Power Series Expansion

- $e^{-t^2} = \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{n!}$ remember: $\underset{\text{error } f^{\underline{n}}}{\Phi(x)} = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt$

- Integrating from 0 to x and multiplying by $\frac{2}{\sqrt{\pi}}$ we get:

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x \sum_{n=0}^{\infty} \frac{(-1)^n t^{2n}}{n!}\, dt = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^x t^{2n}\, dt$$

$$\int_0^x t^{2n}\, dt = \left[\frac{t^{2n+1}}{2n+1}\right]_0^x = \frac{x^{2n+1}}{2n+1}$$

$$\Rightarrow \boxed{\Phi(x) = \frac{2}{\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(2n+1)} x^{2n+1}} \quad (1)$$ converges for all x

Convergence and practical use

- For small $|x|$, this series converges quite rapidly.
- However, for large $|x|$, you need many terms before you get a stable answer due to slow convergence of the power series away from $x = 0$.
- In practical numeric code, one usually limits use of this series to a moderate range of x (e.g., $|x| \leq 1.5$ or so) where it converges rapidly.

- The 1st few terms of the Taylor series expansion:

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \left(x - \frac{x^3}{3} + \frac{x^5}{10} - \frac{x^7}{42} + \frac{x^9}{216} - \dots \right) \quad (2)$$

Convergence of the Series

Root test: $a_n = \frac{(-1)^n x^{2n+1}}{n!(2n+1)}$

The ratio of successive terms:

$$\left|\frac{a_{n+1}}{a_n}\right| = \left| \frac{(-1)^{n+1} x^{2(n+1)+1}}{(n+1)!(2(n+1)+1)} \cdot \frac{n!(2n+1)}{(-1)^n x^{2n+1}} \right|$$

$$= \left| \frac{x^2(2n+1)}{(n+1)(2n+3)} \right|.$$

Assuming x is finite, as $n \to \infty$ the ratio approaches zero, confirming the series converges for all x.

Derivation of the Complementary Error Function

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) = 1 - \left(\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt\right) \quad (3)$$

It is a known result that

$$\int_0^\infty e^{-t^2}\,dt = \frac{\sqrt{\pi}}{2} \quad (4)$$

$$\Rightarrow 1 = \operatorname{erf}(\infty) = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-t^2}\,dt$$

$$\Rightarrow \operatorname{erfc}(x) = \left(\frac{2}{\sqrt{\pi}}\int_0^\infty e^{-t^2}\,dt\right) - \left(\frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt\right)$$

$$\Rightarrow \operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\left(\int_0^\infty e^{-t^2}\,dt - \int_0^x e^{-t^2}\,dt\right) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt$$

where we used the property of definite integrals:

$$\int_0^\infty (\cdot)\,dt - \int_0^x (\cdot)\,dt = \int_x^\infty (\cdot)\,dt \quad (5)$$

$$\Rightarrow \boxed{\operatorname{erfc}(x) = \frac{2}{\sqrt{x}}\int_x^\infty e^{-t^2}\,dt} \quad (6)$$

Derivation of the Asymptotic Expansion for erfc(x)

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt \qquad \text{let } t = x + u,\ dt = du$$

Then when $t = x$, $u = 0$, and as $t \to \infty$, $u \to \infty$.

$$\Rightarrow \operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-(x+u)^2}\,du$$

$$= \frac{2}{\sqrt{\pi}} e^{-x^2}\int_0^\infty e^{-2xu-u^2}\,du. \quad (7)$$

For large x, the main contribution to the integral comes from small u. Therefore, we expand the factor e^{-u^2} in a Taylor series:

$$e^{-u^2} = 1 - u^2 + \frac{u^4}{2!} - \frac{u^6}{3!} + \dots \quad (8)$$

Subst. into (7)

$$\Rightarrow \int_0^\infty e^{-2xu-u^2} = \int_0^\infty e^{-2xu}\left(1 - u^2 + \frac{u^4}{2!} - \frac{u^6}{3!} + \dots\right)$$

