The parabolic cylinder function in elastodynamic problems

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INTRODUCTION

When comparing the synthetic response obtained using a zero-order, high-frequency approximation method with that obtained from a highly numerically accurate method, such as the Alekseev-Mikhailenko Method (AMM) (Mikhailenko, 1985), the largest disparities usually appear near critical reflection points of a ray. This difference between the two methods occurs in both the pre- and post-critical offset range near the critical (branch) point. The reason this occurs is that the zero-order, high-frequency method takes only the saddle point contribution corresponding to the reflected arrival and neglects any effects from the branch point which gives rise to the critically refracted (head-wave) arrival. This problematic area has been discussed in several texts on seismology, notably, Brekhovskikh (1960) and Cerveny and Ravindra (1970), where it is shown that higher order approximations for both the reflected arrival and the associated critically refracted arrival, which increases the accuracy of the high frequency solution, may be written in terms of the frequency-dependent parabolic cylinder functions (PCF).

Assuming a band-limited source wavelet, computation time is increased, as all frequency points where the spectrum of the wavelet is non-zero should be included. Another obstacle is the numerical computation of the parabolic cylinder function required in the higher order high-frequency solution. The particular PCF related to this problem is of order $-3/2$. (In actuality, the PCF of order $1/2$ is also required, but may be obtained from the PCF of order $-3/2$, as they are both linearly dependent solutions of an ordinary differential equation.).

THEORETICAL AND NUMERICAL ANALYSIS

An arbitrary PCF of order p and complex argument, z, may be defined in terms of the confluent hypergeometric function, Φ, (Abramowitz and Stegun, 1970) as

$$D_p(z) = 2^{p/2}\, e^{-z^2/4} \left\{ \frac{\pi^{1/2}}{\Gamma\left[(1-p)/2\right]} \Phi\left[-p/2, 1/2; z^2/2\right] - \frac{(2\pi)^{1/2} z}{\Gamma\left[-p/2\right]} \Phi\left[(1-p)/2, 3/2; z^2/2\right] \right\} \tag{1}$$

where

$$\Phi[a,b;u] = 1 + \frac{au}{b} + \frac{(au)_2\, u^2}{(b)_2\, 2!} + \cdots \frac{(au)_n\, u^n}{(b)_n\, n!} + \cdots \tag{2}$$

with

$$(a)_n = a(a+1)(a+2)\cdots(a+n-1), \quad (a)_0 = 1 . \tag{3}$$

In the problem under consideration here, the complex argument, z, is of a special type, specifically, $z=(1+i)y$, where y is a real quantity. The PCF is required for all combinations of positive and negative z and its complex conjugate. Algorithms currently available for the evaluation of the confluent hypergeometric function become unstable near the imaginary axis, which is the case for the argument used here. Consequently, an alternative method, or combinations thereof, are required to obtain an accurate and stable method of determining the value of the PCF with this particular argument type. The problem is simplified somewhat in that, if a solution can be obtained for $D_{-3/2}\left[(1+i)y\right],\ y \geq 0$, all other required order types, specifically $v = 1/2$, may be obtained using the following

$$D_p\left(z^*\right) = D_p^*(z) \quad \text{and} \quad D_p(-z) = (-1)^p D_p(z) \tag{4}$$

together with the functional relation,

$$D_p(z) = \frac{\Gamma(p+1)}{(2\pi)^{1/2}}\left[e^{i\pi p/2} D_{-p-1}(iz) + e^{i\pi p/2} D_{-p-1}(-iz)\right] \tag{5}$$

with "*" indicating the complex conjugate (Gradshteyn and Rhyzik, 1980).

Previous experience has indicated that numerical accuracy is critical in two areas related to this problem. The first is that, in seismological applications, the real argument y is very sensitive in that it is often the difference of two small numbers. Secondly, a numerical solution for the parabolic cylinder function is usually unstable for small values of the argument, $|z| \approx 0$, if a proper numerical solution technique is not chosen.

