Chebyshev Approximation of \((1 + 2x)\exp(x^2)\erfc x\) in \(0 \leq x < \infty\)

By M. M. Shepherd and J. G. Laframboise

Abstract. We have obtained a single Chebyshev expansion of the function \(f(x) = (1 + 2x)\exp(x^2)\erfc x\) in \(0 < x < \infty\), accurate to 22 decimal digits. The presence of the factors \((1 + 2x)\exp(x^2)\) causes \(f(x)\) to be of order unity throughout this range, ensuring that the use of \(f(x)\) for approximating \(\erfc x\) will give uniform relative accuracy for all values of \(x\).

I. Introduction. The functions \(\erfc x = \frac{2}{\sqrt{\pi}} \int_x^\infty \exp(-t^2) \, dt\) and \(\exp(x^2)\erfc x\) occur frequently in kinetic theory of gases and related subjects. Calculation of these functions using the identity \(\erfc x = 1 - \erf x\), together with available approximations [1] for \(\erf x\), usually results in large relative errors for large \(x\) because \(\erf x \to 1\) as \(x \to \infty\). To overcome this difficulty, Clenshaw [2], Luke [3], [4], and Schonfelder [5] have presented Chebyshev approximations in which the range \(0 < x < \infty\) is split into two ranges \(0 < x < c\) and \(c < x < \infty\), with \(\erf x\) being Chebyshev-approximated in \(0 < x < c\), and \(x \exp(x^2)\erfc x\) being Chebyshev-approximated in \(c < x < \infty\). Clenshaw [2] uses \(c = 4\), 33 terms for \(x < 4\) and 18 terms for \(x > 4\), and obtains an accuracy of twenty decimal places (20D). Corresponding figures for Luke [3], [4] and Schonfelder [5] are \(c = 3\), 25 and 22 terms, and 20D; and \(c = 2\), 27 and 43 terms, and 30D. These authors use various transformations \(t(x)\) to map \(c < x < \infty\) into \(-1 < t < 1\). Use of the identity \(\erfc(-x) = 2 - \erfc x\) eliminates the need to approximate \(\erfc x\) for negative \(x\).

Schonfelder [5] has also presented a single 43-term Chebyshev expansion of \(\exp(x^2)\erfc x\) for the entire interval \(0 < x < \infty\), using a relation of the form \(t = (x - k)/(x + k)\) to map this interval into \(-1 < t < 1\). Oldham [6] has presented a simple approximation of \(\sqrt{\pi} x \exp(x^2)\erfc x\), having a maximum relative error of one part in 7000 and suitable for hand calculation.

Whenever a function to be Chebyshev-approximated has a zero within its interval of definition or at either end of it, such an approximation is likely to give large relative errors near such a zero because the usual procedures for calculating Chebyshev coefficients minimize maximum absolute error. Accordingly, it is advantageous to multiply \(\erfc x\) by factors which yield a product of order unity for all \(x\) in \((0, \infty)\) and then to Chebyshev-approximate this product function, because one will then obtain good uniformity of relative as well as absolute error. Our chosen function, \(f(x) = (1 + 2x)\exp(x^2)\erfc x\), satisfies this criterion. It has limiting values

Received April 14, 1980.

of 1 and $2/\sqrt{\pi} \approx 1.13$ at $x = 0$ and $x \to \infty$, respectively. In comparison, Schonfelder's function $\exp(x^2)\text{erfc} \ x$ approaches 0 as $x \to \infty$. Furthermore, our choice contains no irrational coefficients, in contrast with the more obvious choice $(1 + \sqrt{\pi}x)\exp(x^2)\text{erfc} \ x$, which $\to 1$ at $x = 0$ and $x \to \infty$. A graph of $f(x)$ appears in Figure 1.

![Graph of the function $F(t)$ defined by the relation $f(x) = (1 + 2x)\exp(x^2)\text{erfc} \ x$ together with the mapping $t = (x - 3.75)/(x + 3.75)$.](image)

We have used the same transformation as that of Schonfelder [5], i.e. $t = (x - k)/(x + k)$ with $k = 3.75$, to map $0 < x < \infty$ into $-1 < t < 1$. Tests of various $k$ values for our $f(x)$ yielded results similar to his, namely that this value gives near-optimum convergence of the resulting Chebyshev series over the precision range of greatest interest, i.e. 8D to 18D. Our calculations were done in IBM quadruple precision, which yields a machine precision of 34D.

II. Calculation of Chebyshev Coefficients. We have used the usual [7] form of an $m$th-order Chebyshev expansion. Thus, the Chebyshev polynomials $T_j(t)$ are given by

$$T_j(t) = \cos(j \arccos t); \quad j = 0, 1, 2, \ldots$$

The above-mentioned $f(x)$ and transformation from $x$ to $t$ define a function $F(t)$ which is expanded as follows:

$$F(t) = \sum_{j=0}^{m} c_j T_j(t),$$

where

$$c_j = \frac{\sum_{k=0}^{m} F(t_k)T_j(t_k)}{\|T_j\|^2},$$

License or copyright restrictions may apply to redistribution; see https://www.ams.org/journal-terms-of-use
(4) \( t_k = \cos \left( \frac{2k + 1 + \pi}{2m + 1} \right) ; \quad k = 0, 1, 2, \ldots, m, \)

(5) \( \| T_0 \|^2 = m + 1; \quad \| T_i \|^2 = \frac{1}{2}(m + 1) \) for \( i > 0. \)

In order to calculate the required values of \( f(x) \), we note that the Taylor expansion

\[
\text{erfc } x = 1 - \frac{2}{\sqrt{\pi}} \left( t - \frac{t^3}{3} + \frac{t^5}{5 \cdot 2!} - \frac{t^7}{7 \cdot 3!} + \frac{t^9}{9 \cdot 4!} - \cdots \right)
\]

can be rearranged [8] into the form

\[
\exp(x^2)\text{erfc } x = \exp(x^2) - \frac{2x}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{2^n x^{2n}}{1 \cdot 3 \cdot 5 \cdots (2n + 1)},
\]

the use of which is less sensitive to roundoff errors.

