Section 15: Solution of Partial Differential Equations; the Diffusion equation

15. 1. Wave equation continued

First we finish off our calculation of the Green function for the wave equation we have

$$G(\underline{x}-\underline{x}', t-t') = \begin{cases} 0 & t < t' \\ -\frac{c}{4\pi|\underline{x}-\underline{x}'|}\,\delta(|\underline{x}-\underline{x}'| - c|t-t'|) & t > t' \end{cases}$$

Thus for the inhomogeneous wave equation

$$\nabla^2 u(\underline{x}, t) - \frac{1}{c^2}\frac{\partial^2 u(\underline{x}, t)}{\partial t^2} = f(\underline{x}, t)$$

a particular solution is

$$\begin{aligned} u(\underline{x}, t) &= \int d^3x'\, dt'\, f(\underline{x}', t')G(\underline{x}-\underline{x}', t-t') \\ &= -\frac{1}{4\pi}\int d^3x'\, \frac{f(\underline{x}', t-\frac{1}{c}|\underline{x}-\underline{x}'|)}{|\underline{x}-\underline{x}'|} \end{aligned}$$

Note that $t - \frac{1}{c}|\underline{x}-\underline{x}'|$ is the time required for a signal to propagate from $\underline{x}'$ to $\underline{x}$.

Now let us return to the point of how we bypass the poles on the ω integration contour.

In this example, by going *above* the poles we made sure our system was causal thus we obtained the **retarded** Green function i.e. it is a response to a disturbance in the past.

If instead we went *below* the poles then they would only contribute for $t < 0$ thus we would obtain the **advanced** Green function.

Aside: In some circumstances one goes below one pole (e.g. at $\omega = -|kc|$) and above the other, leading to the half advanced/half retarded Green function. This is relevant for example in Quantum Electrodynamics where it descibes a positive energy electron going forwards in time plus a negative energy electron going backwards in time, which is the same as a positron going forwards in time.

15. 2. Diffusion/ heat conduction equation

This is our canonical example of a parabolic equation. These types of equation have one real characteristic and we should specify Dirichlet or Neumann b.c. on an open surface.

In one space dimension the equation reads

$$\frac{\partial^2 u(\underline{x}, t)}{\partial x^2} - \frac{1}{D}\frac{\partial u(\underline{x}, t)}{\partial t} = 0$$

where D is the diffusion constant. Here the real characteristic is just $x = constant$ i.e. lines propagating forward in time.

As we shall see information propagates *forward* in time and an initial $u(x, t)$ is smoothed out as t increases. Conversely if we run time backwards singularities will appear from an initially smooth function. Thus 'the arrow of time' is inherent within the diffusion equation.

There are two types of 'physical' boundary conditions commonly encountered

a) We specify $u(x, t_0)$ (usually $t_0 = 0$) for all $-\infty < x < \infty$

b) We specify $u(x, t_0)$ over some range beginning/ending at finite x e.g.: $a < x < b$. Then in addition we specify $u(a, t)$ (Dirichlet problem) or $u'(a, t)$ (Neumann problem) on the finite x boundary (or boundaries).

15. 3. Green function for infinite x domain

We first consider one space dimension. Since the x domain is infinite we Fourier transform

$$F(k,t) = F[u(x,t)] \quad = \quad \int_{-\infty}^{\infty} u(x,t) e^{-ikx}$$

$$\text{yielding} \quad -k^2 F(k,t) = \quad \frac{1}{D}\frac{\partial F(k,t)}{\partial t} \quad \Rightarrow \quad F(k,t) = A(k) e^{-k^2 Dt}$$

If the boundary condition is $u(x, 0) = f(x)$ then $A(k) = F[f(x)]$ and

$$F[u(x,t)] = F[u(x,0)] e^{-k^2 Dt}$$

Now

$$F^{-1}\left[e^{-k^2 Dt}\right] = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{-k^2 Dt + ikx} = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \exp\left\{-Dt\left(k - \frac{ix}{2Dt}\right)^2 - \frac{x^2}{4Dt}\right\} = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

where in the big curly brackets we have completed the square and then use a Gaussian integral identity (see tutorial 2.1). Thus invoking the convolution theorem

$$u(x,t) = \int_{-\infty}^{\infty} dx' u(x',0) G(x,t;x')$$

$$\text{where} \quad G(x,t;x') = \frac{1}{\sqrt{4\pi Dt}} \exp\left\{-\frac{(x-x')^2}{4Dt}\right\} \theta(t)$$

$G(x, t; x')$ is the initial value Green function (i.e. response at x, t to initial condition at x').