There are a number of ways to approach this problem, some of which will be discussed here. The PCF may be written in the form of an initial value problem of second-order ordinary differential equation. For an arbitrary order p and argument z the following equation is valid

$$\frac{d^2 D_p}{dz^2} + \left(p + 1/2 - z^2/4\right) D_p = 0 \quad , \tag{6}$$

subject to the initial conditions

$$D_p(0) = \frac{2^{p/2}\pi^{1/2}}{\Gamma\left[(1-p)/2\right]} \tag{7}$$

and

$$\frac{dD_p(0)}{dz} = -\frac{2^{p/2}(2\pi)^{1/2}}{\Gamma[-p/2]} \tag{8}$$

Differential equation problems of this special formulation may be simplified for solution purposes if the following changes of variables are made

$$D_p(z) = u(z) + i\,v(z)\,, \tag{9}$$

u and v real functions of y, and

$$z = (1+i)\,y\,, \tag{10}$$

y a real variable. The above variable changes yield the following initial value problem involving a system of first-order ordinary differential equations

$$\frac{dr}{dy} = 2\,(p+1/2)\,v - y^2 u \tag{11}$$

$$\frac{ds}{dy} = -2\,(p+1/2)\,u - y^2 v \tag{12}$$

$$\frac{du}{dy} = r \tag{13}$$

$$\frac{dv}{dy} = s \tag{14}$$

The initial conditions for this problem at $y = 0$ are

$$u(0) = \frac{2^{p/2}\pi^{1/2}}{\Gamma[(1-p)/2]} \tag{15}$$

$$v(0) = 0 \tag{16}$$

$$\frac{du(0)}{dy} = \frac{dv(0)}{dy} = -\frac{2^{p/2}(2\pi)^{1/2}}{\Gamma[-p/2]} \tag{17}$$

After an evaluation of numerical ODE solvers, Gear's method (Gear, 1971) for the numerical solution of systems of ordinary differential equations (initial value problems) was chosen as it provides acceptable results, partially as a result of the fact that the Jacobian used in the solution of equation (9) may be obtained analytically. As an adaptive finite-difference grid method is used, a reasonably accurate solution in the problematic area, $y \approx 0$, can be expected. There are a number of routines in various mathematical computing libraries based on the above method, which produce little variation in the results and require about equal amounts of computational time. The algorithm used here is the IMSL routine DGEAR.

This approach of solving an initial value problem comprised of first-order ordinary differential equations (ODEs) produces accurate results. Rather than compute the solution once for a range of values, tabulate the results, and write to an external device for later recall, it is more efficient to compute the function values as required and enhance computational speed by using the restart option contained in most of the algorithms. Apart from an independent check of the accuracy of the ODE solver, alternative methods are sought; if not in the full range of interest of the independent variable, then at least in part, and the ODE solution used as required in all other areas.

It has been found that by retaining the first three terms in the asymptotic expansion of $D_{-3/2}\left[(1+i)y\right]$, for $y \geq 4.0$, and using a 64-bit word in the calculations for both the ODE method and the asymptotic expansion, 10 to 13 floating-point digits of accuracy are obtained. The asymptotic expansion, valid in the first quadrant of the complex z-plane for $|z| >> 1$, $|z| >> p$ is (Gradshteyn and Rhyzik, 1980)

$$D_p(z) \approx e^{-z^2/4} z^p \left(1 - \frac{p(p+1)}{2z^2} + \frac{p(p-1)(p-2)(p-3)}{2 \cdot 4 z^4} - \cdots \right) \quad . \tag{18}$$

In the region $\varepsilon < y < y_T$, numerical integration, although computationally slow, produced results comparable to those obtained using the ODE method. Here, ε was chosen to be equal to 0.1 and y_T to 4.0, as a check on the validity of the ODE solver in this region. The choice of $y_T = 4.0$, as previously stated, was based on a numerical test to determine at what value of y equation (18) produced the same accuracy as the ODE algorithm.

