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The equivalence between two techniques of angular interpolation for the discrete-ordinates method

E.S. Chalhoub[a], R.D.M. Garcia[b,c,*]

[a]*Instituto Nacional de Pesquisas Espaciais, Laboratório Associado de Computação e Matemática Aplicada, 12201-970 São José dos Campos, SP, Brazil*

[b]*HSH Scientific Computing, Rua Carlos de Campos 286, 12242-540 São José dos Campos, SP, Brazil*

[c]*Centro Técnico Aeroespacial, Instituto de Estudos Avançados, Caixa Postal 6044, 12231-970 São José dos Campos, SP, Brazil*

Abstract

In this work, two techniques of angular interpolation for the discrete-ordinates method in radiation transport, namely the source-function integration technique and a technique based on the inclusion of dummy nodes in the quadrature scheme, are studied. It is shown that these techniques are equivalent (i.e., they yield the same results) in plane geometry. In addition, numerical studies carried out for two model problems in atmospheric radiative transfer are used to show that the technique based on inclusion of dummy nodes can be implemented in a way that makes it more economical than the source-function integration technique.

1. Introduction

The discrete-ordinates method for solving transport problems was introduced by Wick [1] and Chandrasekhar [2] in the 1940s, following and generalizing the original concept of the two-stream approximation of Schuster [3] and Schwarzschild [4]. The original version of the method, which became known in the literature as the Wick–Chandrasekhar method, is based on approximating the angular integral in the scattering term of the transport equation by a numerical quadrature and analytically solving the resulting set of ordinary differential equations for the particle distribution

* Correspondence address: Centro Técnico Aeroespacial, Instituto de Estudos Avançados, Caixa Postal 6044, 12231-970 São José dos Campos, SP, Brazil. Tel.: 0055-12-347-5480; fax: 0055-12-344-1177.

E-mail address: rdgarcia@ieav.cta.br (R.D.M. Garcia)

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function at the quadrature nodes. The method has been extensively developed by Chandrasekhar [5] and used by several authors for solving problems in radiative transfer, as discussed, for example, by Lenoble [6] in a review that includes a list of references covering the period from the inception of the method up to 1974. Other valuable sources of information on the fundamental aspects of the method and its application to atmospheric radiative-transfer problems are the review by Hansen and Travis [7], the book by Liou [8] and the reprint collection edited by Kattawar [9]. More recent works have focused mainly on computational aspects of the method [10–12], on efficient approaches for treating problems defined by general sources that may depend on space and angle [13,14], and on the extension of the method to accomodate polarization effects [15].

The most obvious difficulty with the discrete-ordinates method is that situations may exist (e.g., remote-sensing applications) where the particle distribution function may have to be computed for directions of particle travel not included in the approximating quadrature. A simple way of overcoming this difficulty is to use some kind of interpolative technique to compute the particle distribution function for any direction, given the discrete-ordinates solution. Indeed, a few such angular interpolation techniques have been developed and reported in the literature, as discussed next.

Chandrasekhar [2] was the first to use the so-called *source-function integration technique*, hereafter referred to as the SFI technique, in the context of the discrete-ordinates method. This technique is based on integrating the equation of transfer in space separately for the positive and the negative ranges of the cosine of the polar angle (μ), with the scattering term being expressed in terms of the (supposedly known) discrete-ordinates solution. The resulting formulas for the particle distribution function are continuous functions of μ in each of the half-intervals $[-1, 0]$ and $[0, 1]$.

In the 1960s and 1970s, a substantial effort was directed towards the development of computer codes based on the discrete-ordinates approximation [16–18]. Because these codes were intended primarily for neutron and gamma-ray transport calculations, and in these fields of study solutions are also required for problems formulated in one-dimensional curvilinear geometries (spheres and infinite cylinders), as well as in two and three dimensions, the fact that analytical solutions of the discrete-ordinates equations were abandoned in favor of a numerical formulation resulted, in part, from the need of using spatial discretization to cope with the more complex form of the streaming operator in these geometries. There are two reasons why *dummy nodes*, i.e. nodes associated with zero weights, are usually included in the quadrature schemes used by these codes. The first is that, sometimes, the inclusion of certain dummy nodes is a requirement of the numerical scheme being used to solve the discretized equations (e.g., the node $\mu = -1$ in spherical geometry [16,17]). The second is of particular interest to us: the inclusion of dummy nodes provides a way of computing the particle distribution function for ordinates not included as regular nodes in the quadrature scheme used by the discrete-ordinates approximation [19].

A few other angular interpolation techniques for the discrete-ordinates method have also been investigated. In addition to the SFI technique, Karp [20] has considered Lagrange and cubic-spline interpolation techniques. As a matter of fact, Karp's analysis was performed for the spherical-harmonics method, but it can be easily extended [20] to equivalent forms of the discrete-ordinates method [21,22]. His conclusions were: (i) the SFI technique is by far the most accurate of these techniques; (ii) Lagrange interpolation is completely inadequate because it can be very innacurate; and (iii) spline interpolation, although less accurate than the SFI technique, is more economical and produces reasonable results, particularly if supplemented with particle

distribution functions computed at a few selected values of the angular variable with the SFI technique. Stamnes [23] has investigated the SFI technique and two different ways of implementing interpolation by cubic splines into the discrete-ordinates method. As before [20], the SFI technique was found to yield much better results than spline interpolation [23].

Our work has two purposes. First, we report in Sections 4 and 5 our proof that the SFI technique and the technique based on dummy-node inclusion (referred to as the DNI technique in this paper) both give the same results when implemented as angular interpolation techniques for the Wick–Chandrasekhar method in plane geometry. This equivalence has been observed numerically in a recent work [24]. Secondly, we discuss in Section 6 the results of our application of both of these techniques to some model problems in atmospheric radiative transfer that led us to conclude that the DNI technique can be implemented in a more efficient way than the SFI technique.

2. Formulation of the problem

We consider a problem where the particle distribution function $G(\tau, \xi)$ satisfies, for $\tau \in (0, \tau_0)$ and $\xi \in [-\gamma, \gamma]$, the equation of transfer [13]

$$\xi \frac{\partial}{\partial \tau} G(\tau, \xi) + G(\tau, \xi) = \sum_{l=0}^{L} f_l \Pi_l(\xi) \int_{-\gamma}^{\gamma} \Psi(\xi') \Pi_l(\xi') G(\tau, \xi') \, \mathrm{d}\xi' + Q(\tau, \xi) \tag{1}$$

and the boundary conditions, for $\xi \in (0, \gamma]$,

$$G(0, \xi) = L(\xi) \tag{2a}$$

and

$$\mathrm{G}(\tau_0, -\xi) = R(\xi). \tag{2b}$$

Here, the source term $Q(\tau, \xi)$ and the incident distributions $L(\xi)$ and $R(\xi)$ are assumed to be known.

We note that in this work, by adopting the general formulation introduced in Ref. [13] to define our problem, we are covering all of the Fourier-component ($m \geq 0$) problems basic to the standard (azimuthally dependent) problem in radiative transfer [5] and a model used in studies of scattering with complete energy redistribution [25,26], with the exception of the conservative case [13]. For brevity, we do not elaborate on the functions $\Psi(\xi)$ and $\{\Pi_l(\xi)\}$ and the constants γ and $\{f_l\}$ that appear in Eq. (1); we believe that the meaning of these functions and constants for the intended applications has been made sufficiently clear in the cited works.

To define our discrete-ordinates version of the problem posed by Eqs. (1) and (2), we begin by introducing a quadrature of order N with nodes $\{\xi_j\}$ and weights $\{w_j\}$ to approximate the integral in Eq. (1). As in Ref. [13], we do not impose any restrictions on the adopted quadrature scheme, so that we can have, for example, a non-symmetrical quadrature or, in the more general case, a composite scheme where the integration interval $[-\gamma, \gamma]$ is subdivided into any number of sub-intervals of arbitrary size, with a quadrature of arbitrary order assigned to each of them. Our only restricting assumption is that the adopted quadrature scheme should not contain a null node.

