Chapter 2

Poisson's Equation

2.1 Physical Origins

Poisson's equation,

$$\boxed{\nabla^2\Phi = \sigma(\mathbf{x}),}$$

arises in many varied physical situations. Here $\sigma(\mathbf{x})$ is the "source term", and is often zero, either everywhere or everywhere bar some specific region (maybe only specific points). In this case, Laplace's equation,

$$\boxed{\nabla^2\Phi = 0,}$$

results.

The Diffusion Equation

Consider some quantity $\Phi(\mathbf{x})$ which diffuses. (This might be say the concentration of some (dilute) chemical solute, as a function of position $\mathbf{x}$, or the temperature T in some heat conducting medium, which behaves in an entirely analogous way.) There is a corresponding *flux*, $\mathbf{F}$, of Φ – that is, the amount crossing an (imaginary) unit area per unit time. Experimentally, it is known that, in the case of a solute, the flux is given by $\mathbf{F} = -k\nabla\Phi$ where k is the *diffusivity*; in the case of temperature, the flux *of heat* is given by $\mathbf{F} = -k\nabla T$ where k is the *coefficient of heat conductivity*. (Note that the minus sign occurs because the flux is directed towards regions of lower concentration.)

The governing equation for this diffusion process is

$$\frac{\partial\Phi}{\partial t} = k\nabla^2\Phi$$

where k is referred to, generically, as the diffusion constant. If we are interested in the *steady-state* distribution of solute or of temperature, then $\partial\Phi/\partial t = 0$ and Laplace's equation, $\nabla^2\Phi = 0$, follows.

When there are *sources* $S(\mathbf{x})$ of solute (for example, where solute is piped in or where the solute is generated by a chemical reaction), or of heat (e.g., an exothermic reaction), the steady-state diffusion is governed by Poisson's equation in the form

$$\boxed{\nabla^2\Phi = -\frac{S(\mathbf{x})}{k}.}$$

The diffusion equation for a solute can be derived as follows. Let $\Phi(\mathbf{x})$ be the concentration of solute at the point $\mathbf{x}$, and $\mathbf{F}(\mathbf{x}) = -k\nabla\Phi$ be the corresponding flux. (We assume here that there is no advection of Φ by the underlying medium.)

Let V be a fixed volume of space enclosed by an (imaginary) surface S. In a small time δt, the quantity of solute leaving V is given by

$$\iint_S \mathbf{F}\delta t \,.\, \mathbf{n}\,\mathrm{d}S.$$

Hence

$$\Big[\iiint_V \Phi\,\mathrm{d}V\Big]_t^{t+\delta t} = -\iint_S \mathbf{F}\,.\,\mathbf{n}\,\mathrm{d}S\,\delta t.$$

Dividing by δt and taking the limit as $\delta t \to 0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}\iiint_V \Phi\,\mathrm{d}V = -\iint_S \mathbf{F}\,.\,\mathbf{n}\,\mathrm{d}S = \iint_S k\nabla\Phi\,.\,\mathbf{n}\,\mathrm{d}S,$$

and hence by the Divergence Theorem,

$$\iiint_V \frac{\partial\Phi}{\partial t}\,\mathrm{d}V = \iiint_V \nabla\,.\,(k\nabla\Phi)\,\mathrm{d}V.$$

As this is true for *any* fixed volume V, we must have

$$\frac{\partial\Phi}{\partial t} = \nabla\,.\,(k\nabla\Phi)$$

everywhere. Assuming that k is constant, we obtain the *diffusion equation*

$$\frac{\partial\Phi}{\partial t} = k\nabla^2\Phi.$$

If there are also *sources* (or *sinks*) of solute, then an additional source term results:

$$\frac{\partial \Phi}{\partial t} = k\nabla^2\Phi + S(\mathbf{x})$$

where $S(\mathbf{x})$ is the quantity of solute (per unit volume and time) being added to the solution at the location $\mathbf{x}$. Poisson's equation for steady-state diffusion with sources, as given above, follows immediately.

The *heat diffusion equation* is derived similarly. Let $T(\mathbf{x})$ be the temperature field in some substance (not necessarily a solid), and $H(\mathbf{x})$ the corresponding heat field. We have the relation $H = \rho c T$ where ρ is the density of the material and c its specific heat. The corresponding heat flux is $-k\nabla T$. A similar argument to the above applies again, resulting in

$$\frac{\partial H}{\partial t} = k\nabla^2 T + S(\mathbf{x})$$

where S represents possible sources of heat. Hence

$$\frac{\partial T}{\partial t} = \kappa\nabla^2 T + (\rho c)^{-1} S(\mathbf{x})$$

where $\kappa = k/\rho c$ is the *coefficient of thermal diffusivity*. The equation for steady-state heat diffusion with sources is as before.

Electrostatics

The laws of electrostatics are

$$\nabla \,.\, \mathbf{E} = \rho/\epsilon_0 \qquad\qquad \nabla \times \mathbf{E} = \mathbf{0}$$

$$\nabla \,.\, \mathbf{B} = 0 \qquad\qquad \nabla \times \mathbf{B} = \mu_0 \mathbf{J}$$

where ρ and $\mathbf{J}$ are the electric charge and current fields respectively. Since $\nabla \times \mathbf{E} = \mathbf{0}$, there is an electric potential Φ such that $\mathbf{E} = -\nabla\Phi$; hence $\nabla \,.\, \mathbf{E} = \rho/\epsilon_0$ gives Poisson's equation

$$\boxed{\nabla^2\Phi = -\rho/\epsilon_0.}$$

In a region where there are no charges or currents, ρ and $\mathbf{J}$ vanish. Hence we obtain Laplace's equation

$$\nabla^2\Phi = 0.$$

Also $\nabla \times \mathbf{B} = \mathbf{0}$ so there exists a magnetostatic potential ψ such that $\mathbf{B} = -\mu_0\nabla\psi$; and $\nabla^2\psi = 0$.

Gravitation

Consider a mass distribution with density $\rho(\mathbf{x})$. There is a corresponding gravitational field $\mathbf{F}(\mathbf{x})$ which we may express in terms of a gravitational potential $\Phi(\mathbf{x})$. Consider an arbitrary fixed volume V with surface S containing a total mass $M_V = \iiint_V \rho(\mathbf{x})\,\mathrm{d}V$.

Gauss showed that the flux of the gravitational field through S is equal to $-4\pi GM_V$. Hence

$$\iint_S \mathbf{F} \,.\, \mathbf{n}\, \mathrm{d}S = -4\pi G M_V$$

$$\implies \quad -\iint_S \nabla\Phi \,.\, \mathbf{n}\, \mathrm{d}S = -4\pi G \iiint_V \rho(\mathbf{x})\, \mathrm{d}V$$

$$\implies \quad \iiint_V \nabla \,.\, (\nabla\Phi)\, \mathrm{d}V = 4\pi G \iiint_V \rho(\mathbf{x})\, \mathrm{d}V.$$

This is true for all volumes V, so we must have

$$\boxed{\nabla^2\Phi = \nabla \,.\, (\nabla\Phi) = 4\pi G\rho.}$$

Other applications

These include the motion of an inviscid fluid; Schrödinger's equation in Quantum Mechanics; and the motion of biological organisms in a solution.