The asymptotic expansion

\[
\exp(x^2)\text{erfc } x = \frac{1}{x\sqrt{\pi}} \left( 1 - \frac{1}{2x^2} + \frac{1 \cdot 3}{(2x^2)^2} - \frac{1 \cdot 3 \cdot 5}{(2x^2)^3} + \cdots \right)
\]

is of limited use when \( x \) is large. The continued-fraction expansion

\[
\sqrt{\pi} x \exp(x^2)\text{erfc } x = \frac{1}{1 + \frac{1}{1 + \frac{2}{1 + \frac{2}{1 + \cdots}}}},
\]

(Perron [9]) yields better precision. Perron [10] gives the following algorithm for use of (9).

We define

\[
A_{-1} = 1, \quad A_0 = b_0, \quad B_{-1} = 0, \quad B_0 = 1;
\]

\[
a_i = i/ (2x^2), \quad b_i = 1 \quad \text{for } i = 0, 1, 2, 3, \ldots ;
\]

\[
b_0 + \frac{a_1}{b_1} + \frac{a_2}{b_2} + \cdots + \frac{a_n}{b_n} = \frac{A_n}{B_n}.
\]

Then \( A_n \) and \( B_n \) are given recursively by the relations

\[
A_n = b_n A_{n-1} + a_n A_{n-2}, \quad B_n = b_n B_{n-1} + a_n B_{n-2}, \quad n = 1, 2, 3, \ldots.
\]

At smaller values of \( x \), the convergence of (9) becomes slower. To overcome this, we have used double Aitken \( \delta^2 \) extrapolation (Burden et al. [11, pp. 56–57]) as follows. If \( y_j \) is the approximation obtained by taking \( j \) terms of (9), then the sequences of numbers

\[
y_j' = y_j - (y_j - y_{j-1})^2 / (y_j - 2y_{j-1} + y_{j-2}),
\]

\[
y_j'' = y_j' - (y_j' - y_{j-1})^2 / (y_j' - 2y_{j-1}' + y_{j-2}'),
\]

converge progressively faster to (9). Use of (12) with (9)–(11) improved the fit of the Chebyshev approximation by about five orders of magnitude.

We have used (7) for \( x < 2.83 \) and (9)–(12) for \( x > 2.83 \). This yielded values of \( f(x) \) accurate to at least 23D for all \( x \). The resulting Chebyshev coefficients,
generated by (3)--(5), are shown in Table 1. Use of these in (2) gives an approximation which reproduces $f(x)$ to at least 22D for all $x$. Schonfelder [5] generates Chebyshev coefficients using a different method [12], [13] in which an expression equivalent to (2) is substituted into a linear differential equation satisfied by the given function. Together with the boundary conditions satisfied by the same function, this procedure generates an infinite set of simultaneous linear equations for the $c_j$, a truncated version of which is then solved.

### Table 1

<table>
<thead>
<tr>
<th>$Y = (1 + 2X) \cdot \exp(X^2) \cdot \text{erfc}(X)$</th>
<th>$T = (1 + X)/(1 + X)$</th>
<th>$x = (0, \infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>ORD</strong></td>
<td><strong>C(N)</strong></td>
<td><strong>N</strong></td>
</tr>
<tr>
<td>0</td>
<td>0.1177578934567401754086 G-01</td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.859054580646877331 G-02</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>0.592099399819809495 G-02</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>0.8250866843530752277 G-01</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>0.4907775836525800632 G-03</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>-0.241316354017608191 G-02</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>-0.69169733025012604 G-04</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>0.4139327986073010 G-05</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0.7743383036619849 G-06</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>0.1076499945671616 G-07</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>0.4521959811261 G-08</td>
<td></td>
</tr>
<tr>
<td>11</td>
<td>0.775440028830 G-09</td>
<td></td>
</tr>
<tr>
<td>12</td>
<td>-0.63108534099 G-10</td>
<td></td>
</tr>
<tr>
<td>13</td>
<td>0.286679501 G-10</td>
<td></td>
</tr>
<tr>
<td>14</td>
<td>-0.194556850 G-12</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>-0.965469675 G-12</td>
<td></td>
</tr>
<tr>
<td>16</td>
<td>-0.325254813 G-13</td>
<td></td>
</tr>
<tr>
<td>17</td>
<td>-0.134781190 G-13</td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>-0.18645630 G-14</td>
<td></td>
</tr>
<tr>
<td>19</td>
<td>-0.12507950 G-14</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>-0.741820 G-16</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>0.509910 G-16</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>-0.21070 G-17</td>
<td></td>
</tr>
<tr>
<td>23</td>
<td>0.276 G-19</td>
<td></td>
</tr>
<tr>
<td>24</td>
<td>0.3 G-20</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>-0.3 G-20</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>-0.3 G-20</td>
<td></td>
</tr>
<tr>
<td>27</td>
<td>-0.3 G-20</td>
<td></td>
</tr>
</tbody>
</table>

### III. Acknowledgments

We wish to thank Y. L. Luke, G. Dahlquist, and S.-Å. Gustavson for valuable discussions and comments. This work was supported by the Natural Sciences and Engineering Research Council of Canada under grants A-4638 and A-4749.

Department of Computer Science
York University
Toronto, Ontario, Canada M3J 1P3

Department of Physics
York University
Toronto, Ontario, Canada M3J 1P3