Continuing, we set $\xi = \xi_j$, $j = 1, 2, \ldots, N$, in Eq. (1) to write the discrete-ordinates equations

$$\xi_j \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \xi_j) + G(\tau, \xi_j) = \sum_{l=0}^{L} f_l \Pi_l(\xi_j) \sum_{i=1}^{N} w_i \Psi(\xi_i) \Pi_l(\xi_i) G(\tau, \xi_i) + Q(\tau, \xi_j), \quad j = 1, 2, \ldots, N. \tag{3}$$

Finally, to specify the boundary conditions needed to complete the definition of our discrete-ordinates version of the problem, we assume that the nodes of the quadrature scheme are ordered in such a way that the first J nodes are *positive* and the remaining $N - J$ nodes are *negative*. Thus, we can write our discrete-ordinates versions of Eqs. (2) as

$$G(0, \xi_j) = L(\xi_j), \quad j = 1, 2, \ldots, J, \tag{4a}$$

and

$$G(\tau_0, \xi_j) = R(-\xi_j), \quad j = J + 1, J + 2, \ldots, N. \tag{4b}$$

3. The discrete-ordinates solution

Making use of the elementary solutions of the discrete-ordinates equations and their orthogonality property developed in Ref. [13], we can now write the general discrete-ordinates solution of order N to the problem formulated by Eqs. (3) and (4) in the form

$$\begin{aligned} G(\tau, \xi_j) = & \sum_{k=1}^{K} A_k \Phi(\nu_k, \xi_j) \mathrm{e}^{-\tau/\nu_k} + \sum_{k=K+1}^{N} B_k \Phi(-\nu_k, \xi_j) \mathrm{e}^{-(\tau_0 - \tau)/\nu_k} \\ & + \sum_{k=1}^{K} \mathfrak{A}_k(\tau) \Phi(\nu_k, \xi_j) + \sum_{k=K+1}^{N} \mathfrak{B}_k(\tau) \Phi(-\nu_k, \xi_j) \end{aligned} \tag{5}$$

for $j = 1, 2, \ldots, N$. Here, ν_k, $k = 1, 2, \ldots, K$, and $-\nu_k$, $k = K + 1, K + 2, \ldots, N$, denote, respectively, the inverses of the *positive* and the *negative* eigenvalues of the $N \times N$ matrix $\mathbf{\Xi}^{-1}(\mathbf{I} - \mathbf{W})$, where $\mathbf{\Xi} = \mathrm{diag}\{\xi_1, \xi_2, \ldots, \xi_N\}$, $\mathbf{I}$ is the identity matrix of order N, and $\mathbf{W}$ is an $N \times N$ matrix with elements

$$W_{i,j} = w_j \Psi(\xi_j) \sum_{l=0}^{L} f_l \Pi_l(\xi_i) \Pi_l(\xi_j). \tag{6}$$

In passing, we note that the analysis of Ref. [13] that we follow here is valid only under the assumption that none of the $\{\nu_k\}$ or the $\{-\nu_k\}$ coincides with one of the nodes $\{\xi_j\}$. In addition, the elementary solutions $\Phi(\nu_k, \xi_j)$ and $\Phi(-\nu_k, \xi_j)$ that appear in Eq. (5) are, respectively, the jth components of the eigenvectors $\mathbf{\Phi}(\nu_k)$ and $\mathbf{\Phi}(-\nu_k)$, associated, respectively, with the eigenvalues $1/\nu_k$ and $-1/\nu_k$. Finally, the coefficients of the particular solution to Eq. (3), $\{\mathfrak{A}_k(\tau)\}$ and $\{\mathfrak{B}_k(\tau)\}$, can be expressed as [13]

$$\mathfrak{A}_k(\tau) = \frac{1}{N(\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(\nu_k, \xi_i) \int_0^{\tau} Q(x, \xi_i) \mathrm{e}^{-(\tau - x)/\nu_k} \, \mathrm{d}x \quad \text{and} \tag{7a}$$

$$\mathfrak{B}_k(\tau) = -\frac{1}{N(-\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(-\nu_k, \xi_i) \int_{\tau}^{\tau_0} Q(x, \xi_i) \mathrm{e}^{-(x - \tau)/\nu_k} \, \mathrm{d}x \tag{7b}$$

with

$$N(\pm\nu_k)=\sum_{i=1}^{N} w_i\xi_i\Psi(\xi_i)[\Phi(\pm\nu_k,\xi_i)]^2 \tag{8}$$

and the coefficients of the homogeneous solution $\{A_k\}$ and $\{B_k\}$ can be found by solving the system of N linear algebraic equations obtained from the requirement that the general solution expressed by Eq. (5) satisfies the boundary conditions expressed by Eqs. (4), viz.,

$$\sum_{k=1}^{K} A_k\Phi(\nu_k,\xi_j)+\sum_{k=K+1}^{N} B_k\Phi(-\nu_k,\xi_j)\mathrm{e}^{-\tau_0/\nu_k}=L(\xi_j)-\sum_{k=K+1}^{N}\mathfrak{B}_k(0)\Phi(-\nu_k,\xi_j) \tag{9a}$$

for $j=1,2,\ldots,J$, and

$$\sum_{k=1}^{K} A_k\Phi(\nu_k,\xi_j)\mathrm{e}^{-\tau_0/\nu_k}+\sum_{k=K+1}^{N} B_k\Phi(-\nu_k,\xi_j)=R(-\xi_j)-\sum_{k=1}^{K}\mathfrak{U}_k(\tau_0)\Phi(\nu_k,\xi_j) \tag{9b}$$

for $j=J+1,J+2,\ldots,N$. We conclude this section by pointing out that once the linear system formulated by Eqs. (9a) and (9b) is solved for $\{A_k\}$ and $\{B_k\}$, we have at hand all quantities necessary to evaluate Eq. (5) for any $\tau\in[0,\tau_0]$.

4. The SFI technique

As discussed in the Introduction, the source-function integration (SFI) technique provides a way of evaluating the particle distribution function $G(\tau,\xi)$ whenever ξ does not coincide with any of the nodes in the approximating quadrature. To obtain the desired result for $G(\tau,\xi)$, we need to consider the cases $\xi\in[0,\gamma]$ and $\xi\in[-\gamma,0]$ separately.

Starting with $\xi\in[0,\gamma]$, we can use the general discrete-ordinates solution expressed by Eq. (5) on the right-hand side of the equation that is obtained by using our quadrature scheme to approximate the integral in Eq. (1) and integrate the resulting equation over space from 0 to τ to obtain, for $\tau\in[0,\tau_0]$ and $\xi\in[0,\gamma]$,

$$\begin{aligned}G(\tau,\xi)=L(\xi)\mathrm{e}^{-\tau/\xi}+\frac{1}{\xi}\int_0^{\tau}Q(x,\xi)\mathrm{e}^{-(\tau-x)/\xi}\,\mathrm{d}x+\sum_{i=1}^{N}w_i\Psi(\xi_i)\left[\sum_{l=0}^{L}f_l\Pi_l(\xi_i)\Pi_l(\xi)\right]\\ \times\left\{\sum_{k=1}^{K}\nu_kA_k\Phi(\nu_k,\xi_i)C(\tau:\nu_k,\xi)+\sum_{k=K+1}^{N}\nu_kB_k\Phi(-\nu_k,\xi_i)\mathrm{e}^{-(\tau_0-\tau)/\nu_k}S(\tau:\nu_k,\xi)\right.\\ +\frac{1}{\xi}\sum_{k=1}^{K}\frac{\Phi(\nu_k,\xi_i)}{N(\nu_k)}\sum_{j=1}^{N}w_j\Psi(\xi_j)\Phi(\nu_k,\xi_j)\int_0^{\tau}\int_0^{x}Q(x',\xi_j)\mathrm{e}^{-(x-x')/\nu_k}\,\mathrm{d}x'\mathrm{e}^{-(\tau-x)/\xi}\,\mathrm{d}x\\ -\frac{1}{\xi}\sum_{k=K+1}^{N}\frac{\Phi(-\nu_k,\xi_i)}{N(-\nu_k)}\sum_{j=1}^{N}w_j\Psi(\xi_j)\Phi(-\nu_k,\xi_j)\\ \left.\times\int_0^{\tau}\int_x^{\tau_0}Q(x',\xi_j)\mathrm{e}^{-(x'-x)/\nu_k}\,\mathrm{d}x'\mathrm{e}^{-(\tau-x)/\xi}\,\mathrm{d}x\right\},\end{aligned} \tag{10}$$

where

$$C(\tau : \nu, \xi) = \frac{e^{-\tau/\nu} - e^{-\tau/\xi}}{\nu - \xi} \tag{11a}$$

and

$$S(\tau : \nu, \xi) = \frac{1 - e^{-\tau/\nu} e^{-\tau/\xi}}{\nu + \xi}. \tag{11b}$$

