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LLNL-JRNL-753609

A TEST PROBLEM FOR CODES SOLVING THE DISCRETIZED DIFFUSION EQUATION IN CARTESIAN GEOMETRY DERIVED VIA DISCRETE GREEN'S FUNCTIONS

N. A. Gentile, J. C. Hayes

June 25, 2018

Journal of Computational and Theoretical Transport

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A TEST PROBLEM FOR CODES SOLVING THE DISCRETIZED DIFFUSION EQUATION IN CARTESIAN GEOMETRY DERIVED VIA DISCRETE GREEN'S FUNCTIONS

N. A. Gentile
Lawrence Livermore National Laboratory
L-38
7000 East Avenue
Livermore, CA 94551
gentile1@llnl.gov
and

John Hayes
Lawrence Livermore National Laboratory
L-95
7000 East Avenue
Livermore, CA 94551
hayes37@llnl.gov

ABSTRACT

We obtain a solution to a zone-centered discretization of the one dimensional time-dependent diffusion equation with arbitrary initial conditions and source, constant absorption and scattering opacity, and constant zone size and time step. The solution is obtained using the discrete Green's functions of the discretized equation. The solution of the discretized equation is useful in the testing of computer codes, because the code can be expected to agree with the solution to the discrete equation, to within small errors caused by roundoff. This is in contrast to solutions of the differential equation, with which the code results only approximately agree. The usefulness of the solution for tests of an inertial confinement fusion code is demonstrated.

1. INTRODUCTION

The diffusion equation is often used to model radiation transport in opaque media, so computational approximations to the diffusion equation are frequently employed. Analytic or semi-analytic solutions to the diffusion equation are often used in order to verify the correctness of computer codes used to solve the diffusion equation. Since the codes usually involve some approximation to the diffusion equation, such as a finite difference approximation, the results of the numerical simulation have discretization error. This prevents the code from producing results that are identical to the known solutions. Instead, the convergence of the numerical results to the known solution as the mesh and time step are decreased is investigated. If the theoretical rate of convergence is achieved, the test results are considered to validate the code.

In this paper, we describe a technique for finding solutions to a discretized form of the one dimensional diffusion equation. This discretized equation is a zone-centered finite difference

approximation to the diffusion equation; it represents the radiation energy density as a zone-centered variable. We require constant absorption and scattering opacities, since our solution technique requires that the difference equation be linear. We also require that all zones be the same size and that the time step remain fixed. Although these requirements are restrictive, we believe the test problem is useful for testing codes that solve the diffusion equation, since many of the frequently-employed discretization techniques reduce to a zone-centered finite difference discretization for one dimensional problems.

Our solution also does not simulate the interaction of radiation with matter. In other words, we do not model thermal emission in our solution. In effect, we are describing a case where the matter temperature $T \approx 0$ and the heat capacity c_v is very large. In this case there is very little thermal emission and the matter temperature remains small. We need to apply this restriction because our solution technique requires that the radiation source be independent of the radiation intensity.

A solution to the discretized diffusion equation is useful for code comparisons because we can expect exact agreement between code results and the solution. This is in contrast to the comparison of code results to an analytic solution of the diffusion equations. In that case, the code is solving a discrete approximation to the equation, and we only expect that the code result will tend to approach the solution of the differential equation as the zone size and time step are decreased. The solution we are presenting has discretization error built-in, in effect. In practice, we will see small differences due to roundoff error between the code results and the results of the solution of the discretized equation.

In the second section of this paper, we will give a brief overview of the solution of the diffusion equation using Green's functions. This short summary of well-known results is provided to illustrate techniques that will be used to obtain the solution of the discretized solution. The third section describes the solution of the discretized equation in terms of a discrete version of Green's functions. These discrete Green's functions satisfy difference equations with Kronecker delta sources instead of differential equations with Dirac delta function sources. The discrete Green's functions are expressed in terms of an integral which can be performed analytically; this is described in the fourth section. The discrete Green's functions allow us to generate analytic solutions for the discretized diffusion equation for arbitrary sources and initial conditions. The last section compares the solution of the discretized diffusion equation, for a test problem with specific sources and initial conditions, to the results of a computational simulation.

A note on notation: where there is the possibility of confusion between continuous quantities and their discrete analogs, we will use a circumflex for continuous quantities to distinguish them from discrete quantities. For example, $\hat{\phi}(x,t)$ denotes the solution of the diffusion equation, with ϕ being a function of the continuous variables x and t, while $\phi(j,n)$ will denote the solution of the discretized diffusion equation, with ϕ being a function of the discrete variables j and n, with $x = j\Delta x$ and $t = n\Delta t$. Since the majority of the symbols in this work represent discrete quantities, this convention seems to provide the most clarity with the least amount of clutter.

2. GREEN'S FUNCTIONS FOR THE ONE-DIMENSIONAL DIFFUSION EQUATION

The diffusion equation with a radiation source and constant absorption opacity σ_a and scattering opacity σ_s is [1]

$$\frac{\partial\hat{\phi}}{\partial t} - cD\frac{\partial^2\hat{\phi}}{\partial x^2} + c\sigma_a\hat{\phi} = \hat{S}(x,t) \ , \tag{1}$$

with the diffusion coefficient $D = \frac{1}{3(\sigma_a+\sigma_s)}$ and $\hat{S}(x,t)$ an arbitrary source function. We take $\hat{\phi}(t=0) = \hat{\phi}_0(x)$. We choose the domain of x to be $[-\infty,\infty]$, so that there are no boundary conditions; we expect that $\hat{\phi}$ will go to zero at large x on physical grounds. This equation is linear in the radiation energy density $\hat{\phi}$, so we can use Green's functions to express the solution as the sum of two integrals, one over the source $\hat{S}(x,t)$ and the other over the initial condition $\hat{\phi}_0(x)$.

The determination of the Green's function for Eq.(1), and the use of these Green's functions to express then solution of Eq.(1), are well-known pieces of mathematical physics. However, we will present a quick overview of the calculation in this section, because it will aid us in developing a similar solution of the discretized version of Eq.(1) in the next section. The following draws heavily from Butkov, pp. 299-301 [2].

We can express the solution of Eq.(1) with the stated initial conditions as

$$\hat{\phi}(x,t) = \int_{-\infty}^{\infty} \mathrm{d}x'\hat{G}_i(x,t,x')\hat{\phi}_0(x') + \int_0^t \mathrm{d}t' \int_{-\infty}^{\infty} \mathrm{d}x'\hat{G}_s(x,t,x',t')\hat{S}(x',t'). \tag{2}$$

Here $\hat{G}_i(x,t,x')$ is the initial condition Green's function which satisfies

$$\frac{\partial\hat{G}_i(x,t,x')}{\partial t} - cD\frac{\partial^2\hat{G}_i(x,t,x')}{\partial x^2} + c\sigma_a\hat{G}_i(x,t,x') = 0 \tag{3}$$

and the initial condition

$$\hat{G}_i(x,0,x') = \delta(x-x') \ . \tag{4}$$

$\hat{G}_s(x,t,x',t')$ is the source Green's function which satisfies the differential equation

$$\frac{\partial\hat{G}_s(x,t,x',t')}{\partial t} - cD\frac{\partial^2\hat{G}_s(x,t,x',t')}{\partial x^2} + c\sigma_a\hat{G}_s(x,t,x',t') = \delta(x-x')\delta(t-t') \tag{5}$$

with the initial condition

$$\hat{G}_s(x,t,x',t') = 0, t \le t'. \tag{6}$$

The fact that Eq.(2) satisfies Eq.(1), when $\hat{G}_i$ satisfies Eqs.(3)-(4) and $\hat{G}_s$ satisfies Eq.(5), is easily shown by direct substitution.

Solving Eq.(1) via Eq.(2) requires us to solve Eq.(3) and Eq.(5). We will solve Eq.(3) first. We do this by trying to satisfy Eq.(3) with a solution that is the product of a function of t only and a function of x only; that is, we try a solution of the form $\hat{T}(t)\hat{X}(x)$. Substituting this into Eq.(3) and dividing by $cD\hat{T}\hat{X}$ yields

$$\frac{1}{Dc\hat{T}}\frac{\partial\hat{T}}{\partial t} + \frac{\sigma_a}{D} = \frac{1}{\hat{X}}\frac{\partial^2\hat{X}}{\partial x^2} \ . \tag{7}$$

Since the right side of Eq.(7) depends only on t and the left side depends only on x, each side must equal a constant, which we will choose to be negative and denote by $-k^2$, where $k \in (-\infty, \infty)$. Then $\hat{T}$ satisfies

$$\frac{\partial \hat{T}}{\partial t} + (c\sigma_a + cDk^2)\hat{T} = 0, \tag{8}$$

the solution of which is

$$\hat{T}(k,t) = e^{-(c\sigma_a + cDk^2)t} \ . \tag{9}$$

$\hat{X}$ satisfies

$$\frac{\partial^2 \hat{X}}{\partial x^2} = -k^2 \hat{X}(x) \ , \tag{10}$$

the solution of which are the familiar Fourier functions $\hat{X}(k,x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$. These functions satisfy the orthogonality relationships

$$\int_{-\infty}^{\infty} \mathrm{d}k \frac{1}{2\pi} \hat{X}^*(k,x')\hat{X}(k,x) = \int_{-\infty}^{\infty} \mathrm{d}k \frac{1}{2\pi} e^{ik(x-x')} = \delta(x-x') \tag{11}$$

and

$$\int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{2\pi} \hat{X}^*(k,x)\hat{X}(k',x) = \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{2\pi} e^{i(k-k')x} = \delta(k-k') \ , \tag{12}$$

where * denotes complex conjugation.

With these functions $\hat{X}$ and $\hat{T}$, a general solution to Eq.(3) can be written as an integral over k:

$$\hat{G}_i(x,t,x') = \int_{-\infty}^{\infty} \mathrm{d}k \hat{A}_b(k,x')\hat{T}(k,t)\hat{X}(k,x) \ , \tag{13}$$

where $\hat{A}_b(k,x')$ is determined by the initial condition Eq.(4):

$$\hat{G}_i(x,0,x') = \int_{-\infty}^{\infty} \mathrm{d}k \hat{A}_b(k,x')\hat{X}(k,x) = \delta(x-x') \ . \tag{14}$$

Multiplying both sides of Eq.(14) by $\hat{X}^*(k',x)$ and integrating over $[-\infty,\infty]$ in x yields

$$\begin{aligned} \int_{-\infty}^{\infty} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{d}k \hat{A}_b(k,x')\hat{X}^*(k',x)\hat{X}(k,x) &= \int_{-\infty}^{\infty} \mathrm{d}x \hat{X}^*(k',x)\delta(x-x') \\ \int_{-\infty}^{\infty} \mathrm{d}k \hat{A}_b(k,x')\delta(k-k') &= \hat{A}_b(k',x') = \hat{X}^*(k',x') \ , \end{aligned} \tag{15}$$

where we have used the orthogonality relationship Eq.(12) and assumed that we can exchange the order of integration. Using the value of $\hat{A}_b(k,x)$ from Eq.(15) in Eq.(13) yields

$$\begin{aligned} \hat{G}_i(x,t,x') &= \int_{-\infty}^{\infty} \mathrm{d}k \hat{T}(k,t)\hat{X}^*(k,x')\hat{X}(k,x) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k e^{-(c\sigma_a + cDk^2)t} e^{ik(x-x')} \\ &= \frac{1}{\sqrt{4\pi cDt}} e^{\left[\frac{-(x-x')^2}{4cDt} - c\sigma_a t\right]} \ . \end{aligned} \tag{16}$$

Now we turn to finding an expression for $\hat{G}_s(x,t,x',t')$. First we expand $\hat{G}_s(x,t,x',t')$ in terms of $\hat{X}(k,x)$:

$$\hat{G}_s(x,t,x',t') = \int_{-\infty}^{\infty} \mathrm{d}k \hat{A}_s(k,t,x',t')\hat{X}(k,x). \tag{17}$$

Then we can write

$$\frac{\partial \hat{G}_s(x,t,x',t')}{\partial t} = \int_{-\infty}^{\infty} \frac{\partial \hat{A}_s(k,t,x',t')}{\partial t}\hat{X}(k,j)\mathrm{d}k \ , \tag{18}$$

and

$$\frac{\partial^2 \hat{G}_s(x,t,x',t')}{\partial x^2} = \int_{-\infty}^{\infty} \mathrm{d}k \left[-k^2 \hat{A}_s(k,t,x',t')\hat{X}(k,x)\right]. \tag{19}$$

We insert these expressions into Eq.(5), and use Eq.(11) to represent $\delta(x-x')$. This yields

$$\int_{-\infty}^{\infty} \mathrm{d}k \frac{1}{c}\frac{\partial \hat{A}_s}{\partial t}\hat{X} + Dk^2\hat{A}_s\hat{X} + \sigma_a\hat{A}_s\hat{X} = \int_{-\infty}^{\infty} \mathrm{d}k\hat{X}(k,x)\hat{X}^*(k,x')\delta(t-t') \ . \tag{20}$$