We know the standard Laplace integral:

$$\int_0^\infty u^n e^{-2xu}\, du = \frac{n!}{(2x)^{n+1}} \quad (9)$$

Thus we can compute the terms:

$$\int_0^\infty e^{-2xu}\, du = \frac{1}{2x}$$

$$\int_0^\infty u^2 e^{-2xu}\, du = \frac{2!}{(2x)^3} = \frac{1}{4x^3}$$

$$\int_0^\infty u^4 e^{-2xu}\, du = \frac{4!}{(2x)^5} = \frac{3}{4x^5}$$

$$\int_0^\infty u^6 e^{-2xu}\, du = \frac{6!}{(2x)^7} = \frac{15}{8x^7}$$

Thus, the series for the integral becomes

$$\int_0^\infty e^{-2xu-u^2} = \frac{1}{2x} - \frac{1}{4x^3} + \frac{1}{2}\frac{3}{4x^5} - \frac{1}{6}\frac{15}{8x^7} + \dots$$

$$= \frac{1}{2x} - \frac{1}{4x^3} + \frac{3}{8x^5} - \frac{15}{48x^7} + \dots \quad (10)$$

Subst. (10) back into the expession for erfc(x):

$$\mathrm{erfc}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}\left[\frac{1}{2x} - \frac{1}{4x^3} + \frac{3}{8x^5} - \frac{15}{48x^7} + \dots\right]$$

$$= \frac{e^{-x^2}}{x\sqrt{\pi}}\left[1 - \frac{1}{2x^2} + \frac{3}{(2x^2)^2} - \frac{15}{(2x^2)^3} + \dots\right] \quad (11)$$

Thus we arrive at the asymptotic expansion:

$$\boxed{\mathrm{erfc}(x) \sim \frac{e^{-x^2}}{x\sqrt{\pi}}\left(1 - \frac{1}{2x^2} + \frac{3}{(2x^2)^2} - \frac{15}{(2x^2)^3} + \dots\right)} \quad (12)$$

approximate symbol used to indicate that the series provides an approximation that becomes increasingly accurate as x grows larger.

This can be written in an alternative form which expresses the series in terms of a general term:

$$\operatorname{erfc}(x) \sim \frac{e^{-x^2}}{x\sqrt{\pi}} \sum_{n=0}^{\infty} \frac{(-1)^n (2n-1)!!}{(2x^2)^n} \qquad (13)$$

where the double factorial $(2n-1)!!$ is defined recursively by:

$$(2n-1)!! = \begin{cases} 1, & n=0, \\ (2n-1)(2n-3)!!, & n \geq 1 \end{cases} \qquad (14)$$

def$^{\underline{n}}$ of $n!!$: if n is an odd +ve integer:

$$(2k-1)!! = (2k-1)\cdot(2k-3)\cdot \ldots \cdot 3 \cdot 1.$$

e.g. $5!! = 5 \cdot 3 \cdot 1 = 15$

if n is an even +ve integer:

$$(2k)!! = (2k)\cdot(2k-2)\cdot \ldots \cdot 4 \cdot 2.$$

e.g. $6!! = 6 \cdot 4 \cdot 2 = 48$

By convention, $0!!$ is defined to be 1.

Note: This is not a convergent power series. Instead, it is asymptotic:
- As $x \to \infty$, keeping a finite number N of terms gives you an approximation whose accuracy improves with increasing x.
- For any fixed x, if you keep adding terms, eventually the partial sums may stop getting better and can even get worse.

Because of this nature, there is no single "on/off" boundary where it abruptly becomes valid. Instead, it just tends to do very well for 'sufficiently large' x.

Heat Conduction in a semi-infinite solid

1-D semi-infinite solid occupying $x \geq 0$.
temp. is initialy uniform at T_i. At time $t=0$, the boundary at $x=0$ is abruptly set to a new temp. T_s. The scenario is modelled by the heat eq^n:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (14)$$

subject to initial condition

$$T(x,0) = T_i \quad (x>0),$$

and boundary conditions

$$T(0,t) = T_s \quad (t>0), \quad T(x,t) \to T_i \text{ as } x \to \infty$$

Aim is to find $T(x,t)$ for $x \geq 0$, $t > 0$

- Shifted temperature variable:

$$\theta(x,t) = T(x,t) - T_i$$

Thus, the PDE becomes

$$\frac{\partial \theta}{\partial t} = \alpha \frac{\partial^2 \theta}{\partial x^2} \quad (15)$$

