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A more efficient implementation of the discrete-ordinates method for an approximate model of particle transport in a duct

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ABSTRACT

We consider transport of light, neutrons, or any uncharged particles in a straight duct of circular cross section. This problem first came to fashion some 30 years ago when Pomraning and Prinja formulated their so called "pipe problem". In the years to follow, investigators applied essentially every known method of numerical solution, including MMRW's Wiener–Hopf – except possibly one. This presentation concerns that particular numerical solution, which arguably seems to be the most efficient of all.

1. Introduction

It is hard to believe that it has been 30 years since Jerry Pomraning and then, post doc, Anil Prinja (having recently completed his dissertation at Queen Mary with MMRW) published their classical work on the solution to the 1-D analogue to the 3-D straight duct problem (Prinja and Pomraning, 1984). The origin of the "pipe problem" as it is called, is for a fusion application to eliminate neutral particles from a proposed tokamak design. Their work had all the synergetic features of the collaboration between the two transport theorists—producing a physically and mathematically insightful paper that was to have a life of its own. Ed Larsen then showed (Larsen, 1984) (as only EWL can do), the Pomraning–Prinja model was merely the "tip of the iceberg" and lent itself to a much deeper theory yielding higher order methods that improved upon numerical precision and physical relevance of the model. Not surprisingly, MMRW took up the challenge in an entirely different physical context—light transport in a duct, where he applied his signature Wiener–Hopf technique in a most delightful presentation (Williams, 2007). In the meantime, essentially all the known transport solution methodologies at the time came to bear on this problem (Larsen et al., 1986; Garcia et al., 2000; Jing et al., 2010; Jing and Xiang, 2010; Garcia and Ono, 1999a; Garcia and Ono, 1999b)—save one.

In the following, we apply the method of adding and doubling as a reformulation of the discrete ordinate method in a new response matrix form. While doubling is well known in radiative transfer, it is not so in neutron transport theory, where the duct problem originated. As shown, doubling eliminates the need for sweeps in the directions of particle travel, yet assumes a simple fully discretized form. The method, called the **R**esponse **M**atrix **SN M**ethod (**RMSNM**), is based on the conventional diamond difference algorithm to include doubling to avoid iteratively sweeping back and forth through the duct. The method uniquely applies doubling coupled to convergence acceleration to achieve extreme precision. It features precision through simplicity and will be described in a way that seems to be new, at least to this author and I am sure to others.

Relying on the informative description of the duct transport problem and its mathematical formulation given by Garcia (Garcia, 2013), we first state the appropriate transport equation, followed by a change of "angular variable" to the range [0,1]. Next, a Gauss–Legendre quadrature approximates the scattering integral through contiguous half-ranges. Continuing with a trapezoidal integration over a spatial interval (which gives the diamond difference approximation), the fully discretized discrete ordinates transport equation emerges. One then forms the response matrix for the exiting surface angular and interior distributions as well as for the pipe reflectance and transmittance. Finally, we demonstrate high order numerical performance in comparison to the ADO method.

2. The discrete ordinates balance equation

The deceptively simply looking transport equation in the duct of area A and circumference L reads as:

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$$\left[\xi\frac{\partial}{\partial\tau}+1\right]Y(\tau,\xi)=\int_{-\infty}^{\infty}d\xi'\psi(\xi')Y(\tau,\xi'), \tag{1a}$$

with

$$\psi(\xi)\equiv\frac{2c}{\pi}\frac{1}{(1+\xi^2)^2}, \tag{1b}$$

where τ is the spatially scaled variable

$$\tau\equiv\frac{L}{\pi A}z.$$

The obvious difference between this transport equation and say, the neutron transport equation, is the variable ξ, in $(-\infty,\infty)$, rather than in [−1,1], assuming the role of the "angular variable". A change of the ξ – dependent variable enables transformation to the finite interval [0,1] however.

The duct is of length Z with entering particles in the half-range at the near end and none at the far end according to:

$$\begin{aligned}&Y(0,\xi)=1\\&Y(\tau_0,-\xi)=0,\end{aligned} \tag{1c}$$

where $\xi\in[0,\infty)$ for a pipe of dimensionless length τ_0 and a circular cross section to give

$$\tau_0\equiv\frac{2}{\pi}\frac{Z}{\rho}. \tag{1d}$$

Only an isotropically entering particle distribution is considered here.

2.1. Angular discretization

Writing the scattering integral as:

$$\int_{-\infty}^{\infty}d\xi'\psi(\xi')Y(\tau,\xi')=\int_0^{\infty}d\xi'\psi(\xi')Y(\tau,\xi')+\int_0^{\infty}d\xi'\psi(\xi')Y(\tau,-\xi')$$

gives

$$\int_{-\infty}^{\infty}d\xi'\psi(\xi')Y(\tau,\xi')=\int_0^1 d\mu'\psi(\xi'(\mu'))[Y(\tau,\xi'(\mu'))+Y(\tau,-\xi'(\mu'))] \tag{2}$$

for the change of variable

$$\xi'=\frac{\mu'}{1-\mu'};\quad \mu'\in[0,1].$$

By applying the Nth-order shifted Legendre–Gauss quadrature approximation on interval [0,1], Eq. (2) becomes

$$\int_{-\infty}^{\infty}d\xi'\psi(\xi')Y(\tau,\xi')\simeq\sum_{m'=0}^{2N}\omega_{m'}\psi_{m'}Y_{m'}(\tau), \tag{3a}$$

where for $m=1,\dots,N$

$$\begin{aligned}&\omega_m=\omega_{N+m}=\tfrac{1}{(1-\mu_m)^2}\mathrm{v}_m\\&\xi_m=\tfrac{\mu_m}{1-\mu_m}\\&\xi_{N+m}=-\xi_m.\end{aligned} \tag{3b}$$

