# Mathematics 24: Partial Differential Equations

In this section we will review the solving of a particular class of partial differential equations involving both space and time. The generic problem is:

$$\frac{\partial z}{\partial t}(x,t) = f\left(x, \frac{\partial}{\partial x}\right) z(x,t) \tag{$*$}$$

combined with the initial conditions that $z(x, t=0)$ is known.

To tackle this problem we need to discretise both space and time. We discretise *time* first with:

$$z_j(x) = z(x, j\Delta t)$$

on a grid, $t_j = j\Delta t$. We have a variety of ways to find an approximate solution, in analogy with ordinary differential equations ('Maths20'). The simplest is the Euler method:

$$z_{j+1}(x) = z_j(x) + \Delta t f\left(x, \frac{\partial}{\partial x}\right) z_j(x)$$

and then one can consider multi-step methods and Runge-Kutta methods. Due to the simplicity of the current *linear* equation, however, it is often best to employ an *implicit* method:

$$z_{j+1}(x) = z_j(x) + \frac{\Delta t}{2}\left[f\left(x, \frac{\partial}{\partial x}\right) z_j(x) + f\left(x, \frac{\partial}{\partial x}\right) z_{j+1}(x)\right]$$

which is accurate to order $(\Delta t)^2$, one better than the Euler method at order $\Delta t$. The real reason for using this implicit method, however, is numerical *stability* as we will soon see.

The next task is to discretise the space and then to find an approximation for the spatial derivatives. We use:

$$z_{i,j} = z_j(i\Delta x) = z(i\Delta x, j\Delta t)$$

and then look for a *linear* approximation:

$$\Delta t f\left(x, \frac{\partial}{\partial x}\right) z_{i,j} \sim \sum_l a_l z_{i+l,j}$$

where a collection of derivatives is approximated by a carefully weighted sum of the function at nearby grid points. We choose the $a_l$ to obtain agreement with Taylor's theorem to as high an order 'as possible'.

A general expansion around the point $x$ yields:

$$\sum_m a_m z(x + m\Delta x) = \sum_{l=0}^{\infty} \frac{(\Delta x)^l}{l!}\left[\frac{\partial}{\partial x}\right]^l z(x) \sum_m a_m m^l$$

from which the 'general' expression:

$$\Delta t f\left(x, \frac{\partial}{\partial x}\right) z(x) = \Delta t \sum_{l=0}^{\infty} f_l(x) \left[\frac{\partial}{\partial x}\right]^l z(x)$$

can be recovered by solving:

$$\frac{(\Delta x)^l}{l!} \sum_m a_m m^l = \Delta t f_l(x)$$

for the coefficients $a_m$.

In order to make these ideas concrete, we look initially at the *diffusion equation*:

$$\frac{\partial z}{\partial t} = \frac{\partial^2 z}{\partial x^2}$$

and then we need to solve:

$$\begin{aligned}\sum_m a_m m^l &= 0 \qquad\qquad for \quad l \neq 2 \\ &= 2\frac{\Delta t}{(\Delta x)^2} \equiv 2r \quad for \quad l = 2\end{aligned}$$

By using more and more neighbouring points, we can force more and more derivatives to vanish. This yields a sequence of approximations order by order. The first approximation is:
$a_0^{(1)} = -2r; \quad a_1^{(1)} = a_{-1}^{(1)} = r;$ $\qquad a_n = 0$ other $n$'s

the second approximation is:
$a_0^{(2)} = -\frac{5}{2}r; \quad a_1^{(2)} = a_{-1}^{(2)} = \frac{4}{3}r; \quad a_2^{(2)} = a_{-2}^{(2)} = -\frac{1}{12}r;$ $\qquad a_n = 0$ other $n$'s

the third approximation is:
$a_0^{(3)} = -\frac{49}{18}r; \; a_1^{(3)} = a_{-1}^{(3)} = \frac{3}{2}r; \quad a_2^{(3)} = a_{-2}^{(3)} = -\frac{3}{20}r; \; a_3^{(3)} = a_{-3}^{(3)} = \frac{1}{90}; \quad a_n = 0$ other $n$'s

and so on...

