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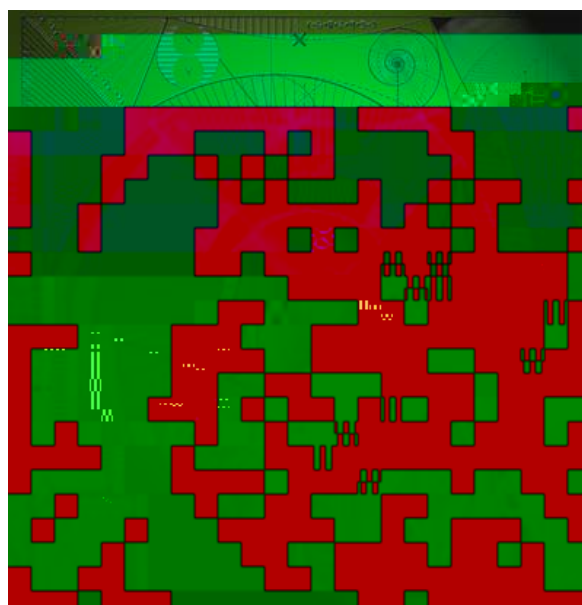
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Computing Fresnel Integrals via Modified Trapezium Rules

by

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Dedicated to David Hunter on the occasion of his 80th birthday

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Abstract In this paper we propose methods for computing Fresnel integrals based on truncated trapezium rule approximations to integrals on the real line, these trapezium rules modified to take into account poles of the integrand near the real axis. Our starting point is a method for computation of the error function of complex argument due to Matta and Reichel (*J. Math. Phys.* **34** (1956), 298{307) and Hunter and Regan (*Math. Comp.* **26** (1972), 539{541). We construct approximations which we prove are exponentially convergent as a function of N , the number of quadrature points, obtaining explicit error bounds which show that accuracies of 10^{-15} uniformly on the real line are achieved with $N = 12$, this confirmed by computations. The approximations we obtain are attractive, additionally, in that they maintain small relative errors for small and large argument, are analytic on the real axis (echoing the analyticity of the Fresnel integrals), and are straightforward to implement. In a last section we explore the implications of our results for the computation of the error function of real and complex argument.

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1 Introduction

Let $C(x)$, $S(x)$, and $F(x)$ be the Fresnel integrals defined by

$$C(x) := \int_0^x \cos \frac{i}{2} t^2 dt; \quad S(x) := \int_0^x \sin \frac{i}{2} t^2 dt; \quad (1)$$

and

$$F(x) := \frac{e^{i\pi/4}}{\sqrt{2}} \int_x^\infty e^{it^2} dt. \quad (2)$$

Our definitions in (1) are those of [2] and [1, x7.2(iii)], and F , C and S are related through

$$\frac{1}{2} e^{i\pi/4} F(x) = \frac{1}{2} i C(x) - \frac{1}{2} S(x)$$

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function f = fresnel(x,N)
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When $x > 0$ is large this approximation is very accurate, indeed is essentially identical to the approximation $F_N(x)$ with N large if the choice

$$h = \frac{1}{4} A_N = \frac{1}{4(N+1/2)} \quad (26)$$

is made. However, this approximation becomes increasingly poor as $x \rightarrow 0$ approaches zero.

In the context of developing methods for evaluating the complementary error function of complex argument (by (20), evaluating $F(x)$ for x real is just a special case of this larger problem), Chiarella and Riechel [7], Matta and Reichel [18], and Hunter and Regan [15] proposed modifications of the trapezium rule that follow naturally from the contour integration argument used to prove that the trapezium rule is exponentially convergent. The most appropriate form of this modification is that in [15] where the modified trapezium rule approximation

$$F(x) \approx \frac{1}{4} \frac{xh}{1/4} e^{i(x^2 + 1/4)} \sum_{k=1}^{\infty} e^{-i \zeta_k^2} \quad 0$$

real line by a discontinuous function (albeit with small discontinuities). This contribution is further to realise that the approximation formula proposed on $0 < x < \sqrt[4]{2}h$ in fact provides a smooth and accurate approximation on the whole real line. The third contribution, the contribution which is most substantial in terms of analysis, is to improve the error bound (28) of [15]. This error bound is unsatisfactory in that it blows up at $x = \sqrt[4]{2}h$ in a way not seen in the numerical results in x4 (though there is some increase observed in the error when x is near this value; see Figure 3). The bounds we prove in x4

2 The approximation of $F(x)$ and its error bounds

In this section we derive the approximation (5) to $F(x)$ and derive (12) and related error bounds for this approximation, these error bounds demonstrating that both the absolute and relative errors in the approximation $F_N(x)$ converge exponentially to zero as N increases, uniformly on the real line, and that $N = 12$ is large enough to achieve errors $< 10^{-15}$.

The first part of our derivation follows in large part Matta and Reichel [18] and Hunter and Regan [15]. From (22) we have that, for $x > 0$,

$$I := \int_{-1}^1 f(t) dt = F(x); \text{ where } f(t) := e^{i(x^2 + \frac{1}{4}t^2)} \frac{x}{2^{1/4}} \frac{e^{it^2}}{x^2 + it^2}; \quad (29)$$

and we have suppressed in our notation the dependence of $f(t)$ on x . Choose a step-size $h > 0$ for the trapezium rule and let

$$g(z) = i \tan(\frac{1}{4}z=h);$$

which is a meromorphic function with simple poles at the points i_k , defined by (25), which has the property that, for $z = X + iH$ with $X \in \mathbb{R}$, $H > 0$,

$$1 + g(z) = \frac{2e^{i2^{1/4}H=h}}{1 - e^{i2^{1/4}H=h}}; \quad (30)$$

The approximation (27) is obtained by considering the integral in the complex plane,

$$J = \int_{\gamma} f(z)(1 + g(z)) dz;$$

where the path of integration is from -1 to 1 along the real axis, except that the path makes small semicircular deformations to pass above each of the simple poles at the points i_k , $k \in \mathbb{Z}$. Explicitly, the k th deformation is the semicircle $\gamma_k = \{z_k + 2e^{i\mu} : \frac{1}{4} \leq \mu \leq \frac{3}{4}\}g$, with 2 in the range $(0; h=2)$ small enough so that the simple pole singularity in $f(z)$ at $z = z_0 := e^{i\frac{1}{4}}x$ lies above γ . Then, since $f(z)g(z)$ is an odd function, we see that

$$J = \int_{\gamma} f(z) dz + \int_{\gamma} f(z)g(z) dz = I + \sum_{k \in \mathbb{Z}} \int_{\gamma_k} f(z)g(z) dz;$$

In the limit $2 \rightarrow 0$, $\int_{\gamma_k} f(z)g(z) dz \rightarrow i \frac{1}{4} \text{Res}(fg; i_k) = i h f(i_k)$, where $\text{Res}(g; i_k)$ denotes the residue of fg at i_k . Thus $J = I + I_h$, where

$$I_h = h \sum_{k \in \mathbb{Z}} f(i_k) = 2h \sum_{k=1}^{\infty} f((k - \frac{1}{2})h) \quad (31)$$

is a trapezium/midpoint rule approximation to I . On the other hand, where $\gamma_H = \{x + iH : x \in \mathbb{R}\}$, by the residue theorem,

$$J = \int_{\gamma_H} f(z)(1 + g(z)) dz + H \sum_{k \in \mathbb{Z}} \text{Res}(f(1 + g); i_k);$$

for $H > 0$, where H is the Heaviside step function and

$$PC_h = 2\frac{1}{2}i \operatorname{Res}(f(1+g); z_0) = \frac{1}{2} (1 + g(z_0)) = \frac{1}{2} (1 + i \tan^{-1} e^{i\frac{3}{4}} x^{\frac{1}{4}} = h) :$$