Next, with the help of the integral inversion formulas

$$\int_0^\tau \int_0^x F(x, x')\,dx'\,dx = \int_0^\tau \int_{x'}^\tau F(x, x')\,dx\,dx' \tag{12a}$$

and

$$\int_0^\tau \int_x^{\tau_0} F(x, x')\,dx'\,dx = \int_0^\tau \int_0^{x'} F(x, x')\,dx\,dx' + \int_\tau^{\tau_0} \int_0^\tau F(x, x')\,dx\,dx', \tag{12b}$$

we can evaluate the integrals over x in Eq. (10) to obtain our final result for $G(\tau, \xi)$, $\tau \in [0, \tau_0]$ and $\xi \in [0, \gamma]$, viz.,

$$\begin{aligned} G(\tau, \xi) = {} & L(\xi) e^{-\tau/\xi} + \frac{1}{\xi} \int_0^\tau Q(x, \xi) e^{-(\tau - x)/\xi}\,dx + \sum_{i=1}^{N} w_i \Psi(\xi_i) \left[\sum_{l=0}^{L} f_l \Pi_l(\xi_i) \Pi_l(\xi) \right] \\ & \times \left\{ \sum_{k=1}^{K} \nu_k A_k \Phi(\nu_k, \xi_i) C(\tau : \nu_k, \xi) + \sum_{k=K+1}^{N} \nu_k B_k \Phi(-\nu_k, \xi_i) e^{-(\tau_0 - \tau)/\nu_k} S(\tau : \nu_k, \xi) \right. \\ & + \sum_{k=1}^{K} \frac{\nu_k \Phi(\nu_k, \xi_i)}{N(\nu_k)} \sum_{j=1}^{N} w_j \Psi(\xi_j) \Phi(\nu_k, \xi_j) \int_0^\tau Q(x, \xi_j) C(\tau - x : \nu_k, \xi)\,dx \\ & - \sum_{k=K+1}^{N} \frac{\nu_k \Phi(-\nu_k, \xi_i)}{N(-\nu_k)} \sum_{j=1}^{N} w_j \Psi(\xi_j) \Phi(-\nu_k, \xi_j) \left[\int_0^\tau Q(x, \xi_j) e^{-(\tau - x)/\xi} S(x : \nu_k, \xi)\,dx \right. \\ & \left. \left. + S(\tau : \nu_k, \xi) \int_\tau^{\tau_0} Q(x, \xi_j) e^{-(x - \tau)/\nu_k}\,dx \right] \right\}. \end{aligned} \tag{13}$$

Similarly, for $\xi \in [-\gamma, 0]$, we can use the general discrete-ordinates solution expressed by Eq. (5) on the right-hand side of the equation that is obtained by changing ξ to $-\xi$ in Eq. (1) and using our quadrature scheme to approximate the integral in that equation, and integrate the resulting equation over space from τ to τ_0, to obtain, for $\tau \in [0, \tau_0]$ and $\xi \in [0, \gamma]$,

$$\begin{aligned} G(\tau, -\xi) = {} & R(\xi) e^{-(\tau_0 - \tau)/\xi} + \frac{1}{\xi} \int_\tau^{\tau_0} Q(x, -\xi) e^{-(x - \tau)/\xi}\,dx + \sum_{i=1}^{N} w_i \Psi(\xi_i) \left[\sum_{l=0}^{L} f_l \Pi_l(\xi_i) \Pi_l(-\xi) \right] \\ & \times \left\{ \sum_{k=1}^{K} \nu_k A_k \Phi(\nu_k, \xi_i) e^{-\tau/\nu_k} S(\tau_0 - \tau : \nu_k, \xi) + \sum_{k=K+1}^{N} \nu_k B_k \Phi(-\nu_k, \xi_i) C(\tau_0 - \tau : \nu_k, \xi) \right. \\ & \left. + \frac{1}{\xi} \sum_{k=1}^{K} \frac{\Phi(\nu_k, \xi_i)}{N(\nu_k)} \sum_{j=1}^{N} w_j \Psi(\xi_j) \Phi(\nu_k, \xi_j) \int_\tau^{\tau_0} \int_0^x Q(x', \xi_j) e^{-(x - x')/\nu_k}\,dx' e^{-(x - \tau)/\xi}\,dx \right. \end{aligned}$$

$$-\frac{1}{\xi}\sum_{k=K+1}^{N}\frac{\Phi(-\nu_k,\xi_i)}{N(-\nu_k)}\sum_{j=1}^{N}w_j\Psi(\xi_j)\Phi(-\nu_k,\xi_j)$$
$$\times\int_{\tau}^{\tau_0}\int_{x}^{\tau_0}Q(x',\xi_j)\mathrm{e}^{-(x'-x)/\nu_k}\,\mathrm{d}x'\mathrm{e}^{-(x-\tau)/\xi}\,\mathrm{d}x\Bigg\}. \tag{14}$$

Again, using the integral inversion formulas

$$\int_{\tau}^{\tau_0}\int_{0}^{x}F(x,x')\,\mathrm{d}x'\,\mathrm{d}x=\int_{0}^{\tau}\int_{\tau}^{\tau_0}F(x,x')\,\mathrm{d}x\,\mathrm{d}x'+\int_{\tau}^{\tau_0}\int_{x'}^{\tau_0}F(x,x')\,\mathrm{d}x\,\mathrm{d}x' \tag{15a}$$

and

$$\int_{\tau}^{\tau_0}\int_{x}^{\tau_0}F(x,x')\,\mathrm{d}x'\,\mathrm{d}x=\int_{\tau}^{\tau_0}\int_{\tau}^{x'}F(x,x')\,\mathrm{d}x\,\mathrm{d}x', \tag{15b}$$

we can evaluate the integrals over x in Eq. (14) to obtain our final result for $G(\tau,-\xi)$, $\tau\in[0,\tau_0]$ and $\xi\in[0,\gamma]$, viz.

$$G(\tau,-\xi)=R(\xi)\mathrm{e}^{-(\tau_0-\tau)/\xi}+\frac{1}{\xi}\int_{\tau}^{\tau_0}Q(x,-\xi)\mathrm{e}^{-(x-\tau)/\xi}\,\mathrm{d}x+\sum_{i=1}^{N}w_i\Psi(\xi_i)\Bigg[\sum_{l=0}^{L}f_l\Pi_l(\xi_i)\Pi_l(-\xi)\Bigg]$$
$$\times\Bigg\{\sum_{k=1}^{K}\nu_kA_k\Phi(\nu_k,\xi_i)\mathrm{e}^{-\tau/\nu_k}S(\tau_0-\tau:\nu_k,\xi)+\sum_{k=K+1}^{N}\nu_kB_k\Phi(-\nu_k,\xi_i)C(\tau_0-\tau:\nu_k,\xi)$$
$$+\sum_{k=1}^{K}\frac{\nu_k\Phi(\nu_k,\xi_i)}{N(\nu_k)}\sum_{j=1}^{N}w_j\Psi(\xi_j)\Phi(\nu_k,\xi_j)\Bigg[S(\tau_0-\tau:\nu_k,\xi)\int_{0}^{\tau}Q(x,\xi_j)\mathrm{e}^{-(\tau-x)/\nu_k}\,\mathrm{d}x$$
$$+\int_{\tau}^{\tau_0}Q(x,\xi_j)\mathrm{e}^{-(x-\tau)/\xi}S(\tau_0-x:\nu_k,\xi)\,\mathrm{d}x\Bigg]$$
$$-\sum_{k=K+1}^{N}\frac{\nu_k\Phi(-\nu_k,\xi_i)}{N(-\nu_k)}\sum_{j=1}^{N}w_j\Psi(\xi_j)\Phi(-\nu_k,\xi_j)\int_{\tau}^{\tau_0}Q(x,\xi_j)C(x-\tau:\nu_k,\xi)\,\mathrm{d}x\Bigg\}. \tag{16}$$

In conclusion, we note that our results for $G(\tau,\pm\xi)$, $\tau\in[0,\tau_0]$ and $\xi\in[0,\gamma]$, expressed by Eqs. (13) and (16), could be made more explicit by introducing into these equations the specific representations of the source $Q(\tau,\xi)$ for the two classes of problems considered in this work and by performing the indicated integrations analytically, when possible. However, since in this work we are interested mainly in demonstrating the equivalence between the SFI and the DNI techniques and, as we will see, this equivalence is independent on the specific form of the source term, we do not report here the simplifications of Eqs. (13) and (16) that can be worked out for our intended applications.

5. The DNI technique

As mentioned in the Introduction, this technique is based on adding a set of nodes associated with zero weights, denoted here as ξ_j, $j=N+1,N+2,\ldots,N+M$, to the regular quadrature

scheme of order N adopted in Section 2. Thus, in addition to Eqs. (3) subject to Eqs. (4), we consider

$$\xi_j \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \xi_j) + G(\tau, \xi_j) = \sum_{l=0}^{L} f_l \Pi_l(\xi_j) \sum_{i=1}^{N} w_i \Psi(\xi_i) \Pi_l(\xi_i) G(\tau, \xi_i) + Q(\tau, \xi_j) \tag{17}$$

for $j = N+1, N+2, \ldots, N+M$, subject to

$$G(0, \xi_j) = L(\xi_j) \tag{18a}$$

for $j = N+1, N+2, \ldots, N+I$, and

$$G(\tau_0, \xi_j) = R(-\xi_j) \tag{18b}$$

for $j = N+I+1, N+I+2, \ldots, N+M$. Clearly, to write the additional boundary conditions as in Eqs. (18a) and (18b), we have assumed that the M dummy nodes are ordered so that the first I are strictly *positive* and the last $M-I$ strictly *negative*.

