

1. Table of Integrals

This table of integrals presents the results of the computations carried out in Chapter 3. Chapter 2 presents the main results of Chapter 3 in handbook format.

(1.0) Integrals

Fundamental Integrals

	<u>Integral</u>	<u>Ref.</u>
(1.0.1)	$F(x) = \int_0^x \frac{\operatorname{erf}(w)}{w} dw, \quad x \geq 0$	(2.1)
(1.0.2)	$G(x) = \int_x^\infty \frac{\operatorname{erfc}(w)}{w} dw, \quad x > 0$	(2.1)
(1.0.3)	$F(x) = \frac{\gamma}{2} + \ln(2x) + G(x) \quad (\gamma = 0.5772156649015328606\dots)$	(2.1)
(1.0.4)	$\int_0^x e^{-a^2 w^2} \ln w dw = \frac{\sqrt{\pi}}{2a} [\operatorname{erf}(ax) \ln x - F(ax)], \quad x \geq 0$	(2.1)
(1.0.5)	$\int_x^\infty e^{-a^2 w^2} \ln w dw = \frac{\sqrt{\pi}}{2a} [\operatorname{erfc}(ax) \ln x + G(ax)], \quad x > 0$	(2.1)
(1.0.6)	$\int_0^\infty e^{-a^2 w^2} \ln w dw = -\frac{\sqrt{\pi}}{2a} \left[\frac{\gamma}{2} + \ln(2a) \right].$	(2.1)
(1.0.7)	$G_\nu(x) \equiv \int_1^\infty \frac{E_\nu(xw)}{w^\nu} dw = \frac{-\partial E_\nu(x)}{\partial \nu} = \int_1^\infty \frac{e^{-xw} \ln w}{w^\nu} dw, \quad x > 0, \nu > 0$	(2.2)
(1.0.8)	$G_{1/2}(x) = 2\sqrt{\frac{\pi}{x}} G(\sqrt{x}), \quad x > 0$	(2.2)
(1.0.9)	$\int_x^\infty \frac{E_\mu(w)}{w^\nu} dw = \frac{1}{x^{\nu-1}} \frac{E_\nu(x) - E_\mu(x)}{\mu - \nu} \quad \text{or}$	(2.2)
(1.0.10)	$\int_1^\infty \frac{E_\mu(xw)}{w^\nu} dw = \frac{E_\nu(x) - E_\mu(x)}{\mu - \nu}, \quad x > 0, \mu > 0, \nu > 0, \mu \neq \nu$	(2.2)
(1.0.11)	$\int_x^\infty \frac{E_\nu(w)}{w^\nu} dw = \frac{1}{x^{\nu-1}} G_\nu(x), \quad x > 0 \quad \text{or}$	(2.2)
(1.0.12)	$\int_1^\infty \frac{E_\nu(xw)}{w^\nu} dw = G_\nu(x), \quad x > 0, \nu > 0 \quad (\mu = \nu \text{ above})$	(2.2)
(1.0.13)	$\int_1^\infty \frac{E_{1/2}(xw)}{\sqrt{w}} dw = G_{1/2}(x) = 2\sqrt{\frac{\pi}{x}} G(\sqrt{x})$	(2.2)
(1.0.14)	$I_n(b, x) = \int_x^\infty \frac{e^{-b^2 w^2} \ln w}{w^n} dw, \quad n = 0, 1, 2, \dots, \quad x > 0$	(2.2)
(1.0.15)	$I_n(b, x) = \frac{\ln x}{2x^{n-1}} E_{(n+1)/2}(b^2 x^2) + \frac{1}{4x^{n-1}} G_{(n+1)/2}(b^2 x^2), \quad x > 0$	(2.2)
(1.0.16)	$I_0(b, x) = \int_x^\infty e^{-b^2 w^2} \ln w dw = \frac{\sqrt{\pi}}{2b} [\operatorname{erfc}(bx) \ln x + G(bx)]$	(2.2)

$$(1.0.17) \quad \frac{(n+1)}{2b^2} I_{n+2} + I_n = \frac{\ln x}{2b^2} \cdot \frac{e^{-b^2 x^2}}{x^{n+1}} + \frac{1}{4b^2 x^{n+1}} E_{(n+3)/2}(b^2 x^2), \quad n \geq 0 \quad (2.2)$$