Thus

$$I = I_h + H \int_{iH}^Z \frac{f(z)(1+g(z))}{2H + i x} dz : \quad (32)$$

The point here is that the integral over iH can be negligible so that a good approximation is obtained by the modified trapezium rule approximation, $I_h + H \int_{iH}^Z \frac{f(z)(1+g(z))}{2H + i x} dz$. In particular, noting (30) and that, for $z = X + iH$,

$$jx^2 + iz^2j = jz_0 + jzjz_0 + jz, \quad jx = \frac{1}{2} H j jx = \frac{1}{2} + H j = jx^2 = 2 + H^2 j$$

and that $\int_{iH}^Z \frac{1}{2} e^{it^2} dt = \frac{1}{\sqrt{4}}$, we see that

$$\int_{iH}^Z f(z)(1+g(z)) dz = \frac{x e^{H^2 + i 2\frac{1}{4}H=h}}{\frac{1}{\sqrt{4}} j H^2 + x^2 = 2j} \frac{1}{1 + i e^{i 2\frac{1}{4}H=h}} :$$

Choosing $H = \frac{1}{2}h$, to minimise the exponent $H^2 + i 2\frac{1}{4}H=h$, it follows that $I = I_h + H \int_{iH}^Z \frac{f(z)(1+g(z))}{2H + i x} dz + e_h$ with

$$je_h j = \pm_1(x) := \frac{x e^{i \frac{1}{4}h^2}}{\frac{1}{\sqrt{4}} j \frac{1}{4}h^2 = h^2 + x^2 = 2j} \frac{1}{1 + i e^{i \frac{1}{2}h^2}} : \quad (33)$$

Note that $I_h + H \int_{iH}^Z \frac{f(z)(1+g(z))}{2H + i x} dz = I_h + R(h; x)$ is precisely the approximation (27), and that the above bound on e_h is precisely the bound (28) from [15].

Let $I_h^a := I_h + PC_h$ and $e_h^a := I - I_h^a$. Then (33) implies that

$$je_h^a j = \pm_1(x); \text{ for } 0 < x < \frac{1}{2}h : \quad (34)$$

Since, applying (30),

$$jPC_h j = \frac{e^{i \frac{1}{2} \frac{1}{4}x=h}}{1 + i e^{i \frac{1}{2} \frac{1}{4}x=h}};$$

we see that

$$je_h^a j = \pm_3(x) := \pm_1(x) + \frac{e^{i \frac{1}{2} \frac{1}{4}x=h}}{1 + i e^{i \frac{1}{2} \frac{1}{4}x=h}}; \text{ for } x > \frac{1}{2}h : \quad (35)$$

The bounds (34) and (35) both blow up as x approaches $\frac{1}{2}h$. Continuing to choose $H = \frac{1}{4}h$, select $\frac{1}{2}$ in the range $(0; H)$ and consider the case that

$$\frac{X}{2} + H < 2 : \quad (36)$$

In this case we observe that the derivation of (32) can be modified to show that

$$e_h^a = \int_{iH}^Z f(z)(1+g(z)) dz \quad (37)$$

where the contour γ_H^a passes above the pole in f at z_0 ; precisely, γ_H^a is the union of γ^0 and γ^∞ , where $\gamma^0 = \{z \in \mathbb{C} : |z - z_0| = r, \arg(z - z_0) \in [\mu, \mu + 2\pi]\}$ and γ^∞ is the circular arc $\gamma^\infty = \{z_0 + re^{i\mu} : \mu_0 \leq \mu \leq \mu_0 + 2\pi\}$, where $\mu_0 = \sin^{-1}((H - x)/2)$ ($\mu_0 = 2\pi$ if $x = 2$). For $z \in \gamma^0$ it holds that

$$jx^2 + iz^2j = jz_0 - zjjz_0 + zj, \quad jx = \frac{p}{2} + Hj; \quad (38)$$

Thus, and applying (30), similarly to (34) we deduce that

$$\int_{\gamma^0} f(z)(1 + g(z)) dz = \frac{x e^{i\frac{1}{4}\pi} = h^2}{p^{\frac{1}{4}} j^{\frac{1}{4}} = h + x = \frac{p}{2} j} \frac{1}{1 - e^{i\frac{1}{2}\pi} = h^2}}. \quad (39)$$

To bound the integral over γ^∞ we note that, for $z = X + iY = z_0 + re^{i\mu}$, (38) is true and $Y \leq H$. Further, $je^{iz^2}j = e^P$, where

$$P = Y^2 - X^2 = 2x^2 \sin(\mu - \frac{1}{4}\pi) - 2^2 \cos(2\mu) < 2x^2 + 2^2 \leq 2^{\frac{p}{2}} H^2 + (2^{\frac{p}{2}} + 1)^{2^2};$$

using (36). From these bounds and (30), defining $\mathbb{R} = 2^{\frac{p}{2}} H^2 + (2^{\frac{p}{2}} + 1)^{2^2}$, we deduce that

$$\int_{\gamma^\infty} f(z)(1 + g(z)) dz \leq \frac{2x \exp((2^{\frac{p}{2}} \mathbb{R} + (2^{\frac{p}{2}} + 1)^{2^2})^{\frac{1}{4}} = h^2)}{p^{\frac{1}{4}} j^{\frac{1}{4}} = h + x = \frac{p}{2} j} \frac{1}{1 - e^{i\frac{1}{2}\pi} = h^2}}. \quad (40)$$

Choosing $\mathbb{R} = 1$, we can bound e_h^a using (37), (39), (40), and the triangle inequality, to get that

$$je_h^a j \cdot \pm_2(x) := \frac{4hx e^{i\frac{1}{4}\pi} = h^2}{p^{\frac{1}{4}} j^{\frac{1}{4}} = h + x = \frac{p}{2} j} \frac{1}{1 - e^{i\frac{1}{2}\pi} = h^2}} \left(1 + 2^{\frac{p}{4}} e^{i^{-\frac{1}{4}\pi} = h^2} \right); \quad (41)$$

for $x = h$

which, for $x > 0$, is bounded by

$$\begin{aligned}
 |jT_N| &\leq \frac{hx}{2^{1/4}} \sum_{m=N+1}^{\infty} \frac{e^{i\zeta_m^2}}{x^4 + \zeta_m^4} \\
 &\leq \frac{x}{2^{1/4} (x^4 + \zeta_{N+1}^4)} \frac{2he^{i\zeta_{N+1}^2} + 2h}{\zeta_{N+1}} \sum_{m=N+2}^{\infty} e^{i\zeta_m^2} \\
 &\leq \frac{x}{2^{1/4} (x^4 + \zeta_{N+1}^4)} \frac{2he^{i\zeta_{N+1}^2} + 2}{\zeta_{N+1}} \int_{\zeta_{N+1}}^{\infty} e^{it^2} dt \\
 &\leq \frac{x}{2^{1/4} (x^4 + \zeta_{N+1}^4)} \frac{2he^{i\zeta_{N+1}^2} + \frac{e^{i\zeta_{N+1}^2}}{\zeta_{N+1}}}{\zeta_{N+1}} = \frac{(2h\zeta_{N+1} + 1)x}{2^{1/4}\zeta_{N+1} (x^4 + \zeta_{N+1}^4)} e^{i\zeta_{N+1}^2}.
 \end{aligned}$$