Collecting coefficients of $\hat{X}$ establishes that $\hat{A}_s(k,t,x',t')$ satisfies

$$\frac{1}{c}\frac{\partial \hat{A}_s}{\partial t} + Dk^2\hat{A}_s + \sigma_a\hat{A}_s = \hat{X}^*(k,x')\delta(t-t') \ . \tag{21}$$

We now solve this equation for $\hat{A}_s(k,t,x',t')$. On physical grounds, we demand that $\hat{A}_s(k,t,x',t') = 0$ for $t < t'$. This is because $\hat{G}_s(x,t,x',t')$ describes the effect of the source at the point x' at time t' on the solution at the point x at time t, and causality requires that the effect not precede the cause. For $t > t'$, $\hat{A}_s(k,t,x',t')$ satisfies the differential equation

$$\frac{1}{c}\frac{\partial \hat{A}_s}{\partial t} + Dk^2\hat{A}_s + \sigma_a\hat{A}_s = 0 \ , \ t > t' \ , \tag{22}$$

which has the solution

$$\hat{A}_s(k,t,x',t') = \hat{A}_0 e^{[-(cDk^2+c\sigma_a)(t-t')]} \ , \ t > t' \ , \tag{23}$$

where $\hat{A}_0$ is constant with respect to t. To determine the value of $\hat{A}_0$, we integrate Eq.(21) over t from t' to $t' + dt$. This yields $\hat{A}_0 = \hat{X}^*(k,x')$. Using this value in Eq.(23), and inserting that into Eq.(17) allows us to solve for $\hat{G}_s(x,t,x',t')$:

$$\begin{aligned}
\hat{G}_s(x,t,x',t') &= H(t-t')\int_{-\infty}^{\infty} \mathrm{d}k e^{[-(cDk^2+c\sigma_a)(t-t')]}\frac{e^{ik(x-x')}}{2\pi} \\
&= \frac{H(t-t')}{\sqrt{4\pi cD(t-t')}} e^{\left[\frac{-(x-x')^2}{4cD(t-t')} - c\sigma_a(t-t')\right]} \ ,
\end{aligned} \tag{24}$$

where H(t - t') is the Heaviside step function. Then the general solution of Eq.(1) with the stated initial conditions is

$$\begin{aligned}
\hat{\phi}(x,t) &= \int_{-\infty}^{\infty} \mathrm{d}x' \frac{1}{\sqrt{4\pi Dt}} e^{\left[\frac{-(x-x')^2}{4Dt} - c\sigma_a t\right]}\hat{\phi}_0(x') \\
&+ \int_0^t \mathrm{d}t' \int_{-\infty}^{\infty} \mathrm{d}x' \hat{S}(x',t') \frac{1}{\sqrt{4\pi D(t-t')}} e^{\left[\frac{-(x-x')^2}{4D(t-t')} - c\sigma_a(t-t')\right]} \ .
\end{aligned} \tag{25}$$

This may be verified explicitly by substituting this expression for $\hat{\phi}(x,t)$ into Eq.(1).

For future reference, we wish to note that both $\hat{G}_i(x,t,x')$ and $\hat{G}_s(x,t,x',t')$ can be written in terms of the function $\hat{G}_0(x,t)$ defined by

$$\hat{G}_0(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{\left[\frac{-x^2}{4Dt} - c\sigma_a t\right]} \ . \tag{26}$$

In terms of $\hat{G}_0(x,t)$, we have

$$\hat{G}_i(x,t,x') = \hat{G}_0(x-x',t) \tag{27}$$

and

$$\hat{G}_s(x,t,x',t') = H(t-t')\hat{G}_0(x-x',t-t') \ . \tag{28}$$

With $\hat{G}_i(x,t,x')$ and $\hat{G}_s(x,t,x',t')$ determined, we can calculate the solution $\hat{\phi}(x,t)$ of Eq.(1) with arbitrary source $\hat{S}(x,t)$ and arbitrary initial conditions $\hat{\phi}_0(x)$ using Eq.(25). The solution is expressed in terms of integrals, which may or may not have a closed form. But a numerical value for the integrals is sufficient for many purposes.

Solutions of Eq.(1) derived via Eq.(25) are useful in testing a code which solves the diffusion equation. However, these solutions cannot be compared directly to the code output. That is because the code is not solving the differential equation Eq.(1). Instead, it is solving a discretized approximation to this equation. So using solutions of Eq.(1) to verify a code involve determining if the approximate solutions calculated by the code converge, at the expected rate, to the solutions of Eq.(1).

In the next section, we will employ discrete versions of the techniques described above to derive a solution of the discretized version of Eq.(1), which can be compared directly to the output of a code. These solutions will be analytic solutions of the same discretized version of the equation solved by the code. Thus, we expect that the analytic solutions and the output of the code will agree, except for small differences due to roundoff error.

3. GREEN'S FUNCTIONS FOR THE DISCRETE FORM OF THE DIFFUSION EQUATION

We will now examine solutions to a difference equation that is a discrete approximation of the diffusion equation Eq.(1). The difference equation will be written in terms of variables that are defined at discrete values of the time and space variables. These discrete values of time will be defined by integer multiples of a fixed time step: $t = n\Delta t$, with $n \geq 0$. Similarly, the discrete values of position will be defined by $x = j\Delta x$, with j any integer and Δx a constant.

The solutions to the difference equation will be functions of the discrete variables j and n instead of continuous variables x and t. For example, $\phi(j,n)$ means ϕ at grid point j at time n; this is a discrete analog to $\phi(x,t)$, which means ϕ at location x at time t.

Before we examine the difference approximation of the diffusion equation, it will prove useful to examine a simpler single variable differential equation and its discrete approximation. The differential equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} = k\phi \tag{29}$$

has the solution

$$\phi(t) = \phi(0)e^{kt} \ . \tag{30}$$

This differential equation can be approximated by the difference equation

$$\frac{\phi(n+1) - \phi(n)}{\Delta t} = k\phi(n+1) \tag{31}$$

where $\Delta t \equiv t^{n+1} - t^n$. We will assume henceforth that Δt is constant. We can solve Eq.(31) for $\phi(n+1)$, which yields

$$\phi(n+1) = \frac{\phi(n)}{1 - k\Delta t} \ . \tag{32}$$

To get a closed form solution for $\phi(n)$ from Eq.(32), we try a solution of the form $\phi(n) = \tau^n$, with τ unknown. Substituting the conjectured solution into Eq.(32) yields $\tau = 1/(1 - k\Delta t)$, so the solution of Eq.(32) is

$$\phi(n) = \frac{\phi(0)}{(1 - k\Delta t)^n} \ . \tag{33}$$

Since $\Delta t = t/n$, we can write

$$\phi(n) = \frac{\phi(0)}{(1 - kt/n)^n} \ , \tag{34}$$

and since [3]

$$lim_{n\to\infty}(1 - kt/n)^{-n} = e^{kt} \ , \tag{35}$$

we see that the solution of the difference equation Eq.(31) becomes a better approximation to the solution of the differential equation Eq.(29) as we increase the number of time steps n and decrease Δt, while holding $n\Delta t = t$ fixed.

Now we turn our attention to a discrete approximation of the diffusion equation. We discretize the diffusion equation as

$$\frac{\phi(j,n+1) - \phi(j,n)}{\Delta t} - cD\frac{\phi(j+1,n+1) - 2\phi(j,n) + \phi(j-1,n+1)}{\Delta x^2} + c\sigma_a\phi(j,n+1) = S(j,n) \tag{36}$$

with $S(j,n)$ an arbitrary source and arbitrary initial conditions $\phi(j,0)$. We will assume Δt, Δx, D, and σ_a are constant.

Eq.(36) with its source and initial condition is a discrete analog of Eq.(1). It is this equation that a computer code would actually solve, rather than the differential equation Eq.(1). We would like to find a solution analogous to Eq.(2), which would involve discrete versions of Green's functions for this difference equation.

We can express the solution of Eq.(36) with the stated initial conditions as

$$\phi(j,n) = \sum_{j'=-\infty}^{\infty} G_i(j,n,j')\phi_0(j') + \sum_{n'=0}^{n}\sum_{j'=-\infty}^{\infty} G_s(j,n,j',n')S(j',n') \ . \tag{37}$$

Here $G_i(j,n,j')$ is a discrete analog of the initial condition Green's function. $G_i(j,n,j')$ satisfies the difference equation

$$\begin{aligned}\frac{G_i(j,n+1,j') - G_i(j,n,j')}{\Delta t} &- cD\frac{G_i(j+1,n+1,j') - 2G_i(j,n+1,j') + G_i(j-1,n+1,j')}{\Delta x^2} \\ &+ c\sigma_a G_i(j,n+1,j') = 0\end{aligned} \tag{38}$$

and has the initial condition

$$G_i(j,0,j') = \delta_{jj'} \ . \tag{39}$$

$G_s(j,n,j',n')$ is a discrete analog of the source Green's function which satisfies the difference equation

$$\begin{aligned} \frac{G_s(j,n+1,j',n') - G_s(j,n,j',n')}{\Delta t} &- cD\frac{G_s(j+1,n+1,j',n') - 2G_s(j,n+1,j',n') + G_s(j-1,n+1,j',n')}{\Delta x^2} \\ &+ c\sigma_a G_s(j,n+1,j',n') = \delta_{jj'}\delta_{nn'} \end{aligned} \tag{40}$$

with the initial condition

$$G_s(j,n,j',n') = 0 \ , \ n \leq n' \ . \tag{41}$$

The fact that Eq.(37) satisfies Eq.(36), when G_i satisfies Eqs.(38)-(39) and G_s satisfies Eqs.(40)-(41) is easily shown by direct substitution.

Eq.(37) shows that G_i is dimensionless, while G_s has the same dimensions as the quantity $\frac{\phi}{S}$. Since Eq.(36) shows that S has units of ϕ over time, the units of G_s are time.

Inspired by the similarity between the difference equations Eq.(38) and Eq.(40) and the differential equations Eq.(3) and Eq.(5), we will attempt to find solutions for the difference equations Eq.(38) and Eq.(40) using similar techniques.

First, we will attempt to solve Eq.(38) for $G_i(j,n,j')$. As we did in solving Eq.(3), we look for solutions to this equation that are separable into products: $T(n)X(j)$. Applying Eq.(38) to $T(n)X(j)$ and dividing by $cDT(n+1)X(j)$ yields

$$\frac{T(n+1) - T(n)}{Dc\Delta t T(n+1)} + \frac{\sigma_a}{D} = \frac{X(j+1) - 2X(j) + X(j-1)}{\Delta x^2 X(j)} \ . \tag{42}$$

The term on the left side of Eq.(42) depends only on the index n and is independent of j, while the term on the right depends on j but not n. For them to be equal, they must therefore have a constant value (i.e., a value independent of j and n.) We will choose this value to be negative and denote it $-K^2$. Then T will satisfy

$$\frac{T(n+1) - T(n)}{c\Delta t} + \sigma_a T(n+1) + K^2 D T(n+1) = 0 \tag{43}$$

and X will satisfy

$$\frac{X(j+1) - 2X(j) + X(j-1)}{\Delta x^2} = -K^2 X(j) \ . \tag{44}$$

Because of the resemblance between Eq.(43) and Eq.(31), we will again try a solution of the form $T(n) = \tau^n$ for Eq.(43). Inserting this form into Eq.(43), we find that $\tau = (1 + c\sigma_a\Delta t + cK^2 D\Delta t)$, and that

$$T(n) = \frac{1}{(1 + c\sigma_a\Delta t + cK^2 D\Delta t)^n} \ , \tag{45}$$

where we have chosen $T(0) = 1$ for convenience. For physical reasons, we expect $T(n)$ to decrease with time. Eq.(43) is an approximation to a decaying exponential, which is why we chose the constant $-K^2$ to be negative; this choice ensures that the denominator of Eq.(45) is larger than

1. In the limit where $n \to \infty$ and $\Delta t \to 0$ with $n\Delta t \to t$, $T(n) \to e^{(-c\sigma_a t - ck^2 Dt)}$, by virtue of Eq.(35).

Now we turn to Eq.(44). By analogy with the solutions of the differential equation Eq.(10), we expect the solutions to this equation to be oscillatory. Therefore, we attempt to satisfy it with a solution of the form

$$X(j) = Ne^{ikj\Delta x} \tag{46}$$

with k real and N being a normalization constant that we will determine later. Applying Eq.(44) to $Ne^{ikj\Delta x}$ and dividing by $Ne^{ikj\Delta x}$, we get

$$e^{ik\Delta x} - 2 + e^{-ik\Delta x} = -K^2\Delta x^2 \ . \tag{47}$$

Using the definition of cosine in terms of exponentials, this can be written as $2\cos(k\Delta x) - 2 = -K^2\Delta x^2$, so K satisfies

$$K^2(k) = \frac{2(1-\cos(k\Delta x))}{\Delta x^2} \ . \tag{48}$$

As Δx gets small, we get

$$lim_{\Delta x \to 0} K^2(k) = \frac{2(k^2\Delta x^2/2)}{\Delta x^2} = k^2 \ , \tag{49}$$

and since in the limit $j\Delta x \to x$, we also obtain

$$lim_{\Delta x \to 0} X(j) = Ne^{ikx} \ . \tag{50}$$

We see that in the limit of small Δx we recover the familiar Fourier functions.