$$(1.0.18) \quad J_\nu(a, x) = \int_x^\infty \frac{\operatorname{erf}(aw)}{w^\nu} dw = \frac{1}{(\nu-1)x^{\nu-1}} \left[\operatorname{erf}(ax) + \frac{ax}{\sqrt{\pi}} E_{\nu/2}(a^2 x^2) \right], \quad \nu > 1 \quad (2.11)$$

$$(1.0.19) \quad J_\nu^c(a, x) = \int_x^\infty \frac{\operatorname{erfc}(aw)}{w^\nu} dw = \frac{1}{(\nu-1)x^{\nu-1}} \left[\operatorname{erfc}(ax) - \frac{ax}{\sqrt{\pi}} E_{\nu/2}(a^2 x^2) \right], \quad \nu \neq 1 \quad (2.11)$$

$$(1.0.20) \quad J_2(a, x) = \int_x^\infty \frac{\operatorname{erf}(aw)}{w^2} dw = \frac{\operatorname{erf}(ax)}{x} + \frac{a}{\sqrt{\pi}} E_1(a^2 x^2), \quad \nu = 2 \quad (2.11)$$

$$(1.0.21) \quad J_2^c(a, x) = \int_x^\infty \frac{\operatorname{erfc}(aw)}{w^2} dw = \frac{\operatorname{erfc}(ax)}{x} - \frac{a}{\sqrt{\pi}} E_1(a^2 x^2), \quad \nu = 2 \quad (2.11)$$

$$(1.0.22) \quad J_3(a, x) = \int_x^\infty \frac{\operatorname{erf}(aw)}{w^3} dw = \frac{\operatorname{erf}(ax)}{2x^2} + \frac{a}{x} \operatorname{ierfc}(ax), \quad \nu = 3 \quad (2.11)$$

$$(1.0.23) \quad J_3^c(a, x) = \int_x^\infty \frac{\operatorname{erfc}(aw)}{w^3} dw = \frac{\operatorname{erfc}(ax)}{2x^2} - \frac{a}{x} \operatorname{ierfc}(ax) = \frac{2i^2 \operatorname{erfc}(ax)}{x^2}, \quad \nu = 3 \quad (2.11)$$

$$(1.0.24) \quad I_5(a, b, x) = \int_x^\infty e^{-a^2 w^2} \operatorname{erfc}(bw) dw = \frac{1}{2d\sqrt{\pi}} \sum_{k=0}^\infty \frac{(1/2)_k}{k!} \left(\frac{a^2}{d^2} \right)^k E_{k+3/2}(d^2 x^2), \quad a \leq b \quad (2.3)$$

$$(1.0.25) \quad I_5(a, b, x) = \frac{be^{-a^2 x^2}}{a^2 + b^2} \sum_{k=1}^\infty \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} [(k-1)! i^{2k-1} \operatorname{erfc}(bx)], \quad a \leq b \quad (2.3)$$

$$(1.0.26) \quad = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) \operatorname{erfc}(bx) - \frac{b}{a} I_5(b, a, x), \quad d^2 = a^2 + b^2, \quad a > b \quad (2.3)$$

$$(1.0.27) \quad J_5(a, b, x) = \int_x^\infty e^{-a^2 w^2} \operatorname{erf}(bw) dw = \frac{\sqrt{\pi}}{2a} \operatorname{erfc}(ax) - I_5(a, b, x) \quad (2.3)$$

$$(1.0.28) \quad U_5(a, b, x) = \int_0^x e^{-a^2 w^2} \operatorname{erfc}(bw) dw = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{a}{b} - I_5(a, b, x) \quad (2.3)$$

$$(1.0.29) \quad V_5(a, b, x) = \int_0^x e^{-a^2 w^2} \operatorname{erf}(bw) dw = \frac{\sqrt{\pi}}{2a} \operatorname{erf}(ax) - U_5(a, b, x) \\ = \frac{1}{a\sqrt{\pi}} \tan^{-1} \frac{b}{a} - J_5(a, b, x) \quad (2.3)$$

$$(1.0.30) \quad I_2(a, b, T) = \int_0^T \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_1^\infty \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erf}(b/\sqrt{\tau})}{\tau^{3/2}} d\tau, \quad T = \frac{1}{\sqrt{t}} \quad (2.8)$$

$$(1.0.31) \quad I_2^c(a, b, T) = \int_T^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erf}(b/\sqrt{\tau})}{\tau^{3/2}} d\tau \quad (2.8)$$