To arrive at the last line we have used that, for $x > 0$,

$$\int_x^{\infty} e^{it^2} dt = \frac{e^{ix^2}}{x} + \int_x^{\infty} \frac{e^{it^2}}{t^2} dt < \frac{e^{ix^2}}{x}. \quad (45)$$

The choice of h we make is designed to approximately equalise $\phi_h(x)$ and this bound on T_N . We choose h so that $H = \frac{1}{4}h = \zeta_{N+1} = (N+1/2)h$, i.e., we make the choice $h = \frac{1}{4}(N+1/2)$ given by (26), in which case $\zeta_{N+1} = A_N = \frac{1}{4}(N+1/2)$, and $\zeta_k = t_k$, where t_k is defined by (7). With this choice of h it holds that

$$E_N(x) = F(x) - F_N(x) = e_h^a + T_N$$

and that

$$|jT_N| \leq \frac{(2^{1/4} + 1)x}{2^{1/4}A_N (x^4 + A_N^4)} e^{iA_N^2}.$$

Thus we arrive at our main pointwise error bound, that

$$|jE_N(x)| \leq \phi_N(x) := \phi_h(jx) + \frac{(2^{1/4} + 1)x}{2^{1/4}A_N (x^4 + A_N^4)} e^{iA_N^2}; \quad (46)$$

with $h = \frac{1}{4}(N+1/2)$ so that $H = \frac{1}{4}h = A_N$. We have shown this bound for $x > 0$, but the symmetries (16) and (17) imply that $E_N(-x) = -E_N(x)$, so that (46) holds also for $x < 0$, and, by continuity, also for $x = 0$ (and in fact $E_N(0) = \phi_N(0) = 0$). Explicitly, for this choice of h we have that

$$\begin{aligned}
 \phi_h(x) &= \begin{cases} \frac{x e^{iA_N^2}}{2^{1/4}(A_N^2 - x^2)} \frac{1}{1 - i e^{i2A_N^2}}; & 0 < \frac{x}{2} < \frac{3}{4}A_N; \\ \frac{4x e^{iA_N^2}}{2^{1/4}A_N(A_N + x)} \frac{1}{1 + i e^{i2A_N^2}}; & \frac{3}{4}A_N < \frac{x}{2} < \frac{5}{4}A_N; \\ \frac{x e^{iA_N^2}}{2^{1/4}(x^2 - A_N^2)} \frac{1}{1 - i e^{i2A_N^2}} + \frac{e^{i\frac{1}{2}A_N x}}{1 - i e^{i\frac{1}{2}A_N x}}; & \frac{x}{2} > \frac{5}{4}A_N. \end{cases} \quad (47)
 \end{aligned}$$

We will compare $|E_9(x)|$ to the upper bound $\hat{\epsilon}_9(x)$ in Figure 2 below.

Note the factor $\exp(-\frac{1}{2}A^2)$

where

$$c_N^\alpha = 2e^{\frac{1}{4}N} \left(1 + \frac{5}{4} \frac{p}{2^{1/4} A_N} \zeta_h \right) e^{\frac{1}{4} \frac{p}{2} A_N} + \frac{(2^{1/4} + 1)}{2^{1/4}} \frac{e^{i A_N^2}}{A_N} \frac{1}{p^{1/2} A_N} + p^{1/4} \\ = \frac{10 \frac{p}{2} \frac{1}{4} + 5 \frac{p}{2^{1/4} A_N} \zeta_h^3}{9 \frac{p}{1/4} e^{\frac{1}{4}=2} A_N} \frac{1}{1} \frac{1}{e^{i 2 A_N^2}} + \frac{(2^{1/4} + 1)}{1/4 e^{\frac{1}{4}=2} A_N} \frac{1}{p^{1/2} A_N} + p^{1/4} :$$

Note that c_N^α decreases as N increases, with $c_1^\alpha \approx 10.4$ and $\lim_{N \rightarrow \infty} c_N^\alpha = 100e^{\frac{1}{4}=2} \approx 9.2 \cdot 3$. The bound (51) shows exponential convergence of the relative error, $|F_N(x) - F(x)| = |F_N(x)|$, uniformly on the real line, in particular showing that the relative error is $\leq 1.6 \times 10^{-16}$ on the whole real line if $N = 12$ (see Figure 1 below).

The above estimates use (46) and (47) to bound the maximum absolute and relative errors in the approximation $F_N(x)$. Let us note that these inequalities, additionally, imply that $F_N(x)$ is particularly accurate for $|x|$ small. For $|x| \leq \frac{A_N}{2} = \frac{1}{2(N+1)^{1/4}}$, it follows from (46) and (47) that

$$|F(x) - F_N(x)| \leq \epsilon_N |x| \frac{e^{\frac{1}{4}N}}{2N+1} \quad (52)$$

where

$$\epsilon_N = \frac{8}{3^{1/4} 3^{1/2} e^{\frac{1}{4}=2}} \frac{1}{1} \frac{1}{e^{i 2 A_N^2}} + \frac{(2^{1/4} + 1)}{1/4^2 e^{\frac{1}{4}=2} A_N} : \quad (53)$$

Note that ϵ_N decreases as N increases, with $\epsilon_1 \approx 0.17$ and $\lim_{N \rightarrow \infty} \epsilon_N = 8/(3^{1/4} 3^{1/2} e^{\frac{1}{4}=2}) \approx 0.10$.

In §1 we have made claims regarding the analyticity of the approximation $F_N(x)$, considered as a function of x in the complex plane. We justify these claims now. One attractive feature of the modified trapezium rule approximation I_h^α is that, in contrast to I_h , it is entire as a function of x . This is not immediately obvious: $I_h^\alpha = I_h + PC_h$, and PC_h has simple pole singularities at $x = e^{i \frac{1}{4}=4} t_k$, $k \in \mathbb{Z}$. But I_h also has simple poles at the same points and it is an easy calculation to see that the residues add to zero, so that the singularities cancel out. Since $F_N(x) = I_h^\alpha + T_N$, with h given by (26), it follows that the singularities of $F_N(x)$ are those of T_N , i.e., simple poles at $\pm e^{i \frac{1}{4}=4} t_k$, for $k = N+1; N+2; \dots$. Thus $F_N(x)$ is a meromorphic function and, in particular, is analytic in the strip $|\operatorname{Im}(x)| < A_N = \frac{1}{2(N+1)^{1/4}}$ and in the first and third quadrants of the complex plane.

We will note two consequences of this analyticity and the bounds that we have already proved. In these arguments we will use an extension of the maximum principle for analytic functions to unbounded domains, that if $w(z)$ is analytic in an open quadrant in the complex plane, let us say $Q = \{z \in \mathbb{C} : 0 < \arg(z) < \frac{1}{4}=2g\}$, and is continuous and bounded in its closure, then

$$\sup_{z \in Q} |w(z)| \leq \sup_{z \in \partial Q} |w(z)|; \quad (54)$$

where ∂Q denotes the boundary of the quadrant. (This sort of extension of the maximum principle to unbounded domains is due to Phragmen and Lindelöf; see, e.g., [25].)