2.2 Separation of Variables for Laplace's Equation

Plane Polar Coordinates

We shall solve Laplace's equation $\nabla^2\Phi = 0$ in plane polar coordinates (r, θ) where the equation becomes

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} = 0. \tag{1}$$

Consider solutions of the form $\Phi(r, \theta) = R(r)\Theta(\theta)$ where each function R, Θ is a function of one variable only. Then

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) = \frac{\Theta(\theta)}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right)$$

and

$$\frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} = \frac{R(r)}{r^2}\frac{\mathrm{d}^2\Theta}{\mathrm{d}\theta^2}.$$

Hence after rearrangement,

$$\frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) = -\frac{\Theta''}{\Theta}. \tag{2}$$

The LHS is a function of r only, and the RHS of θ only; hence both must be constant, λ say. Then

$$\Theta'' = -\lambda\Theta$$

$$\Longrightarrow \qquad \Theta = \begin{cases} A + B\theta & \lambda = 0 \\ A\cos\sqrt{\lambda}\,\theta + B\sin\sqrt{\lambda}\,\theta & \lambda \neq 0 \end{cases}$$

To obtain a sensible physical solution, replacing θ by $\theta + 2\pi$ should give the same value of $\nabla\Phi$ (see later). This is true only if $\Theta'(\theta + 2\pi) = \Theta'(\theta)\ \forall\,\theta$; i.e., either $\lambda = 0$ or

$$\cos 2\pi\sqrt{\lambda} = 1 \quad \text{and} \quad \sin 2\pi\sqrt{\lambda} = 0$$

which implies $2\pi\sqrt{\lambda} = 2n\pi$ for some integer n. (Note that the possibility that $\lambda < 0$ is ruled out at this stage.) Hence

$$\Theta = \begin{cases} A + B\theta & n = 0 \\ A\cos n\theta + B\sin n\theta & n \neq 0 \end{cases}$$

Returning to (2),

$$\frac{r}{R}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) = \lambda = n^2$$

$$\Longrightarrow \qquad r^2R'' + rR' - n^2R = 0.$$

It is easily shown (either by direct verification or by making the substitution $u = \ln r$) that the solutions of this equation are

$$R = \begin{cases} C + D\ln r & n = 0 \\ Cr^n + Dr^{-n} & n \neq 0 \end{cases}$$

Hence, we obtain possible solutions to (1) as

$$\Phi = R\Theta = \begin{cases} (C + D\ln r)(A + B\theta) & n = 0 \\ (Cr^n + Dr^{-n})(A\cos n\theta + B\sin n\theta) & n \neq 0 \end{cases}$$

We note that the combination $\theta\ln r$ does not satisfy the requirement above for 2π-periodicity of $\nabla\Phi$, and so we exclude it. Equation (1) is linear and so we may form a superposition of the above solutions; in fact the general solution is an arbitrary linear combination of *all* the possible solutions obtained above, that is

$$\boxed{\Phi = A_0 + B_0\theta + C_0\ln r + \sum_{n=1}^{\infty}(A_nr^n + C_nr^{-n})\cos n\theta + \sum_{n=1}^{\infty}(B_nr^n + D_nr^{-n})\sin n\theta}$$

where we have relabelled all the arbitrary constants, e.g., AC has become A_n and BD has become D_n. We can make this expression more compact by defining $A_{-n} = C_n$ and $B_{-n} = D_n$ for $n > 0$; then

$$\Phi = A_0 + B_0\theta + C_0 \ln r + \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} r^n (A_n \cos n\theta + B_n \sin n\theta).$$

Although this is more compact, the first expression is often easier to use.

Notes:

(i) Why did we require that $\nabla\Phi$, rather than Φ itself, be periodic? In many cases (e.g. temperature, diffusion), Φ must clearly be periodic and so we shall further need $B_0 = 0$. But in other cases (e.g. electrostatics, gravitation), Φ is not itself a physical quantity, only a potential; it is $\nabla\Phi$ which has a physical significance (e.g., the force). For example, consider the magnetostatic potential around a wire carrying a current I; here $\psi = -(I/2\pi)\theta$, which is multi-valued, but $\mathbf{B} = -\mu_0\nabla\psi$ (the quantity of physical interest) is of magnitude $\mu_0 I/2\pi r$ and is single valued.

(ii) A common mistake made during separation of variables is to retain too many arbitrary constants; e.g. to write

$$\sum C_n r^n (A_n \cos n\theta + B_n \sin n\theta).$$

For each n, this looks like 3 arbitrary constants (A_n, B_n, C_n); but of course there are really only two arbitrary quantities ($C_n A_n$ and $C_n B_n$, which we have relabelled as A_n and B_n above).

(iii) The above derivation also applies to 3D cylindrical polar coordinates in the case when Φ is independent of z.

Spherical Polar Coordinates: Axisymmetric Case

In spherical polars (r, θ, ϕ), in the case when we know Φ to be axisymmetric (i.e., independent of ϕ, so that $\partial\Phi/\partial\phi = 0$), Laplace's equation becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\Phi}{\partial\theta}\right) = 0.$$

Seek solutions of the form $\Phi(r,\theta) = R(r)\Theta(\theta)$. Then

$$\frac{1}{R}(r^2R')' = -\frac{1}{\Theta\sin\theta}(\Theta'\sin\theta)' \qquad (3)$$

and both sides must be constant, λ say. So

$$(\Theta' \sin\theta)' = -\lambda\Theta \sin\theta.$$

Let $\zeta = \cos\theta$, and use the chain rule to replace $\mathrm{d}/\mathrm{d}\theta$ by $\mathrm{d}/\mathrm{d}\zeta$:

$$\frac{\mathrm{d}}{\mathrm{d}\theta} = \frac{\mathrm{d}\zeta}{\mathrm{d}\theta}\frac{\mathrm{d}}{\mathrm{d}\zeta} = -\sin\theta\,\frac{\mathrm{d}}{\mathrm{d}\zeta}.$$

So

$$-\sin\theta\,\frac{\mathrm{d}}{\mathrm{d}\zeta}\left(-\sin^2\theta\,\frac{\mathrm{d}\Theta}{\mathrm{d}\zeta}\right) = -\lambda\Theta\sin\theta$$

$$\Longrightarrow \qquad \frac{\mathrm{d}}{\mathrm{d}\zeta}\left((1-\zeta^2)\frac{\mathrm{d}\Theta}{\mathrm{d}\zeta}\right) + \lambda\Theta = 0.$$

This is Legendre's equation; for well-behaved solutions at $\zeta = \pm 1$ (i.e., $\theta = 0, \pi$) we need $\lambda = n(n+1)$ for some non-negative integer n, in which case

$$\Theta = CP_n(\zeta) = CP_n(\cos\theta)$$

where C is an arbitrary constant.

Returning to (3),

$$(r^2R')' = \lambda R$$

$$\Longrightarrow \qquad r^2R'' + 2rR' - n(n+1)R = 0,$$

to which the solution is

$$R = Ar^n + Br^{-n-1}.$$

The general solution to Laplace's equation in the axisymmetric case is therefore (absorbing the constant C into A and B)

$$\boxed{\Phi(r,\theta) = \sum_{n=0}^{\infty}(A_n r^n + B_n r^{-n-1})P_n(\cos\theta).}$$

Non-axisymmetric Case [non-examinable]

A similar analysis when Φ may depend on ϕ shows that the general solution is

$$\Phi(r,\theta,\phi) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}(A_{mn}r^n + B_{mn}r^{-n-1})P_n^m(\cos\theta)e^{im\phi}$$

where $P_n^m(\zeta)$ are the associated Legendre functions which satisfy the associated Legendre equation

$$\frac{\mathrm{d}}{\mathrm{d}\zeta}\left((1-\zeta^2)\frac{\mathrm{d}\Theta}{\mathrm{d}\zeta}\right) + \left(n(n+1) + \frac{m}{1-\zeta^2}\right)\Theta = 0$$

when m and n are integers, $n \geq 0$, $-n \leq m \leq n$.

2.3 Uniqueness Theorem for Poisson's Equation

Consider Poisson's equation

$$\nabla^2\Phi = \sigma(\mathbf{x})$$

in a volume V with surface S, subject to so-called *Dirichlet boundary conditions* $\Phi(\mathbf{x}) = f(\mathbf{x})$ on S, where f is a given function defined on the boundary.

From a physical point of view, we have a well-defined problem; say, find the steady-state temperature distribution throughout V, with heat sources given by $\sigma(\mathbf{x})$, subject to a specified temperature distribution on the boundary. No further conditions are required in real life to ensure that there is only one solution. Mathematically, then, can we show that the problem above has a unique solution?