We would like to see if $X(k,j)$ satisfies an orthogonality relationship similar to Eq.(11). The orthogonality of $X(k,j)$ can be established by using Eq.(44). We take $X^*(k',j)$ and multiply it by Eq.(44) applied to $X(k,j)$, and subtract $X(k,j)$ multiplied by Eq.(44) applied to $X^*(k',j)$, and sum over all j. By virtue of the fact that $X(k,j)$ and $X^*(k',j)$ satisfy Eq.(44), we get the following result:

$$\begin{aligned} \sum_{j=-\infty}^{j=\infty} X^*(k',j)\frac{X(k,j+1) - 2X(k,j) + X(k,j-1)}{\Delta x^2} \quad - \\ X(j)\frac{X^*(k',j+1) - 2X^*(k',j) + X^*(k')(j-1)}{\Delta x^2} \quad = \quad (k'^2 - k^2)\sum_{j=-\infty}^{j=\infty} X(k,j)X^*(k') \end{aligned} \tag{51}$$

Next, we apply the Abel's lemma, also known as summation by parts, to the sums on the left side. Abel's lemma is

$$\sum_{j=m}^{n} f_j(g_{j+1} - g_j) = f_{n+1}g_{n+1} - f_m g_m - \sum_{j=m}^{n}(f_{j+1} - f_j)g_{j+1} \ . \tag{52}$$

This is the difference equation analog of integration by parts.

Both terms on the left side of Eq.(51) can be written in a form to which Eq.(52) can be applied. This is because

$$\frac{X(j+1) - 2X(j) + X(j-1)}{\Delta x^2} = \frac{1}{\Delta x}\frac{X(j+1) - X(j)}{\Delta x} - \frac{X(j) - X(j-1)}{\Delta x} \ , \tag{53}$$

with a similar equation applying to the term in $X^*(j)$. Now we apply Eq.(52) to Eq.(51). Since the sum in Eq.(51) is over $j \in (-\infty, \infty)$, the surface terms in Eq.(52) vanish and we get

$$\sum_{j=-\infty}^{j=\infty} \left[\frac{X^*(k',j+1) - X^*(k',j)}{\Delta x} \frac{X(k,j+1) - X(k,j)}{\Delta x} \right. \quad - \\ \left. \frac{X(k,j+1) - X(k,j)}{\Delta x} \frac{X^*(k',j+1) - X^*(k',j)}{\Delta x} \right] \quad = \\ \left[K(k)^2 - K(k')^2 \right] \sum_{j=-\infty}^{j=\infty} X(k,j) X^*(k',j) \ . \tag{54}$$

The left side of Eq.(54) is identically 0 - the expressions we are subtracting are the same - so we must have

$$\sum_{j=-\infty}^{j=\infty} X(k,j) X^*(k',j) = 0 \tag{55}$$

when $k \neq k'$. This means that we can write

$$\sum_{j=-\infty}^{j=\infty} X(k,j) X^*(k') = \delta(k-k'). \tag{56}$$

Eq.(56) can be used to determine the value of the normalization constant N from Eq.(46). To determine the value of N, we integrate Eq.(56) over k from $k = k' - a$ to $k = k' + a$, where $a > 0$ but otherwise arbitrary. This yields

$$\int_{k'-a}^{k'+a} dk \sum_{j=-\infty}^{j=\infty} X(k,j) X^*(k') = 1 \ . \tag{57}$$

Exchanging the order of summation and integration in Eq.(57) results in

$$\begin{aligned} 1 &= \sum_{j=-\infty}^{j=\infty} N^2 e^{-ik'j\Delta x} \int_{k'-a}^{k'+a} dk e^{ikj\Delta x} \\ \frac{1}{N^2} &= \sum_{j=-\infty}^{j=\infty} e^{-ik'j\Delta x} \frac{e^{i(k'+a)j\Delta x} - e^{i(k'-a)j\Delta x}}{ij\Delta x} \\ &= \sum_{j=-\infty}^{j=\infty} \frac{2sin(ja\Delta x)}{j\Delta x} \\ &= 2a + 2\sum_{j=1}^{j=\infty} \frac{2sin(ja\Delta x)}{j\Delta x} \\ &= 2a + \frac{4}{\Delta x}\left[\frac{\pi - a\Delta x}{2}\right] \\ &= \frac{2\pi}{\Delta x}, \end{aligned} \tag{58}$$

which implies that

$$N = \sqrt{\frac{\Delta x}{2\pi}} \tag{59}$$

where we have used [3], p. 38, Eq.(1.1441.1) to evaluate the sum.

With N defined, we can obtain another orthogonality relationship:

$$\begin{aligned}\int_{-\pi/\Delta x}^{\pi/\Delta x} d\mathrm{k} X(k,j)X^*(k,j') &= \frac{\Delta x}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} d\mathrm{k} e^{ik(j-j')\Delta x} \\ &= \frac{\Delta x}{2\pi}\frac{1}{i(j-j')\Delta x}[e^{ik(j-j')\Delta x}]_{-\pi/\Delta x}^{\pi/\Delta x} \\ &= \frac{1}{\pi}\frac{\sin[(j-j')\pi]}{j-j'} = \frac{1}{\pi}\delta_{jj'} \ . \end{aligned} \tag{60}$$

With these properties of $T(k,n)$ and $X(k,j)$ established, we will now return to calculating $G_i(j,n,j')$.

We can write a solution of the difference equation Eq.(38) as an integral of $T(k,n)X(k,j)$. Because $K(k)$, defined by Eq.(48), is periodic in k, we will restrict the values of k to give one cycle of the cosine: $k \in [-\pi/\Delta x, \pi/\Delta x]$. The integral over the allowed values of k is:

$$\begin{aligned} G_i(j,n,j') &= \int_{-\pi/\Delta x}^{\pi/\Delta x} A_b(k,j')T(k,n)X(k,j)\mathrm{d}k \\ &= \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{A_b(k,j')e^{ikj\Delta x}}{[1+c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2} - \frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \ . \end{aligned} \tag{61}$$

$A_b(k,j')$ is obtained by requiring that $G_i(j,n,j')$ satisfy the initial condition Eq.(39). This requires that

$$G_i(j,0,j') = \int_{-\pi/\Delta x}^{\pi/\Delta x} A_b(k,j')X(k,j)\mathrm{d}k = \delta_{jj'} \ . \tag{62}$$

To solve Eq.(62) for $A_b(k)$, we use the orthogonality relationship given by Eq.(57). Multiplying Eq.(62) by $X^*(k')$ and summing over all j yields

$$\sum_{j=-\infty}^{j=\infty} X^*(k',j)\int_{-\pi/\Delta x}^{\pi/\Delta x} A_b(k,j')X(k,j)\mathrm{d}k = \sum_{j=-\infty}^{j=\infty} X^*(k',j)\delta_{jj'} \ . \tag{63}$$

Interchanging the order of integration and summation and using Eq.(57) results in

$$\int_{-\pi/\Delta x}^{\pi/\Delta x} A_b(k,j')\sum_{j=-\infty}^{j=\infty} X^*(k',j)X(k,j)\mathrm{d}k = \int_{-\pi/\Delta x}^{\pi/\Delta x}\frac{2\pi}{\Delta x}\delta(k-k')A_b(k,j') = X^*(k',j') \ , \tag{64}$$

which gives us

$$A_b(k,j) = \frac{\Delta x}{2\pi}X^*(k,j) \ . \tag{65}$$

Inserting this definition of $A_b(k)$ into Eq.(61) yields the solution of our difference equation with the initial condition Eq.(39):

$$\begin{aligned} G_i(j,n,j') &= \frac{\Delta x}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{e^{ik(j-j')\Delta x}}{[1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}-\frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \\ &= \frac{\Delta x}{\pi}\int_{0}^{\pi/\Delta x} \mathrm{d}k \frac{\cos(k(j-j')\Delta x)}{[1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}-\frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \\ &= \frac{1}{\pi}\frac{1}{[1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}]^n}\int_0^\pi \mathrm{d}\omega \frac{\cos((j-j')\omega)}{[1-\gamma\cos(\omega)]^n} \end{aligned} \tag{66}$$

where the dimensionless constant γ is defined by

$$\gamma \equiv \frac{\frac{2cD\Delta t}{\Delta x^2}}{1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}} \ , \tag{67}$$

and $\omega \equiv k\Delta x$ is a dummy variable of integration. Since $\gamma \in [0,1)$ the denominator of the integral can never be less than or equal to zero. The integral in Eq.(66) can be solved analytically using the Residue theorem. This solution will be presented in a later section.

Eq.(66) implies that

$$G_i(j,n,j') = G_i(j-j',n,0) \ , \tag{68}$$

and that

$$G_i(-j,n,0) = G_i(j,n,0) \ . \tag{69}$$

We will now verify that $G_i(j,n,j')$ given by Eq.(66) satisfies the difference equation Eq.(38) and the initial conditions Eq.(39). First, we will show that $G_i(j,n=0,j') = \delta_{jj'}$. In this case, we have:

$$\begin{aligned} G_i(j,0,j') &= \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \cos((j-j')\omega) \\ &= \frac{1}{\pi}\left[\frac{\sin((j-j')\omega}{j-j'}\right]_0^\pi \\ &= \delta_{jj'} \ . \end{aligned} \tag{70}$$

Next, we will verify that $G_i(j,n,j')$ satisfies the difference equation Eq.(38). First, for notational convenience, we define

$$B(\omega) \equiv c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2} - \frac{2cD\Delta t}{\Delta x^2}\cos(\omega) \ . \tag{71}$$

The first term in Eq.(38), representing the approximation to the time derivative, applied to $G_i(j,n,j')$ is

$$\begin{aligned} \frac{G_i(j,n+1,j')-G_i(j,n,j')}{\Delta t} &= \frac{1}{\pi\Delta t}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1}}(1-(1+B(\omega))) \\ &= \frac{-1}{\pi\Delta t}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1}}B(\omega) \ . \end{aligned} \tag{72}$$

The second term in Eq.(36), approximating the space derivative, is

$$\begin{aligned} - & cD\frac{G_i(j+1,n+1,j') - 2G_i(j,n+1,j') + G_i(j-1,n+1,j')}{\Delta x^2} \\ = & -\frac{cD}{\pi\Delta x^2}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j'+1)\omega] - 2\cos[(j-l)\omega] + \cos[(j-j'-1)\omega]}{[1+B(\omega)]^{n+1}} \\ = & \frac{-cD}{\pi\Delta x^2}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega](2\cos(\omega)-2)}{[1+B(\omega)]^{n+1}} \ , \end{aligned} \tag{73}$$

where we have used fact that $\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$ to simplify the numerator. The third term in Eq.(36) is

$$c\sigma_a G_i(j,n+1,j') = \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega c\sigma_a \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1}} \ . \tag{74}$$

Adding Eqs.(72)-(74) together produces

$$\begin{aligned} & \frac{G_i(j,n+1,j') - G_i(j,n,j')}{\Delta t} \\ - & cD\frac{G_i(j+1,n+1,j') - 2G_i(j,n+1,j') + G_i(j-1,n+1,j')}{\Delta x^2} \\ + & c\sigma_a G_i(j,n,j') \\ = & \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1}} \left[\frac{-c\sigma_a\Delta t - \frac{2cD\Delta t}{\Delta x^2} + \frac{2cD\Delta t}{\Delta x^2}\cos(\omega)}{\Delta t} - \frac{2cD}{\pi\Delta x^2}[\cos(\omega)-1] + c\sigma_a \right] \\ & = 0 \ . \end{aligned} \tag{75}$$

Since $G_i(j,n,j')$ satisfies the initial conditions and the difference equation, it is the function we seek as a solution to Eq.(38) with the initial conditions given by Eq.(39).

We will now proceed to obtain $G_s(j,n,j',n')$, which satisfies Eq.(40). This equation is a discrete version of Eq.(5). We will use techniques that parallel those used to solve that equation. The procedure by which we obtained a solution of that equation began with Eq.(17).