If we apply these ideas to Euler's method for the diffusion equation, then this sequence of approximations is progressively more accurate spatially, but there is a price to pay: These approximations have *limited stability* and become progressively *less* stable. To see this we need to pay careful attention to our proposed algorithm:

$$z_{i,j+1} = z_{i,j} + \sum_m a_m z_{i+m,j}$$

The *signs* of these coefficients *oscillate*, and so the contributions add up *maximally* when $z_{i,j} = (-1)^i A_j$. Such a solution is an *eigenstate* for our operator and we find:

$$z_{i,j+1} = (-1)^i \left[1 - \sum_m \mid a_m \mid\right] A_j$$

and so this solution grows exponentially oscillatingly whenever:

$$\sum_m \mid a_m \mid > 2$$

this occurs at a critical value of $r$, $r_c^{(n)}$ say. For the previously developed approximations, this instability occurs when $r > r_c^{(n)}$ with:

$$r_c^{(1)} = \frac{1}{2} \qquad r_c^{(2)} = \frac{3}{8} \qquad r_c^{(3)} = \frac{45}{136}$$

becoming sequentially worse. This restriction therefore requires that:

$$\Delta t < r_c(\Delta x)^2$$

and one requires immensely small time steps for moderate spatial accuracy.

This stability problem is 'solved' by the application of the previously explained *implicit* algorithm. For this new idea we require to solve:

$$z_{i,j+1} = z_{i,j} + \frac{1}{2}\left[\sum_m a_m z_{i+m,j} + \sum_m a_m z_{i+m,j+1}\right]$$

which, if we think of the $i$ label as a 'vector' label and the coefficients $a_m$ as a matrix, $a_{i,i'} = a_{i-i'}$, may be rewritten:

$$(2-a)z_{j+1} = (2+a)z_j$$

which is trivially solved by a matrix inversion to yield:

$$z_{j+1} = Tz_j \equiv (2-a)^{-1}(2+a)z_j$$

The analogue to the stability problem of the Euler method now reveals that:

$$z_{i,j+1} = (-1)^i \frac{2 - \sum_m \mid a_m \mid}{2 + \sum_m \mid a_m \mid} A_j = (-1)^i \frac{r_c - r}{r_c + r} A_j$$

which does not become unstable for any value of $r$.

Our final task is to consider the radial diffusion equation in $d$-dimensions. This problem is simply:

$$\frac{\partial z}{\partial t}(x,t) = \frac{\partial^2 z}{\partial x^2}(x,t) + \frac{d-1}{x}\frac{\partial z}{\partial x}(x,t)$$

where now $x > 0$ is a radial coordinate. Since our procedure for creating our algorithm is *linear*, we may safely restrict attention to finding a sequence of approximations for the first derivative and then adding this to the previous result. This problem amounts to solving:

$$\begin{aligned} \sum_m b_m m^l &= 0 \qquad \textit{for} \quad l \neq 1 \\ &= \frac{\Delta t}{\Delta x} \equiv s \qquad \textit{for} \quad l = 1 \end{aligned}$$

The first few solutions are:
$b_1^{(1)} = -b_{-1}^{(1)} = \frac{1}{2}s;$ $\qquad b_n = 0$ other $n$'s

for the first approximation:
$b_1^{(2)} = -b_{-1}^{(2)} = \frac{2}{3}s;\quad b_2^{(2)} = -b_{-2}^{(2)} = -\frac{1}{12}s;$ $\qquad b_n = 0$ other $n$'s

for the second approximation and:
$b_1^{(3)} = -b_{-1}^{(3)} = \frac{3}{4}s;\quad b_2^{(2)} = -b_{-2}^{(2)} = -\frac{3}{20}s;\quad b_3^{(3)} = -b_3^{(3)} = \frac{1}{60}s;$ $\qquad b_n = 0$ other $n$'s

for the third approximation.