Suppose that there are actually two (or more) solutions $\Phi_1(\mathbf{x})$ and $\Phi_2(\mathbf{x})$. Let $\Psi = \Phi_1 - \Phi_2$. Then

$$\nabla^2\Psi = \nabla^2\Phi_1 - \nabla^2\Phi_2 = \sigma - \sigma = 0 \qquad \text{in } V$$

subject to

$$\Psi = f - f = 0 \qquad \text{on } S.$$

One solution of this problem for Ψ is clearly $\Psi = 0$; is it unique? Consider

$$\begin{aligned}\nabla \cdot (\Psi\nabla\Psi) &= \nabla\Psi \cdot \nabla\Psi + \Psi\nabla \cdot (\nabla\Psi) \\ &= |\nabla\Psi|^2 + \Psi\nabla^2\Psi \\ &= |\nabla\Psi|^2.\end{aligned}$$

Hence

$$\begin{aligned}\iiint_V |\nabla\Psi|^2 \,\mathrm{d}V &= \iiint_V \nabla \cdot (\Psi\nabla\Psi)\,\mathrm{d}V \\ &= \iint_S \Psi\nabla\Psi \cdot \mathbf{n}\,\mathrm{d}S \\ &= 0\end{aligned}$$

because $\Psi = 0$ on S. But $|\nabla\Psi|^2 \geq 0$ everywhere; its integral can only be zero if $|\nabla\Psi|$ is zero everywhere, i.e., $\nabla\Psi \equiv \mathbf{0}$, which implies that Ψ is constant throughout V. But $\Psi = 0$ on S, so $\Psi \equiv 0$ throughout V. Thus $\Phi_1 = \Phi_2$, which demonstrates that our problem has a unique solution, as expected.

A similar theorem holds when instead of Dirichlet boundary conditions we have *Neumann* boundary conditions: that is to say instead of Φ being specified (by the function

f) on the boundary S, $\partial\Phi/\partial n$ is specified on S, where we use the notation

$$\boxed{\frac{\partial \Phi}{\partial n} \equiv \mathbf{n} \,.\, \nabla\Phi.}$$

2.4 Minimum and Maximum Properties of Laplace's Equation

Suppose that Φ satisfies $\nabla^2\Phi = 0$ in a volume V with surface S. Then both the minimum and maximum values of Φ occur somewhere on S (and possibly *also* somewhere inside V).

Why is this? Suppose Φ has a local maximum somewhere in the interior of V. At that point we must have $\partial\Phi/\partial x = \partial\Phi/\partial y = \partial\Phi/\partial z = 0$ (stationary point); and as it is a maximum, $\partial^2\Phi/\partial x^2 < 0$, $\partial^2\Phi/\partial y^2 < 0$, $\partial^2\Phi/\partial z^2 < 0$. But this cannot happen since $0 = \nabla^2\Phi = \partial^2\Phi/\partial x^2 + \partial^2\Phi/\partial y^2 + \partial^2\Phi/\partial z^2$.

The same applies to minima.

This is not a formal proof since it is actually possible for a maximum to have

$$\frac{\partial^2\Phi}{\partial x^2} = \frac{\partial^2\Phi}{\partial y^2} = \frac{\partial^2\Phi}{\partial z^2} = 0,$$

a case we haven't considered: compare with the possibility in 1D that a maximum could have $\mathrm{d}^2y/\mathrm{d}x^2 = 0$. However, the theorem can still be shown to hold.

Example: in the worked example of the steady-state temperature distribution in a cylinder, we can deduce that $|T| \leq T_0$ in $r < a$.

2.5 Green's Function

The Delta Function in 3D

In 1D, $\delta(x - x_0)$ is a function which is zero everywhere except at $x = x_0$, and is infinite there in such a way that

$$\int_a^b \delta(x - x_0)\,\mathrm{d}x = 1$$

whenever $x_0 \in (a, b)$. As a consequence, $\int_a^b f(x)\delta(x - x_0)\,\mathrm{d}x = f(x_0)$. We extend the definition to 3D via

$$\delta(\mathbf{x} - \mathbf{x}_0) = \delta(x - x_0)\delta(y - y_0)\delta(z - z_0)$$

where $\mathbf{x}_0 = (x_0, y_0, z_0)$. Then

$$\boxed{\iiint_V f(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}_0)\,\mathrm{d}V = f(\mathbf{x}_0)}$$

whenever $\mathbf{x}_0 \in V$ (and the integral is 0 otherwise).

Green's Function

Suppose that we wish to solve Poisson's equation in a volume V with surface S on which Dirichlet boundary conditions are imposed. The *Green's function* $G(\mathbf{x};\mathbf{x}_0)$ associated with this problem is a function of two variables: $\mathbf{x}$, the position vector, and $\mathbf{x}_0$, a fixed location. It is defined as the solution to

$$\boxed{\begin{aligned} \nabla^2 G(\mathbf{x};\mathbf{x}_0) &= \delta(\mathbf{x}-\mathbf{x}_0) \qquad && \text{in } V, \\ G &= 0 && \text{on } S. \end{aligned}}$$

(Physically, we can think of G as the "potential" from a point source at $\mathbf{x}_0$ with the boundary held at zero potential.)

It is possible to prove that G is symmetric, i.e., $G(\mathbf{x};\mathbf{x}_0) = G(\mathbf{x}_0;\mathbf{x})$. This can be useful as a check that G has been correctly calculated. Physically, this corresponds to the remarkable fact that the potential at $\mathbf{x}$ due to a source at $\mathbf{x}_0$ is the same as the potential at $\mathbf{x}_0$ due to a source at $\mathbf{x}$, regardless of the shape of S.

When V is all space (i.e., the limit of a sphere whose radius tends to ∞), Green's function is known as the *fundamental solution*.

For a problem with Neumann boundary conditions, $G(\mathbf{x};\mathbf{x}_0)$ is defined to satisfy $\partial G/\partial n = 1/A$ on S, where $A = \iint_S \mathrm{d}S$ is the surface area of S, rather than $G = 0$ there. In many cases S is infinitely large, in which case the boundary condition reduces to $\partial G/\partial n = 0$.

The Fundamental Solution in 3D

Consider first $\mathbf{x}_0 = \mathbf{0}$. Then $\nabla^2 G = \delta(\mathbf{x})$ and $G \to 0$ as $|\mathbf{x}| \to \infty$. The problem is spherically symmetric about the origin, so we expect G to be a function of r alone. Try

$G = g(r)$. By the definition of $\delta(\mathbf{x})$, if V_R is the sphere of radius R with surface S_R,

$$1 = \iiint_{V_R} \delta(\mathbf{x})\,\mathrm{d}V \;= \iiint_{V_R} \nabla \,.\, (\nabla G)\,\mathrm{d}V$$

$$= \iint_{S_R} \nabla G \,.\, \mathbf{n}\,\mathrm{d}S = \iint_{S_R} g'(r)\,\mathrm{d}S$$

($\mathbf{n}$ is just the unit radial vector)

$$= g'(R) \iint_{S_R} \mathrm{d}S \quad = 4\pi R^2 g'(R)$$

$$\Longrightarrow \qquad g'(R) = \frac{1}{4\pi R^2} \qquad \text{for all } R$$

$$\Longrightarrow \qquad g'(r) = \frac{1}{4\pi r^2}$$

$$\Longrightarrow \qquad g(r) = -\frac{1}{4\pi r} + A,$$

where A is a constant. As $r \to \infty$, $G \to 0$, so $A = 0$. Hence the solution is $-1/4\pi|\mathbf{x}|$.