As we did with $\hat{G}_s(x,t,x',t')$ in Eq.(17), we will expand $G_s(j,n,j',n')$ in terms of the eigenvalues of the spatial part of the difference operator of which $G_s(j,n,j',n')$ is a solution. That is, we expand $G_s(j,n,j',n')$ in terms of the $X(k,j)$, which satisfy Eq.(44). This results in

$$G_s(j,n,j',n') = \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k A_s(k,n,j,n')X(k,j) \ . \tag{76}$$

Now we express the time and space differences of $G_s(j,n,j',n')$ in Eq.(40) as integrals involving $A_s(k,n,j,n')$. The time difference of $G_s(j,n,j',n')$ is

$$\frac{G_s(j,n+1,j',n') - G_s(j,n,j',n')}{\Delta t} = \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{A_s(k,n+1,j,n') - A_s(k,n,j,n')}{\Delta t} X(k,j) \tag{77}$$

and the spatial difference is

$$\frac{G_s(j+1,n+1,j',n') - 2G_s(j,n+1,j',n') + G_s(j-1,n+1,j',n')}{\Delta x^2} = \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \left[-K^2 A_s(k,t,x',t')X(k,j)\right] \tag{78}$$

by virtue of Eq.(44). We insert these expressions into Eq.(40), and use Eq.(60) to represent $\delta_{jj'}$. This yields

$$\begin{aligned}\int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \quad & \left[\frac{A_s(k,n+1,j',n') - A_s(k,n,j',n')}{\Delta t} X(k,j)\right. \\ & + \left. cDK^2 A_s(k,n+1,j',n')X(k,j) + c\sigma_a A_s(k,n+1,j',n')X(k,j)\right] \\ & = \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k X(k,j)X^*(k,j')\delta_{nn'} \ . \end{aligned} \tag{79}$$

Eq.(79) establishes that $A_s(k,n,j',n')$ satisfies

$$\frac{A_s(k,n+1,j',n') - A_s(k,n+1,j',n')}{\Delta t} + cDK^2 A_s(k,n+1,j',n') + c\sigma_a A_s(k,n+1,j',n') = X^*(k,j')\delta_{nn'} \ . \tag{80}$$

We now solve this difference equation for $A_s(k,n,j',n')$. In doing so, we will make use of its similarity to Eq.(43). For $n \leq n'$, we demand that $G_s(j,n,j',n') = 0$, and therefore that $A_s(k,n,j',n') = 0$ because $G_s(j,n,j',n')$ describes the effect of a source at position j' at time step n' on the value of ϕ at position j at time step n', and causality requires that the effect not precede the cause. For $n > n'$, $A_s(k,t,x',t')$ satisfies the difference equation

$$\frac{A_s(k,n+1,j',n') - A_s(k,n,j',n')}{\Delta t} + cDK^2 A_s(k,n+1,j',n') + c\sigma_a A_s(k,n+1,j',n') = 0 \ . \tag{81}$$

By comparing Eq.(81) with Eq.(43), we see that

$$A_s(k,n,j',n') = \frac{A_0}{(1 + c\sigma_a\Delta t + cK^2 D\Delta t)^{(n-n')}} \tag{82}$$

for $n > n'$.

We find the value of A_0 by inserting this expression for A_s in this equation into Eq.(80) and setting $n = n'$. Recalling that $A_s(k,n,j',n) = 0$, we obtain

$$\frac{1}{\Delta t}(A_0 - 0) + cDK^2 A_0 + c\sigma_a A_0 = X^*(k,j')[1 + c\sigma_a\Delta t + cK^2 D\Delta t)] \tag{83}$$

which yields

$$A_0(k,j') = \Delta t X^*(k,j') \ . \tag{84}$$

With this value of A_0 we get

$$A_s(k,n,j',n') = \frac{\Delta t X^*(k,j')}{(1 + c\sigma_a\Delta t + cK^2 D\Delta t)^{(n-n')}} \tag{85}$$

and, using this in Eq.(76), we finally find that

$$\begin{aligned} G_s(j,n,j',n') &= \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{\Delta t X(k,j)X^*(k,j')}{(1 + c\sigma_a\Delta t + cK^2 D\Delta t)^{(n-n')}} \\ &= \Delta t \frac{\Delta x}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{c\Delta t e^{i(j-j')\Delta x}}{(1 + c\sigma_a\Delta t + cK^2 D\Delta t)^{(n-n')}}, n > n' \\ &= 0 \ , \ n \leq n' \ . \end{aligned} \tag{86}$$

$G_s(j,n,j',n')$ can be written in a manifestly real form by using the definition of $X(k,j)$ in Eq.(86) and changing the range of integration. Following Eqs.(66-67), it is easily shown that

$$\begin{aligned} G_s(j,n,j',n') &= \Delta t\frac{\Delta x}{\pi}\int_0^{\pi/\Delta x} \mathrm{d}k \frac{\cos[k(j-j')\Delta x]}{[1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}-\frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^{(n-n')}} \\ &= \frac{\Delta t}{[1+c\sigma_a\Delta t+\frac{2cD\Delta t}{\Delta x^2}]^{(n-n')}}\frac{1}{\pi}\int_0^{\pi}\mathrm{d}\omega\frac{\cos((j-j')\omega)}{[1-\gamma\cos(\omega)]^{(n-n')}} \end{aligned} \tag{87}$$

when $n > n'$ and with γ defined in Eq.(67). Note that G_s has units of time, as discussed in the remarks following Eq.(40). Eq.(87) implies that

$$G_s(j,n,j',n') = G_s(j-j',n-n',0,0)\ , \tag{88}$$

and that

$$G_s(-j,n,0,n') = G_s(j,n,0,n')\ . \tag{89}$$

Comparing Eq.(87) and Eq.(66) shows that

$$G_s(j,n,j',n') = \Delta t G_i(j-j',n-,n',0)\ . \tag{90}$$

We will now verify that $G_s(j,n,j',n')$ given by Eq.(86) satisfies the difference equation Eq.(40). Let us first examine the case when $n > n'$. Then the first term in Eq.(40), representing the approximation to the time derivative, applied to $G_s(j,n,j',n')$ is

$$\begin{aligned} \frac{G_s(j,n+1,j',n')-G_s(j,n,j',n')}{\Delta t} &= \frac{1}{\pi}\int_0^{\pi}\mathrm{d}\omega\frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1-n'}}(1-(1+B(\omega))) \\ &= \frac{-1}{\pi}\int_0^{\pi}\mathrm{d}\omega\frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1-n'}}B(\omega)\ . \end{aligned} \tag{91}$$

where we have used the quantity $B(\omega)$ defined in Eq.(71). The second term in Eq.(40), approximating the space derivative, is

$$\begin{aligned} &- cD\frac{G_s(j+1,n+1,j',n')-2G_s(j,n+1,j',n')+G_s(j-1,n+1,j',n')}{\Delta x^2} \\ &= -\frac{cD\Delta t}{\pi\Delta x^2}\int_0^{\pi}\mathrm{d}\omega\frac{\cos[(j-j'+1)\omega]-2\cos[(j-l)\omega]+\cos[(j-j'-1)\omega]}{[1+B(\omega)]^{n+1-n'}} \\ &= \frac{-cD\Delta t}{\pi\Delta x^2}\int_0^{\pi}\mathrm{d}\omega\frac{\cos[(j-j')\omega](2\cos(\omega)-2)}{[1+B(\omega)]^{n+1-n}}\ , \end{aligned} \tag{92}$$

where we have used fact that $\cos(\alpha+\beta)=\cos(\alpha)\cos(\beta)-\sin(\alpha)\sin(\beta)$ to simplify the numerator. The third term in Eq.(40) is

$$c\sigma_a G_s(j,n+1,j',n') = \frac{c\Delta t}{\pi}\int_0^{\pi}\mathrm{d}\omega\sigma_a\frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1-n}}\ . \tag{93}$$

Adding Eqs.(91)-(93) together produces

$$\begin{aligned}
&\frac{1}{c}\frac{G_s(j,n+1,j',n')-G_s(j,n,j',n')}{\Delta t} \\
-\;& D\frac{G_s(j+1,n+1,j',n')-2G_s(j,n+1,j',n')+G_s(j-1,n+1,j',n')}{\Delta x^2} \\
+\;& \sigma_a G_s(j,n,j',n') = \\
&\frac{c\Delta t}{\pi}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1-n'}}\left[\frac{-c\sigma_a\Delta t-\frac{2cD\Delta t}{\Delta x^2}+\frac{2cD\Delta t}{\Delta x^2}\cos(\omega)}{c\Delta t}-\frac{2D}{\pi\Delta x^2}[\cos(\omega)-1]+\sigma_a\right] \\
=\;& \frac{c\Delta t}{\pi}\frac{1}{c\Delta t}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]^{n+1-n'}}\left[-B(\omega)+\frac{2cD\Delta t}{\pi\Delta x^2}-\frac{2cD\Delta t}{\pi\Delta x^2}\cos(\omega)+c\sigma_a\Delta t\right] \\
&= 0\ .
\end{aligned} \tag{94}$$

Now we examine the case when $n = n'$. In this case, $G_s(j,n,j',n) = 0$, and the first term in Eq.(40) is

$$\begin{aligned}
\frac{G_s(j,n+1,j',n)-G_s(j,n,j',n)}{\Delta t} &= \frac{G_s(j,n+1,j',n)-0}{\Delta t} \\
&= \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{1+B(\omega)}\ .
\end{aligned} \tag{95}$$

The second term in Eq.(40) when $n = n'$ is

$$\begin{aligned}
-\;& cD\frac{G_s(j+1,n+1,j',n)-2G_s(j,n+1,j',n)+G_s(j-1,n+1,j',n)}{\Delta x^2} \\
=\;& -\frac{cD\Delta t}{\pi\Delta x^2}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j'+1)\omega]-2\cos[(j-l)\omega]+\cos[(j-j'-1)\omega]}{[1+B(\omega)]} \\
=\;& \frac{-cD\Delta t}{\pi\Delta x^2}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega](2\cos(\omega)-2)}{[1+B(\omega)]}\ ,
\end{aligned} \tag{96}$$

where we have again used fact that $\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$ to simplify the numerator. The third term in Eq.(40) when $n = n'$ is

$$c\sigma_a G_s(j,n+1,j',n) = \frac{c\Delta t}{\pi}\int_0^\pi \mathrm{d}\omega\sigma_a \frac{\cos[(j-j')\omega]}{[1+B(\omega)]}\ . \tag{97}$$

Adding Eqs.(95)-(97) together produces

$$\begin{aligned}
&\frac{G_s(j,n+1,j',n)-G_s(j,n,j',n)}{\Delta t} \\
-\;& cD\frac{G_s(j+1,n+1,j',n)-2G_s(j,n+1,j',n)+G_s(j-1,n+1,j',n)}{\Delta x^2} \\
+\;& c\sigma_a G_s(j,n,j',n) = \\
&\frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]}\left[1-\frac{2cD\Delta t}{\pi\Delta x^2}[\cos(\omega)-1]+c\sigma_a\Delta t\right] \\
=\;& \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \frac{\cos[(j-j')\omega]}{[1+B(\omega)]}\left[1+\frac{2cD\Delta t}{\pi\Delta x^2}-\frac{2cD\Delta t}{\pi\Delta x^2}\cos(\omega)+c\sigma_a\Delta t\right] \\
=\;& \frac{1}{\pi}\int_0^\pi \mathrm{d}\omega \cos[(j-j')\omega] \\
=\;& \delta_{jj'}\ .
\end{aligned} \tag{98}$$

When $n < n'$, $G_s(j,n,j',n') = G_s(j,n+1,j',n') = 0$, so we have, trivially,

$$\frac{G_s(j,n+1,j',n') - G_s(j,n,j',n)}{\Delta t} - cD\frac{G_s(j+1,n+1,j',n') - 2G_s(j,n+1,j',n) + G_s(j-1,n+1,j',n')}{\Delta x^2} + \quad c\sigma_a G_s(j,n,j',n') = 0 \ , \ n < n' \ . \tag{99}$$

Eq.(94), Eq.(98), and Eq.(99) combine to show that, for any n,

$$\frac{G_s(j,n+1,j',n') - G_s(j,n,j',n')}{\Delta t} - cD\frac{G_s(j+1,n+1,j',n') - 2G_s(j,n+1,j',n') + G_s(j-1,n+1,j',n')}{\Delta x^2} + c\sigma_a G_s(j,n+1,j',n') = \delta_{jj'}\delta_{nn'} \ . \tag{100}$$

This means that $G_s(j,n,j',n')$ satisfies Eq.(40), and so it is the function we seek.

Since G_i and G_s satisfy the equations Eq.(38) and Eq.(40) respectively, the general solution to Eq.(36), the discretized diffusion equation with an arbitrary source $S(j,n)$ defined and arbitrary initial conditions $\phi_0(j)$ is given by the sum defined by Eq.(37), with $G_i(j,n,j')$ given by Eq.(66) and $G_s(j,n,j',n')$ given by Eq.(86).