The first consequence is that, from (11), (12), and (18), it follows that (12) holds if x is real or if $x = iY$ with $Y \geq \mathbb{R}$, i.e., the bound (12) holds on both the real and imaginary axes. Further, from (20) and the asymptotics of $\operatorname{erfc}(x)$ in the complex plane [2, (7.1.23)], it follows that $F(x) \neq 0$, uniformly in $\arg(x)$, for $0 \leq \arg(x) \leq \frac{3}{4}\pi$; moreover, it is clear from (6) that the same holds for $F_N(x)$ and hence for $E_N(x)$. Thus (54) implies that (12) holds for $0 \leq \arg(x) \leq \frac{3}{4}\pi$, and (16) and (17) then imply that (12) holds also for $\frac{3}{4}\pi \leq \arg(x) \leq \frac{7}{4}\pi$.

It is clear from the derivations above that, if h is given by (26), then I_h^α also satisfies the bound (12), i.e.,

$$|F(x) - I_h^\alpha| \leq c_N e^{i\frac{3}{4}N} \frac{1}{N+1/2}; \quad (55)$$

this holding in the first instance for real x , then for imaginary x , and finally for all x in the first and third quadrants. The bound (12) cannot hold in the second or fourth quadrant because $E_N(x) = F(x) - F_N(x)$ has poles there. This issue does not apply to $F(x) - I_h^\alpha$, which is an entire function, but (55) cannot hold in the whole complex plane because this, by Liouville's theorem ([25]), would imply that $F(x) - I_h^\alpha$ is a constant. What does hold is that $e^{ix^2}(F(x) - I_h^\alpha)$ is bounded in the second and fourth quadrants, this a consequence of the definition of I_h^α and the asymptotics of $e^{z^2}\operatorname{erfc}(z)$ at infinity. Thus it follows from (54), and since $je^{ix^2}j = 1$ if x is real or pure imaginary, that

$$|F(x) - I_h^\alpha| \leq c_N e^{iXY} \frac{1}{N+1/2}; \quad (56)$$

for $x = X + iY$ in the second and fourth quadrants.

We can use the bound (56) to obtain a bound on $E_N(x)$ in the second and fourth quadrants. Clearly, where T_N is defined by (44), with h given by (26), for $x = X + iY$ in the second and fourth quadrants,

$$|F(x) - F_N(x)| \leq c_N e^{iXY} \frac{1}{N+1/2} + |T_N|;$$

Further, arguing as below (44), if $|Y| \leq A_N = (2\frac{p}{2})$ so that

$$|x^2 + it_k^2| \leq \frac{A_N}{2} + |Y| \leq \frac{A_N}{2} + |Y| \leq \frac{A_N}{2} + \frac{A_N}{2} = A_N, \quad \frac{A_N}{2} \leq |x| \leq \frac{A_N}{2} + |Y| \leq \frac{A_N}{2} + \frac{A_N}{2} = A_N, \quad \frac{A_N}{2} \leq |x| \leq \frac{A_N}{2} + |Y| \leq \frac{A_N}{2} + \frac{A_N}{2} = A_N;$$

which implies that $|x^2 + it_k^2| \leq A_N = (2\frac{p}{2})$, then

$$|T_N| \leq e^{iXY} \frac{(2\frac{p}{2} + 1)^{p/2}}{\frac{1}{4}A_N^2} e^{iA_N^2} = e^{iXY} \frac{(2\frac{p}{2} + 1)^{p/2}}{\frac{1}{4}3^{p/2}(N+1/2)} e^{i\frac{3}{4}N}.$$

Thus, for $x = X + iY$ in the second and fourth quadrants with $|Y| \leq A_N = (2^{p-2})^{1/3}$,

$$|F(x) - F_N(x)| \leq C_N e^{iX} \frac{e^{iY/4}}{(N+1)^{1/2}} \quad (57)$$

where

$$C_N := C_N + \frac{2^{p-2}(2^{1/4} + 1)}{3^{1/2} \exp(1/4)} \frac{1}{(N+1)^{1/2}}. \quad (58)$$

The sequence C_N is decreasing with $C_1 = 1.14$ and $\lim_{N \rightarrow \infty} C_N = \lim_{N \rightarrow \infty} C_N = 0.208$.

We observe above that the bound (12) on $E_N(x) = F(x) - F_N(x)$ holds for all complex x

and are given explicitly in (8) and (9). We note the similarity between (8) and (9) and the formulae [1, (7.5.3)-(7.5.4)]

$$C(x) = \frac{1}{2} + f(x) \sin i \frac{1}{2} \frac{1}{4} x^2 \zeta + g(x) \cos i \frac{1}{2} \frac{1}{4} x^2 \zeta; \quad (62)$$

$$S(x) = \frac{1}{2} + f(x) \cos i \frac{1}{2} \frac{1}{4} x^2 \zeta + g(x) \sin i \frac{1}{2} \frac{1}{4} x^2 \zeta; \quad (63)$$

which express $C(x)$ and $S(x)$ in terms of the auxiliary functions, $f(x)$ and $g(x)$