Shifting the origin to a non-zero $\mathbf{x}_0$, we see that in general the fundamental solution in 3D is

$$\boxed{G(\mathbf{x};\mathbf{x}_0) = -\frac{1}{4\pi|\mathbf{x}-\mathbf{x}_0|}.}$$

Example: an electron located at $\mathbf{x}_0$ is an electrostatic point source, so the charge distribution in space is $\rho(\mathbf{x}) = -e\,\delta(\mathbf{x}-\mathbf{x}_0)$. Hence the electrostatic potential obeys

$$\nabla^2\Phi = (e/\epsilon_0)\,\delta(\mathbf{x}-\mathbf{x}_0)$$

using a result from §2.1. The solution Φ is therefore just a factor e/ϵ_0 times the fundamental solution, i.e., $-e/4\pi\epsilon_0|\mathbf{x}-\mathbf{x}_0|$. This is the standard formula for the potential due to an electron.

The Fundamental Solution in 2D

Again, we solve $\nabla^2 G = \delta(\mathbf{x})$, where the delta-function is now in 2D. We will see that a solution with $G \to 0$ as $|\mathbf{x}| \to \infty$ is impossible; instead we will find a solution such that $|\nabla G| \to 0$.

As before, $G = g(r)$ (where r is now the plane polar radius). Applying the Divergence

Theorem in 2D to a circle of radius R,

$$1 = \iint_{r\le R} \delta(\mathbf{x})\,\mathrm{d}V \;= \iint_{r\le R} \nabla\,.\,(\nabla G)\,\mathrm{d}V$$

$$= \oint_{r=R} \nabla G\,.\,\mathbf{n}\,\mathrm{d}l = \oint_{r=R} g'(r)\,\mathrm{d}l$$

$$= 2\pi R g'(R)$$

$$\Longrightarrow \qquad g'(r) = \frac{1}{2\pi r}$$

$$\Longrightarrow \qquad g(r) = \frac{1}{2\pi}\ln r + \text{constant}.$$

(Note that $g'(r) \to 0$ as $r \to \infty$, but $g(r) \to \infty$, whatever the constant.)

Shifting the origin, we see that the fundamental solution in 2D is

$$\boxed{G(\mathbf{x};\mathbf{x}_0) = \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_0| + \text{constant}.}$$

Example: consider an infinitely long charged wire in three dimensions lying along the z-axis, with a charge density of μ per unit length. What is the electric potential Φ around the wire?

We assume the wire to be mathematically perfect, i.e., of infinitesimal width. Then the electric charge distribution, in 3D, is $\rho = \mu\delta(x)\delta(y)$. (Check that this gives the correct result for the amount of charge in a unit length of the wire.) But it is clear that this problem is fundamentally two-dimensional, with $\rho = \mu\delta(\mathbf{x})$ where $\mathbf{x} = (x, y)$; and the potential satisfies $\nabla^2\Phi = -\mu\delta(\mathbf{x})/\epsilon_0$. Hence the potential is (up to an arbitrary additional constant) just given by an appropriate multiple of the two-dimensional fundamental solution, namely

$$\Phi = -\frac{\mu}{2\pi\epsilon_0}\ln|\mathbf{x}| = -\frac{\mu}{2\pi\epsilon_0}\ln\sqrt{x^2+y^2} = -\frac{\mu}{2\pi\epsilon_0}\ln r$$

where r is the perpendicular distance to the wire (i.e., the "r" of cylindrical polar coordinates rather than of spherical polars).

2.6 The Method of Images

We can use the fundamental solution to find Green's function in some simple geometries, using the "method of images". We shall find *a* function which satisfies the equation and the boundary conditions; by uniqueness, this must be *the* Green's function.

Example: A 3D half-space $x > 0$

Suppose that the domain D is the half-space of $\mathbb{R}^3$ with $x > 0$. The Green's function obeys

$$\begin{aligned} \nabla^2 G &= \delta(\mathbf{x} - \mathbf{x}_0) \qquad && \forall\, \mathbf{x} \in D, \\ G &= 0 && \text{on } x = 0, \\ G &\to 0 && \text{as } |\mathbf{x}| \to \infty,\ \mathbf{x} \in D. \end{aligned}$$

Consider the solution in *all space* for the point source at $\mathbf{x} = \mathbf{x}_0$ together with another (imaginary) source of strength -1 at the "image point" $\mathbf{x} = \mathbf{x}_1$ as shown:

$$\Phi = -\frac{1}{4\pi|\mathbf{x} - \mathbf{x}_0|} - \frac{-1}{4\pi|\mathbf{x} - \mathbf{x}_1|}$$

and

$$\nabla^2 \Phi = \delta(\mathbf{x} - \mathbf{x}_0) - \delta(\mathbf{x} - \mathbf{x}_1)$$

by superposition of the two fundamental solutions. This certainly satisfies the requirement $\nabla^2\Phi = \delta(\mathbf{x} - \mathbf{x}_0)$ for all $\mathbf{x} \in D$, because $\delta(\mathbf{x} - \mathbf{x}_1) \equiv 0\ \forall\, \mathbf{x} \in D$. It also satisfies $\Phi \to 0$ as $|\mathbf{x}| \to \infty$; and on $x = 0$, $|\mathbf{x} - \mathbf{x}_0| = |\mathbf{x} - \mathbf{x}_1|$ so that $\Phi = 0$. Hence by uniqueness,

$$G(\mathbf{x}; \mathbf{x}_0) = \Phi = -\frac{1}{4\pi}\left(\frac{1}{|\mathbf{x} - \mathbf{x}_0|} - \frac{1}{|\mathbf{x} - \mathbf{x}_1|}\right).$$

Example: A 2D quarter-plane $x > 0, y > 0$

In this case, we need to find G such that

$$\nabla^2 G = \delta(\mathbf{x} - \mathbf{x}_0) \qquad \forall\, \mathbf{x} \in D$$

with $G = 0$ on both $x = 0$ and $y = 0$. We find that we need *3* image sources as shown: $\mathbf{x}_1$ and $\mathbf{x}_2$ with strength -1, and $\mathbf{x}_3$ with strength $+1$. Then

$$\begin{aligned} G &= \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_0| - \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_1| - \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_2| + \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_3| + \text{constant} \\ &= \frac{1}{2\pi}\ln\frac{|\mathbf{x}-\mathbf{x}_0|\,|\mathbf{x}-\mathbf{x}_3|}{|\mathbf{x}-\mathbf{x}_1|\,|\mathbf{x}-\mathbf{x}_2|} + \text{constant}. \end{aligned}$$

Clearly $\nabla^2 G = \delta(\mathbf{x}-\mathbf{x}_0)$ in D (all the other delta-functions are zero there); on $x = 0$, $|\mathbf{x}-\mathbf{x}_0| = |\mathbf{x}-\mathbf{x}_1|$ and $|\mathbf{x}-\mathbf{x}_2| = |\mathbf{x}-\mathbf{x}_3|$, so choosing the constant to be zero ensures that $G = 0$; similarly on $y = 0$. By uniqueness, then, this is the required Green's function.

Further extensions to this idea are possible; e.g., planes inclined at 60° to each other, or a pair of parallel planes.

Example: Heat flow from a source in a 3D half-space with a wall at constant temperature

Suppose that the ambient temperature is T_0 and that a wall at $x = 0$ is held at that temperature, with a heat source of strength Q at $\mathbf{x}_0$. Then

$$T = T_0 - \frac{Q}{k}G(\mathbf{x};\mathbf{x}_0),$$

where G is the Green's function for the 3D half-space $x > 0$. (Why? Because we need to solve $\nabla^2 T = -\frac{Q}{k}\delta(\mathbf{x}-\mathbf{x}_0)$ here.)

What is the total heat flux across the wall S? It is

$$\iint_S (-k\nabla T)\,.\,\mathbf{n}\,\mathrm{d}S = k\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial T}{\partial x}\,\mathrm{d}y\,\mathrm{d}z = -Q\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\partial}{\partial x}G(\mathbf{x};\mathbf{x}_0)\bigg|_{x=0}\mathrm{d}y\,\mathrm{d}z$$

which we can evaluate with some effort (see the worked example in the next section for an example of this sort of evaluation).