Thus, the initial and boundary conditions become:

$$\theta(x,0) = 0, \ \theta(0,t) = T_s - T_i, \ \theta(x,t) \to 0 \text{ as } x \to \infty$$

We seek sol^n of the form $\theta(x,t) = \Phi(\eta)$, where

$$\eta = \frac{x}{2\sqrt{\alpha t}}$$

$$\frac{\partial \theta}{\partial x} = \Phi'(\eta)\frac{d\eta}{dx} = \Phi'(\eta)\frac{1}{2\sqrt{\alpha t}},$$

$$\frac{\partial \theta}{\partial x^2} = \frac{\partial}{\partial x}\left[\Phi'(\eta)\frac{1}{2\sqrt{\alpha t}}\right] = \Phi''(\eta)\left(\frac{1}{2\sqrt{\alpha t}}\right)^2$$

Similarly

$$\frac{\partial \theta}{\partial t} = \Phi'(\eta)\frac{\partial \eta}{\partial t}$$

But $\eta = \frac{x}{2\sqrt{\alpha t}} \Rightarrow \frac{\partial \eta}{\partial t} = \frac{\partial}{\partial t}\left(\frac{x}{2\sqrt{\alpha}} t^{-1/2}\right) = -\frac{x}{4\sqrt{\alpha}} t^{-3/2} = -\eta \frac{1}{2t}$

Hence $\frac{\partial \theta}{\partial t} = \Phi'(\eta)\left(-\eta\frac{1}{2t}\right)$.

Subst. into (15)

$$\frac{\partial \theta}{\partial t} = \alpha\frac{\partial^2 \theta}{\partial x^2} \Rightarrow \Phi'(\eta)\left(-\eta\frac{1}{2t}\right) = \alpha\,\Phi''(\eta)\left(\frac{1}{2\sqrt{\alpha t}}\right)^2$$

Rearrange:

$$-\Phi'(\eta)\frac{\eta}{2t} = \alpha\,\Phi''(\eta)\frac{1}{4\alpha t} \Rightarrow -\Phi'(\eta)\eta = \frac{1}{4}\Phi''(\eta)$$

$\times -4$ both sides:

$$4\eta\,\Phi'(\eta) = -\Phi''(\eta)$$

$$\Rightarrow \Phi''(\eta) + 4\eta\,\Phi'(\eta) = 0$$

This ODE can be simplified further by known transformations, but it is well-known that its sol^{n} leads to an erf or erfc function.

The original boundary conditions for θ translate to:

$$\theta(0,t) = \Phi(0) = T_s - T_i\,; \quad \theta(\infty,t) = \Phi(\infty) = 0,$$

$\theta(x,0)$ is satisfied automatically by the limiting behavious as $t \to 0^+$

Hence we want $\Phi(0) = T_s - T_i$ and $\Phi(\infty) = 0$.

A standard result is that:

$$\Phi(\eta) = (T_s - T_i)\,\mathrm{erfc}(\eta)\,,\ \text{where } \mathrm{erfc}(\eta) = 1 - \mathrm{erf}(\eta)$$

Indeed, $\mathrm{erfc}(0) = 1$ matches $\Phi(0) = T_s - T_i$, and $\mathrm{erf}(\infty) = 0$ gives $\Phi(\infty) = 0$.

Thus, $\theta(x,t) = T(x,t) - T_i = (T_s - T_i)\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right)$

Re-expressing in terms of T,

$$T(x,t) = T_i + (T_s - T_i)\,\mathrm{erfc}\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

$$\Rightarrow T(x,t) = T_s + (T_i - T_s)\,\mathrm{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right)$$

Both forms satisfy exactly the same initial/boundary conditions because

$T_s + (T_i - T_s)\,\mathrm{erf}(z) = T_i - (T_i - T_s)\,\mathrm{erfc}(z)$.

Final Solution

Thus, the temp. field in the semi-infinite solid is

$$\boxed{T(x,t) = T_s + (T_i - T_s)\,\mathrm{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right)}$$

which satisfies

$$T(0,t) = T_s\,, \quad T(\infty,t) = T_i\,, \quad T(x,0) = T_i.$$

Physically, $\mathrm{erf}\left(\frac{x}{2\sqrt{\alpha t}}\right)$ captures how the thermal disturbance diffuses away from the boundary over time.