μ_m,v_m are the Gauss-quadrature abscissae and weights respectively. The abscissae μ_m come from

$$P_N(x_m)=0,\ x_m\equiv 2\mu_m-1,\quad m=1,\dots,N,$$

where $P_l(x)$ is the lth order shifted Legendre polynomial satisfying the usual recurrence

$$\frac{l+1}{2l+1}P_{l+1}(x)=xP_l(x)-\frac{l}{2l+1}P_{l-1}(x);\ P_0(x)\equiv 1,\ P_{-1}(x)\equiv 0.$$

Therefore, the recurrence in vector form is

$$\boldsymbol{AP}_m=x_m\boldsymbol{P}_m-\frac{N}{2N-1}\boldsymbol{S}_m;\quad m=1,\dots,N \tag{4a}$$

with

$$\boldsymbol{A}\equiv\begin{bmatrix}0&1&0&\dots&&&0\\1/3&0&2/3&\dots&&&\dots\\0&2/5&0&3/5&&\dots&\\\dots&&&\dots&&&0\\&&&\dots&0&&(N-1)/(2N-3)\\0&\dots&&0&(N-1)/(2N-1)&&0\end{bmatrix} \tag{4b}$$

and

$$\begin{aligned}&\boldsymbol{P}_m\equiv[P_0(x_m)\quad P_1(x_m)\quad\dots\quad P_{N-1}(x_m)]^T\\&\boldsymbol{S}_m\equiv[0\quad 0\quad\dots\quad P_N(x_m)]^T.\end{aligned}$$

The abscissae, therefore, are the eigenvalues of matrix $\boldsymbol{A}$

$$[\boldsymbol{A}-x_m\boldsymbol{I}]\boldsymbol{P}_m=0;\quad m=1,\dots,N \tag{5a}$$

giving

$$\mu_m=\frac{1}{2}(1+x_m) \tag{5b}$$

and the weights are (Stegun and Abramowitz, 1994)

$$\mathrm{v}_m=\frac{2(1-x_m^2)}{(N+1)^2[P_{N+1}(x_m)]^2}. \tag{5c}$$

On substitution of the scattering integral approximation of Eq. (3a) at the abscissae, Eq. (1a) becomes the following angularly discretized approximation to the transport equation for the angular flux

$$\left[\xi_m\frac{d}{d\tau}+1\right]Y_m(\tau)=\sum_{m'=0}^{2N}\omega_{m'}\psi_{m'}Y_{m'}(\tau), \tag{6}$$

where

$$Y(\tau,\xi_m)=Y_m(\tau)+\varepsilon(\tau,\xi_m)$$

with the combined quadrature and discretization error $\varepsilon(\tau,\xi_m)$ neglected. Note that since the Gauss Quadrature converges to the exact integral for a sufficiently smooth integrand as O(N^{-4}), $Y_m(\tau)$ also converges to the exact solution for every m.

More conveniently, Eq. (6), in vector form for the bi-angular flux vectors in the negative and positive directions, becomes

$$\begin{aligned}&\left[-\tfrac{d}{d\tau}+\boldsymbol{M}^{-1}(\boldsymbol{I}-\boldsymbol{C})\right]\boldsymbol{Y}^-(\tau)=\boldsymbol{M}^{-1}\boldsymbol{CY}^+(\tau)\\&\left[\tfrac{d}{d\tau}+\boldsymbol{M}^{-1}(\boldsymbol{I}-\boldsymbol{C})\right]\boldsymbol{Y}^+(\tau)=\boldsymbol{M}^{-1}\boldsymbol{CY}^-(\tau)\end{aligned} \tag{7a, b}$$

with

$$\begin{aligned}&\boldsymbol{Y}^+(\tau)\equiv[Y_1(\tau)\quad Y_2(\tau)\quad\dots\quad Y_N(\tau)]^T\\&\boldsymbol{Y}^-(\tau)\equiv[Y_{N+1}(\tau)\quad Y_{N+2}(\tau)\quad\dots\quad Y_{2N}(\tau)]^T\end{aligned} \tag{7c, d}$$

and

$$\begin{aligned}&\boldsymbol{C}\equiv\boldsymbol{\psi W}\\&\boldsymbol{\psi}\equiv\{\psi_m;\quad i,m=1,\dots,N\}\\&\boldsymbol{W}\equiv diag\{\omega_m;\quad m=1,\dots,N\}\\&\boldsymbol{M}\equiv diag\{\xi_m;\quad m=1,\dots,N\}.\end{aligned} \tag{7e, f, g, h}$$

2.2. Spatial discretization and single layer response

Uniformly discretizing the interval $[0,\tau_0]$ into n intervals with $h\equiv\tau_0/n$ characterizes the spatial variation with an additional trapezoidal rule integration of Eqs. (7a,b) over interval $[\tau_j,\tau_{j+1}]$ to give