Alternatively, we can use the Divergence Theorem on the surface consisting of the wall plus the hemisphere at ∞. Since ∇T tends to zero on the hemisphere,

$$\begin{aligned}\iint_S (-k\nabla T)\,.\,\mathbf{n}\,\mathrm{d}S &= -\iiint_V \nabla\,.\,(k\nabla T)\,\mathrm{d}V \\ &= -k\iiint_V \nabla^2 T\,\mathrm{d}V \\ &= -k\iiint_V \left(-\frac{Q}{k}\delta(\mathbf{x}-\mathbf{x}_0)\right)\mathrm{d}V \\ &= Q,\end{aligned}$$

so the total heat radiated across the wall is Q.

Example: A point charge near an earthed boundary plate

Here

$$\Phi = -\frac{e}{\epsilon_0}G(\mathbf{x};\mathbf{x}_0)$$

where G is the Green's function for the 3D half-space $x > 0$.

Now the surface charge density induced on the plate is $\mu = \epsilon_0 E_x$ (standard result from electrostatics, where E_x is the x-component of $\mathbf{E}$). The normal force (per unit area) on the plate, towards the charge, is

$$\tfrac{1}{2}\mu E_x = \tfrac{1}{2}\epsilon_0 E_x^2 = \tfrac{1}{2}\epsilon_0\left(-\frac{\partial\Phi}{\partial x}\right)^2 = \frac{e^2}{2\epsilon_0}\left(\frac{\partial G}{\partial x}\right)^2,$$

and we calculate $\partial G/\partial x$ as in the worked example in the next section. We can integrate this over the whole plate (with considerable effort) to obtain the total force:

$$\frac{e^2}{2\epsilon_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{x_0^2}{4\pi^2\left(x_0^2+(y-y_0)^2+(z-z_0)^2\right)^3}\,\mathrm{d}y\,\mathrm{d}z = \cdots = \frac{e^2}{16\pi\epsilon_0 x_0^2}.$$

The force *on* the charge *from* the plate is equal and opposite, i.e., $e^2/4\pi\epsilon_0(2x_0)^2$ towards the wall. Note that we could also have found this directly by considering the force on the charge due to the image charge, ignoring the plate!

Example: Images in a sphere

What is Green's function for the domain $r < a$ in 3D? We need

$$\begin{aligned}\nabla^2 G &= \delta(\mathbf{x}-\mathbf{x}_0) \qquad &&\text{in } r < a,\\ G &= 0 &&\text{on } r = a.\end{aligned}$$

The image point turns out to be at the *inverse point*

$$\mathbf{x}_1 = \frac{a^2}{|\mathbf{x}_0|^2}\,\mathbf{x}_0$$

(so that $a/|\mathbf{x}_1| = |\mathbf{x}_0|/a$) with strength $-a/|\mathbf{x}_0|$, so Green's function is

$$G(\mathbf{x};\mathbf{x}_0) = \frac{1}{4\pi}\left(-\frac{1}{|\mathbf{x}-\mathbf{x}_0|} + \frac{a/|\mathbf{x}_0|}{|\mathbf{x}-\mathbf{x}_1|}\right).$$

(Check this by first showing that $|\mathbf{x}-\mathbf{x}_1|^2 = (\mathbf{x}-\mathbf{x}_1)\,.\,(\mathbf{x}-\mathbf{x}_1) = (a^2/|\mathbf{x}_0|^2)|\mathbf{x}-\mathbf{x}_0|^2$ when $|\mathbf{x}| = a$.)

Note that the same result holds if we consider the domain $r > a$ instead.

Example: Images in a circle

This is the 2D equivalent of the above. The image point is at $\mathbf{x}_1 = (a^2/|\mathbf{x}_0|^2)\mathbf{x}_0$ as before, but now the strength of the image is just -1, so the Green's function is

$$G(\mathbf{x};\mathbf{x}_0) = \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_0| - \frac{1}{2\pi}\ln|\mathbf{x}-\mathbf{x}_1| + \text{constant}$$

$$= \frac{1}{2\pi}\ln\frac{|\mathbf{x}-\mathbf{x}_0|}{|\mathbf{x}-\mathbf{x}_1|} + \text{constant}.$$

Choosing the constant correctly, we can ensure that $G = 0$ on the circle $r = a$.

2.7 The Integral Solution of Poisson's Equation

The most important application of Green's function is that it can be used to find the solution of Poisson's equation with an arbitrary source distribution.

Green's Identity

For any smooth functions Φ and Ψ, Green's Identity is

$$\boxed{\iiint_V (\Phi\nabla^2\Psi - \Psi\nabla^2\Phi)\,\mathrm{d}V = \iint_S (\Phi\nabla\Psi - \Psi\nabla\Phi)\,.\,\mathbf{n}\,\mathrm{d}S}$$

where V is a volume with surface S. Prove this by applying the Divergence Theorem to the vector field $\mathbf{F} = \Phi\nabla\Psi - \Psi\nabla\Phi$, and using $\nabla \cdot (\Phi\nabla\Psi) = \nabla\Phi \cdot \nabla\Psi + \Phi\nabla^2\Psi$.

The RHS is also written

$$\iint_S \left(\Phi\frac{\partial\Psi}{\partial n} - \Psi\frac{\partial\Phi}{\partial n}\right) \mathrm{d}S.$$

The Integral Solution

Consider the general problem of Poisson's equation with Dirichlet boundary conditions:

$$\nabla^2\Phi = \sigma \qquad \text{in } V,$$

$$\Phi = f \qquad \text{on } S.$$

Apply Green's Identity, taking Ψ to be the Green's function $G(\mathbf{x};\mathbf{x}_0)$ for the problem:

$$\iiint_V (\Phi\nabla^2 G - G\nabla^2\Phi)\,\mathrm{d}V = \iint_S (\Phi\nabla G - G\nabla\Phi)\cdot\mathbf{n}\,\mathrm{d}S$$

$$\delta(\mathbf{x}-\mathbf{x}_0) \quad \sigma \qquad\qquad f \qquad 0$$

$$\implies \qquad \iiint_V \Phi\delta(\mathbf{x}-\mathbf{x}_0)\,\mathrm{d}V = \iiint_V G\sigma\,\mathrm{d}V + \iint_S f\frac{\partial G}{\partial n}\,\mathrm{d}S$$

$$\implies \qquad \boxed{\Phi(\mathbf{x}_0) = \iiint_V \sigma(\mathbf{x})G(\mathbf{x};\mathbf{x}_0)\,\mathrm{d}V + \iint_S f(\mathbf{x})\frac{\partial G}{\partial n}\,\mathrm{d}S.}$$

This is the Integral Solution of Poisson's equation.

Notes:

(i) We can also use the integral solution to solve Laplace's equation with Dirichlet boundary conditions, by taking $\sigma(\mathbf{x}) = 0$.

(ii) A similar result (but with technical differences) can be derived for Neumann boundary conditions, in which case G is defined differently (see §2.5).

(iii) We sometimes wish to take V to be "all space", by taking the limit of a sphere whose radius tends to ∞. In this case we simply use the fundamental solution for G; but (strictly speaking) we need to ensure that the surface integral tends to zero (by requiring, for example, that on the surface of the sphere, $\Phi(\mathbf{x}) \to 0$ sufficiently quickly as the radius increases). Then

$$\Phi(\mathbf{x}_0) = \iiint_{\mathbb{R}^3} \sigma(\mathbf{x})G(\mathbf{x};\mathbf{x}_0)\,\mathrm{d}V.$$

This latter result is easy to understand in many physical situations. For instance, consider an arbitrary electrostatic charge distribution $\rho(\mathbf{x})$. Then

$$\nabla^2\Phi = -\rho/\epsilon_0 \qquad \text{in } \mathbb{R}^3,$$

$$\Phi \to 0 \qquad \text{as } |\mathbf{x}| \to \infty.$$

(We assume here that the charge distribution decays rapidly far from the origin.) Using the integral solution of Poisson's equation, with $V = \mathbb{R}^3$, and setting G to be the fundamental solution in 3D,

$$\Phi(\mathbf{x}_0) = \iiint_{\mathbb{R}^3} \frac{\rho(\mathbf{x})}{4\pi\epsilon_0|\mathbf{x}-\mathbf{x}_0|}\,\mathrm{d}V.$$

We can interpret this physically as the superposition of many infinitesimal charge elements $\rho(\mathbf{x})\,\mathrm{d}V$. Each of these is effectively a point charge, and the potential at $\mathbf{x}_0$ from such a point charge (using the standard formula for the electrostatic potential due to a point charge) is just $\rho(\mathbf{x})\,\mathrm{d}V/4\pi\epsilon_0|\mathbf{x}-\mathbf{x}_0|$. Summing over all such infinitesimal elements gives the above result.