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function [C,S] = fresnelCS(x,N)
% Evaluates approximations to the Fresnel integrals C(x) and S(x).
% x is a real scalar or matrix,
% N is a positive integer controlling accuracy (suggest N=12),
% C and S are the scalars/matrices of the same size as x approximating C(x) and S(x).
h = sqrt(pi/(N+0.5));
t = h*((N:-1:1)-0.5); AN = pi/h; rootpi = sqrt(pi);
t2 = t.*t; t4 = t2.*t2; et2 = exp(-t2);
x2pi2 = (pi/2)*x.*x; x4 = x2pi2.*x2pi2;
a = et2(1)./(x4+t4(1)); b = t2(1)*a;
for n = 2:N
    term = et2(n)./(x4+t4(n));
    a = a + term; b = b + t2(n)*term;
end
a = a.*x2pi2;
mx = (rootpi*AN)*x; Mx = (rootpi/AN)*x;
Chalf = 0.5*sign(mx); Shalf = Chalf;
select = abs(mx)<39;
if any(select)
    mxs = mx(select); shx = sinh(mxs); sx = sin(mxs);
    den = 0.5./(cos(mxs)+cosh(mxs));
    Chalf(select) = (shx+sx).*den;
    ssdiff = shx-sx;
    select2 = abs(mxs)<1;
    if any(select2)
        mxs = mxs(select2); mxs3 = mxs.*mxs.*mxs; mxs4 = mxs3.*mxs;
        ssdiff(select2) = mxs3.*(1/3 + mxs4.*(1/2520 ...
            + mxs4.*((1/19958400)+(0.001/653837184)*mxs4)));
    end
    Shalf(select) = ssdiff.*den;
end
cx2 = cos(x2pi2); sx2 = sin(x2pi2);
C = Chalf + Mx.*(a.*sx2-b.*cx2); S = Shalf - Mx.*(a.*cx2+b.*sx2);

```

Table 2 Matlab code to evaluate $C_N(x)$ and $S_N(x)$ given by (8) and (9). See x3 for details.

applied. In particular, from (50) and (52) it follows that both $jC(x) - C_N(x)$ and $jS(x) - S_N(x)$ are

$$\leq 2c_N e^{\frac{i}{4}N} \frac{1}{2N+1}; \quad \text{for } x \in \mathbb{R}; \quad (65)$$

and

$$\leq e_N \frac{1}{4} \frac{e^{\frac{i}{4}N}}{2N+1}; \quad \text{for } |x| \leq \frac{1}{N+1/2}. \quad (66)$$

Here $c_N < 0.83$ and $e_N < 0.18$ are the decreasing sequences of positive numbers defined by (8) and (53), respectively.

These bounds show that $C_N(x)$ and $S_N(x)$ are exponentially convergent as $N \rightarrow \infty$, uniformly on the real line, so that very accurate approximations can be obtained with very small values of N ((65) shows that both $jC_N(x) - C(x)$ and $jS_N(x) - S(x)$ are $\leq 1.4 \times 10^{-16}$ on the real line for $N \geq 11$). In x4 we will confirm the effectiveness of these approximations by numerical experiments,

checking the accuracy of (8) and (9) by comparison with the power series [1, x7.6(i)]

$$C(x) = \sum_{n=0}^{\infty} \frac{(i-1)^n i^{\frac{1}{2}n} \zeta_{2n} x^{4n+1}}{(2n)!(4n+1)}; \quad S(x) = \sum_{n=0}^{\infty} \frac{(i-1)^n i^{\frac{1}{2}n} \zeta_{2n+1} x^{4n+3}}{(2n+1)!(4n+3)}. \quad (67)$$

It follows from the analyticity of $F_N(x)$ in the complex plane, discussed in x2, that $F_N(x)$ has a Maclaurin series convergent in $|x| < A_N = \frac{1}{2}$, and from (61) that $C_N(x)$ and $S_N(x)$ have convergent Maclaurin series representations in $|x| < A_N = \frac{1}{4}$. From the observations below (19) it is clear that, echoing (67), these take the form

$$C_N(x) = \sum_{n=0}^{\infty} c_n x^{4n+1}; \quad S_N(x) = \sum_{n=0}^{\infty} s_n x^{4n+3}. \quad (68)$$

Further, it follows from (61) and (59) that the coefficients c_n and s_n are close to the corresponding coefficients of $C(x)$ and $S(x)$, with the difference having absolute value

$$\leq \frac{2^{-N} e^{i \frac{1}{4}(N-1)}}{N+1}; \quad (69)$$

for $N \geq 4$, where $\hat{c}_N = \hat{c}_4 < 0.77$ is the decreasing sequence of positive numbers given by (58). This implies that, near zero, where $C(x)$ has a simple zero and $S(x)$ a zero of order three, the approximations $C_N(x)$ and $S_N(x)$ retain small relative error. For $C_N(x)$ this follows already from (66) but to see this for $S_N(x)$ we need the stronger bound implied by (69) that, for $|x| < 1$,

$$|S_N(x) - S(x)| \leq \frac{2^{-N}}{N+1} \quad (\text{but}) \quad |S_N(x) - S(x)| \leq \frac{2^{-N}}{N+1} \quad \text{for } |x| < 1. \quad (70)$$

Methods for evaluation of $w(z)$ based on continued fraction representations for larger complex z (which can be applied to evaluate $F(x)$ and hence $C(x)$ and $S(x)$) are also discussed in Gautschi [11] and are finely tuned, to form TOMS "Algorithm 680", in Poppe and Wijers [21,22], which achieves relative errors of 10^{-14} over "nearly all" the complex plane by using Taylor expansions of degree up to 20 in an ellipse around the origin, convergents of up to order 20 of continued fractions outside a larger ellipse, and a more expensive mix of Taylor expansion and continued fraction calculations in between.

Weideman [29] presents an alternative method of computation (the derivation starts from the integral representation (21)) which approximates $w(z)$ by the polynomial

$$w_M(z) = \frac{2}{L^2 + z^2} \sum_{n=0}^M a_n z^n i$$

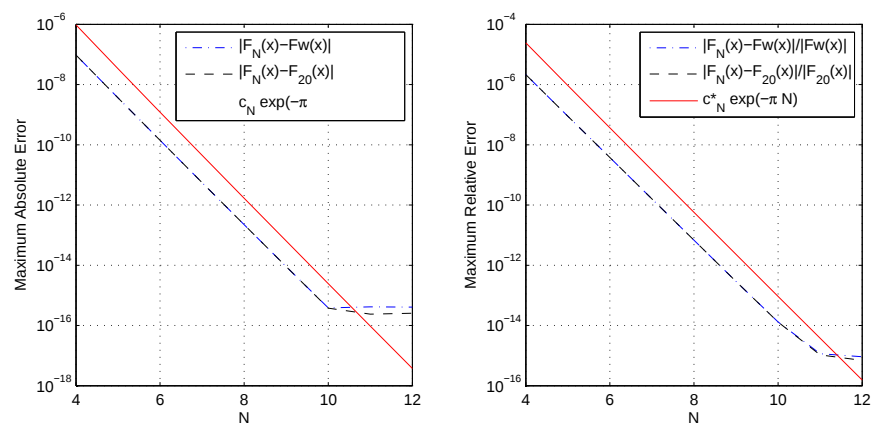


Fig. 1 Left hand side: maximum error, $\max_{x \in [0, 1]} |F(x) - F_N(x)|$, and its upper bound (12) (13), plotted against N , where $F(x)$ is approximated by $Fw(x) := e^{ix^2} w_{36}(e^{i\pi/4} x) = 2$ with $w_{36}(x) = \frac{1}{2} \left(e^{ix^2} + e^{-ix^2} \right)$.

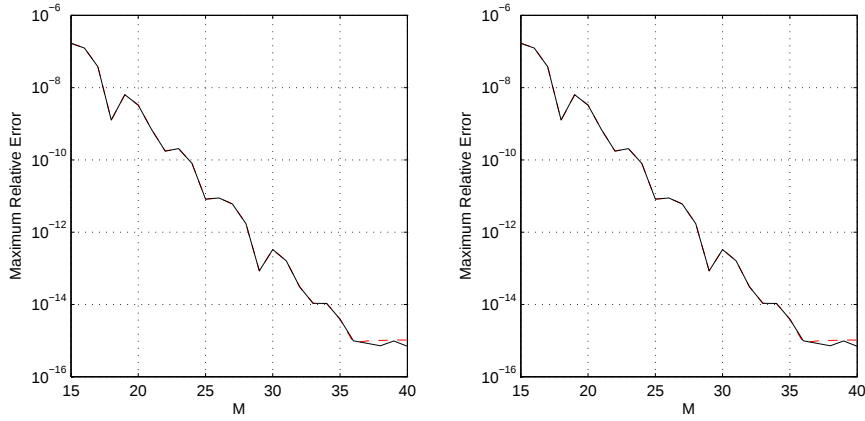


Fig. 2 Left hand side: maximum error, $\max_{x \in [0, 1]} |F(x) - Fw(x)|$, where $Fw(x) := e^{ix^2} w_M(e^{i\pi/4} x)$ with $w_M(z)$ given by (71), plotted against M . Right hand side: same, but maximum relative error, $\max_{x \in [0, 1]} |F(x) - Fw(x)|/|F(x)|$, is plotted against M . In each plot the two curves correspond to different methods for approximating the exact value of $F(x)$, either $F(x) \approx F_{20}(x)$ given by (5) (blue), or $F(x) \approx Fw(x)$ with $M = 50$ (red).