Note the 'diffusive scaling' i.e. after time t the inital condition at x' affects points x which are distance of order $t^{1/2}$ away.

To see this explicitly consider $u(x, 0) = u_0\, \delta(x)$. Then

$$u(x,t) = \frac{u_0}{\sqrt{4\pi Dt}} \exp\left\{-\frac{x^2}{4Dt}\right\} \theta(t) \; .$$

Consider $u(x, t)$ as the density of some substance. At $t = 0$ the substance is concentrated at the origin; as time proceeds the density profile smoothes out and is of width $\sim t^{1/2}$. You should plot this.

Now we consider three space dimensions and define a Green function through

$$\nabla^2 G(\underline{x} - \underline{x}', t - t') - \frac{1}{D}\frac{\partial G(\underline{x} - \underline{x}', t - t')}{\partial t} = \delta(\underline{x} - \underline{x}')\delta(t - t') \qquad (1)$$

Wlog we set $\underline{x}'=0$, $t'=0$. Again because we have an infinite $\underline{x}$ domain we Fourier transform, with the convention

$$\widetilde{G}(\underline{k},t)=\int_{-\infty}^{\infty}d^3x\int_{-\infty}^{\infty}dt\,u(\underline{x},t)e^{-i\underline{k}\cdot\underline{x}+i\omega t}$$

Thus (1) yields

$$-k^2\widetilde{G}+\frac{i\omega}{D}\widetilde{G} \quad = \quad 1 \quad \Rightarrow \quad \widetilde{G}=\frac{D}{i(\omega+iDk^2)}$$

$$\text{and} \qquad G(\underline{x},t)=D\int\frac{d^3k}{(2\pi)^3}\int\frac{d\omega}{2\pi}\frac{e^{i(\underline{k}\cdot\underline{x}-\omega t)}}{i(\omega+iDk^2)}\,.$$

Note that in the ω integral there is only one pole at $\omega=-iDk^2$. Thus for $t<0$, when the contour is closed in the upper half plane, there is no singularity within the closed contour and $G=0$. For $t>0$, when the contour is closed in the lower half plane, the pole is within the integration contour and using the residue theorem (note clockwise contour)

$$G(\underline{x},t)=-D\int_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}e^{-k^2Dt+i\underline{k}\cdot\underline{x}}=-\int_{-\infty}^{\infty}\frac{d^3k}{2\pi}\exp\left\{-Dt\left(\underline{k}-\frac{i\underline{x}}{2Dt}\right)^2-\frac{r^2}{4Dt}\right\}$$

$$=-\frac{D}{(2\pi)^3}\left[\int_{\infty}^{\infty}dke^{-Dtk^2}\right]^3\exp\left\{-\frac{r^2}{4Dt}\right\}=-\frac{D}{(2\pi)^3}\left(\frac{\pi}{Dt}\right)^{3/2}\exp\left\{-\frac{r^2}{4Dt}\right\}\theta(t)$$

Note again the diffusive scaling where the region affected by the disturbance at $x=0$ has a radius of order $r\sim t^{1/2}$. In $2d$ the Green function is a 'bell shaped' curve—you should sketch this.

15. 4. Finite x boundary condition

As an example we consider the *semi-infinite rod.* The boundary condition is $u(x,0)$ given for $x>0$ and $u(0,t)=f(t)$ i.e. u is prescribed at the boundary $x=0$.