Before proceeding with our presentation, we note that, since the dummy nodes are associated with zero weights, they do not contribute to the scattering term in Eqs. (17). Therefore, if the problem were solved in two steps, i.e. first for the regular ordinates, exactly as done in Section 3, and then for the dummy ordinates, by simply integrating Eqs. (17) over space and using the boundary conditions expressed by Eqs. (18a) and (18b), the DNI technique could be viewed as a mere discretized version of the SFI technique discussed in the preceding section. The equivalence between these techniques would then be evident. Here, however, we are interested in investigating what happens when the problem is solved *simultaneously* for the regular and the dummy ordinates, as is the case with transport codes based on numerical implementations of the discrete-ordinates method.

Defining the particle-distribution vectors

$$\mathbf{G}(\tau) = (G(\tau, \xi_1) \quad G(\tau, \xi_2) \quad \cdots \quad G(\tau, \xi_N))^{\mathrm{T}} \tag{19a}$$

and

$$\hat{\mathbf{G}}(\tau) = (G(\tau, \xi_{N+1}) \quad G(\tau, \xi_{N+2}) \quad \cdots \quad G(\tau, \xi_{N+M}))^{\mathrm{T}}, \tag{19b}$$

the source vectors

$$\mathbf{Q}(\tau) = (Q(\tau, \xi_1) \quad Q(\tau, \xi_2) \quad \cdots \quad Q(\tau, \xi_N))^{\mathrm{T}} \tag{20a}$$

and

$$\hat{\mathbf{Q}}(\tau) = (Q(\tau, \xi_{N+1}) \quad Q(\tau, \xi_{N+2}) \quad \cdots \quad Q(\tau, \xi_{N+M}))^{\mathrm{T}}, \tag{20b}$$

the diagonal matrix $\hat{\boldsymbol{\Xi}} = \mathrm{diag}\{\xi_{N+1}, \xi_{N+2}, \ldots, \xi_{N+M}\}$, the $M \times N$ matrix $\hat{\mathbf{W}}$ with elements

$$\hat{W}_{i,j} = w_j \Psi(\xi_j) \sum_{l=0}^{L} f_l \Pi_l(\xi_{N+i}) \Pi_l(\xi_j) \tag{21}$$

for $i = 1, 2, \ldots, M$ and $j = 1, 2, \ldots, N$, and using the matrices $\boldsymbol{\Xi}$ and $\mathbf{W}$ defined in Section 3, we can write our enlarged set of discrete-ordinates equations consisting of Eqs. (3) and (17) in matrix-block notation as

$$\begin{pmatrix} \boldsymbol{\Xi} & \mathbf{0} \\ \mathbf{0} & \hat{\boldsymbol{\Xi}} \end{pmatrix} \frac{\mathrm{d}}{\mathrm{d}\tau} \begin{pmatrix} \mathbf{G}(\tau) \\ \hat{\mathbf{G}}(\tau) \end{pmatrix} + \begin{pmatrix} \mathbf{I} - \mathbf{W} & \mathbf{0} \\ -\hat{\mathbf{W}} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{G}(\tau) \\ \hat{\mathbf{G}}(\tau) \end{pmatrix} = \begin{pmatrix} \mathbf{Q}(\tau) \\ \hat{\mathbf{Q}}(\tau) \end{pmatrix}. \tag{22}$$

Now, trying exponential solutions of the form [13]

$$\begin{pmatrix}\mathbf{G}_h(\tau)\\ \hat{\mathbf{G}}_h(\tau)\end{pmatrix}=\begin{pmatrix}\mathbf{\Phi}(\nu)\\ \hat{\mathbf{\Phi}}(\nu)\end{pmatrix}\mathrm{e}^{-\tau/\nu} \tag{23}$$

for the homogeneous version of Eq. (22), we find that the separation constant ν and the enlarged vector of elementary solutions

$$\mathbf{F}(\nu)=\begin{pmatrix}\mathbf{\Phi}(\nu)\\ \hat{\mathbf{\Phi}}(\nu)\end{pmatrix} \tag{24}$$

must satisfy the enlarged eigensystem of order $N+M$

$$\begin{pmatrix}\mathbf{\Xi}^{-1}(\mathbf{I}-\mathbf{W}) & \mathbf{0}\\ -\hat{\mathbf{\Xi}}^{-1}\hat{\mathbf{W}} & \hat{\mathbf{\Xi}}^{-1}\end{pmatrix}\mathbf{F}(\nu)=\frac{1}{\nu}\mathbf{F}(\nu). \tag{25}$$

As Eq. (25) is equivalent to

$$\mathbf{\Xi}^{-1}(\mathbf{I}-\mathbf{W})\mathbf{\Phi}(\nu)=\frac{1}{\nu}\mathbf{\Phi}(\nu) \tag{26a}$$

and

$$\hat{\mathbf{\Xi}}^{-1}[\hat{\mathbf{\Phi}}(\nu)-\hat{\mathbf{W}}\mathbf{\Phi}(\nu)]=\frac{1}{\nu}\hat{\mathbf{\Phi}}(\nu) \tag{26b}$$

and Eq. (26a) is precisely the eigensystem that must be solved when dummy nodes are not present, we conclude that the first N of a total of $N+M$ separation constants we are looking for are those of Section 3, i.e. the union of the set of positive separation constants ν_k, $k=1,2,\ldots,K$, with the set of negative separation constants $-\nu_k, k=K+1,K+2,\ldots,N$. Using Eq. (26b), we can show that the corresponding enlarged vectors of elementary solutions are given by

$$\mathbf{F}(\nu_k)=\begin{pmatrix}\mathbf{\Phi}(\nu_k)\\ \hat{\mathbf{D}}(\nu_k)\hat{\mathbf{W}}\mathbf{\Phi}(\nu_k)\end{pmatrix} \tag{27a}$$

for $k=1,2,\ldots,K$, and

$$\mathbf{F}(-\nu_k)=\begin{pmatrix}\mathbf{\Phi}(-\nu_k)\\ \hat{\mathbf{D}}(-\nu_k)\hat{\mathbf{W}}\mathbf{\Phi}(-\nu_k)\end{pmatrix} \tag{27b}$$

for $k=K+1,K+2,\ldots,N$. In these equations, $\mathbf{\Phi}(\nu_k)$, $k=1,2,\ldots,K$, and $\mathbf{\Phi}(-\nu_k)$, $k=K+1,K+2,\ldots,N$, are the eigenvectors that satisfy Eq. (26a), respectively, for the *positive* eigenvalues $\{1/\nu_k\}$ and for the *negative* eigenvalues $\{-1/\nu_k\}$ (see Section 3), and $\hat{\mathbf{D}}(\nu)$ is a M-diagonal matrix defined as $\hat{\mathbf{D}}(\nu)=\mathrm{diag}\{\nu/(\nu-\xi_{N+1}),\nu/(\nu-\xi_{N+2}),\ldots,\nu/(\nu-\xi_{N+M})\}$.