$$(1.0.32) \quad I_2^c(a, b, 0) = \int_0^\infty \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{(2/\sqrt{\pi})}{a+b+\sqrt{a^2+b^2}} \quad (2.8)$$

$$(1.0.33) \quad I_9(a, b, T) = \int_0^T w \operatorname{erf}(aw) \operatorname{erf}(bw) dw = \frac{1}{2} \int_1^\infty \frac{\operatorname{erf}(a/\sqrt{u}) \operatorname{erf}(b/\sqrt{u})}{u^2} du \quad (2.8)$$

$$(1.0.34) \quad I_9^c(a, b, T) = \int_T^\infty w \operatorname{erfc}(aw) \operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{u}) \operatorname{erfc}(b/\sqrt{u})}{u^2} du \quad (2.8)$$

$$(1.0.35) \quad I_{20}(a, b, T) = \int_T^\infty e^{-a^2 x^2} \operatorname{erf}(bx) \ln x dx, \quad (2.4)$$

$$(1.0.36) \quad I_{20}^c(a, b, T) = \int_T^\infty e^{-a^2 x^2} \operatorname{erfc}(bx) \ln x dx, \quad (2.4)$$

$$(1.0.37) \quad P(a, b, T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w} dw \quad (2.5)$$

$$(1.0.38) \quad P^c(a, b, T) = \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w} dw \quad (2.5)$$

$$(1.0.39) \quad Q(a, b, T) = \int_T^\infty e^{-a^2 w^2} E_1(b^2 w^2) dw \quad (2.5)$$

Results in Terms of Fundamental Integrals (1.0.1)-(1.0.39), $T = 1/\sqrt{t}$

$$(1.0.40) \quad \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erf}(b/\sqrt{u})/\sqrt{u} du = I_1(a, b, T) \quad (2.6)$$

$$= \frac{e^{-a^2 T^2} \operatorname{erf}(bT)}{T} + \frac{b}{\sqrt{\pi}} E_1[T^2(a^2 + b^2)] - 2a^2 J_5(a, b, T) \quad (2.6)$$

$$(1.0.41) \quad \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erfc}(b/\sqrt{u})/\sqrt{u} du = I_1^c(a, b, T) \quad (2.6)$$

$$= \frac{e^{-a^2 T^2} \operatorname{erfc}(bT)}{T} - \frac{b}{\sqrt{\pi}} E_1[T^2(a^2 + b^2)] - 2a^2 I_5(a, b, T) \quad (2.6)$$

$$(1.0.42) \quad \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erf}(bw)}{w^3} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erf}(b/\sqrt{u}) du = I_{13}(a, b, T) \quad (2.7)$$

$$= \frac{e^{-a^2 T^2}}{2T^2} \operatorname{erf}(bT) + \frac{b}{T} i \operatorname{erfc}(T\sqrt{a^2 + b^2}) - a^2 P(a, b, T)$$

$$(1.0.43) \quad \int_T^\infty \frac{e^{-a^2 w^2} \operatorname{erfc}(bw)}{w^3} dw = \frac{1}{2} \int_0^t e^{-a^2/u} \operatorname{erfc}(b/\sqrt{u}) du = I_{13}^c(a, b, T) \quad (2.7)$$

$$= \frac{1}{2T^2} E_2(a^2 T^2) - I_{13}(a, b, T)$$

$$(1.0.44) \quad \int_0^T \frac{\operatorname{erf}(aw) \operatorname{erf}(bw)}{w} dw = \frac{1}{2} \int_t^\infty \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erf}(b/\sqrt{\tau})}{\tau} d\tau = I_{19}(a, b, T) \quad (2.9)$$

$$(1.0.45) \quad \int_T^\infty \frac{\operatorname{erfc}(aw) \operatorname{erfc}(bw)}{w} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{\tau}) \operatorname{erfc}(b/\sqrt{\tau})}{\tau} d\tau = I_{19}^c(a, b, T) \quad (2.9)$$

$$(1.0.46) \quad \int_T^\infty \frac{\operatorname{erf}(aw) \operatorname{erfc}(bw)}{w} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erfc}(b/\sqrt{\tau})}{\tau} d\tau = G(bT) - I_{19}(a, b, T) \quad (2.9)$$