2.8 Numerical Solution of Poisson's Equation

Finite Differences

Applying Taylor's theorem to any smooth function f we obtain

$$f(x+\delta x) = f(x) + \delta x\, f'(x) + \tfrac{1}{2}\delta x^2 f''(x) + \tfrac{1}{6}\delta x^3 f'''(x) + O(\delta x^4),$$

$$f(x-\delta x) = f(x) - \delta x\, f'(x) + \tfrac{1}{2}\delta x^2 f''(x) - \tfrac{1}{6}\delta x^3 f'''(x) + O(\delta x^4).$$

We deduce that

$$f'(x) = \frac{f(x+\delta x) - f(x)}{\delta x} + O(\delta x);$$

hence $\big(f(x+\delta x) - f(x)\big)/\delta x$ is a *first order forward finite difference* approximation to $f'(x)$. (First order because the error term, known as the *truncation error*, is $O(\delta x)$.) Similarly, by subtracting the two Taylor expansions above, we obtain

$$f'(x) = \frac{f(x+\delta x) - f(x-\delta x)}{2\delta x} + O(\delta x^2),$$

giving us a second order *central finite difference*.

The same reasoning allows us to find approximants for higher derivatives: for example, a second order central finite difference for the second derivative which we shall use for Poisson's equation is

$$\boxed{f''(x) \approx \frac{f(x+\delta x) - 2f(x) + f(x-\delta x)}{\delta x^2}.}$$

We can use this reasoning to find approximants of as high an order as we like: for instance

$$f'(x) = \frac{-f(x+2\delta x) + 8f(x+\delta x) - 8f(x-\delta x) + f(x-2\delta x)}{12\delta x} + O(\delta x^4).$$

Discretization of Poisson's Equation

Suppose we wish to solve Poisson's equation, $\nabla^2\Phi = \sigma$, in two dimensions in some rectangular domain $a \le x \le b$, $c \le y \le d$. We cover the domain with a regular *grid* (or *mesh*) given by $x_i = a + i\delta x$, $y_j = c + j\delta y$ for $i = 0, \ldots, m$, $j = 0, \ldots, n$: here $\delta x = (b-a)/m$ and $\delta y = (d-c)/n$ are the grid spacings in the x- and y-directions respectively.

At each grid point (i, j) the exact value of the solution Φ is $\Phi(x_i, y_j)$; we shall find an approximate solution at that grid point which we denote $\Phi_{i,j}$. Using second order central finite differences for both the derivatives $\partial^2\Phi/\partial x^2$ and $\partial^2\Phi/\partial y^2$ we obtain the discretization of Poisson's equation on the grid,

$$\frac{\Phi_{i+1,j} - 2\Phi_{i,j} + \Phi_{i-1,j}}{\delta x^2} + \frac{\Phi_{i,j+1} - 2\Phi_{i,j} + \Phi_{i,j-1}}{\delta y^2} = \sigma(x_i, y_j)$$

at each of the *interior* points $0 < i < m$, $0 < j < n$. In addition, we will have boundary conditions (Dirichlet, Neumann, or a mixture of the two) at $i = 0, m$ and $j = 0, n$.

We therefore have a large number of simultaneous linear equations: at every point of the grid, both interior and on the boundary, there is a corresponding equation, so that we have a total of $(m+1)(n+1)$ equations to solve.

It is usual to take $\delta x = \delta y$, which we shall assume from now on, in which case the discretization at interior points reduces to

$$\boxed{\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 4\Phi_{i,j} = \sigma(x_i, y_j)\delta x^2.}$$

This can also be denoted using a *stencil* (or *template*) as

What do we do for non-rectangular domains? Suppose we wish to find the steady-state temperature T in an annulus $a \le r \le b$. There are two possible simple approaches. The first is to change coordinates to plane polar coordinates (r, θ), whereupon the grid becomes rectangular: $0 \le \theta \le 2\pi$, with an extra boundary condition that $T(r, 0) = T(r, 2\pi)$. The second approach is to approximate the boundary of the annulus using short line segments in only the x- and y-directions. More advanced techniques can use grids with non-rectangular elements.

Example: suppose we wish to solve Poisson's equation in $0 \le x \le 1$, $0 \le y \le 1$ with $\sigma = 2y$ and boundary conditions $\Phi(x, 0) = 0$, $\Phi(0, y) = 0$, $\Phi(1, y) = y$ (Dirichlet) and $\frac{\partial \Phi}{\partial y}(x, 1) = x^2$ (Neumann). We shall use a grid spacing of $\frac{1}{3}$ in both directions (and will not expect to obtain very accurate results because of the large spacing!).

At each of the four interior points we apply the stencil. On the lower, left and right boundaries we have simply

$$\Phi_{0,0} = \Phi_{1,0} = \Phi_{2,0} = \Phi_{3,0} = 0; \qquad \Phi_{0,1} = \Phi_{0,2} = \Phi_{0,3} = 0;$$

$$\Phi_{3,1} = \tfrac{1}{3}, \quad \Phi_{3,2} = \tfrac{2}{3}, \quad \Phi_{3,3} = 1$$

respectively. On the top boundary we must use a finite difference approximation for $\partial\Phi/\partial y$ to obtain

$$\Phi_{1,3} - \Phi_{1,2} = x_1^2 \delta y = \tfrac{1}{27}, \qquad \Phi_{2,3} - \Phi_{2,2} = x_2^2 \delta y = \tfrac{4}{27}.$$

We can therefore gather together the 16 simultaneous equations representing each point of the grid in a single equation involving a 16×16 matrix as follows:

$$\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & -4 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\Phi_{0,0} \\ \Phi_{1,0} \\ \Phi_{2,0} \\ \Phi_{3,0} \\ \Phi_{0,1} \\ \Phi_{1,1} \\ \Phi_{2,1} \\ \Phi_{3,1} \\ \Phi_{0,2} \\ \Phi_{1,2} \\ \Phi_{2,2} \\ \Phi_{3,2} \\ \Phi_{0,3} \\ \Phi_{1,3} \\ \Phi_{2,3} \\ \Phi_{3,3}
\end{pmatrix}
=
\begin{pmatrix}
0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{2}{27} \\ \frac{2}{27} \\ \frac{1}{3} \\ 0 \\ \frac{4}{27} \\ \frac{4}{27} \\ \frac{2}{3} \\ 0 \\ \frac{1}{27} \\ \frac{4}{27} \\ 1
\end{pmatrix}$$

In theory, the problem is now solved: we simply use Gaussian elimination to obtain

$$\Phi_{0,3} = 0, \qquad \Phi_{1,3} = \tfrac{1}{9}, \qquad \Phi_{2,3} = \tfrac{4}{9}, \qquad \Phi_{3,3} = 1,$$

$$\Phi_{0,2} = 0, \qquad \Phi_{1,2} = \tfrac{2}{27}, \qquad \Phi_{2,2} = \tfrac{8}{27}, \qquad \Phi_{3,2} = \tfrac{2}{3},$$

$$\Phi_{0,1} = 0, \qquad \Phi_{1,1} = \tfrac{1}{27}, \qquad \Phi_{2,1} = \tfrac{4}{27}, \qquad \Phi_{3,1} = \tfrac{1}{3},$$

$$\Phi_{0,0} = \Phi_{1,0} = \Phi_{2,0} = \Phi_{3,0} = 0,$$

which is our approximate solution to Poisson's equation.