As was the case with $\hat{G}_i(x,t,x')$ and $\hat{G}_s(x,t,x',t')$, $G_i(x,t,x')$ and $G_s(x,t,x',t')$ can both be written in terms of a single function $G_0(m,n)$. $G_0(m,n)$ is defined by

$$G_0(m,n) \equiv \frac{\Delta x}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{e^{ikm\Delta x}}{[1 + c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2} - \frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \ . \tag{101}$$

From Eq.(66), we see that

$$G_i(j,n,j') = G_0(j-j',n) \ , \tag{102}$$

and from Eq.(90), we see that

$$G_s(j,n,j',n') = \Delta t G_0(j-j',n-n') \ . \tag{103}$$

With $G_i(j,n,j')$ and $G_s(j,n,j',n')$ determined, we can calculate the solution $\phi(j,n)$ of the discretized diffusion equation Eq.(36), for an arbitrary source function $S(j,n)$ and arbitrary initial conditions $\phi(j,0)$. The solution is given for any j and n by Eq.(37). The utility of this solution in code validation is that we expect a code solving the difference equation Eq.(36) to produce results which agree with the solution of Eq.(37) within roundoff. To generate such a solution, we need to compute the integral in Eq.(101) analytically. A closed-form solution for this integral will be derived in the next section.

4. THE ANALYTIC SOLUTION OF THE INTEGRAL IN THE DEFINITION OF G_0

The difference equations satisfied by G_i and G_s (Eq.(38) and Eq.(40) respectively) are discrete first-order approximations to the differential equations satisfied by $\hat{G}_i$ and $\hat{G}_s$ (Eq.(3) and Eq.(5) respectively). Thus it is reasonable to suppose that G_i and G_s are first-order approximations to $\hat{G}_i$ and $\hat{G}_s$ respectively. Before developing analytic expressions for G_i and G_s, we will demonstrate this.

We note again that the purpose of displaying the convergence of G_i to $\hat{G}_i$ and G_s to $\hat{G}_d$ is not done to suggest that G_i and G_s are useful for approximating to $\hat{G}_i$ and $\hat{G}_s$, or that G_i and G_s are useful in obtaining approximate solutions to the differential equation Eq.(1). G_i and G_s are used in this paper to obtain exact solutions to the difference equation Eq.(36) for the purposes of code verification.

Both $\hat{G}_i$ and $\hat{G}_s$ can be represented in terms of $\hat{G}_0$ defined by Eq.(26), and both G_s and G_i can be represented in terms of G_0 defined by Eq.(101). Thus the convergence we seek to demonstrate can be shown by demonstrating that G_0 converges to $\hat{G}_0$ in the appropriate limit.

The limit we wish to take is $m \to \infty$, $\Delta x \to 0$ with $m\Delta x \to x$ and $n \to \infty$, $\Delta t \to 0$ with $n\Delta t \to t$. In this limit, the quantity in brackets in the denominator of the integral in Eq.(101) becomes

$$\begin{aligned}
[1 + c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2}(1 - \cos(k\Delta x))] &= [1 + c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2}(\frac{1}{2}k^2\Delta x^2 + O(\Delta x^4)] \\
&= [1 + c\sigma_a\Delta t + cD\Delta t k^2 + O(\Delta x^2)] \\
&= [1 + c\frac{\sigma_a t + cDtk^2}{n} + O(\Delta x^2)] \; . \qquad (104)
\end{aligned}$$

The limit of $\frac{G_0(m,n)}{\Delta x}$ then becomes

$$\begin{aligned}
lim_{m\to\infty n,\, \to\infty}\frac{G_0(m,n)}{\Delta x} &= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \frac{e^{ikx}}{[1 + c\frac{\sigma_a t + cDtk^2}{n}}{}^n \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \frac{e^{ikx}}{e^{-c\sigma_a t + cDtk^2}} \\
&= \frac{1}{\sqrt{4\pi Dt}} e^{\left[\frac{-x^2}{4Dt} - c\sigma_a t\right]} \\
&= \hat{G}_0(x,t) \; . \qquad (105)
\end{aligned}$$

We see that as Δx and Δt become small, the discrete Green's function $G_0(m,n)$ becomes a better and better approximation to $\hat{G}_0(x,t)\Delta x$. The reason for the seemingly extraneous factor of Δx comes from the fact that we chose the source terms in Eq.(38) and Eq.(40 to be $\delta_{jj'}$ and $\delta_{jj'}\delta_{nn'}$ respectively. Had we chosen to make them $\frac{\delta_{jj'}}{\Delta x}$ and $\frac{\delta_{jj'}\delta_{nn'}}{\Delta x \Delta t}$, then $G_0(m,n)$ would be normalized so that in the limit it would approach $\hat{G}_0(x,t)$. In that case, the sum over G_i in Eq.(37) would be multiplied by Δx and the sum over G_s would be multiplied by $\Delta x \Delta t$. This choice is a matter of convention.

We will now describe a method for obtaining an analytic expression for the discrete Green's functions $G_i(j,n,j')$ and $G_s(j,n,j',n')$. Both quantities can be obtained from $G_0(m,n)$ defined by Eq.(101). From Eq.(66), we see that $G_i(j,n,j') = G_0(j-j',n)$, and from Eq.(90), we see that $G_s(j,n,j',n') = \Delta t G_0(j-j',n-n')$. Eqs.(102)-(103) show that we need only generate values of $G_0(m,n)$. Eq.(68)-(90) show that need only generate values of $G_0(m,n)$ with $m \geq 0$.

We can obtain closed-form expressions for $G_0(m,n)$ by performing the integral in Eq.(101) using

the Residue theorem [2]. Repeating the definition of $G_0(m,n)$ from Eq.(101), we have

$$\begin{aligned} G_0(m,n) &= \frac{\Delta x}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{d}k \frac{e^{ikm\Delta x}}{[1+c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2} - \frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}\omega \frac{e^{im\omega}}{[1+c\sigma_a\Delta t + \frac{2cD\Delta t}{\Delta x^2} - \frac{2cD\Delta t}{\Delta x^2}\cos(k\Delta x)]^n} \\ &= \frac{1}{2\pi}\gamma^n\left(\frac{\Delta x^2}{2cD\Delta t}\right)^n \int_{-\pi}^{\pi} \mathrm{d}\omega \frac{e^{im\omega}}{[1-\gamma\cos\omega]^n} \end{aligned} \tag{106}$$

with γ defined by Eq.(67). Using the definition of cosine in terms of exponentials, G_0 can also be written as

$$G_0(m,n) = \frac{1}{\pi}\gamma^n\left(\frac{\Delta x^2}{2cD\Delta t}\right)^n \int_0^{\pi} \mathrm{d}\omega \frac{cos(m\omega)}{[1-\gamma\cos(\omega)]^n} \ . \tag{107}$$

In this form, it is apparent that, as already stated, $G_0(m,n)$ is real for real m and n, and that $G_0(-m,n) = G_0(m,n)$.

Using the substitution

$$z = e^{i\omega} \tag{108}$$

which results in

$$\mathrm{d}\omega = \frac{dz}{iz}, cos(\omega) = \frac{1}{2}\left(z + \frac{1}{z}\right) \tag{109}$$

in Eq.(106), we obtain

$$G_0(m,n) = \frac{1}{2\pi i}(-1)^n 2^n \left(\frac{\Delta x^2}{2cD\Delta t}\right)^n \oint_C \mathrm{d}z \frac{z^{m+n-1}}{\left[z^2 - \frac{2}{\gamma} + 1\right]^n} \ , \tag{110}$$

where the contour C is the unit circle in the complex plane traversed in a counterclockwise direction. This integral expresses $G_0(m,n)$ in a form to which the Residue theorem can be applied. The Residue theorem states that

$$\frac{1}{2\pi i}\oint_C \mathrm{d}z f(z) = \mathrm{Res}(z') \ , \tag{111}$$

where z' is the only pole of the function f enclosed by the contour C.

We will take $n \geq 0$ and, exploiting the symmetry shown in Eq.(107), that $m \geq 0$. When $n = 0$, we have

$$G_0(m,0) = \frac{1}{2\pi i}\oint_C \mathrm{d}z z^{m-1} \ , \tag{112}$$

which has a pole of order 1 a t $z = 0$ when $m = 0$, and does not have a pole otherwise. When $m = 0$, the value of the residue is 1, so we obtain

$$G_0(m,0) = \delta_{m0} \tag{113}$$

which is consistent with Eq.(39).

When $n > 0$, the denominator of the integrand in Eq.(110) has zeros at $z = \frac{1}{\gamma} \pm \sqrt{\frac{1}{\gamma^2} - 1}$. Denoting the 2 roots as z_- and z_-, we see that $\gamma > 0$ implies that only z_- is enclosed by the contour C. Thus the integrand has a pole of order n at $z = z_-$.

With

$$f \equiv \frac{z^{m+n-1}}{\left[z^2 - \frac{2}{\gamma} + 1\right]^n} = \frac{z^{m+n-1}}{[(z-z_+)(z-z_-)]^n} \ , \tag{114}$$

$G_0(m,n)$ is given by

$$G_0(m,n) = \frac{1}{2\pi i}(-1)^n 2^n \left(\frac{\Delta x^2}{2cD\Delta t}\right)^n \oint_C \mathrm{d}z f(z) \ , \tag{115}$$

and thus

$$G_0 = -1^n 2^n \left(\frac{\Delta x^2}{2cD\Delta t}\right)^n \mathrm{Res} f(z_-) \ . \tag{116}$$

We seek the residue of f at z_-, which is a pole of order n. The value of the residue is given by [2] p. 85:

$$\begin{aligned} \mathrm{Res} f(z_-) &= \frac{1}{(n-1)!} lim_{z\to z_-} \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}}[(z-z_-)^n f(z)]\right] \\ &= \frac{1}{(n-1)!} lim_{z\to z_-} \left[\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}} \frac{z^{m+n-1}}{(z-z_+)^n}\right] \ . \end{aligned} \tag{117}$$

Using the fact that

$$\frac{\mathrm{d}^p}{\mathrm{d}z^p} z^{m+n-1} = \frac{(m+n-1)!}{(m+n-1-p)!} z^{m+n-1-p)} \tag{118}$$

for $m+n-1>0$ and, with $n>0$,

$$\frac{\mathrm{d}^p}{\mathrm{d}z^p}(z-z_+)^{-n} = (-1)^p \frac{(n+i-1)!}{(n-1)!}(z-z_+)^{-(n+i)} \ , \tag{119}$$

which implies that

$$\frac{\mathrm{d}^{n-1-p}}{\mathrm{d}z^{n-1-p}}(z-z_+)^{-n} = (-1)^{n-1-p} \frac{(2n-2-p)!}{(n-1)!}(z-z_+)^{-(2n-p-1)} \ , \tag{120}$$

the derivative term can be expanded:

$$\begin{aligned} &\frac{\mathrm{d}^{n-1}}{\mathrm{d}z^{n-1}} \frac{z^{m+n-1}}{(z-z_+)^n} = \sum_{p=0}^{n-1} \frac{(n-1)!}{p!(n-1-p)!} \frac{\mathrm{d}^p}{\mathrm{d}z^p}[z^{m+n-1}] \frac{\mathrm{d}^{n-1-p}}{\mathrm{d}z^{n-1-p}} \left[\frac{1}{(z-z_+)^n}\right] \\ = &\sum_{p=0}^{n-1} \frac{(n-1)!}{p!(n-1-p)!} \frac{(m+n-1)!}{(m+n-1-p)!} z^{m+n-1-p} (-1)^{n-1-p} \frac{(2n-2-p)!}{(n-1)!}(z-z_+)^{-(2n-p-1)} \\ = &(-1)^{n-1} \frac{z^{m+n-1}}{(z-z_+)^{2n-1}} \sum_{p=0}^{n-1} (-1)^p \frac{(m+n-1)!(2n-2-p)!}{p!(n-1-p)!(m+n-1-p)!} \left(\frac{z-z_+}{z}\right)^p \ . \end{aligned} \tag{121}$$

Evaluating this at z_-, substituting the result into Eq.(117), and using the fact that $z_- - z_+ < 0$, we obtain

$$\mathrm{Res} f(z_-) = (-1)^n \frac{z_-^{m+n-1}}{(z_+ - z_-)^{2n-1}} \sum_{p=0}^{n-1} \frac{(m+n-1)!(2n-2-p)!}{p!(n-1-p)!(m+n-1-p)!(n-1)!} \left(\frac{z_+ - z_-}{z_-}\right)^p \tag{122}$$

which yields, via Eq.(116)

$$G_0(m,n) = \left(\frac{\Delta x^2}{2cD\Delta t}\right)^n 2^n \frac{z_-^{m+n-1}}{(z_+ - z_-)^{2n-1}} \sum_{p=0}^{n-1} \frac{(m+n-1)!(2n-2-p)!}{p!(n-1-p)!(m+n-1-p)!(n-1)!} \left(\frac{z_+ - z_-}{z_-}\right)^p . \tag{123}$$

Using the fact that $z_+ - z_- = 2\sqrt{\frac{1}{\gamma^2} - 1}$, we obtain

$$\begin{aligned} G_0(m,n) &= \left(\frac{\Delta x^2}{2cD\Delta t}\right)^n z_-^{m+n-1} \left(\frac{\gamma}{\sqrt{1-\gamma^2}}\right)^{2n-1} \times \\ &\sum_{p=0}^{n-1} \frac{1}{2^{n-1-p}} \frac{(m+n-1)!(2n-2-p)!}{p!(n-1-p)!(m+n-1-p)!(n-1)!} \left(\frac{\sqrt{1-\gamma^2}}{1-\sqrt{1-\gamma^2}}\right)^p . \end{aligned} \tag{124}$$

The factorial coefficient $C(m,n,p)$ defined by

$$C(m,n,p) \equiv \frac{(m+n-1)!(2n-2-p)!}{p!(n-1-p)!(m+n-1-p)!(n-1)!} \tag{125}$$

satisfies

$$C(m,n,0) = \frac{(m+n-1)!(2n-2)!}{(n-1)!(m+n-1)!(n-1)!} = \frac{(2n-2)!}{[(n-1)!]^2} \tag{126}$$

and is independent of m when $p = 0$. $C(m,n,0)$ satisfies the recurrence relation

$$C(m,n,0) = C(m,n-1,0)\frac{2(2n-3)}{n-1} \tag{127}$$

for $n > 1$. Using the fact that $C(m,1,0) = 1$, we can compute values of $C(m,n,0)$ for any n with less concern for overflows that can result from calculating the factorials of large numbers that would be required in calculating $C(m,n,0)$ using Eq.(125).