$$(1.0.47) \quad \int_T^\infty \frac{\operatorname{erf}(aw) \operatorname{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erf}(b/\sqrt{\tau})}{\tau^{1/2}} d\tau = I_6(a, b, T) \quad (2.10)$$

$$(1.0.48) \quad \int_T^\infty \frac{\operatorname{erfc}(aw) \operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erfc}(a/\sqrt{\tau}) \operatorname{erfc}(b/\sqrt{\tau})}{\tau^{1/2}} d\tau = I_6^c(a, b, T) \quad (2.10)$$

$$(1.0.49) \quad \int_T^\infty \frac{\operatorname{erf}(aw) \operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t \frac{\operatorname{erf}(a/\sqrt{\tau}) \operatorname{erfc}(b/\sqrt{\tau})}{\tau^{1/2}} d\tau \quad (2.10)$$

$$= J_2(a, T) - I_6(a, b, T) = J_2(b, T) - I_6^c(a, b, T)$$

$$(1.0.50) \quad \int_T^\infty \frac{\operatorname{erf}(aw) \operatorname{erf}(bw)}{w^3} dw = \frac{1}{2} \int_0^t \operatorname{erf}(a/\sqrt{\tau}) \operatorname{erf}(b/\sqrt{\tau}) d\tau = W_3(a, b, T) \quad (2.11)$$

$$(1.0.51) \quad \int_T^\infty \frac{\operatorname{erfc}(aw)\operatorname{erfc}(bw)}{w^3} dw = \frac{1}{2} \int_0^t \operatorname{erfc}(a/\sqrt{\tau})\operatorname{erfc}(b/\sqrt{\tau}) d\tau = W_3^c(a, b, T) \quad (2.11)$$

$$(1.0.52) \quad \int_T^\infty \frac{\operatorname{erf}(aw)\operatorname{erfc}(bw)}{w^3} dw = \frac{1}{2} \int_0^t \operatorname{erf}(a/\sqrt{\tau})\operatorname{erfc}(b/\sqrt{\tau}) d\tau \quad (2.11)$$

$$= J_3(a, T) - W_3(a, b, T) = J_3^c(b, T) - W_3^c(a, b, T)$$

$$(1.0.53) \quad \int_T^\infty e^{-c^2 w^2} \operatorname{erf}(aw)\operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erf}(a/\sqrt{u})\operatorname{erf}(b/\sqrt{u})}{u^{3/2}} du = I_3(a, b, c, T) \quad (2.12)$$

$$(1.0.54) \quad \int_T^\infty e^{-c^2 w^2} \operatorname{erfc}(aw)\operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erfc}(a/\sqrt{u})\operatorname{erfc}(b/\sqrt{u})}{u^{3/2}} du \quad (2.12)$$

$$= J_3(a, b, c, T) = I_3^c(a, b, c, T)$$

$$(1.0.55) \quad \int_T^\infty w e^{-c^2 w^2} \operatorname{erf}(aw)\operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erf}(a/\sqrt{u})\operatorname{erf}(b/\sqrt{u}) du = J_4(a, b, c, T) \quad (2.13)$$

$$(1.0.56) \quad \int_T^\infty w e^{-c^2 w^2} \operatorname{erf}(aw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erf}(a/\sqrt{u}) du = J_4(a, \infty, c, T) \quad (2.13)$$

$$(1.0.58) \quad \int_T^\infty w e^{-c^2 w^2} \operatorname{erfc}(aw)\operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erfc}(a/\sqrt{u})\operatorname{erfc}(b/\sqrt{u}) du = J_4^c(a, b, c, T) \quad (2.13)$$

$$(1.0.59) \quad \int_T^\infty w e^{-c^2 w^2} \operatorname{erfc}(aw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^2} \operatorname{erfc}(a/\sqrt{u}) du = J_4^c(a, 0, c, T) \quad (2.13)$$

$$(1.0.60) \quad \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erf}(aw)\operatorname{erf}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erf}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erf}\left(\frac{b}{\sqrt{u}}\right) du = I_4(a, b, c, T) \quad (2.13)$$

$$(1.0.61) \quad \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erf}(aw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erf}\left(\frac{a}{\sqrt{u}}\right) du = I_4(a, \infty, c, T) \quad (2.13)$$