is large enough in (71). Exploring this in more detail, in Figure 2 the maximum absolute and relative errors in the approximation $Fw(x) = e^{ix^2} w_M(e^{i\pi/4} x)$ for $F(x)$, with $w_M(z)$ given by (71), are plotted against M . (The maxima, as in Figure 1, are taken over 40,000 equally spaced points between 0 and 1,000.) In each of the plots in Figure 2 the trend is one of exponential convergence, but the convergence is not monotonic and is slower than that in Figure 1.

In Figure 3 we plot against x the absolute and relative errors in $F_N(x)$ for $N = 9$. On the same graphs we plot the upper bounds $\epsilon_N(x)$ and $2(1 + \frac{1}{4}x)\epsilon_N(x)$, respectively, with $\epsilon_N(x)$ defined by (46). We see that the theoretical error bounds are upper bounds as claimed, and that these bounds appear to capture the x -dependence of the errors fairly well, for example that $E_N(x) = O(x)$ as $x \rightarrow 0$, $\epsilon_N(x) = O(x^{1/2})$ as $x \rightarrow 1$, and that $E_N(x)$ reaches a maximum at about $x = \sqrt{2} A_N = \sqrt{2} \frac{1}{4}(2N + 1)$ (i.e. 7.7 when $N = 9$).

The above figures explore the accuracy of the approximation $F_N(x)$. Let us comment now on efficiency. Most straightforward is a comparison of the Matlab function $F(x, N)$ in Table 1 with computation of $F(x)$ via the Matlab code $\exp(i*x.^2) .* \text{cef}(\exp(i*\pi/4)*x, 36)/2$ that uses `cef.m` from [29] which implements (71). Both $F(x, N)$ and `cef(x, M)` are optimised for efficiency when x is a large vector. Assuming that the time for computation in `cef` of the coefficients a_n in (71) is negligible, the main cost in computation of $F(x)$ via `cef` when x is a large vector is a complex vector exponential (for e^{ix^2}), slightly more than M complex vector multiplications and M additions, and 2 complex vector divisions (all vector operations componentwise). The major part of this computation is that required to evaluate the polynomial (71) of degree M us-

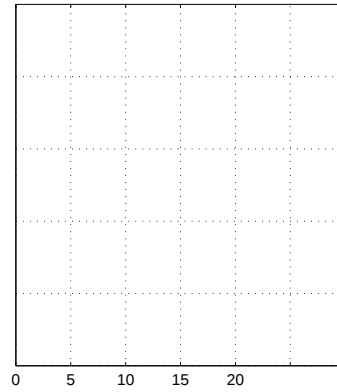


Fig. 3 Left hand side: absolute error, $|F(x) - F_N(x)|$ (red), and its upper bound $\hat{\epsilon}_N(x)$ given by (46) (blue), plotted against x . Right hand side: relative error, $|F(x) - F_N(x)|/|F(x)|$ (red), and its upper bound $2(1 + \sqrt{1/4}x)\hat{\epsilon}_N(x)$ (blue), plotted against x . In both plots $N = 9$ and $F(x)$ is approximated by $F_{20}(x)$.

ing Horner's algorithm. In comparison, evaluation of $F(x)$ using the function $F(x, N)$ in Table 1 requires 2 complex vector exponentials, one complex vector division, and slightly more than N real vector multiplications/divisions, real vector additions, complex vector multiplications, and complex vector additions. From Figures 1 and 2 we read off that to achieve absolute and relative errors below 10^{-8} requires $N = 6$ and $M = 18$; to achieve errors below 10^{-15} requires $N = 12$ and $M = 36$. Thus it seems clear that computing $F(x)$ via $F(x, N)$ requires a substantially lower operation count than computing via cef . (We note, moreover, as discussed in x3.1 and in x7 of [29], that, at least for intermediate values of x ($1.5 \cdot x \cdot 5$), the operation counts via cef are lower than those required via the method for $w(z)$ of [21, 22].)

To test whether $F(x, N)$ is faster we have compared computation times in Matlab (version 7.8.0.347 (R2009a), running on a laptop with dual 2.4GHz P8600 Intel processors) between $\exp(i \cdot x.^2) \cdot \text{cef}(\exp(i \cdot \pi/4) \cdot x, 36)/2$ and $F(x, 12)$ when x is a length 10^7 vector of equally spaced numbers between 0 and 1,000. The elapsed times (average of 10 executions) were 11.1 and 15.6 seconds, respectively, so that $F(x, 12)$ is a little less than 50% faster.

Turning to $C(x)$ and $S(x)$, these can of course be computed using $F(x, N)$ to calculate $F_N(x)$, and then using (61) which incurs negligible additional computation. This is entirely satisfactory except for small x , where this method fails to maintain small relative errors. As discussed in x3, the Matlab function `fresnelCS.m` in Table 2 directly implements (8) and (9), taking care in the evaluation of $\sinh$ & $\sin$ in (9) so as to achieve the high accuracy of $S_N(x)$ for small $|x|$ predicted in (70). To test the efficiency and accuracy of the implementation in Table 2 we have compared evaluation of $C_{12}(x)$ and $S_{12}(x)$ via `fresnelCS` with their evaluation via $F(x, 12)$ and (61), computing

$C_{12}(x)$ and $S_{12}(x)$ at 10^7 equally spaced x -values between 0 and 20. The values of $C_{12}(x)$ and $S_{12}(x)$ computed by these slightly different methods differ by $\approx 4.5 \times 10^{-15}$; this good but not perfect agreement is because there is a difference between $\exp(i(\sqrt{1/4}x)^2)$ and $\exp(i\sqrt{1/4}x^2)$ in floating point arithmetic. In this test fresnelCS requires only 67% of the computation time of computing via $F(x, 12)$, this because the real arithmetic in fresnelCS is faster and because the expressions (64), with $t = \sqrt{2}A_N x$, are evaluated (efficiently and accurately) in fresnelCS as $\text{sign}(t)$ when $|t| \geq 39$ (corresponding to $x \geq 3.51$ for $N = 12$), as discussed in x3.

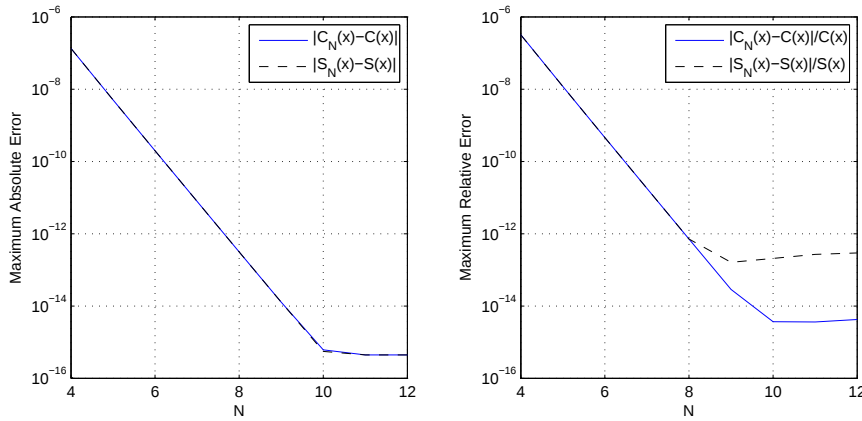


Fig. 4 Left hand side: maximum values of $|jC_N(x) - C(x)|$ and $|jS_N(x) - S(x)|$ on $0 \leq x \leq 20$. Right hand side: maximum values of $|jC_N(x) - C(x)|/C(x)$ and $|jS_N(x) - S(x)|/S(x)$ on $0 \leq x \leq 20$.

These small absolute errors in $C_N(x)$ and $S_N(x)$, evaluated by fresnelCS, do not guarantee small relative errors near the only zero of $C(x)$ and $S(x)$ at $x = 0$. Near zero, from (67), $C(x) \approx \sqrt{1/4}x$ and $S(x) \approx \sqrt{1/4}x^3/6$, so very accurate calculations are needed to maintain small relative errors. The bounds (66) and (70) do, in fact, guarantee small relative errors near zero in in-