To determine the remaining M separation contants, we find it convenient to consider the transposed eigensystem. Thus, denoting as $(\mathbf{X}(\nu)\ \hat{\mathbf{X}}(\nu))$ a left eigenvector of the matrix in Eq. (25), we consider the auxiliary eigensystem

$$\begin{pmatrix}(\mathbf{I}-\mathbf{W}^{\mathrm{T}})\mathbf{\Xi}^{-1} & -\hat{\mathbf{W}}^{\mathrm{T}}\hat{\mathbf{\Xi}}^{-1}\\ \mathbf{0} & \hat{\mathbf{\Xi}}^{-1}\end{pmatrix}\begin{pmatrix}\mathbf{X}(\nu)\\ \hat{\mathbf{X}}(\nu)\end{pmatrix}=\frac{1}{\nu}\begin{pmatrix}\mathbf{X}(\nu)\\ \hat{\mathbf{X}}(\nu)\end{pmatrix}, \tag{28}$$

which can also be written as

$$(\mathbf{I} - \mathbf{W}^{\mathrm{T}})\boldsymbol{\Xi}^{-1}\mathbf{X}(\nu) - \hat{\mathbf{W}}^{\mathrm{T}}\hat{\boldsymbol{\Xi}}^{-1}\hat{\mathbf{X}}(\nu) = \frac{1}{\nu}\mathbf{X}(\nu) \tag{29a}$$

and

$$\hat{\boldsymbol{\Xi}}^{-1}\hat{\mathbf{X}}(\nu) = \frac{1}{\nu}\hat{\mathbf{X}}(\nu). \tag{29b}$$

Eq. (29b) shows clearly that the dummy nodes themselves provide the remaining M separation constants required, i.e. $\nu_{N+k} = \xi_{N+k}$ for $k = 1, 2, \ldots, M$. In regard to the corresponding enlarged vectors of elementary solutions, we first note that the eigenvectors $\{\hat{\mathbf{X}}(\nu_{N+k})\}$ associated with the eigenvalues $\{1/\nu_{N+k}\}$ in Eq. (29b) have their kth component equal to unity and all other components equal to zero. In addition, on comparing Eqs. (26b) and (29b) and considering Eq. (26a), we can easily see that $\boldsymbol{\Phi}(\nu_{N+k}) = \mathbf{0}$, and so $\hat{\boldsymbol{\Phi}}(\nu_{N+k}) = \hat{\mathbf{X}}(\nu_{N+k})$, for $k = 1, 2, \ldots, M$. Thus, the enlarged vectors of elementary solutions associated with the separation constants that coincide with the dummy nodes are given, for $k = 1, 2, \ldots, M$, by

$$\mathbf{F}(\nu_{N+k}) = \begin{pmatrix} \mathbf{0} \\ \boldsymbol{\Delta}_k \end{pmatrix}, \tag{30}$$

where the M-vector $\boldsymbol{\Delta}_k$ is defined as $\boldsymbol{\Delta}_k = (\delta_{k,1}\ \ \delta_{k,2}\ \ \cdots\ \ \delta_{k,M})^{\mathrm{T}}$.

Summarizing our results for the separation constants and the elementary solutions required to implement the discrete-ordinates method in the presence of dummy nodes, we have shown that the determination of these quantities can be reduced to the solution of the eigensystem for the case where dummy nodes are absent and the calculation of the vector blocks $\hat{\mathbf{D}}(\pm\nu_k)\hat{\mathbf{W}}\boldsymbol{\Phi}(\pm\nu_k)$ in Eqs. (27a) and (27b), to complement the elementary solutions reported in Ref. [13] and used in Section 3. We have also shown that the new separation constants arising from the inclusion of dummy nodes are the dummy nodes themselves and that the corresponding elementary solutions can be readily expressed by means of Eq. (30). We note that similar results are reported in a recent work that uses the discrete-ordinates method for solving a class of problems in rarefied-gas dynamics [27].

In view of the form of the vector $\mathbf{F}(\nu_{N+k})$ given by Eq. (30), we conclude that the general discrete-ordinates solution at a regular node is not affected by the dummy-node modes and therefore is still given by Eq. (5), with the coefficients A_k and $\mathfrak{A}_k(\tau)$, for $k = 1, 2, \ldots, K$, and B_k and $\mathfrak{B}_k(\tau)$, for $k = K+1, K+2, \ldots, N$, being computed as discussed in Section 3. On the other hand, defining $\zeta_j = |\xi_j|$ for $j = N+1, N+2, \ldots, N+M$, we conclude that the general discrete ordinates solution at a *positive* dummy node $\xi_j = \zeta_j$, $j = N+1, N+2, \ldots, N+I$, can be written as

$$\begin{aligned} G(\tau, \zeta_j) = {} & \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, \zeta_j) \mathrm{e}^{-\tau/\nu_k} + \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, \zeta_j) \mathrm{e}^{-(\tau_0 - \tau)/\nu_k} + A_j \mathrm{e}^{-\tau/\zeta_j} \\ & + \sum_{k=1}^{K} \mathfrak{A}_k(\tau) \hat{\Phi}(\nu_k, \zeta_j) + \sum_{k=K+1}^{N} \mathfrak{B}_k(\tau) \hat{\Phi}(-\nu_k, \zeta_j) + \mathfrak{A}_j(\tau) \end{aligned} \tag{31a}$$

and at a *negative* dummy node $\xi_j = -\zeta_j$, $j = N+I+1, N+I+2, \ldots, N+M$, as

$$G(\tau, -\zeta_j) = \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, -\zeta_j) e^{-\tau/\nu_k} + \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, -\zeta_j) e^{-(\tau_0-\tau)/\nu_k} + B_j e^{-(\tau_0-\tau)/\zeta_j} + \sum_{k=1}^{K} \mathfrak{A}_k(\tau) \hat{\Phi}(\nu_k, -\zeta_j) + \sum_{k=K+1}^{N} \mathfrak{B}_k(\tau) \hat{\Phi}(-\nu_k, -\zeta_j) + \mathfrak{B}_j(\tau). \tag{31b}$$

Here, the elementary solutions $\hat{\Phi}(\pm\nu_k, \pm\zeta_j)$ can be computed by using $\nu = \nu_k$ or $-\nu_k$ and $\zeta = \zeta_j$ or $-\zeta_j$, as required, in the expression

$$\hat{\Phi}(\nu, \zeta) = \frac{\nu}{\nu - \zeta} \sum_{i=1}^{N} w_i \Psi(\xi_i) \left[\sum_{l=0}^{L} f_l \Pi_l(\xi_i) \Pi_l(\zeta) \right] \Phi(\nu, \xi_i), \tag{32}$$

which denotes a component of the vector block $\hat{\mathbf{D}}(\nu)\hat{\mathbf{W}}\boldsymbol{\Phi}(\nu)$ that appears in Eqs. (27a) and (27b). In addition, as already noted, the coefficients A_k and $\mathfrak{A}_k(\tau)$, for $k = 1, 2, \ldots, K$, and B_k and $\mathfrak{B}_k(\tau)$, for $k = K+1, K+2, \ldots, N$, can be determined as discussed in Section 3. Thus, only the coefficients $A_j, B_j, \mathfrak{A}_j(\tau)$ and $\mathfrak{B}_j(\tau)$ are still unknown in Eqs. (31a) and (31b).

The coefficients $\mathfrak{A}_j(\tau)$, for $j = N+1, N+2, \ldots, N+I$, and $\mathfrak{B}_j(\tau)$, for $j = N+I+1, N+I+2, \ldots, N+M$, can be found by modifiying the infinite-medium Green's function solution reported in Ref. [13] to take into account the presence of dummy nodes (see a detailed derivation of the required modifications in the appendix). The resulting expressions for $\mathfrak{A}_j(\tau)$ and $\mathfrak{B}_j(\tau)$ can be written as

$$\mathfrak{A}_j(\tau) = \frac{1}{\zeta_j} \int_0^{\tau} Q(x, \zeta_j) e^{-(\tau-x)/\zeta_j} \, dx - \sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, \zeta_j)}{N(\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(\nu_k, \xi_i) \int_0^{\tau} Q(x, \xi_i) e^{-(\tau-x)/\zeta_j} \, dx - \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, \zeta_j)}{N(-\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(-\nu_k, \xi_i) \int_0^{\tau} Q(x, \xi_i) e^{-(\tau-x)/\zeta_j} \, dx \tag{33a}$$

for $j = N+1, N+2, \ldots, N+I$, and

$$\mathfrak{B}_j(\tau) = \frac{1}{\zeta_j} \int_{\tau}^{\tau_0} Q(x, -\zeta_j) e^{-(x-\tau)/\zeta_j} \, dx + \sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, -\zeta_j)}{N(\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(\nu_k, \xi_i) \int_{\tau}^{\tau_0} Q(x, \xi_i) e^{-(x-\tau)/\zeta_j} \, dx + \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, -\zeta_j)}{N(-\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(-\nu_k, \xi_i) \int_{\tau}^{\tau_0} Q(x, \xi_i) e^{-(x-\tau)/\zeta_j} \, dx \tag{33b}$$

for $j = N+I+1, N+I+2, \ldots, N+M$.

The coefficients A_j, for $j = N+1, N+2, \ldots, N+I$, and B_j, for $j = N+I+1, N+I+2, \ldots, N+M$, can be determined by imposing that the solution expressed by Eq. (31a)

satisfies Eq. (18a) for $\tau = 0$ and that the solution expressed by Eq. (31b) satisfies Eq. (18b) for $\tau = \tau_0$. We find

$$A_j = L(\zeta_j) - \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, \zeta_j) - \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, \zeta_j) e^{-\tau_0/\nu_k} - \sum_{k=K+1}^{N} \mathfrak{B}_k(0) \hat{\Phi}(-\nu_k, \zeta_j) \tag{34a}$$

for $j = N+1, N+2, \ldots, N+I$, and

$$B_j = R(\zeta_j) - \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, -\zeta_j) e^{-\tau_0/\nu_k} - \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, -\zeta_j) - \sum_{k=1}^{K} \mathfrak{U}_k(\tau_0) \hat{\Phi}(\nu_k, -\zeta_j) \tag{34b}$$

for $j = N+I+1, N+I+2, \ldots, N+M$.