$$(1.0.62) \quad \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erfc}(aw)\operatorname{erfc}(bw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erfc}\left(\frac{a}{\sqrt{u}}\right) \operatorname{erfc}\left(\frac{b}{\sqrt{u}}\right) du = I_4^c(a, b, c, T) \quad (2.13)$$

$$(1.0.63) \quad \int_T^\infty w^2 e^{-c^2 w^2} \operatorname{erfc}(aw) dw = \frac{1}{2} \int_0^t \frac{e^{-c^2/u}}{u^{5/2}} \operatorname{erfc}\left(\frac{a}{\sqrt{u}}\right) du = I_4^c(a, 0, c, T) \quad (2.13)$$

$$(1.0.64) \quad \int_T^\infty e^{-c^2 w^2} \frac{\operatorname{erf}(aw)\operatorname{erf}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erf}(a/\sqrt{u})\operatorname{erf}(b/\sqrt{u})}{\sqrt{u}} du = I_{14}(a, b, c, T) \quad (2.14)$$

$$(1.0.65) \quad \int_T^\infty e^{-c^2 w^2} \frac{\operatorname{erfc}(aw)\operatorname{erfc}(bw)}{w^2} dw = \frac{1}{2} \int_0^t e^{-c^2/u} \frac{\operatorname{erfc}(a/\sqrt{u})\operatorname{erfc}(b/\sqrt{u})}{\sqrt{u}} du = I_{14}^c(a, b, c, T) \quad (2.14)$$

Let

$$(1.0.66) \quad Y_n(a, b, T) = \int_T^\infty e^{-a^2 w^2} i^n \operatorname{erfc}(bw) dw, \quad V_n(a, b, T) = \int_T^\infty w e^{-a^2 w^2} i^n \operatorname{erfc}(bw) dw, \quad n \geq -1 \quad (2.3)$$

$$(1.0.67) \quad Y_{-1}(a, b, T) = \frac{\operatorname{erfc}(T\sqrt{a^2 + b^2})}{\sqrt{a^2 + b^2}}, \quad Y_0(a, b, T) = I_5(a, b, T),$$

$$(1.0.68) \quad V_{-1}(a, b, T) = \frac{e^{-(a^2 + b^2)T^2}}{(a^2 + b^2)\sqrt{\pi}}, \quad V_0(a, b, T) = \frac{1}{2a^2} \left[e^{-a^2 T^2} \operatorname{erfc}(bT) - \frac{b}{\sqrt{a^2 + b^2}} \operatorname{erfc}(T\sqrt{a^2 + b^2}) \right]$$

$$(1.0.69) \quad 2nY_n - \left(1 + \frac{b^2}{a^2}\right)Y_{n-2} = \frac{-b}{a^2} e^{-a^2 T^2} i^{n-1} \operatorname{erfc}(bT), \quad V_n = \frac{1}{2a^2} \left[e^{-a^2 T^2} i^n \operatorname{erfc}(bT) - bY_{n-1} \right], \quad n \geq 1$$

In particular,

$$(1.0.70) \quad Y_1(a, b, T) = \int_T^\infty e^{-a^2 w^2} ierfc(bw) dw = \frac{1}{2a^2} \left[\sqrt{a^2 + b^2} \operatorname{erfc}(T\sqrt{a^2 + b^2}) - be^{-a^2 T^2} \operatorname{erfc}(bT) \right]$$

$$(1.0.71) \quad V_1(a, b, T) = \int_T^\infty we^{-a^2 w^2} ierfc(bw) dw = \frac{1}{2a^2} \left[e^{-a^2 T^2} ierfc(bT) - bI_5(a, b, T) \right]$$

$$(1.0.72) \quad Y_n(a, b, T) = \frac{be^{-a^2 T^2}}{a^2 + b^2} \sum_{k=1}^\infty \left(\frac{4a^2}{a^2 + b^2} \right)^{k-1} \frac{\Gamma(n/2 + k)}{\Gamma(n/2 + 1)} i^{n+2k-1} \operatorname{erfc}(bT), \quad n \geq 0, \quad a \leq b$$

$$(1.0.73) \quad Y_n(a, b, T) = \frac{\sqrt{\pi}}{2a} \sum_{k=0}^n (-1)^k \left(\frac{b}{a} \right)^k i^k \operatorname{erfc}(aT) i^{n-k} \operatorname{erfc}(bT) + (-1)^{n+1} \left(\frac{b}{a} \right)^{n+1} Y_n(b, a, T), \quad a > b$$