errors are $\approx 4.5 \times 10^{-16}$ for $N = 11$, the maximum relative error in $C_N(x)$ is $\approx 3.6 \times 10^{-15}$ for $N = 11$ and that in $S_N(x)$ as large as 2.7×10^{-13} . These errors may be entirely acceptable, but the truncated power series (67) must achieve smaller errors for small x , and may be cheaper to evaluate. (In fact, evaluating at 10^7 equally spaced points between 0 and 1.5 takes 2.9 times longer in Matlab with `fresnelCS` than evaluating 15 terms of both the series (67) via Horner's algorithm.)

5 Extensions and Concluding Remarks

To conclude, we have presented in this paper new approximations for the Fresnel integrals, derived from and inspired by modified trapezium rule approximations previously suggested for the complementary error function of complex argument in [18,15]. These approximations are simple to implement (Matlab codes are included in Tables 1 and 2): the computation of $F_N(x)$ requires a couple of complex exponentiations and a short summation to compute a quadrature sum, and that of $C_N(x)$ and $S_N(x)$ evaluation of trigonometric and hyperbolic functions and a similar short summation. The numerical methods are proven to converge exponentially (in absolute and relative error), approximately in proportion to $\exp(-\frac{1}{4}N)$ where N is the number of quadrature points used. Simple explicit error bounds are provided, and the predicted exponential convergence is precisely observed in practice. The approximation $F_N(x)$ with N

With respect to this hope, most obviously the results in this paper suggest a revisit of the methods of [18, 15] for $\operatorname{erfc}(z)$. Clearly, (20) suggests $\operatorname{erfc}_N(z) := 2F_N(e^{i\frac{1}{4}}z)$, given explicitly as

$$\operatorname{erfc}_N(z) = \frac{2}{e^{2A_N z} + 1} + \frac{2z}{A_N} e^{i z^2} \sum_{k=1}^N \frac{e^{i t_k^2}}{z^2 + t_k^2}; \quad (72)$$

as an approximation for $\operatorname{erfc}(z)$. (For $0 < \operatorname{Re}(z) < A_N$, this is precisely the approximation of [15] truncated to N quadrature points and with the particular choice (26) for h made.) The results of x2 show that (12) holds for $0 < \arg(x) < \frac{1}{4}\pi$ and for $\frac{1}{4}\pi < \arg(x) < \frac{3}{4}\pi$ which implies that

$$|\operatorname{erfc}(z) - \operatorname{erfc}_N(z)| \leq 2c_N \frac{e^{i\frac{1}{4}N}}{N+1} < 2 \frac{e^{i\frac{1}{4}N}}{N+1}; \quad (73)$$

for $\frac{1}{4}\pi < \arg(z) < \frac{3}{4}\pi$ and $\frac{3}{4}\pi < \arg(z) < \frac{5}{4}\pi$. This is a strong result in $\frac{3}{4}\pi < \arg(z) < \frac{5}{4}\pi$, where it is known that $|\operatorname{erfc}(z)| \leq 1$ so that (73) is a bound on both the absolute and relative error. However, in $\frac{1}{4}\pi < \arg(z) < \frac{3}{4}\pi$ the bound (73) is less satisfactory. In particular, since $\operatorname{erfc}(x) \gg e^{-x^2} = (e^{-\frac{1}{4}x})^2$ as $x \rightarrow +1$, for larger $x > 0$ (73) does not guarantee small relative errors. Indeed, $\operatorname{erfc}_N(x) \gg 2e^{i\frac{1}{4}N}$ has the wrong asymptotic behaviour as $x \rightarrow +1$.

A large part of a possible fix and analysis is already in [18] and [15] (see equations (7)-(8) in [15] and cf. (27), [19]), namely to discard the first term in (73) for $\operatorname{Re}(z) > A_N$, so that $\operatorname{erfc}(z)$ is approximated by

$$\operatorname{erfc}_N^0(z) = R_N(z) + \frac{2z}{A_N} e^{i z^2} \sum_{k=1}^N \frac{e^{i t_k^2}}{z^2 + t_k^2}; \quad (74)$$

where

$$R_N(z) := \begin{cases} \frac{1}{2}(e^{2A_N z} + 1); & \operatorname{Re}(z) \leq A_N; \\ 0; & \operatorname{Re}(z) > A_N; \end{cases}$$

Figure 5 plots the supremum, on $0 \leq x \leq 25$, of the absolute and relative errors in $\operatorname{erfc}_N^0(x)$ against N , computing $\operatorname{erfc}(x)$ with the inbuilt Matlab function erfc , and with $\operatorname{erfc}_{20}^0$. Clearly, both plots show exponential convergence at a rate approximately proportional to $e^{i\frac{1}{4}N}$. The absolute error in erfc_N^0 is $< 4.5 \times 10^{-16}$ for $N \geq 10$ and the relative error $< 6.7 \times 10^{-16}$ for $N \geq 12$, while the maximum relative error of the standard Matlab function is limited to about 5.7×10^{-14} . We have not computed $D[(NTJ/F7e3-450(\cos 369.97(v)^2(e)-289(n(e)-289)-289)-289-289) \cdot 1w239.96f7.56 \cdot 5TD[(;)]TJ/F29.96f-91.24D[(;)]TJ/F2959.96f-9$

In the right hand figure we plot this lower bound which accurately predicts the maximum error, this suggests that the small size of error present is associated with the discontinuity in erfc_N^0 .

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A Appendix

In this appendix we prove the bounds

$$\frac{1}{2} \leq |jF(x)| \leq \frac{1}{2} \frac{1}{e^{i\pi/4} + e^{\pi/4} x} = \frac{1}{2} \frac{1}{1 + e^{\pi/4} x + \frac{1}{4} x^2} \leq \frac{1}{2 + 2e^{\pi/4} x}; \quad (76)$$

for $x \geq 0$. The lower bounds in (76), which appear to be new, are used in [2] to prove an upper bound on the relative error in the approximation $F_N(x)$ to $F(x)$. From (76) and (16) we immediately deduce bounds for negative arguments which are also used in [2], that

$$\frac{3}{2} \leq |jF(-ix)| \leq \frac{1}{2}; \quad \text{for } x \geq 0; \quad (77)$$

We can also immediately deduce bounds on the version of the Fresnel integral defined by (4), and on the complementary error function of argument $e^{i\pi/4} x$ (via (20) and that $\text{erfc}(z) = \text{erfc}(\bar{z})$), for example that