Finally, on substituting Eqs. (7a), (7b), (33a) and (34a) into Eq. (31a), we find that the general discrete-ordinates solution at a *positive* dummy node ζ_j can be written as

$$\begin{aligned} G(\tau, \zeta_j) = {} & L(\zeta_j) e^{-\tau/\zeta_j} + \frac{1}{\zeta_j} \int_0^{\tau} Q(x, \zeta_j) e^{-(\tau - x)/\zeta_j} \, dx + \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, \zeta_j) [e^{-\tau/\nu_k} - e^{-\tau/\zeta_j}] \\ & + \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, \zeta_j) e^{-(\tau_0 - \tau)/\nu_k} [1 - e^{-\tau/\nu_k} e^{-\tau/\zeta_j}] \\ & + \sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, \zeta_j)}{N(\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(\nu_k, \xi_i) \int_0^{\tau} Q(x, \xi_i) [e^{-(\tau - x)/\nu_k} - e^{-(\tau - x)/\zeta_j}] \, dx \\ & - \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, \zeta_j)}{N(-\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(-\nu_k, \xi_i) \\ & \times \left\{ \int_0^{\tau} Q(x, \xi_i) e^{-(\tau - x)/\zeta_j} [1 - e^{-x/\nu_k} e^{-x/\zeta_j}] \, dx \right. \\ & \left. + [1 - e^{-\tau/\nu_k} e^{-\tau/\zeta_j}] \int_{\tau}^{\tau_0} Q(x, \xi_i) e^{-(x - \tau)/\nu_k} \, dx \right\} \end{aligned} \tag{35}$$

for $j = N+1, N+2, \ldots, N+I$. Similarly, on substituting Eqs. (7a), (7b), (33b) and (34b) into Eq. (31b), we find that the general discrete-ordinates solution at a *negative* dummy node $-\zeta_j$ can be written as

$$\begin{aligned} G(\tau, -\zeta_j) = {} & R(\zeta_j) e^{-(\tau_0 - \tau)/\zeta_j} + \frac{1}{\zeta_j} \int_{\tau}^{\tau_0} Q(x, -\zeta_j) e^{-(x - \tau)/\zeta_j} \, dx + \sum_{k=1}^{K} A_k \hat{\Phi}(\nu_k, -\zeta_j) e^{-\tau/\nu_k} \\ & \times [1 - e^{-(\tau_0 - \tau)/\nu_k} e^{-(\tau_0 - \tau)/\zeta_j}] + \sum_{k=K+1}^{N} B_k \hat{\Phi}(-\nu_k, -\zeta_j) [e^{-(\tau_0 - \tau)/\nu_k} - e^{-(\tau_0 - \tau)/\zeta_j}] \\ & + \sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, -\zeta_j)}{N(\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(\nu_k, \xi_i) \left\{ [1 - e^{-(\tau_0 - \tau)/\nu_k} e^{-(\tau_0 - \tau)/\zeta_j}] \int_0^{\tau} Q(x, \xi_i) \right. \\ & \left. \times e^{-(\tau - x)/\nu_k} \, dx + \int_{\tau}^{\tau_0} Q(x, \xi_i) e^{-(x - \tau)/\zeta_j} [1 - e^{-(\tau_0 - x)/\nu_k} e^{-(\tau_0 - x)/\zeta_j}] \, dx \right\} \end{aligned}$$

$$- \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, -\zeta_j)}{N(-\nu_k)} \sum_{i=1}^{N} w_i \Psi(\xi_i) \Phi(-\nu_k, \xi_i)$$

$$\times \int_{\tau}^{\tau_0} Q(x, \xi_i) [e^{-(x-\tau)/\nu_k} - e^{-(x-\tau)/\zeta_j}] \, dx \tag{36}$$

for $j = N + I + 1, N + I + 2, \ldots, N + M$.

Clearly, if we use Eq. (32) to express the hatted elementary solutions that appear in Eqs. (35) and (36) in terms of the non-hatted elementary solutions, we can conclude that the resulting equations are the same as the equations obtained from Eqs. (13) and (16) when the continuous variable $\pm \xi$ is restricted to the set of dummy nodes $\{\pm \zeta_j\}$ in these equations. Thus, the equivalence between the DNI technique and the SFI technique is established.

6. The computational efficiency of the techniques

Having concluded that SFI and DNI are formally equivalent techniques of angular interpolation when applied to the Wick–Chandrasekhar method in plane-parallel geometry, we now report in this section the results of a study aimed at determining the most efficient of these techniques, computationally speaking. However, before discussing our findings, we believe it important to give the reader an idea of the main aspects of our computational implementation.

We begin by noting that the implementation of the SFI technique consists essentially in introducing the expressions given by Eqs. (13) and (16) into the discrete-ordinates code being used. Of course, for computational efficiency, some care must be exercised in order to properly nest the "DO" loops that translate into computer language the summations that appear in these equations, but, in general, the task is straightforward.

On the other hand, in regard to the DNI technique, there are various possible ways of performing its implementation. We have found that the most efficient of these ways makes use of some of the simplifying results developed in Section 5. Thus, in our computer code, instead of considering the enlarged eigensystem expressed by Eq. (25), we considered the smaller eigensystem expressed by Eq. (26a), used the fact that the additional separation constants that show up when dummy nodes are introduced into the quadrature scheme are the dummy nodes themselves, and used the expressions for the enlarged vectors of elementary solutions provided by Eqs. (27a), (27b) and (30). However, to determine the additional coefficients of the homogeneous solution that are required when dummy nodes are present, i.e. A_j, $j = N + 1, N + 2, \ldots, N + I$, and B_j, $j = N + I + 1, N + I + 2, \ldots, N + M$, we prefer to add Eqs. (34a) and (34b) to the linear system defined by Eqs. (9a) and (9b) and solve the enlarged linear system thus obtained for all of the coefficients. We have found that this, in general, requires less computer time than solving the linear system defined by Eqs. (9a) and (9b) and then using the explicit expressions provided by Eqs. (34a) and (34b) to compute the additional coefficients of the homogeneous solution. Finally, the desired interpolated solutions are computed with Eqs. (31a) and (31b), where the additional coefficients of the particular solution required, i.e. $\mathfrak{A}_j$, $j = N + 1, N + 2, \ldots, N + I$, and $\mathfrak{B}_j$, $j = N + I + 1$, $N + I + 2, \ldots, N + M$, are given by Eqs. (33a) and (33b).

Two test problems in atmospheric radiative transfer (see Table 1) were solved in order to evaluate the computational performance of the SFI and DNI techniques. The scattering models that define these problems were first used in a comparison exercise promoted by the Radiation Commission of the International Association of Meteorology and Atmospheric Physics more than 20 years ago [6], and for this reason we keep the original denominations *Haze L* and *Cloud* C_1. The phase functions that define the *Haze L* and the *Cloud* C_1 problems are described by Legendre expansions with 83 and 300 terms, respectively. As discussed in Ref. [28], the coefficients of these Legendre expansions were computed independently by J.F. de Haan and A.H. Karp, as a way of establishing complete confidence in their accuracy, and are tabulated in Refs. [28,29]. The quadrature scheme selected to solve these problems is the double quadrature of order $N = 2n$ obtained by applying a standard Gauss–Legendre scheme of order n to each of the half-intervals $[-1, 0]$ and $[0, 1]$. Since the selected quadrature is symmetric, a reduction in the order of the eigenvalue problem to one half of the original size (i.e., n instead of N) can be achieved [14,30] and was used in our computational implementation. The quadrature orders shown in Table 1 were chosen so that the particle distribution functions obtained for both problems turned out to be accurate to within ± 1 in the fifth significant figure, when compared to highly accurate numerical results reported in other works that considered these same problems — in particular, Ref. [29] for the *Haze L* problem and Ref. [14] for the *Cloud* C_1 problem.