The integral chosen for numerical integration was (Gradshteyn and Rhyzik, 1980)

$$D_{-p-1}\left[(1+i)y\right] = \frac{e^{-iy^2/2}}{2^{(p-1)/2}\,\Gamma\left[(p+1)/2\right]} \int_0^\infty \frac{e^{-ix^2y^2} x^p}{\left(1+x^2\right)^{1+p/2}}\,dx$$

$$\left[\mathrm{Re}(p) > -1,\ \mathrm{Re}\left(iz^2\right) \geq 0\right] \tag{19}$$

The numerical integration was computed using a modified trapezoidal algorithm with x sampled at $\Delta x = 0.000001$. ODE results agreed to an average of about 12 floating-point digits in this region. The asymptotic expansion, equation (18), produced the same degree of accuracy, in agreement with the ODE solution: the onset of $y = 4$ was chosen such that this would be the case.

The ODE solution to the parabolic cylinder function was sought at increments of $\Delta y = 0.01$ in the range $0.0 < y \leq 8.0$. The user-supplied (estimated) $\Delta y_{\min}$ was set to 1.0×10^{-04}, which the routine DGEAR modified to 1.0×10^{-07} in the vicinity of $y \approx 0.0$. Over the range, $0 < y \leq 8.0$, Δy never became larger than 5.0×10^{-03}. This is partially, but not totally, due to the value of the user-specified relative tolerance, initially set to 1.0×10^{-12}. After experimentation, it was reset to 1.0×10^{-10}, producing the same results as the previous tolerance. In the region, $0.0 < y \leq 0.1$, the solution was assumed to be as accurate as the remainder of the range, based on the initial values of the problem at $y = 0.0$ and the corresponding Taylor series expansion in $u(y)$ and $v(y)$ near $y = 0$, the numerical integration-ODE solutions agreement near $y = 0.1$, and the smoothness of the displayed solution (Figure 1) in the range $0 < y < 0.1$.

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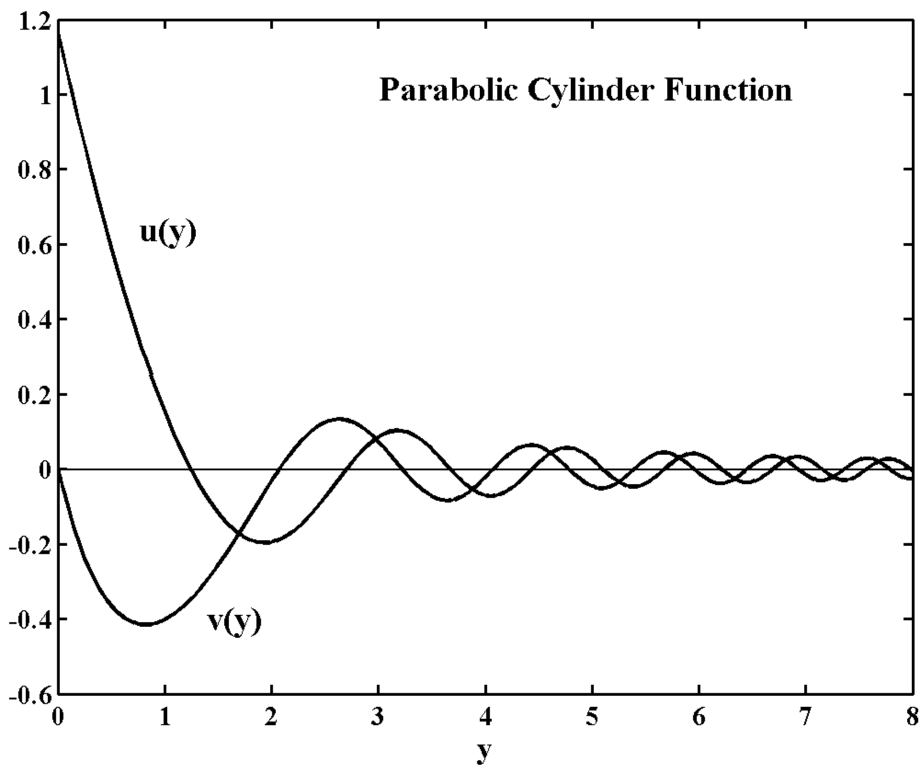

FIG. 1. Real, *u(y),* and imaginary, *v(y),* parts of the parabolic cylinder function, $D_{-3/2}\left[(1+i)y\right]$, for the range of the dimensionless variable 0<y<8. Only the ODE solution is shown as the others overlay.