$$|jF(x)| \leq \frac{1}{2 + \frac{1}{4} x} \quad \text{and} \quad \frac{3}{2} \leq \text{erfc}(e^{i\pi/4} x) \leq \frac{1}{1 + e^{\pi/4} x}; \quad \text{for } x \geq 0; \quad (78)$$

The remainder of this appendix is the proof of (76). But note first that both

$$L_1(x) := \frac{1}{2} \frac{1}{1 + e^{\pi/4} x + \frac{1}{4} x^2} \quad \text{and} \quad L_2(x) := \frac{1}{2 + 2e^{\pi/4} x} \quad (79)$$

are sharp lower bounds for $|jF(x)|$ for $x = 0$ (since $|jF(0)| = L_1(0) = L_2(0) = \frac{1}{2}$) and in the limit $x \rightarrow +1$ (since $|jF(x)| \gg (2e^{\pi/4} x)^{-1}$ as $x \rightarrow +1$, and $L_1(x)$ and $L_2(x)$

where, for $n = 0; 1; \dots$:

$$g_n(x) := \int_0^x \frac{e^{i x^2 u^2} u^{2n}}{1 + u^4} du.$$

Clearly, $g_n(x) > 0$ is well-defined for all n and all $x > 0$ by this definition, and also for $x = 0$ for $n = 0; 1$, with (this computation done, e.g., by contour integration) $g_0(0) = g_1(0) = \frac{1}{4} \sqrt{\frac{\pi}{2}}$. Further, for $x > 0$ (and $x = 0$ for $n = 0$),

$$g_n'(x) = i 2x g_{n+1}(x) < 0; \quad (81)$$

so that

$$g_n(x) < g_n(0) = \frac{1}{4} \sqrt{\frac{\pi}{2}}; \quad \text{for } x > 0 \text{ and } n = 0; 1; \quad (82)$$

Using this last inequality in (80) gives $|f(x)| < \frac{1}{2}$, for $x > 0$. Moreover, (80) implies that

$$\begin{aligned} 2^{-i\frac{\pi}{4}} + \frac{1}{4} \sqrt{\frac{\pi}{2}} x^{-i\frac{\pi}{4}} |f(x)| &\leq G(x) := \frac{1}{2^{i\frac{\pi}{4}}} \operatorname{Re} \left(1 + \frac{p}{2^{i\frac{\pi}{4}}} x + i (g_0(x) - i g_1(x)) \right) \\ &= \frac{1}{2^{i\frac{\pi}{4}}} \left(1 + \frac{p}{2^{i\frac{\pi}{4}}} x + g_0(x) + g_1(x) \right). \end{aligned} \quad (83)$$

Clearly, (76) will follow if we can show that $G(x) \geq 1$ for $x > 0$.

Now, for $x > 0$,

$$g_0(x) + g_2(x) = \int_0^x e^{i x^2 u^2} du = \frac{p}{x}; \quad (84)$$

so that, for $x > 0$,

$$g_1'(x) = i 2x g_2(x) = i 2 \frac{p}{x} + 2x g_0(x)$$

and

$$g_0(x) = g_0(0) + \int_0^x g_0'(t) dt = \frac{1}{4} \sqrt{\frac{\pi}{2}} + \int_0^x i 2 t g_1(t) dt; \quad (85)$$

$$g_1(x) = g_1(0) + \int_0^x g_1'(t) dt = \frac{1}{4} \sqrt{\frac{\pi}{2}} + \int_0^x \left(2 \frac{p}{t} + 2 t g_0(t) \right) dt. \quad (86)$$

From (82) we see that $g_0(x) \leq \frac{1}{4} \sqrt{\frac{\pi}{2}}$, and then from (86) that

$$g_1(x) \leq \frac{1}{4} \sqrt{\frac{\pi}{2}} + \int_0^x \left(2 \frac{p}{t} + 2 t g_0(t) \right) dt.$$

It follows from (85) that

$$g_0(x) \leq \frac{1}{4} \sqrt{\frac{\pi}{2}} + \int_0^x \left(\frac{1}{2} x^2 + \frac{4}{3} \frac{p}{x^3} + \frac{1}{2} \frac{p}{x^2} x^4 \right) dt; \quad (87)$$

and then from (86) that

$$g_1(x) \leq \frac{1}{4} \sqrt{\frac{\pi}{2}} + \int_0^x \left(2 \frac{p}{t} + \frac{1}{2} x^2 + \frac{1}{2} \frac{p}{x^2} x^4 + \frac{8}{15} \frac{p}{x^5} + \frac{1}{12} \frac{p}{x^6} \right) dt; \quad (88)$$

all these bounds holding for $x \geq 0$. Using these lower bounds in (83) we see that, for $x \geq 0$,

$$\begin{aligned} G(x) &\geq 1 + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + 2 \right) x + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{4}{3} \right) x^3 + \frac{5}{6} x^4 + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{4}{15} \right) x^5 + \frac{x^6}{12} \\ &= 1 + \frac{x}{p^{\frac{1}{2\frac{1}{4}}}} h_0(x); \end{aligned}$$

where

$$h_0(x) = \left(\frac{1}{4} + 2 \right) x + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{4}{3} \right) x^3 + \frac{5}{6} x^4 + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{8}{15} \right) x^5 + \frac{p^{\frac{1}{2\frac{1}{4}}}}{12} x^6.$$

We will show now that $h_0(x) > 0$ for $0 \leq x \leq 1$ which will show that $G(x) \geq 1$ for $0 \leq x \leq 1$. To see this we observe that $h_0^0(x) = x h_1(x)$ where

$$\begin{aligned} h_1(x) &= \left(\frac{1}{4} + 2 \right) x + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{4}{3} \right) x^3 + \frac{5}{2} x + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(\frac{1}{4} + \frac{32}{15} \right) x^2 + \frac{5}{12} \frac{p^{\frac{1}{2\frac{1}{4}}}}{x^3} x^3 \\ &< \left(\frac{10}{3} + 7x \right) + 4x^2 = \left(\frac{10}{3} + 7x \right) + 4x^2 = \left(\frac{10}{3} + 7x \right) + \frac{1}{15} + \frac{1}{3} < 0; \end{aligned}$$

so that $h_0^0(x) < 0$ for $x > 0$. Thus, for $0 \leq x \leq 1$,

$$h_0(x) \geq h_0(1) = \frac{3}{4} + \frac{1}{2} + \frac{2}{15} > 0.$$

We have shown that $G(x) \geq 1$ for $0 \leq x \leq 1$. It remains to show that $G(x) \geq 1$ for $x > 1$. To see this we make use of (83) and (84) which give that, for $x > 0$,

$$\begin{aligned} G(x) &> \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(1 + \frac{p^{\frac{1}{2\frac{1}{4}}}}{x} \right) + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} g_2(x) \\ &= 1 + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} \left(1 + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} + \frac{p^{\frac{1}{2\frac{1}{4}}}}{2x} \right) + \frac{1}{p^{\frac{1}{2\frac{1}{4}}}} g_2(x) \end{aligned}$$

To show that $G(x) \leq 1$ for $1 < x < \sqrt{2}$ we need a sharper upper bound on $g_2(x)$ than (90). To obtain this upper bound we write

$$xg_2(x) = I := \int_{-1}^1 \frac{e^{it^2} t^4}{x^4 + t^4} dt;$$

and approximate this integral by the trapezium rule as

$$I_h = h \sum_{n=-j}^j \frac{e^{in^2h^2} n^4 h^4}{x^4 + n^4 h^4} = 2h \sum_{n=1}^j \frac{e^{in^2h^2} n^4 h^4}{x^4 + n^4 h^4}.$$

Arguing as in x2 (or see [24, x5.1.4]), the error in this trapezium rule approximation is $I - I_h = PC_h + E_h^a$, where PC_h , a pole contribution, and E_h^a are given by

$$PC_h = 2\pi i(r_0 + r_1) \text{ and } E_h^a = \int_{iH}^Z f(z)(1 + g(z)) dz;$$

Here, $f(z) = e^{iz^2} z^4$

provided that $H > x$. In particular, for $1 < x < p_-$