We report in Tables 2 and 3 the CPU times spent by our code on an IBM compatible personal computer equipped with a Pentium 233-MHz processor, using the SFI and the DNI techniques to

Table 1
The test problems

Parameter	Description	Haze L	Cloud C_1
ϖ	Single-scattering albedo	0.9	0.9
τ_0	Optical thickness of the layer	1.0	64
μ_0	Cosine of the polar angle of incidence	0.5	0.2
φ_0	Azimuthal angle of incidence	0.0	0.0
L	Scattering order	82	299
N	Selected quadrature order	42	220

Table 2
CPU times (s) and % gain for the *Haze L* problem

($N = 42$, $Z = 6$)				($N = 42$, $M = 16$)			
M	t_{SFI}	t_{DNI}	%	Z	t_{SFI}	t_{DNI}	%
2	2.8	2.7	4	1	2.9	2.9	0
4	3.1	2.8	10	2	3.1	2.9	6
8	3.7	2.9	22	4	4.0	3.0	25
16	4.8	3.1	35	6	4.8	3.1	35
32	7.3	3.6	51	8	5.7	3.2	44
64	12.6	4.6	63	10	6.6	3.2	52

Table 3
CPU times (min) and % gain for the *Cloud* C_1 problem

($N = 220$, $Z = 6$)				($N = 220$, $M = 32$)			
M	t_{SFI}	t_{DNI}	%	Z	t_{SFI}	t_{DNI}	%
4	22.6	22.9	−1	2	23.3	23.7	−2
8	22.8	23.1	−1	4	24.6	23.8	3
16	23.9	23.3	3	6	26.0	23.9	8
32	26.0	23.9	8	8	27.4	24.0	12
64	30.0	24.8	17	10	28.9	24.0	17
128	38.3	27.7	28	20	35.6	24.1	32

compute the particle distribution function for the *Haze L* and the *Cloud* C_1 problems, respectively. In these tables, M and Z denote, respectively, the number of polar angles and the number of spatial positions at which the particle distribution function was computed and the % gain for the DNI technique is defined as

$$\% \text{ gain} = \frac{t_{SFI} - t_{DNI}}{t_{SFI}} \times 100, \tag{37}$$

where t_{SFI} and t_{DNI} denote the CPU times for the SFI and DNI techniques, respectively. It is important to note that these are the *total* CPU times needed to solve the problems, not just the CPU times for performing angular interpolation.

Clearly, we can conclude from the CPU times shown in Tables 2 and 3 that, except for very low values of M and/or Z, the DNI technique is more economical than the SFI technique, specially for the *Haze L* problem, and that the % gain displays a sharp increase with increasing values of M and Z for both problems. We should add that, for values of M and Z above those shown in the tables, we have observed a tendency of the % gain to saturate, followed by a slight decline.

7. Concluding remarks

In this work, we have studied two techniques of angular interpolation for the Wick–Chandrasekhar method in plane-parallel geometry: the source-function integration (SFI) technique and the dummy-node inclusion (DNI) technique. These techniques differ mainly in the way their results are expressed. The SFI technique yields expressions for the particle distribution function which are continuous functions of the angular variable, while the DNI technique expresses the particle distribution function at selected points. We believe that the main result of this work is the proof that the results of the SFI technique coincide with those of the DNI technique at the selected points, thus establishing a formal equivalence between both techniques. Looking at these techniques from the perspective of computational efficiency, we have concluded that the DNI technique can be implemented in a way that makes it more economical than the SFI technique.

Finally, we note that we expect soon to be able to extend our equivalence proof to the case where the boundaries are reflective. Since the expressions for the particle distribution function resulting from the application of the SFI technique for this case are more complicated than those reported in Section 4, we believe that the DNI technique will also prove to be more efficient than the SFI technique for this class of problems.

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Appendix

The form of the particular solution at a dummy node

In this appendix, we report the modifications that we had to introduce into the infinite-medium Green's function formalism of Ref. [13], in order to be able to develop all of the particular solutions required in Section 5 of our work. As in Section 5, we assume that ξ_j, $j = 1, 2, \ldots, N$, are regular quadrature nodes (i.e., nodes associated with nonzero weights), $\xi_j = \zeta_j$, $j = N + 1$, $N + 2, \ldots, N + I$, are *positive* dummy nodes and $\xi_j = -\zeta_j, j = N + I + 1, N + I + 2, \ldots, N + M$, are *negative* dummy nodes. As shown in Section 5, the form of the particular solution at a regular node reported in Ref. [13] is not affected by the inclusion of dummy nodes in the quadrature scheme, and so, to avoid unnecessary repetition, we restrict this appendix to our derivation of the form of the particular solution at a dummy node.

In our derivation of the required extension of the infinite-medium Green's function, we seek a solution, for $j = N + 1, N + 2, \ldots, N + M$ and $\alpha = 1, 2, \ldots, N + M$, of

$$\xi_j \frac{\mathrm{d}}{\mathrm{d}\tau} G(\tau, \xi_j : x, \xi_\alpha) + G(\tau, \xi_j : x, \xi_\alpha) = \sum_{l=0}^{L} f_l \Pi_l(\xi_j) \sum_{i=1}^{N} w_i \Psi(\xi_i) \Pi_l(\xi_i) G(\tau, \xi_i : x, \xi_\alpha), \tag{A.1}$$

subject to the "jump" condition

$$\xi_j \lim_{\varepsilon \to 0} [G(x + \varepsilon, \xi_j : x, \xi_\alpha) - G(x - \varepsilon, \xi_j : x, \xi_\alpha)] = \delta_{j,\alpha} \tag{A.2}$$

and bounded as $\tau \to \pm \infty$. Using the results for the separation constants and elementary solutions that were derived in Section 5, we find that we can write the infinite-medium Green's function for a *positive* dummy node ζ_j as

$$G(\tau, \zeta_j : x, \xi_\alpha) = \sum_{k=1}^{K} A_{k,\alpha} \hat{\Phi}(\nu_k, \zeta_j) \mathrm{e}^{-(\tau - x)/\nu_k} + A_{j,\alpha} \mathrm{e}^{-(\tau - x)/\zeta_j}, \quad \tau > x, \tag{A.3a}$$

and

$$G(\tau, \zeta_j : x, \xi_\alpha) = -\sum_{k=K+1}^{N} B_{k,\alpha} \hat{\Phi}(-\nu_k, \zeta_j) \mathrm{e}^{-(x - \tau)/\nu_k}, \quad \tau < x. \tag{A.3b}$$

On substituting Eqs. (A.3) into Eq. (A.2) for $\xi_j = \zeta_j$, we obtain

$$\zeta_j \sum_{k=1}^{K} A_{k,\alpha}\hat{\Phi}(\nu_k, \zeta_j) + \zeta_j A_{j,\alpha} + \zeta_j \sum_{k=K+1}^{N} B_{k,\alpha}\hat{\Phi}(-\nu_k, \zeta_j) = \delta_{j,\alpha}, \tag{A.4}$$

where the coefficients $A_{k,\alpha}$, $k = 1, 2, \ldots, K$, and $B_{k,\alpha}$, $k = K+1, K+2, \ldots, N$, have been determined in Ref. [13] and are given by

$$A_{k,\alpha} = \frac{w_\alpha \Psi(\xi_\alpha)\Phi(\nu_k, \xi_\alpha)}{N(\nu_k)} \tag{A.5a}$$

and

$$B_{k,\alpha} = \frac{w_\alpha \Psi(\xi_\alpha)\Phi(-\nu_k, \xi_\alpha)}{N(-\nu_k)} \tag{A.5b}$$

with $N(\pm\nu_k)$ as defined by Eq. (8) of Section 3. It follows that Eq. (A.4) can be solved for $A_{j,\alpha}$, and thus we have, for $j = N+1, N+2, \ldots, N+I$,

$$A_{j,\alpha} = \frac{\delta_{j,\alpha}}{\zeta_j} - w_\alpha \Psi(\xi_\alpha)\left[\sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, \zeta_j)\Phi(\nu_k, \xi_\alpha)}{N(\nu_k)} + \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, \zeta_j)\Phi(-\nu_k, \xi_\alpha)}{N(-\nu_k)}\right]. \tag{A.6}$$

In a similar way, we can write the infinite-medium Green's function for a *negative* dummy node $-\zeta_j$ as

$$G(\tau, -\zeta_j : x, \xi_\alpha) = \sum_{k=1}^{K} A_{k,\alpha}\hat{\Phi}(\nu_k, -\zeta_j)\mathrm{e}^{-(\tau - x)/\nu_k}, \quad \tau > x, \tag{A.7a}$$

and

$$G(\tau, -\zeta_j : x, \xi_\alpha) = -\sum_{k=K+1}^{N} B_{k,\alpha}\hat{\Phi}(-\nu_k, -\zeta_j)\mathrm{e}^{-(x-\tau)/\nu_k} - B_{j,\alpha}\mathrm{e}^{-(x-\tau)/\zeta_j}, \quad \tau < x, \tag{A.7b}$$

and substitute these equations into Eq. (A.2) for $\xi_j = -\zeta_j$ to obtain

$$-\zeta_j \sum_{k=1}^{K} A_{k,\alpha}\hat{\Phi}(\nu_k, -\zeta_j) - \zeta_j \sum_{k=K+1}^{N} B_{k,\alpha}\hat{\Phi}(-\nu_k, -\zeta_j) - \zeta_j B_{j,\alpha} = \delta_{j,\alpha}. \tag{A.8}$$

