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LETTER TO THE EDITOR

Why does the double-Gauss approach perform well in slab transport problems?

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Abstract. The double-Gauss approach in transport calculations performs well because it is a full-range type formulation.

The traditional discrete-ordinates (S_N) method does not perform well for relatively high absorption cases when the order of approximation is not too large. The discrepancy may be attributed to the use of orthogonal polynomials $P_N(\mu)$ in $(-1, 1)$ to evaluate Gauss–Legendre quadrature coefficients. This process regularizes the singular eigenfunction in the transient range according to the classical polynomial theory, which, however, does not produce a natural basis for use in transport theory. Intriguingly, the double-Gauss method, which uses the Legendre polynomials in the half-range, performs very well for slab problems [1]. The reason for this is due to the fact that the double-Gauss approach is a full-range type formulation [2] like the F_N method. We demonstrate this in the following with an example of double S_2. The conclusion is, however, true for any order of approximation.

We have observed that any attempt to use basis functions other than the Case eigenfunctions or a suitable approximate set of these functions may not always produce optimal results. Recently, the singular eigenfunctions have, indeed, been approximated by regular rational functions [3]. However, it is useful to be in the framework of ordinary differential equations as in the usual spherical harmonics or discrete-ordinates method from a computational point of view. An indirect approach [2, 4] to solve the transient integral problem involving the singular eigenfunction is, therefore, important. Siewert's work on the F_N method [2] and then its generalization by Sengupta [5] demonstrate the importance of the full-range weight function μ to solve the half-range transport problem. The F_N method was originally derived from the Plackzek lemma, which relates the solution of the half-space problem to an infinite medium problem.

In the framework of discrete-ordinates, we can derive the full-range formulation by choosing the zeros of orthogonal polynomials with respect to μ in $(0, 1)$ followed by a reflection of the zeros on the other half $(-1, 0)$. This ensures that the entire range of the independent variable has been used together with the full-range weight function μ, with respect to which the complete set of eigenfunctions of the full-range problem are orthogonal. The weights in the quadrature formula may then be obtained in a Gaussian way. For example, the quadrature coefficients for double-S_2 type formulation are obtained from:

$$\sum_{i=1}^{2} w_i \mu_i^n = \int_0^1 (\mu) \cdot \mu^n \, d\mu \qquad n = 0, 1, 2, 3$$

i.e.

$$w_1+w_2=\tfrac{1}{2} \tag{1}$$

$$w_1\mu_1+w_2\mu_2=\tfrac{1}{3} \tag{2}$$

$$w_1\mu_1^2+w_2\mu_2^2=\tfrac{1}{4} \tag{3}$$

$$w_1\mu_1^3+w_2\mu_2^3=\tfrac{1}{5}. \tag{4}$$

The solution of (1)–(4) yields $\mu_{1,2}=(6\pm\sqrt{6})/10$ and $w_{1,2}=(3\sqrt{6}\pm2)/12\sqrt{6}$. The direction-cosines are zeros of $10\mu^2-12\mu+3=0$, which is orthogonal to μ in $(0,1)$. The numerical solution based on these quadrature coefficients is, however, not satisfactory. The reason is the following. When we use the quadrature formula $\int_0^1 f(\mu)\,d\mu=\Sigma_{i=1}^2 (w_i/\mu_i)f(\mu_i)$, we obtain $W_1+W_2=0.8888$, where $W_i=w_i/\mu_i$, $i=1,2$. We observe that the formulation does not satisfy the conservation condition

$$W_1+W_2=1 \tag{5}$$

which is an important property of discrete-ordinates. If we now replace (4) by (5), we obtain the new set

$$W_1+W_2=1$$

$$W_1\mu_1+W_2\mu_2=\tfrac{1}{2}$$

$$W_1\mu_1^2+W_2\mu_2^2=\tfrac{1}{3}$$

$$W_1\mu_1^3+W_2\mu_2^3=\tfrac{1}{4}$$

which *coincides* with the double-Gauss formula based on Legendre polynomial orthogonal with respect to unity in $(0,1)$. The direction cosines are zeros of $\mu^2-\mu+\frac{1}{6}=0$, a second-order orthogonal polynomial with respect to unity in $(0,1)$. This set performs remarkably well for 'sum' results for all c (number of secondaries per primary), including both highly absorbing and scattering cases. For example, the leakage values for the constant source problem (source = 1) are 0.5433 and 2.6058 for $c=0.1$ and $c=0.9$ respectively. For the traditional discrete-ordinates S_4, these values are 0.5654 and 2.6401, where as the exact results are 0.5435 and 2.6103. The performance of the double-Gauss set is equally satisfactory for the albedo problem. This is explained by the fact that the double-Gauss approach is a full-range formulation (like the F_N method), with the inclusion of the conservation condition.

However, the eigenvalues of the double-Gauss get worse compared to the traditional S_N method. For example, the asymptotic eigenvalues with flux representation of the form $\exp(-x/\nu)$ are: $\nu_0(\text{double } S_2)=2.0765$, $\nu_0(S_4)=1.9027$, $\nu_0(\text{exact})=1.9032$ for $c=0.9$. This calls for a theory based on the quadrature set, dependent on the medium [6]. Further work in this direction is in progress.

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