Integrals Related To the Function $U(a, b, t)$

$$U(a, b, t) = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$$a > 0, \quad b > 0, \quad c > 0, \quad d > 0, \quad t > 0$$

$$(1.0.74) \quad V(a, b, t) = \int_0^t U(a, b, \tau) d\tau, \quad (2.15)$$

$$(1.0.75) \quad I_{21}(a, b, c, t) = \int_0^t U(a, b, \tau) \operatorname{erf}(c/\sqrt{\tau}) d\tau \quad (2.15)$$

$$(1.0.76) \quad I_{21}^c(a, b, c, t) = \int_0^t U(a, b, \tau) \operatorname{erfc}(c/\sqrt{\tau}) d\tau \quad (2.15)$$

$$(1.0.77) \quad J_{21}(a, b, c, t) = \int_0^t \frac{U(a, b, \tau) e^{-c^2/\tau}}{\tau^{3/2}} d\tau \quad (2.15)$$

$$(1.0.78) \quad I_{22}(a, b, c, t) = \int_0^t U(a, b, \tau) \frac{e^{-c^2/\tau}}{\sqrt{\tau}} d\tau \quad (2.16)$$

$$(1.0.79) \quad J_{22}(a, b, c, t) = \int_0^t U(a, b, \tau) \sqrt{\tau} e^{-c^2/\tau} d\tau \quad (2.16)$$

$$(1.0.80) \quad I_{24}(a, b, c, t) = \int_0^t \tau U(a, b, \tau) \operatorname{erf}\left(\frac{c}{\sqrt{\tau}}\right) d\tau, \quad (2.17)$$

$$(1.0.81) \quad I_{24}^c(a, b, c, t) = \int_0^t \tau U(a, b, \tau) \operatorname{erfc}\left(\frac{c}{\sqrt{\tau}}\right) d\tau, \quad (2.17)$$

$$(1.0.82) \quad J_{24}(a, b, t) = \int_0^t \tau U(a, b, \tau) d\tau, \quad (2.17)$$

$$(1.0.83) \quad V_{24}(a, b, t) = \int_0^t V(a, b, \tau) d\tau, \quad (2.17)$$

$$(1.0.84) \quad I_{25}(a, b, c, d, t) = \int_0^t U(a, b, \tau) U(c, d, \tau) d\tau \quad (2.18)$$

$$(1.0.85) \quad I_{26}(a, b, c, d, t) = \int_0^t \tau U(a, b, \tau) U(c, d, \tau) d\tau \quad (2.19)$$

$$(1.0.86) \quad J = \int e^{(a^2 - b^2)x} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) dx \quad (2.20)$$

$$(1.0.87) \quad I = \int x e^{(a^2 - b^2)x} \operatorname{erfc}\left(a\sqrt{x} + \frac{c}{\sqrt{x}}\right) dx \quad (2.20)$$

Miscellaneous Integrals $x \geq 0$

$$(1.0.88) \quad H_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) \frac{dv}{\sqrt{v}} \quad (2.21)$$

$$(1.0.89) \quad I_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) dv \quad (2.21)$$

$$(1.0.90) \quad J_{23}(x) = \int_0^x e^{w^2} \operatorname{erfc}(w) w^2 dw = \frac{1}{2} \int_0^{x^2} e^v \operatorname{erfc}(\sqrt{v}) \sqrt{v} dv \quad (2.21)$$

Reduction formula ending in H_{23} or I_{23}

$$(1.0.91) \quad \int_0^x e^{w^2} \operatorname{erfc}(w) w^\alpha dw = \frac{x^{\alpha-1}}{2} e^{x^2} \operatorname{erfc}(x) + \frac{x^\alpha}{\alpha\sqrt{\pi}} - \frac{(\alpha-1)}{2} \int_0^x e^{w^2} \operatorname{erfc}(w) w^{\alpha-2} dw \quad (2.21)$$

$\alpha = 2n \text{ or } 2n+1, \quad n = 1, 2, \dots$

$$(1.0.92) \quad G_n(a, b, x) = \int_x^\infty \frac{e^{-a^2 w^2} i^n \operatorname{erfc}(bw)}{w^n} dw, \quad n = 1, 2, \dots, a > 0, \quad b > 0 \quad (2.15)$$

$$(1.0.93) \quad I(a, b, x) = \int_x^\infty e^{-at-b/t} dt, \quad a > 0, \quad b > 0, \quad x > 0 \quad (2.22)$$