$C(m,n,p)$ satisfies the recurrence relation

$$C(m,n,p) = C(m,n,p-1)\frac{(m+n-p)(n-p)}{p(2n-1-p)}. \tag{128}$$

The sum in Eq.(124) consists of terms of the form

$$T(m,n,p) \equiv \frac{2^p}{2^{n-1}} C(m,n,p) \left(\frac{\sqrt{1-\gamma^2}}{1-\sqrt{1-\gamma^2}}\right)^p \tag{129}$$

with

$$T(m,n,0) = \frac{1}{2^{n-1}} C(m,n,0) \ . \tag{130}$$

Defining

$$y \equiv \frac{\sqrt{1-\gamma^2}}{1-\sqrt{1-\gamma^2}} \tag{131}$$

and using Eq.(128), it can be seen that $T(m,n,p)$ satisfies the recurrence relation

$$\begin{aligned} T(m,n,p) &= 2\frac{2^{p-1}}{2^{n-1}}C(m,n,p-1)\frac{C(m,n,p)}{C(m,n,p-1)}y^{p-1}y \\ &= 2y\frac{(m+n-p)(n-p)}{p(2n-1-p)}T(m,n,p-1)\ . \end{aligned} \tag{132}$$

This recurrence, starting with $p=0$, can be used to calculate $T(m,n,p)$ for any value of p. The first value, $T(m,n,0)$, is calculated using Eq.(130). Note that explicitly calculated values of $C(m,n,p)$ other than $C(m,n,0)$ are not required to calculate $T(m,n,p)$.

Eq.(124), with the sum over p performed using the $T(m,n,p)$ calculated using the recurrence Eq.(132), yields values of $G_0(m,n)$ for any values of $m >= 0$ and $n > 0$. Values with $m < 0$ are obtained by applying the fact that $G_0(-m,n) = G_0(m,n)$. For $n = 0$, we use $G_0(0,n) = \delta_{m0}$.

We will now display results for $G_0(n,m)$ computed with particular values of σ_s, σ_a, etc. We compare the computed values to approximate values obtained by solving the linear system given by Eq.(38) with the initial condition Eq.(39). This is done to establish the correctness of the analytic solution. We also compare the convergence of the discrete Green's function $G_0(m,n)$ to the continuous Green's function for the diffusion equation $\hat{G}(x,t)$, which is given by Eq.(26).

In the following, we use the following values: $c=1, \sigma_a = 0.1, \sigma_s = 50.0, \Delta x = 0.05$, and $\Delta t = 0.1$. The values of σ_a and σ_s result in $D \equiv \frac{1}{3(\sigma_a+\sigma_s)} = 0.00665336$.

Eq.(38) with the initial condition Eq.(39) describes a tridiagonal system of equations for $G_i(j,n,j')$. Eq.(102) allows us to define G_0 in terms of G_i. Setting $j' = 0$ in Eq.(38) and Eq.(39), we see that $G_0(m,n)$ satisfies the difference equation

$$\begin{aligned} \frac{G_0(m,n+1)-G_0(m,n)}{\Delta t} &- cD\frac{G_0(m+1,n+1)-2G_0(m,n+1)+G_0(m-1,n+1)}{\Delta x^2} \\ &+ c\sigma_a G_0(m,n+1) = 0 \end{aligned} \tag{133}$$

with the initial condition

$$G_0(m,0) = \delta_{m0}\ . \tag{134}$$

Eq.(133) with Eq.(134) define an infinite tridiagonal system that relates the values of $G_0(m+1,n+1), G_0(m,n+1)$ and $G_0(m-1,n+1)$ to the value $G_0(m,n)$. Because the value of $G_0(m,0)$ is zero everywhere except at $m=0$, we expect that the value of $G_0(m,n)$ is very weakly dependent on the value of $G_0(m',n-1)$, where $|m'-n|$ is large compared to $D/\Delta x$. So we can construct a finite linear system by confining allowed values of m to the range $[-M,M]$, where M is a large integer.

The finite tridiagonal system resulting from this approximation can be solved by standard methods, such as those described in [4]. Solving this system repeatedly for $G_0(m,n+1)$ in terms of $G_0(m,n+1)$ gives us a series of approximate values of G_0.

Fig.(1) compares $G_0(m,n)$ computed from the analytic solution given by Eq.(124) to the approximate values computed via the solution of Eq.(133) and Eq.(134) truncated with $M = 500$. The results of the linear system solution are shows as black crosses, while the analytic solutions are shown as lines. For small n, both solutions start out with large values near $m = 0$; as n increases, the solutions spread out to larger values of m, and decline in magnitude. This is

expected, since the solutions should behave similarly to the decaying Gaussian solutions given by $\hat{G}_0$ in Eq.(26). Fig.(2) shows the same data as Fig.(1) plotted on a log scale. Both figures indicate that the agreement between the two values is very good.

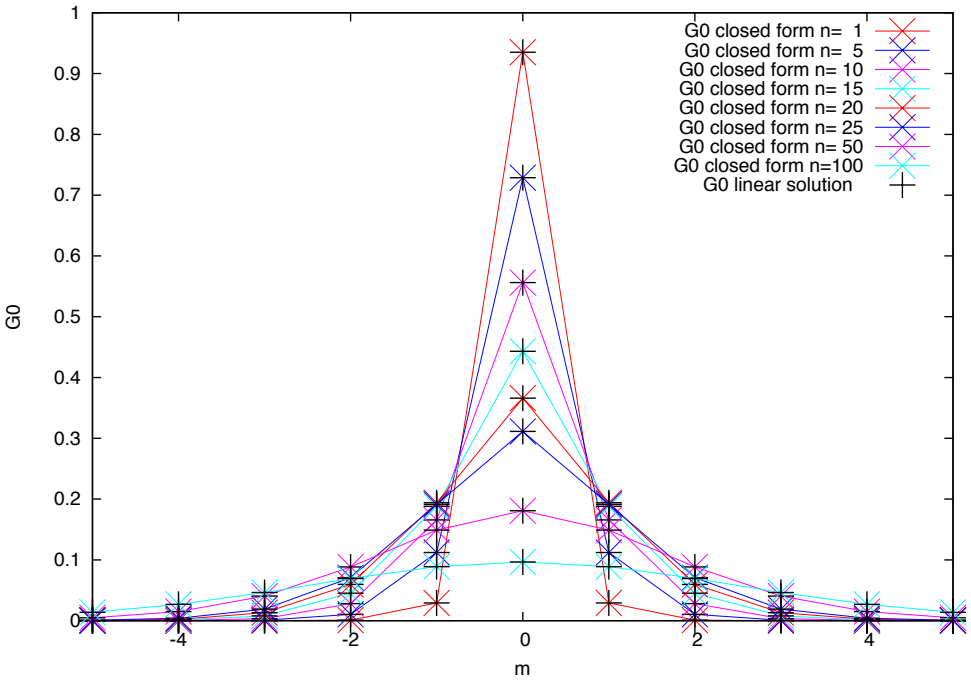

Figure 1: Plot of $G_0(n,m)$ for various values of m and n computed by Eq.(124) compared with approximate values obtained by solving the linear system given by Eq.(133). The values computed with the analytic solution Eq.(124) agree well with the approximate values obtained by solving Eq.(133) and Eq.(134).

Next we show that the difference between G_0 computed with Eq.(124) and the approximate G_0 computed by solving a linear system is small. Fig.(3) shows that, for a wide range of n and m, the absolute value of the difference between the two computed values of G_0 is always smaller than 1.5×10^{-14}.

Another estimate of the error in the values of $G_0(m,n)$ calculated with Eq.(124) is provided by substituting these values into the difference equation that these values should satisfy. This equation is

$$\frac{G_0(m,n+1)-G_0(m,n)}{\Delta t} - cD\frac{G_0(m+1,n+1)-2G_0(m,n+1)+G_0(m-1,n+1)}{\Delta x^2} + c\sigma_a G_0(m,n+1) = 0 \; . \tag{135}$$

$G_0(m,n)$ satisfies Eq.(135) because $G_0(m,n) = G_i(m,n,0)$ as implied by Eq(66). Eq.(135) is obtained by applying Eq.(38) to $G_i(m,n,0)$. We will define the error$E(m,n)$ in our value of

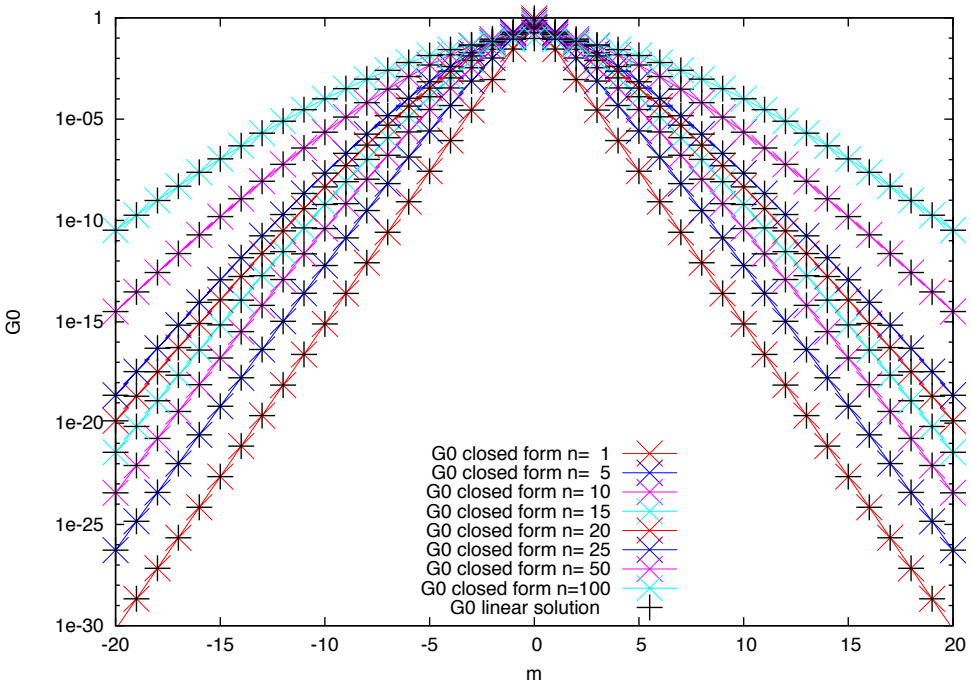

Figure 2: The same data plotted in Fig.(1) with a log scale on the y axis.

$G_0(m,n)$ via

$$E(m,n) = \frac{G_0(m,n+1) - G_0(m,n)}{\Delta t} - cD\frac{G_0(m+1,n+1) - 2G_0(m,n+1) + G_0(m-1,n+1)}{\Delta x^2} + c\sigma_a G_0(m,n+1) \tag{136}$$

and examine the absolute value of $E(m,n)$ for various values of m and n. Fig.(4) shows that this quantity is always smaller than 1.5×10^{-14}. The small values of the values plotted in Fig.(3) and Fig.(136) establish that Eq.(124) is an accurate means of evaluating $G_0(m,n)$.