The linearised approximation for the spatial problem is therefore:

$$\Delta t \frac{\partial^2 z}{\partial x^2}(x,t) + \Delta t \frac{d-1}{x}\frac{\partial z}{\partial x}(x,t) \mapsto \sum_m \left( a_m + b_m \frac{d-1}{x_i} \right) z_{i+m,j}$$

We also need to understand the permissible *boundary conditions.* In order to understand these, it is useful to rewrite the diffusion equation as:

$$\frac{\partial z}{\partial t} = x^{1-d}\frac{\partial}{\partial x}\left[ x^{d-1}\frac{\partial z}{\partial x}\right]$$

and then with a corresponding 'measure':

$$M(f) = S(d)\int_{x_1}^{x_2} dx x^{d-1} f(x)$$

where $S(d) = 2\pi^{d/2}\left[\Gamma(d/2)\right]^{-1}$ and $n! = \Gamma(n+1)$ is the usual definition, we find a description of a 'particle' number:

$$N(x_1, x_2; t) = S(d)\int_{x_1}^{x_2} dx x^{d-1} z(x,t)$$

for the number of particles in the interval $x \in (x_1, x_2)$. There is a corresponding 'flux' of particles through the 'point' $x$:

$$\phi(x) = S(d) x^{d-1}\frac{\partial z}{\partial x}$$

and a conservation law:

$$\frac{\partial N}{\partial t}(x_1, x_2; t) = \frac{\partial}{\partial t} S(d)\int_{x_1}^{x_2} dx x^{d-1} z(x,t) = \left[ S(d) x^{d-1}\frac{\partial z}{\partial x}\right]_{x_1}^{x_2} = \phi(x_2) - \phi(x_1)$$

and the number of particles in a region is altered by incoming and outgoing fluxes.

*Reflecting* boundary condition involve a *vanishing* flux and hence the boundary condition is:

$$\frac{\partial z}{\partial x}(x^*, t) = 0$$

or equivalently, and more useful numerically, symmetry at the point $x^*$:

$$z(x^* + x, t) = z(x^* - x, t)$$

A second plausible boundary condition involves a vanishing particle density:

$$z(x^*, t) = 0$$

or equivalently, and more useful numerically, anti-symmetry at the point $x^*$:

$$z(x^* + x, t) = -z(x^* - x, t)$$

Note that for this boundary condition there is a flux 'across' the point $x^*$ which acts as a *source* or *sink* for particles.

Due to the fact that the 'volume' associated with the limit $x \mapsto 0$ vanishes faster than $x$ in other than one dimension, the boundary condition at the origin is *subtle*. In *real* diffusion there is an *underlying* velocity of the particles which is indirectly related to the diffusive properties. A surface which permits particles to pass in only one direction reacts to this underlying velocity. If this velocity is independent of density, then we would expect such a surface to extract a particle number proportional to the density. If we had such a surface at 'radius' $x^*$, then we would expect a boundary condition of the form:

$$S(d)\,[x^*]^{d-1}\,\frac{\partial z}{\partial x}(x^*, t) = \alpha z(x^*, t)$$

in terms of a parameter $\alpha$, which when increased extracts a higher number of particles, since:

$$\frac{\partial N}{\partial t}(x^*, \infty; t) = \phi(\infty) - \phi(x^*) = -\alpha z(x^*, t)$$

and hence:

$$N(x^*, \infty; t) = N_0(x^*, \infty) - \alpha \int_0^t dt' z(x^*, t')$$

Note that this analysis becomes *singular* as $x^* \mapsto 0$, as previously suggested, leading to doubts over the previous suggestion of anti-symmetric boundary conditions at $x = 0$.

Finally, the point $x = 0$ is one of the boundaries of the system, and we need to consider the equation:

$$\frac{\partial z}{\partial t} = \frac{\partial^2 z}{\partial x^2} + \frac{d-1}{x}\frac{\partial z}{\partial x}$$

in the limit that $x \mapsto 0$. For vanishing particle density there is a sink for particles, so this equation is *not* valid. For reflecting boundary conditions, we have $\frac{\partial z}{\partial x} \mapsto 0$ as $x \mapsto 0$, and so:

$$\frac{\partial z}{\partial t} \mapsto d\frac{\partial^2 z}{\partial x^2}\,|_{x=0}$$

completing the description.