Inverse LaPlace Transform:

$$(1.0.94) \quad L^{-1} \left[\frac{e^{-2b\sqrt{p}}}{\sqrt{p}(\sqrt{p}+a)^{n+1}} \right] = (2\sqrt{t})^n e^{a^2 t + 2ab} i^n \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t})$$

$n=0$ gives

$$(1.0.95) \quad L^{-1} \left[\frac{e^{-2b\sqrt{p}}}{\sqrt{p}(\sqrt{p}+a)} \right] = e^{a^2 t + 2ab} \operatorname{erfc}(a\sqrt{t} + b/\sqrt{t}) = U(a, b, t)$$

Useful expansions for small aT (See (1.0.68) and (1.0.70) and Chapter 3, Folder 9):

$$(1.0.96) \quad \operatorname{erfc}(T\sqrt{a^2 + b^2}) = e^{-a^2 T^2} \sum_{k=0}^{\infty} (-2)^k i^k \operatorname{erfc}(bT) (bT\phi)^k, \quad bT\phi = \frac{a^2 T}{b + \sqrt{a^2 + b^2}}$$

$$(1.0.97) \quad i \operatorname{erfc}(T\sqrt{a^2 + b^2}) = e^{-a^2 T^2} i \operatorname{erfc}(bT) + e^{-a^2 T^2} \sum_{k=2}^{\infty} (-2)^{k-1} k i^k \operatorname{erfc}(bT) (bT\phi)^{k-1}$$

The general case is:

$$(1.0.98) \quad i^n \operatorname{erfc}(T\sqrt{a^2 + b^2}) = e^{-a^2 T^2} i^n \operatorname{erfc}(bT) + e^{-a^2 T^2} \sum_{k=n+1}^{\infty} (-2)^{k-n} C_n^k i^k \operatorname{erfc}(bT) (bT\phi)^{k-n}$$

where C_n^k is a binomial coefficient.

Reciprocal relations for $E_{n+1/2}(x^2)$ and $i^n \operatorname{erfc}(x)$ (See Chapter 3, Folder 28):

$$A(n, k) = (-1)^{k-1} 2^{2k-1} (k-1)! C_{k-1}^{n-1} = \frac{(-1)^{k-1} 2^{2k-1} (n-1)!}{(n-k)!}, \quad 1 \leq k \leq n, \quad n \geq 1$$

$$B(n, k) = \frac{(-1)^{k-1} C_{k-1}^{n-1}}{2^{2n-1} (n-1)!} = \frac{(-1)^{k-1}}{2^{2n-1} (k-1)! (n-k)!}, \quad 1 \leq k \leq n, \quad n \geq 1$$

$$(1.0.99) \quad \frac{1}{\sqrt{\pi}} E_{n+1/2}(x^2) = \sum_{k=1}^n A(n, k) i^{2k-1} \operatorname{erfc}(x) , \quad n \geq 1$$

$$(1.0.100) \quad i^{2n-1} \operatorname{erfc}(x) = \sum_{k=1}^n B(n, k) [E_{k+1/2}(x^2) / \sqrt{\pi}] , \quad n \geq 1 ,$$

$$(1.0.101) \quad \frac{2x}{\sqrt{\pi}} E_{n+1/2}(x^2) = \sum_{k=0}^n A(n+1, k+1) i^{2k} \operatorname{erfc}(x) , \quad n \geq 0$$

$$(1.0.102) \quad i^{2n} \operatorname{erfc}(x) = 2x \sum_{k=0}^n B(n+1, k+1) [E_{k+1/2}(x^2) / \sqrt{\pi}] , \quad n \geq 0$$