Next, we will compare $\frac{G_0(m,n)}{\Delta x}$ to $\hat{G}_0(x,t)$. This demonstrates the convergence of $\frac{G_0(m,n)}{\Delta x}$ to $\hat{G}_0(x,t)$. This convergence is an illustration of the results of Eq.(105). Fig.(5) plots $\frac{G_0(m,n)}{\Delta x}$ for various values of Δx and Δt, along with $\hat{G}_0(x,t)$, at a fixed time $t = 1$. In this figure, for fixed values of x and t, n and m have been increased while both Δx and Δt have been decreased, to keep x and t constant. Fig.(5) shows that $\frac{G_0(m,n)}{\Delta x}$ becomes closer to $\hat{G}_0(x,t)$ as we increase the resolution of our discretization.

Fig.(6) shows the decrease in the absolute value of the difference between the values of $\frac{G_0(m,n)}{\Delta x}$ and $\hat{G}_0(x,t)$ that were plotted in Fig.(5). This difference becomes smaller as we increase the resolution of our discretization.

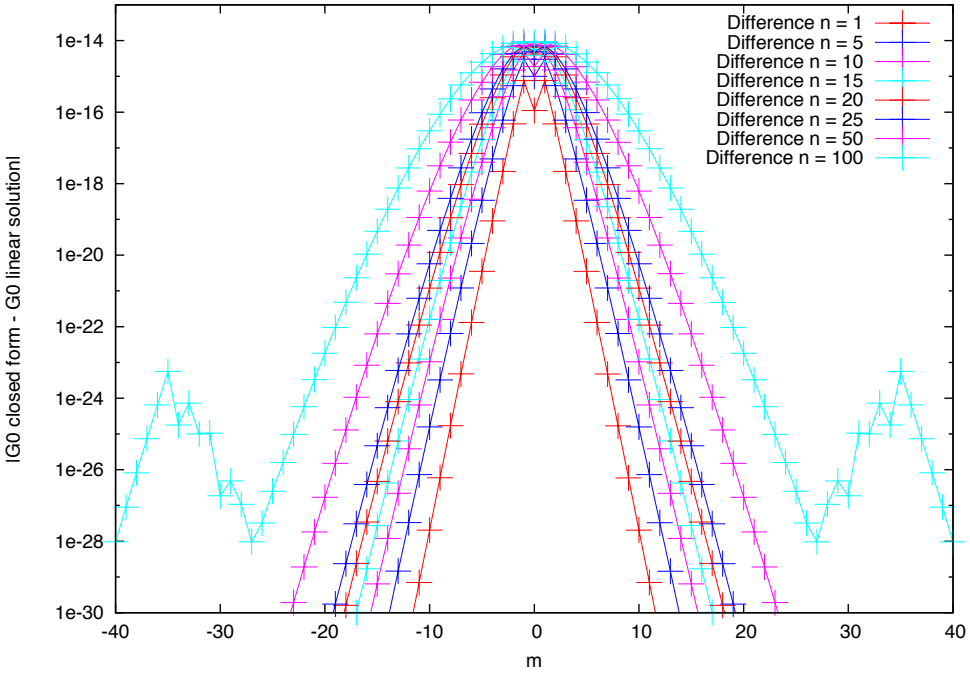

Figure 3: Absolute value of the differences between the values calculated by the closed form solution Eq.(124) and the solution of the linear system. This is the difference of the colored lines and the black lines plotted in Figs.(1)-(2). The magnitude of the difference between the analytic values and the approximate values is less than 1.5×10^{-14}.

We wish to point out we do not claim that $G_0(m,n)$ is useful as an approximation to $\hat{G}_0(x,t)$ that can be used to generate approximate solutions to the differential equation Eq.(1). The usefulness of the expression for $G_0(m,n)$ is that it can be used to calculate exact values for $G_i(j,n,j')$ and $G_s(j,n,j',n')$ for any j and n. These in turn allow us, via Eq.(37), to calculate exact solutions to the difference equation Eq.(36) for arbitrary source $S(j,n)$ and arbitrary initial conditions $\phi_0(j)$. In the next section, we will select a specific source and initial conditions, and compare the solution of Eq.(36) with the output of the diffusion package of an inertial confinement fusion code.

5. COMPARISON OF ANALYTIC RESULTS AND CODE RESULTS FOR A SPECIFIC TEST PROBLEM

With the values of $G_i(j,n,j')$ and $G_s(j,n,j',n')$ obtained by the techniques described in section 4., Eq.(37) allows us to calculate the solution $\phi(j,n)$ of Eq.(36) for arbitrary initial conditions $\phi_0(j)$ and source $S(j,n)$. In this section, we will compare the value of $\phi(j,n)$ obtained for specific choices of initial conditions $\phi_0(j)$ and source $S(j,n)$ to that obtained by a computer code which

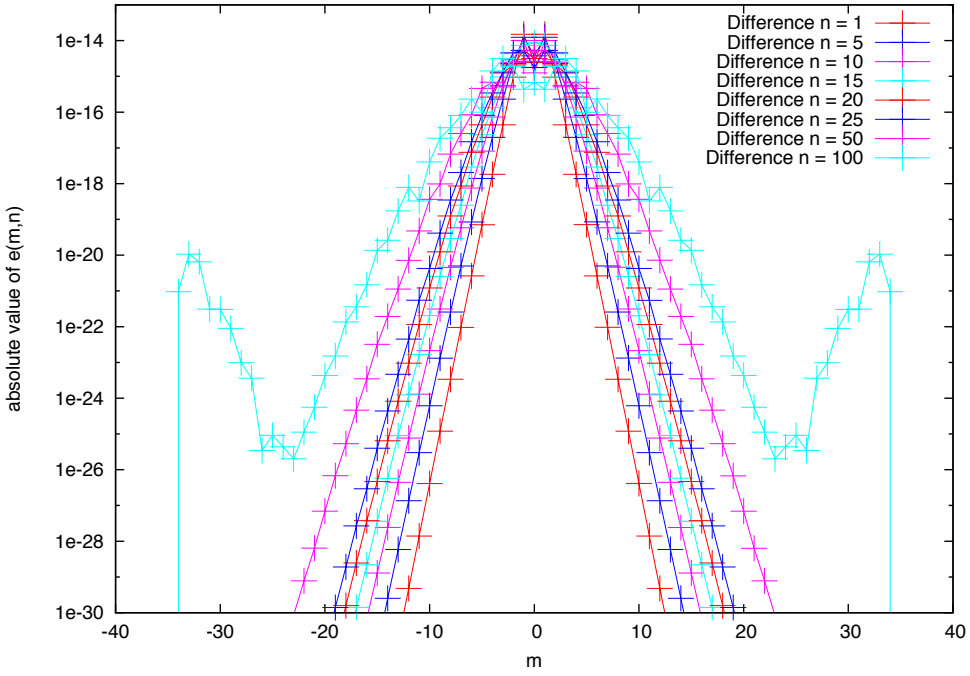

Figure 4: Absolute value of the error in our expression for $G_0(m,n)$ for various values of m and n. The error $E(m,n)$ is defined by Eq.(136). The analytic solution for $G_0(m,n)$ satisfies the difference equation Eq.(133) with an accuracy greater than 2×10^{-14} .

solves Eq.(36).

The computer code to which we will compare our solution is the inertial confinement fusion code Ares [5]. The Ares code radiation diffusion package solves coupled difference equations for radiation energy density ϕ and matter temperature T_m. On a one-dimensional Cartesian grid, Ares represents both of these quantities as arrays holding values for ϕ and T_m in zone j for time step n. The equation satisfied by $\phi(j,n)$ in Ares is

$$\frac{\phi(j,n+1)-\phi(j,n)}{\Delta t} - cD\frac{\phi(j+1,n+1)-2\phi(j,n)+\phi(j-1,n+1)}{\Delta x^2} + c\sigma_a\phi(j,n+1) = c\sigma_a a T_m^4 + S(j,n) \tag{137}$$

and the equation satisfied by $T_m(j,n)$ in Ares is

$$\frac{e_m(j,n+1)-e_m(j,n)}{\Delta t} = c\sigma_a\phi(j,n+1) - c\sigma_a a T_m(j,n+1)^4 \tag{138}$$

where e_m is the matter energy density. In general, e_m is related to the mass density ρ and T_m by a function called the equation of state. Inverting the equation of state numerically allows the code to calculate $T_m(j,n+1)$ from $e_m(j,n+1)$.

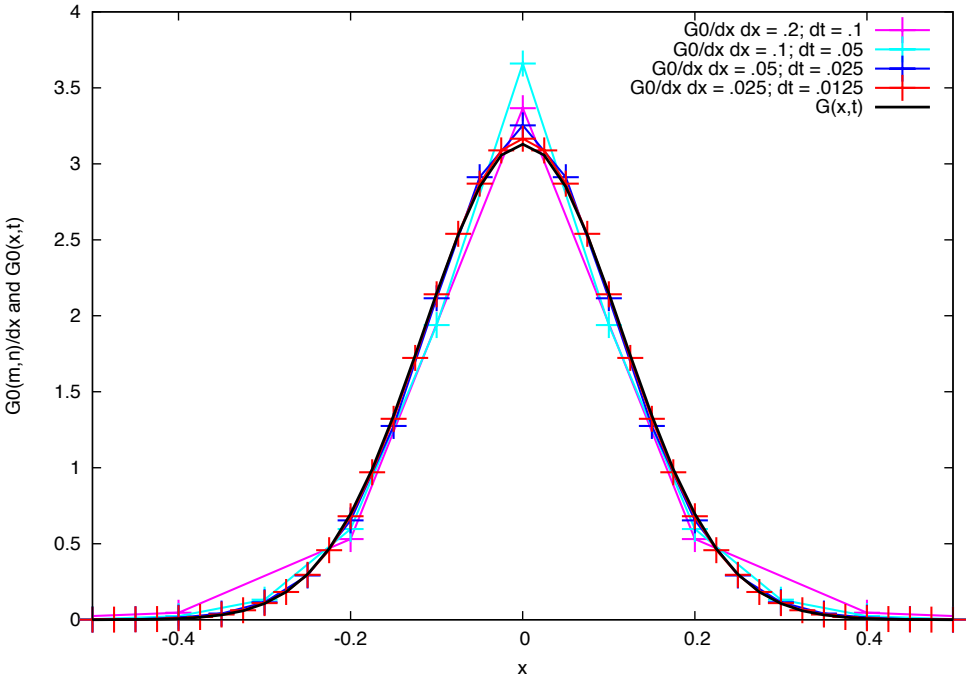

Figure 5: $\frac{G_0(m,n)}{\Delta x}$ computed with various values of Δx and Δt, compared to $\hat{G}_0(x,t)$ at fixed values of x and $t = 1$. As we decrease Δx and Δt and increase m and n to keep x and t fixed, the shape of $G_0(m,n)$ becomes more like that of the Gaussian $\hat{G}_0(x,t)$ given by Eq.(26).

To compare to the analytic results, we use the equation of state $e_m(j,n) = c_v T_m(j,n)$, with $c_v = 10^{22} \frac{\text{erg}}{\text{cm}^3-\text{keV}}$ and $T_m(j,0) = 0.0$. With this large value of c_v and small initial matter temperature, T_m remains negligibly small for all n. With T_m small, the temperature term in Eq.(137) vanishes. In this case, Eq.(137) reduces to Eq.(36).

Since $\phi(j,n)$ in Ares satisfies Eq.(36) to a very good approximation, we can compare the results for ϕ from Ares to the results of an analytic solution of Eq.(36) obtained from Eq.(37).

Our specific test problem used $\Delta x = 0.05$ cm. and $\Delta t = 3.0 \times 10^{-13}$ sec. It was run on a grid of 1000 equal-width zones. The large number of zones was employed in the calculation so that the boundaries would be very far away, rendering the influence of boundary conditions negligible.

