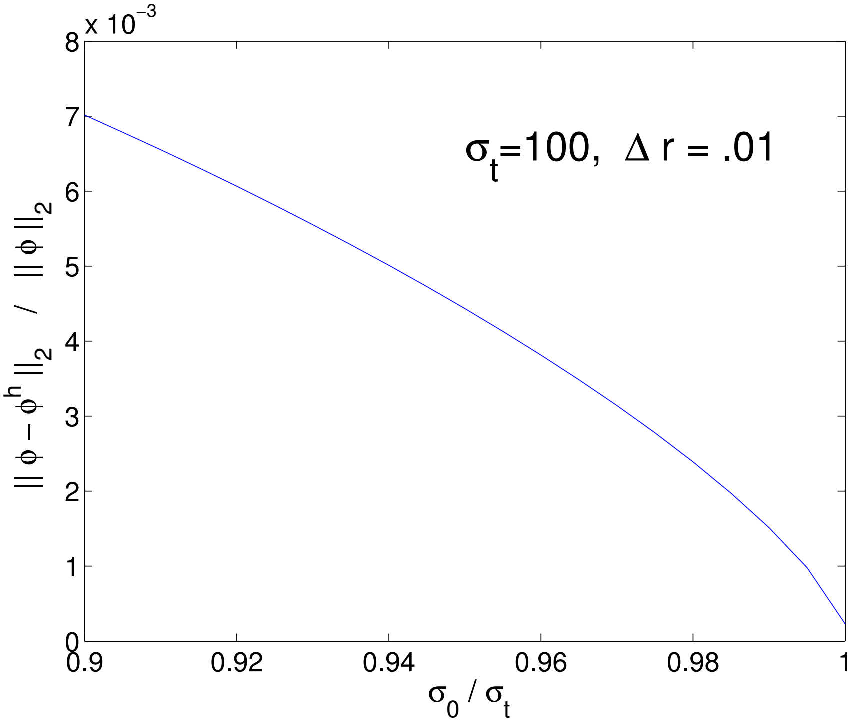

FIG. 2.4. *These results are similar to those of Fig. 2.3 but were calculated with* $\Delta r = .01$.