(1.1) Comments on the Use of Quadrature

Introduction

The main thrust of this work is directed toward the development of forms suitable for high accuracy computation (double precision arithmetic). It is not uncommon to find that representations of the desired integral break down computationally over some parameter ranges and a suitable alternative cannot be found. In these cases, a numerical quadrature is used as a default even though a quadrature is generally computationally more expensive. The quadratures used for this study are done on integrals whose integrands are analytic over the range of integration. This is achieved by a change of variable or a change in representation since the natural form of heat conduction solutions in the time variable often involves arguments of a square root or reciprocal square root. Historically, analytic forms (their Taylor series exist) are a kind of standard because a lot of work has been done to approximate these integrals by integration of polynomial approximations of the integrand (locally, a truncated Taylor series is a polynomial). Consequently, there are robust codes which will do the integration automatically without excessive programmer intervention. In these codes, only a subroutine for the function, the limits of integration, and an error tolerance REL need be specified. DGAUS8 written by R. E. Jones is one such routine which can be found on the SLATEC library and is used as part of this work. This subroutine was developed for high accuracy (double precision) applications and is well tested. It is adaptive, meaning that an 8-point Gauss formula is applied on subintervals where an error estimate is made for a given interval. If the estimate meets the required accuracy, then this interval is excluded from further subdivision and the routine moves on to test and subdivide until all subintervals meet the requirements or a specified limit is reached. Furthermore, one can expect significant digits from non-negative integrands because the 8-point Gauss formula has positive coefficients and losses of significant digits by differences of nearly equal quantities cannot occur. It is also assumed that a suitable double precision library of special functions is available to compute the integrand to the required accuracy.

Computing With DGAUS8 and DQUAD8

We apply DGAUS8 in a special way on infinite integrals to construct a routine called DQUAD8. To be a candidate for DQUAD8, the integral should converge rapidly. In these cases it is important to estimate a scale of integration in order to do the computation efficiently and not let the routine search for the region where most of the work needs to be done. Many of the integrands which result in quadratures are dominated by an exponential. In these cases, the scale of integration can be estimated by a “standard deviation”, σ . To be precise, we consider integrals of the form

$$(1.1.1) \quad I = \int_x^\infty f(x)dx$$

with

$$f(x) = g(x)e^{-ax} \quad \text{or} \quad f(x) = g(x)e^{-a^2x^2}$$

where $g(x)$ is slowly varying and the estimate for σ is given by

$$(1.1.2) \quad \sigma = \frac{m}{a}, \quad m = 4 \text{ or } 5 \quad \text{or} \quad \sigma = \frac{m}{a\sqrt{2}}, \quad m=3 \text{ or } 4.$$

Notice that when a is small then the scale of integration can be very large and when a is large the scale of integration can be very small. Then the quadrature proceeds according to the formula

$$(1.1.3) \quad I_K = \sum_{k=1}^K Q_k, \quad Q_k = \int_{X+(k-1)\sigma}^{X+k\sigma} f(x)dx,$$

and Q_k is computed by DGAUS8 with the REL parameter to specify the accuracy. The sum is terminated in DQUAD8 on a relative error test

$$(1.1.4) \quad |Q_K / I_K| \leq REL$$

This termination procedure is not rigorous, but it can be made rigorous by estimating the truncation error. Thus, if $g(x)$ is bounded by M for $x > R$, then the truncation at R gives an estimate

$$(1.1.5) \quad |T_R| \leq \frac{M}{a} e^{-aR} = B_R \quad \text{or} \quad |T_R| \leq \frac{M(\sqrt{\pi}/2)\text{erfc}(aR)}{a} < \frac{M}{2a^2 R} e^{-a^2 R^2} = B_R, \quad R > X,$$

where we have used an estimate of Mill's ratio to estimate $\text{erfc}(aR)$ [A&S, 7.1.13]:

$$\frac{\text{erfc}(x)}{e^{-x^2}} \leq \frac{2/\sqrt{\pi}}{x + \sqrt{x^2 + 4/\pi}} < \frac{1}{x\sqrt{\pi}}.$$

DQUAD8 returns not only an answer I_K but also the end point of the quadrature, $X_K = X + K\sigma$, after K applications of DGAUS8. Because DQUAD8 can also be called repeatedly with no change in the call list, DQUAD8 can be put into a loop. On each return from DQUAD8, the truncation error can be estimated by one of the formulas above with $R = X_K$. If the inequality

$$(1.1.6) \quad |B_R / I_K| \leq REL$$

is satisfied, then exit from the loop; otherwise, the looping continues until the estimate is satisfied or the maximum loop index is reached. Experience has indicated that the truncation error estimate is almost always satisfied on the first time through DQUAD8.

While the main thrust of DQUAD8 is to compute quadratures on infinite intervals, one can use this stepping procedure on finite intervals also. The details are given in the APPENDIX of Folder 21 in Chapter 3.

References: Chapter 3, Folder 21, APPENDIX