In fact the exact solution of this problem is $\Phi = x^2 y$, and we see that our approximate solution is quite unexpectedly exact! This is linked to the fact that the exact solution contains only powers of x and y no higher than cubes, and the finite difference formula for second derivatives is exact for such functions.

However, in real applications Gaussian elimination is simply not possible. There are $N = (m+1)(n+1)$ unknowns $\Phi_{i,j}$; the matrix in the problem has N^2 elements, and the number of calculations required to perform a full Gaussian elimination is $O(N^3)$. For

even a modest grid size (say 100×100) the number of calculations required would be around 10^{12}, which is unreasonable.

Fortunately, we note that the matrix has a *band diagonal* (or *banded*) structure: beyond a certain distance from the leading diagonal, all entries are zero, so that only a small number of the diagonals in the matrix are non-zero. Because of the widespread need to solve Poisson's and related equations efficiently, many specialised algorithms have been developed for such matrices, taking advantage of the large number of zeros to optimise the elimination process. The number of calculations required by these algorithms is typically only $O(N)$.

2.9 Relaxation Techniques for Poisson's Equation

Another approach to solving the discretized form of Poisson's equation is to use an iterative method. These so-called *relaxation* methods start with some initial guess at the solution (which does not need to be a good guess: it could be simply all zeros!) which is then allowed to move slowly towards the true solution. Note that such methods therefore involve two kinds of errors: those caused by the fact that the finite differences used in the discretization are not exact, and those caused by the fact that the initial guess never quite reaches the true solution.

Relaxation methods are typically a little slower than the matrix methods discussed above, but require significantly less computer memory. This can be an important consideration when high accuracy is required and a small grid spacing is being used.

The Jacobi Method

This is the simplest of the relaxation methods. For Poisson's equation in two dimensions using the standard discretization above the algorithm is as follows:

1. Initialise each $\Phi_{i,j}$ to some initial guess.
2. Apply the boundary conditions.
3. For every interior grid point, calculate the quantity

$$\Phi^*_{i,j} = \tfrac{1}{4}(\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - \sigma(x_i, y_j)\delta x^2).$$

4. For every interior grid point, replace the old approximation $\Phi_{i,j}$ with $\Phi^*_{i,j}$.
5. Repeat from step 2 until the difference between the latest two approximations is smaller than some set tolerance everywhere.

Once the tolerance has been reached, we have that

$$\Phi_{i,j} \approx \tfrac{1}{4}(\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - \sigma(x_i, y_j)\delta x^2),$$

i.e.

$$\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 4\Phi_{i,j} \approx \sigma(x_i, y_j)\delta x^2.$$

We therefore have an approximate solution to our original simultaneous equations (which were themselves an approximation to Poisson's equation).

Unfortunately, although each iteration of the Jacobi method is quick and easy, it is very slow to converge, especially for large grids. It is therefore impractical, but it forms the basis for other more useful methods.

The Gauss–Seidel Method

This is very similar to the Jacobi method, except that steps 3 and 4 of the algorithm are combined: as soon as $\Phi^*_{i,j}$ has been calculated for a particular grid point it is *immediately* used to replace $\Phi_{i,j}$. The advantages of this method are that at any time it is only necessary to store the value of $\Phi^*_{i,j}$ at one grid point, rather than at all of them; and the convergence turns out to be somewhat faster (though it is still quite slow).

Successive Over-Relaxation (SOR)

The errors in solutions obtained using either the Jacobi or Gauss–Seidel iterations decrease only slowly, and often in a monotonic manner. We can therefore improve on those methods by over-correcting our solution at each step using a different formula for $\Phi^*_{i,j}$:

$$\Phi^*_{i,j} = (1-\omega)\Phi_{i,j} + \tfrac{1}{4}\omega(\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - \sigma(x_i, y_j)\delta x^2)$$

where ω is the relaxation parameter. The value $\omega = 1$ gives the Gauss–Seidel method again; $\omega < 1$ would produce *under*-relaxation, where we keep a proportion of the old solution; and $\omega > 1$ produces *over*-relaxation where we actually move further away from the old solution than we would using Gauss–Seidel.

The best value to use for ω depends on the particular problem being solved, and may also vary as the iterative process proceeds. However, values in the range 1.2 to 1.4 typically produce good results, and in some cases it is possible to determine an optimal value analytically. The number of iterations required using SOR is significantly less than for either Jacobi or Gauss-Seidel, and for large grids it is often the most practical of all methods of solution.

More advanced methods exist with even better convergence rates, such as the multigrid method which simultaneously uses a number of different grids with different grid

spacings. However, the programming effort required becomes much greater, and so these advanced methods are usually implemented using "black box" routines written by experts in numerical analysis.

2.10 Numerical Solution of the Diffusion Equation

The methods developed for numerical solution of Poisson's equation are easily extended to the diffusion equation

$$\frac{\partial \Phi}{\partial t} = k\nabla^2\Phi.$$

For simplicity we shall consider a rectangular two-dimensional domain $0 \leq x \leq 1$, $0 \leq y \leq 1$, with some initial value for $\Phi(x, y, t)$ at $t = 0$.

We first introduce a spatial grid just as for Poisson's equation, with $\delta x = \delta y$, and denote our approximation to $\Phi(x_i, y_j, t)$ by $\Phi_{i,j}(t)$. Using the standard finite difference formulae for the spatial second derivatives we obtain

$$\frac{\mathrm{d}\Phi_{i,j}}{\mathrm{d}t} = k(\Phi_{i+1,j} + \Phi_{i-1,j} + \Phi_{i,j+1} + \Phi_{i,j-1} - 4\Phi_{i,j})/\delta x^2$$

at each interior point. Thus we have $(n-1)^2$ coupled ordinary differential equations, which we can solve using various methods. However, we need to take care to ensure that the method we use leads to a *stable* solution.

The Euler Method

To solve these differential equations we can use a first order forward finite difference in time. Introduce a time-step δt, and let $\Phi_{i,j}^{(k)}$ denote our approximation to $\Phi(x_i, y_j, k\delta t)$. Then using

$$\frac{\Phi_{i,j}^{(k+1)} - \Phi_{i,j}^{(k)}}{\delta t}$$

for the finite difference approximation to $\partial\Phi/\partial t$, we obtain the iterative scheme

$$\boxed{\Phi_{i,j}^{(k+1)} = \Phi_{i,j}^{(k)} + \mu(\Phi_{i+1,j}^{(k)} + \Phi_{i-1,j}^{(k)} + \Phi_{i,j+1}^{(k)} + \Phi_{i,j-1}^{(k)} - 4\Phi_{i,j}^{(k)})}$$

where

$$\boxed{\mu = \frac{k\,\delta t}{\delta x^2}}$$

is the *Courant number*. We can now, starting from the known values of $\Phi_{i,j}^{(0)}$, *step forward* in time to $\Phi_{i,j}^{(1)}$ and so on.

We shall see that the stability of this method depends on μ.

To analyse the stability, we examine the behaviour of our approximate solution $\Phi_{i,j}^{(k)}$ as $k \to \infty$. In the exact solution, Φ remains bounded as $t \to \infty$; that is, it does not grow ever larger with time (Φ is simply diffusing from one place to another, and there are no source terms). Will this also be true of our approximate solution?

Before we can make progress we need to introduce the concept of a *Fourier mode*. Any function $f(x)$ can be expressed using Fourier transforms as

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widetilde{f}(k) e^{ikx} \, \mathrm{d}k;$$

that is, as an sum (in fact, an integral) of individual modes of the form e^{ikx}, each weighted by the appropriate factor $\widetilde{f}(k)/2\pi$. By taking a double Fourier transform in both x and y, we can therefore write the initial value $\Phi(x, y, 0)$ as a weighted sum of individual modes of the form $e^{i\alpha x} e^{i\beta y}$ where α and β are the wavenumbers in the x- and y-directions respectively. We shall investigate the evolution of each such mode individually. If any one mode grows uncontrollably with time then the complete solution (the sum of the weighted modes) will do too.