There are two approaches to solving the problem

1. Use Fourier transform wrt x, but since range is 0 to ∞ we use sine/cosine transforms defined by

$$g(k)=2\int_0^{\infty}dx\,f(x)\left\{\begin{array}{l}\sin(xk)\\ \cos(xk)\end{array}\right. \qquad f(x)=\frac{1}{\pi}\int_0^{\infty}dk\,g(k)\left\{\begin{array}{l}\sin(xk)\\ \cos(xk)\end{array}\right.$$

   This leads to

$$B(t)-k^2g(k,t)=\frac{1}{D}\frac{\partial g(k,t)}{\partial t}$$

   where the boundary term is $B(t)=ku(0,t)$ for the sine transform and $B(t)=-\partial u(0,t)/\partial x$ for the cosine transform. We thus choose whichever transform suits the given b.c. then integrate to find $g(k,t)$ and invert; details are left to tutorial.

2. Use Laplace transform wrt t:

$$F(x,s)=\int_0^{\infty}dtu(x,t)e^{-st} \qquad \text{and recall} \qquad \int_0^{\infty}dt\left(\frac{\partial u(x,t)}{\partial t}\right)e^{-st}=u(x,0)+sF(x,s)$$

As an example of the Laplace transform approach consider the heat conduction problem on the semi-infinite rod where the temperature T is initially 0 for $x > 0$ and the boundary ($x = 0$) is kept at constant temperature T_0 then

$$\frac{\partial^2 T}{\partial x^2} - \frac{1}{D}\frac{\partial T}{\partial t} = 0 \qquad T(x,0) = 0 \quad T(0,t) = T_0$$

Taking the Laplace transform yields

$$\frac{\partial^2 F(x,s)}{\partial x^2} - \frac{sF(x,s)}{D} = 0 \qquad \text{and} \quad F(0,s) = \frac{T_0}{s}$$

$$\Rightarrow F(x,s) = \frac{T_0}{s} \exp\left(-\sqrt{s/D}\; x\right)$$

where we have discarded the solution $\exp\left(+\sqrt{s/D}\; x\right)$ since it is not bounded as $x \to \infty$. The easiest way to invert the Laplace transform is to look up tables and note that

$$L\left[\operatorname{erfc}\left(\frac{a}{2\sqrt{t}}\right)\right] = \frac{\exp(-a\sqrt{s})}{s} \qquad \Rightarrow \quad T(x,t) = T_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{D\,t}}\right)$$

$$\text{where} \quad \operatorname{erfc}(z) = 1 - \operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty du \, \exp(-u^2)$$

$$\text{for small } z \qquad \operatorname{erfc}(z) \sim 1 - \frac{2}{\sqrt{\pi}}\left(z - \frac{z^3}{3} + \frac{z^5}{5} - \cdots\right)$$

$$\text{for large } z \qquad \operatorname{erfc}(z) \sim \frac{e^{-z^2}}{\sqrt{\pi}}\left(\frac{1}{z} - \frac{1}{2z^2} + \cdots\right)$$

You should make a sketch of $\operatorname{erfc}(z)$.

One can invert the LT by the inversion integral but it is a bit nasty to dig out the erfc (see tutorial). However, as usual, the integration contour allows easy evaluation of the large t behaviour as we now show.

We note that $F(x,s)$ has a branch point at $s = 0$ and we take the branch cut along the negative real axis. Then, when we close the contour to the left we introduce a 'loop integral' or 'Hankel type contour' C around the branch cut and our inversion is given (see section 12) by

$$T(x,t) = \frac{T_0}{2\pi i} \int_C \frac{ds}{s} \exp\left(-\sqrt{s/D}\; x\right) e^{st}$$

The large t behaviour is given by the singularity furthest to the right (i.e. $s = 0$) so we expand

$$\frac{T_0}{s} \exp\left(-\sqrt{s/D}\; x\right) = \frac{T_0}{s} - \frac{T_0}{\sqrt{D}} \frac{x}{s^{1/2}} + \cdots$$

and recalling (see section 12) $\displaystyle \frac{1}{2\pi i}\int_C ds\, s^{-\nu} e^{st} = \frac{t^{\nu-1}}{\Gamma(\nu)}$ and $\Gamma(1/2) = \sqrt{\pi}$ we obtain

$$T(x,t) = T_0\left[1 - \frac{x}{\sqrt{\pi D}\, t^{1/2}} + \cdots\right]$$