As the coefficients $A_{k,\alpha}$, $k = 1, 2, \ldots, K$, and $B_{k,\alpha}$, $k = K+1, K+2, \ldots, N$, are explicitly known [see Eqs. (A.5a) and (A.5b)] for $B_{j,\alpha}$ to find

$$B_{j,\alpha} = -\frac{\delta_{j,\alpha}}{\zeta_j} - w_\alpha \Psi(\xi_\alpha)\left[\sum_{k=1}^{K} \frac{\hat{\Phi}(\nu_k, -\zeta_j)\Phi(\nu_k, \xi_\alpha)}{N(\nu_k)} + \sum_{k=K+1}^{N} \frac{\hat{\Phi}(-\nu_k, -\zeta_j)\Phi(-\nu_k, \xi_\alpha)}{N(-\nu_k)}\right]. \tag{A.9}$$

Having found all quantities necessary to construct the infinite-medium Green's function at a dummy node, we can now express our particular solution to Eq. (17) of Section 5 for positive and negative dummy nodes $\pm\zeta_j$ as

$$G_p(\tau, \pm\zeta_j) = \int_0^{\tau_0} \sum_{\alpha=1}^{N+M} G(\tau, \pm\zeta_j : x, \xi_\alpha) Q(x, \xi_\alpha)\, \mathrm{d}x. \tag{A.10}$$

For a positive dummy node ζ_j, we substitute Eqs. (A.3) into Eq. (A.10) and use Eqs. (A.5) and (A.6) in the resulting equation to obtain

$$G_p(\tau,\zeta_j)=\sum_{k=1}^{K}\mathfrak{A}_k(\tau)\hat{\Phi}(\nu_k,\zeta_j)+\sum_{k=K+1}^{N}\mathfrak{B}_k(\tau)\hat{\Phi}(-\nu_k,\zeta_j)+\mathfrak{A}_j(\tau), \tag{A.11}$$

where $\mathfrak{A}_k(\tau)$ and $\mathfrak{B}_k(\tau)$ are given by Eqs. (7a) and (7b) of Section 3, and

$$\begin{aligned}\mathfrak{A}_j(\tau)=&\frac{1}{\zeta_j}\int_0^{\tau}Q(x,\zeta_j)\mathrm{e}^{-(\tau-x)/\zeta_j}\,\mathrm{d}x\\&-\sum_{k=1}^{K}\frac{\hat{\Phi}(\nu_k,\zeta_j)}{N(\nu_k)}\sum_{\alpha=1}^{N}w_\alpha\Psi(\xi_\alpha)\Phi(\nu_k,\xi_\alpha)\int_0^{\tau}Q(x,\xi_\alpha)\mathrm{e}^{-(\tau-x)/\zeta_j}\,\mathrm{d}x\\&-\sum_{k=K+1}^{N}\frac{\hat{\Phi}(-\nu_k,\zeta_j)}{N(-\nu_k)}\sum_{\alpha=1}^{N}w_\alpha\Psi(\xi_\alpha)\Phi(-\nu_k,\xi_\alpha)\int_0^{\tau}Q(x,\xi_\alpha)\mathrm{e}^{-(\tau-x)/\zeta_j}\,\mathrm{d}x.\end{aligned} \tag{A.12}$$

For a negative dummy node $-\zeta_j$, we substitute Eqs. (A.7) into Eq. (A.10) and use Eqs. (A.5) and (A.9) in the resulting equation to obtain

$$G_p(\tau,-\zeta_j)=\sum_{k=1}^{K}\mathfrak{A}_k(\tau)\hat{\Phi}(\nu_k,-\zeta_j)+\sum_{k=K+1}^{N}\mathfrak{B}_k(\tau)\hat{\Phi}(-\nu_k,-\zeta_j)+\mathfrak{B}_j(\tau), \tag{A.13}$$

where, again, $\mathfrak{A}_k(\tau)$ and $\mathfrak{B}_k(\tau)$ are given by Eqs. (7a) and (7b) of Section 3, and

$$\begin{aligned}\mathfrak{B}_j(\tau)=&\frac{1}{\zeta_j}\int_{\tau}^{\tau_0}Q(x,-\zeta_j)\mathrm{e}^{-(x-\tau)/\zeta_j}\,\mathrm{d}x\\&+\sum_{k=1}^{K}\frac{\hat{\Phi}(\nu_k,-\zeta_j)}{N(\nu_k)}\sum_{\alpha=1}^{N}w_\alpha\Psi(\xi_\alpha)\Phi(\nu_k,\xi_\alpha)\int_{\tau}^{\tau_0}Q(x,\xi_\alpha)\mathrm{e}^{-(x-\tau)/\zeta_j}\,\mathrm{d}x\\&+\sum_{k=K+1}^{N}\frac{\hat{\Phi}(-\nu_k,-\zeta_j)}{N(-\nu_k)}\sum_{\alpha=1}^{N}w_\alpha\Psi(\xi_\alpha)\Phi(-\nu_k,\xi_\alpha)\int_{\tau}^{\tau_0}Q(x,\xi_\alpha)\mathrm{e}^{-(x-\tau)/\zeta_j}\,\mathrm{d}x.\end{aligned} \tag{A.14}$$

Eqs. (A.12) and (A.14) are the results that were used without proof in Section 5.

References

[1] Wick GC. Z Phys 1943;120:702.
[2] Chandrasekhar S. Astrophys J 1944;100:76.
[3] Schuster A. Astrophys J 1905;21:1.
[4] Schwarzschild K. Göttinger Nachr Math-Phys Klasse 1906;195:41.
[5] Chandrasekhar S. Radiative transfer. London: Oxford University Press, 1950.
[6] Lenoble J, editor. Standard procedures to compute atmospheric radiative transfer in a scattering atmosphere. Boulder, CO: National Center for Atmospheric Research, 1977.
[7] Hansen JE, Travis LD. Space Sci Rev 1974;16:527.
[8] Liou KN. An introduction to atmospheric radiation. New York: Academic Press, 1980.
[9] Kattawar GW, editor. Selected papers on multiple scattering in plane parallel atmospheres and oceans: methods. SPIE Milestone Series, vol. MS 42. Bellingham, WA: SPIE — The International Society for Optical Engineering, 1991.

[10] Stamnes K, Conklin P. JQSRT 1984;31:273.
[11] Stamnes K, Tsay SC, Nakajima T. JQSRT 1988;39:415.
[12] Stamnes K, Tsay SC, Wiscombe W, Jayaweera K. Appl Opt 1988;27:2502.
[13] Barichello LB, Garcia RDM, Siewert CE. Particular solutions for the discrete-ordinates method. JQSRT 2000;64:219.
[14] Siewert CE. A concise and accurate solution to Chandrasekhar's basic problem in radiative transfer. JQSRT 2000;64:227.
[15] Siewert CE. A discrete-ordinates solution for radiative-transfer models that include polarization effects. JQSRT, in press, 1999.
[16] Carlson BG, Lathrop KD. Transport theory, the method of discrete ordinates. In: Greenspan H, Kelber CN, Okrent D. Editors. Computing methods in reactor physics. Gordon & Breach, New York: 1968, p. 166.
[17] Lathrop KD. Reactor Technol 1972;15:107.
[18] Sanchez R, McCormick NJ. Nucl Sci Engng 1982;80:481.
[19] Chalhoub ES, Garcia RDM. Ann Nucl Energy 1997;24:1069.
[20] Karp AH. JQSRT 1981;25:403.
[21] Karp AH, Petrack S. JQSRT 1983;30:351.
[22] Barichello LB, Siewert CE. Nucl Sci Engng 1998;132:79.
[23] Stamnes K. JQSRT 1982;28:47.
[24] Chalhoub ES. The discrete-ordinates method for solving azimuthally-dependent transport problems. Sc D thesis, Instituto de Pesquisas Energéticas e Nucleares, São Paulo, Brazil, 1997 [in Portuguese].
[25] Hummer DG. Mon Not Roy Astron Soc 1968;138:73.
[26] McCormick NJ, Siewert CE. Astrophys J 1970;162:633.
[27] Siewert CE. J Comput Phys 1999;152:251.
[28] Benassi M, Garcia RDM, Karp AH, Siewert CE. Astrophys J 1984;280:853.
[29] Garcia RDM, Siewert CE. Transp Theory Stat Phys 1985;14:437.
[30] Stamnes K, Swanson RA. J Atmos Sci 1981;38:387.