In cgs units, $c = 2.9979 \times 10^{10} \frac{\text{cm}}{\text{s}}$ and $a = 1.372^{14} \frac{\text{erg}}{\text{keV}^4-\text{cm}^3}$. The initial conditions, at n = 0, were given by

$$\begin{aligned} \phi_0(j) &= 6.86 \times 10^{13} \frac{\text{erg}}{\text{cm}^3}, \ j \in [-20, 0], \\ &= 0, \ j \notin [-20, 0]. \end{aligned} \tag{139}$$

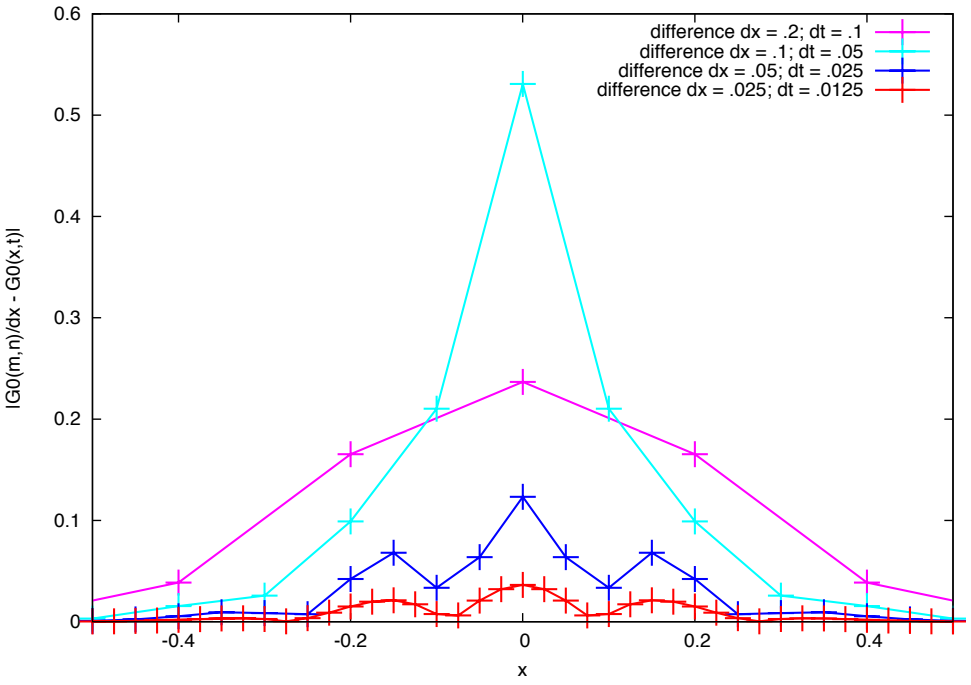

Figure 6: Absolute value of the difference between $\frac{G_0(m,n)}{\Delta x}$ computed with various values of Δx and Δt and $\hat{G}_0(x,t)$, at fixed values of x and $t = 1$. This plot depicts the convergence of $\frac{G_0(m,n)}{\Delta x}$ to $\hat{G}_0(x,t)$ as the grid and time step are refined.

The value of $S(j,n)$ was given by

$$\begin{aligned} S(j,n) &= S_0[n+\frac{1}{2}]\ ,\ n \in [0,20],\ j \in [5,25]\ , \\ &= S_0[40-(n+\frac{1}{2})]\ ,\ n \in [0,20],\ j \in [5,25] \\ &= 0,\ j \notin [5,25]\ , \end{aligned} \tag{140}$$

where $S_0 = 6.667 \times 10^{-7} \frac{\text{erg}}{\text{cm}^3-\text{sec}}$.

Both the initial conditions and the source function have large differences between adjacent values of zone index j, and the source is a function of both j and time step n. This provides us with a challenging test problem for both the Ares diffusion package and for our analytic solution technique.

In Fig.(7) we compare the results of the Ares code and the analytic results generated at various values of zone index j and time step n. We show results for $j \in [-75,75]$ and $n = [0,25,50,...200,250]$. Fig.(8) shows the same data in a log plot. The agreement between the results is excellent at all values of j and n shown.

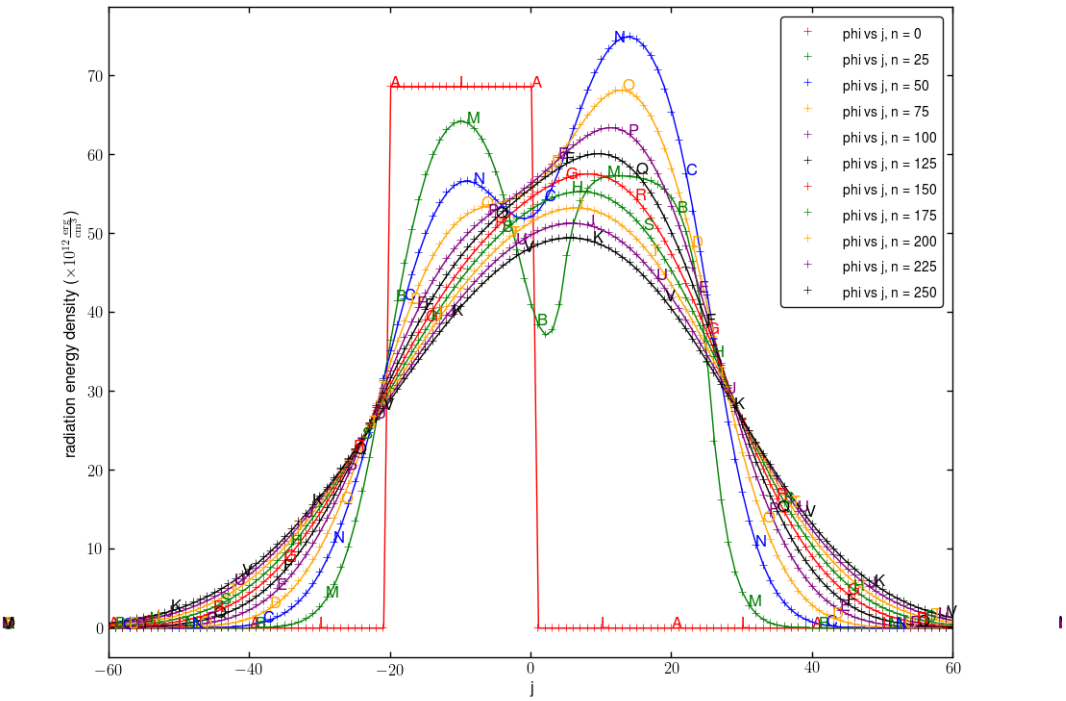

Figure 7: Comparison of radiation energy density vs spatial index j computed by Ares with the results of an analytic solution calculated using discrete Green's functions via Eq.(37) for various values of time step n. The results shown are for the test problem described in the text. Solid lines are Ares code results; symbols are discrete Green's function results.

Fig.(9) shows the absolute difference between the Ares code results and the discrete Green's function results plotted in Figs.(7)-(8). That is, the plot is of the value of the analytic result subtracted from the code result for each value of j and n. For all values of j and n shown, the magnitude of the difference between the code results and the analytic solution is less than 10^{-11}. This demonstrates that the agreement between the solution of Eq.(36) by the Ares code and the solution of Eq.(36) by discrete Green's functions using Eq.(37) is very small. This level of agreement between the code results and the solution of Eq.(36) is evidence that the diffusion package in Ares is correctly solving the difference equation Eq.(137 in regimes in which Eq.(137) reduces to Eq.(36).

6. CONCLUSIONS

A diffusion equation in one-dimensional Cartesian coordinates for a quantity ϕ with constant coefficients, and with arbitrary initial conditions and an arbitrary source, can be solved by use of Green's functions, as described in standard mathematical physics texts. We have shown that the discretized version of such a diffusion equation can be solved by similar techniques. We have given an analytic expression for the Green's function for the discretized diffusion equation in one-

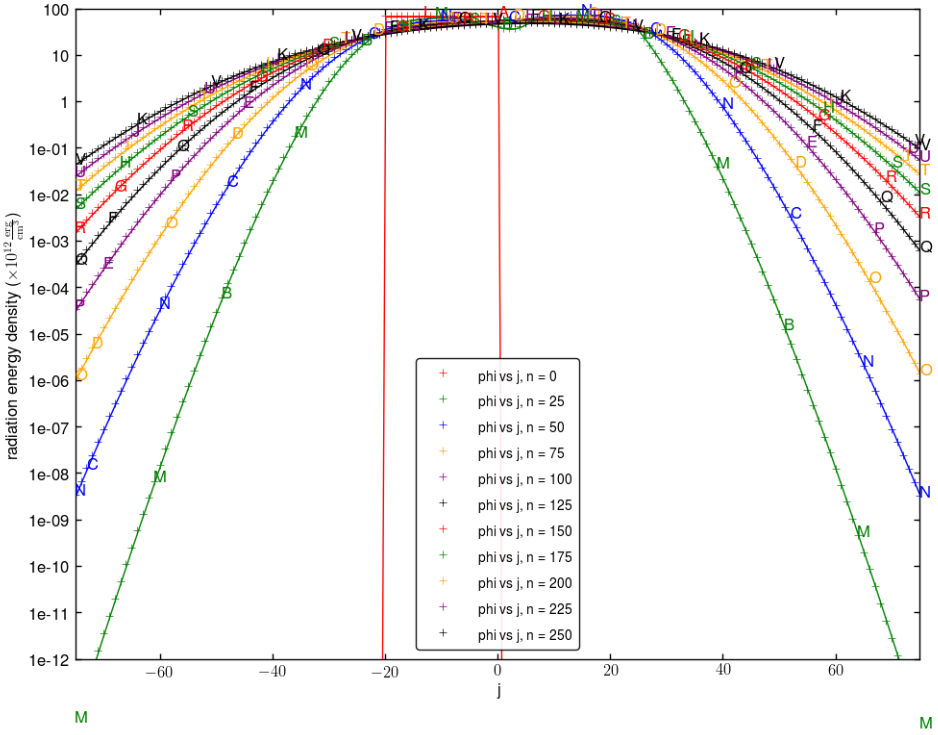

Figure 8: The same data shown in Fig.(7) plotted on a log scale. Solid lines are Ares code results; symbols are discrete Green's function results.

dimensional Cartesian coordinates. This allows us to obtain solutions to the discretized diffusion equation for arbitrary initial conditions and an arbitrary source. We have compared the analytic solution for the discrete Green's function to the Green's function of the differential equation, and shown that the discrete Green's function converges to the continuous Green's function as expected. We have compared a solution of the discretized diffusion equation obtained using the discrete Green's function, with a specified source and initial conditions, to the solution of the discretized diffusion equation obtained from a radiation transport code and shown that the solutions agree to better than one part in 10^{11}.

ACKNOWLEDGMENTS

The work of the both authors was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, L.L.C. under Contract DE-AC52-07NA27344. The first author would like to thank Charlie Cerjan for for helpful conversations.

REFERENCES

1. G. C. Pomraning, "Equations of Radiation Hydrodynamics", in International Series of Monographs in Natural Philosophy, edited by D. ter Harr (Pergamon, New York, 1973),

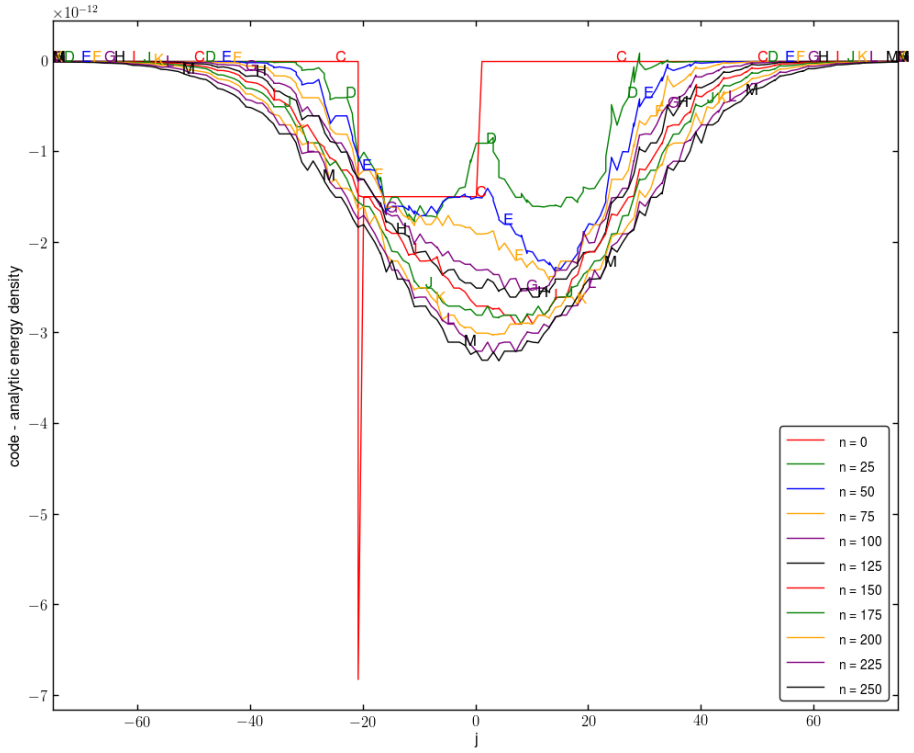

Figure 9: Absolute difference between the Ares code results and the discrete Green's function results plotted in Figs.(7)-(8). The magnitude of the difference is always less than 10^{-11}.

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2. Eugene Butkov, "Mathematical Physics", Addison-Wesley, Reading, MA, (1968)

3. I. S. Gradshteyn and I. M. Ryzhik, "Table of Integrals, Series, and Products" fourth edition, Academic Press, San Diego, CA, (1980)

4. W. H. Press, et. al, "Numerical Recipes, Second Edition", Cambridge University Press, New York, N. Y., (2002)

5. G. Bazan, in "Proceedings from the 2nd International Workshop on Laboratory Astrophysics with Intense Lasers", edited by B. A Remington (Lawrence Livermore National Laboratory, Livermore, 1998), UCRL-ID-131978, pp. 42-63