This approach works because the diffusion equation $\partial\Phi/\partial t = \nabla^2\Phi$ is linear, which means that individual modes do not interfere with each other. In a nonlinear system, modes could interact and so it would be impossible to investigate them individually. For example, consider the ordinary differential equation $y' = y^2$; if we tried using a sum of Fourier modes then the y^2 term would introduce lots of cross-products (because, for example, $(e^{ik_1 x} + e^{ik_2 x})^2$ is not the same as just the sum of the squares of the individual two modes $e^{ik_1 x}$ and $e^{ik_2 x}$).

So how would $\Phi_{i,j}^{(0)} = e^{i\alpha x_i} e^{i\beta y_j}$ evolve? We see that

$$\begin{aligned}
\Phi_{i,j}^{(1)} &= e^{i\alpha x_i} e^{i\beta y_j} + \mu(e^{i\alpha x_{i+1}} e^{i\beta y_j} + e^{i\alpha x_{i-1}} e^{i\beta y_j} + e^{i\alpha x_i} e^{i\beta y_{j+1}} + e^{i\alpha x_i} e^{i\beta y_{j-1}} - 4e^{i\alpha x_i} e^{i\beta y_j}) \\
&= \big(1 + \mu(e^{i\alpha\delta x} + e^{-i\alpha\delta x} + e^{i\beta\delta y} + e^{-i\beta\delta y} - 4)\big) e^{i\alpha x_i} e^{i\beta y_j} \\
&= \big(1 + 2\mu(\cos\alpha\delta x - 1) + 2\mu(\cos\beta\delta x - 1)\big) \, \Phi_{i,j}^{(0)} \\
&= \xi \Phi_{i,j}^{(0)}
\end{aligned}$$

where the *amplification factor* ξ is given by

$$\xi = 1 - 4\mu \sin^2 \tfrac{1}{2}\alpha\delta x - 4\mu \sin^2 \tfrac{1}{2}\beta\delta x.$$

Applying this repeatedly, we see that

$$\Phi_{i,j}^{(k)} = \xi^k \Phi_{i,j}^{(0)}.$$

Now, if $\mu \le \frac{1}{4}$ then $-1 \le \xi \le 1$ for all α and β; so as the mode evolves it does not grow in amplitude. However, if $\mu > \frac{1}{4}$ then for some values of α and β we have $|\xi| > 1$, so that as

the mode evolves it grows larger and larger in amplitude, eventually tending to infinity as $k \to \infty$. Hence we deduce that the condition for stability of the Euler method for the diffusion equation in two dimensions is $\mu \leq \frac{1}{4}$: this is known as the *Courant condition*.

A similar analysis in one dimension leads to the Courant condition $\mu \leq \frac{1}{2}$. It is easy to extend the method, and the stability analysis, to n dimensions.

In practice, we find that it is difficult to ensure stability using the Euler method if we want both accuracy and a reasonable speed of calculation. Recall that $\mu = k\,\delta t/\delta x^2$; if δx is small then we will require an *extremely* small value of δt to ensure stability. Such a small value means that a very large number of iterations will be required to calculate the solution at a given time t.

We have ignored in this discussion the boundary conditions. These do, of course, have an effect on the evolution of the solution, but in general their effect is of subsidiary importance if the method we are using is unstable. Because of the way the finite difference equations have been set up, at $k = 1$ only those points in the grid which are immediately next to a boundary will have been affected by the boundary conditions. At later times, for general k, only points in the grid which are k or fewer points away from a boundary will have been affected. By the time the effect of the boundaries reaches a point in the interior of the grid, therefore, the instability of the solution caused by the factor ξ^k will generally have already taken hold. Nevertheless, it is *possible* for unusual boundary conditions to turn a method which would otherwise have been stable into an unstable method.

Error Analysis for the Euler Method

Suppose that we wish to find the values of Φ throughout the grid at some time $t = T > 0$, starting from the given initial conditions. We will choose δx and δt so that the Courant condition is satisfied and the Euler method is stable; but it is useful to have some idea of how accurate our results will be.

Recall that we used a first order approximation for $\partial\Phi/\partial t$, but a second order one for the spatial partial derivatives, thereby introducing errors of $O(\delta t)$ and $O(\delta x^2)$ respectively. In deriving our iterative scheme (i.e., the equation which gives $\Phi_{i,j}^{(k+1)}$ in terms of the values of $\Phi_{i,j}^{(k)}$), we multiplied by δt; so the *local truncation error* of the Euler method is $O(\delta t^2) + O(\delta x^2 \delta t)$. The word "local" here refers to the fact that this is the truncation error introduced into $\Phi_{i,j}^{(k+1)}$ by a *single* step.

To iterate all the way to $t = T$ we will need to carry out $T/\delta t$ steps of the iteration, and at each step we will accumulate the above local error. The *global error* of the method, i.e., the total error in the solution at $t = T$, is therefore

$$\big(T/\delta t\big)\big(O(\delta t^2) + O(\delta x^2 \delta t)\big) = O(\delta t) + O(\delta x^2).$$

Recalling that $\mu = k\,\delta t/\delta x^2$, we see that if μ is fixed, δt and δx^2 are of the same order; so the global error can be written simply as $O(\delta t)$.

The above errors, caused by our numerical method itself, would be the only errors in a "perfect" computer implementation of the Euler method. However, for any real computer there will also be *rounding errors*, caused by the computer's inability to store real numbers with infinite precision. These rounding errors are usually significantly smaller than the truncation error; but if the step-size is reduced too far, rounding errors may become significant. Hence it may be impossible to get the precision we desire, however small we make the step-size.

The Crank–Nicholson Method

The Crank–Nicholson method is a much better way of solving the diffusion equation in one dimension, though it is rather tricky to use in higher dimensions. We shall therefore illustrate its application to the one-dimensional equation

$$\frac{\partial \Phi}{\partial t} = k \frac{\partial^2 \Phi}{\partial x^2}.$$

We still use a forward finite difference for $\partial\Phi/\partial t$, but instead of simply using a central finite difference at time t for $\partial^2\Phi/\partial x^2$ we use the *average* of a central finite difference at time t and one at time $t + \delta t$. This leads to

$$\frac{\Phi_i^{(k+1)} - \Phi_i^{(k)}}{\delta t} = \frac{k}{2}\left(\frac{\Phi_{i+1}^{(k)} - 2\Phi_i^{(k)} + \Phi_{i-1}^{(k)}}{\delta x^2} + \frac{\Phi_{i+1}^{(k+1)} - 2\Phi_i^{(k+1)} + \Phi_{i-1}^{(k+1)}}{\delta x^2} \right)$$

or equivalently

$$\Phi_i^{(k+1)} - \frac{\mu}{2}\left(\Phi_{i+1}^{(k+1)} - 2\Phi_i^{(k+1)} + \Phi_{i-1}^{(k+1)} \right) = \Phi_i^{(k)} + \frac{\mu}{2}\left(\Phi_{i+1}^{(k)} - 2\Phi_i^{(k)} + \Phi_{i-1}^{(k)} \right).$$

This is an implicit method: to find the values of $\Phi_i^{(k+1)}$ from the values of $\Phi_i^{(k)}$ we will need to solve a system of coupled linear equations. However, the system is (fortunately) tridiagonal, and so quick solvers exist for the problem.

To test the stability of the Crank–Nicholson method, we again investigate the evolution of a single Fourier mode $e^{i\alpha x}$. An analysis very similar to the one above, left as an exercise for the reader, leads to

$$\Phi_i^{(k)} = \left(\frac{1 - 2\mu \sin^2 \frac{1}{2}\alpha\delta x}{1 + 2\mu \sin^2 \frac{1}{2}\alpha\delta x} \right)^k \Phi_i^{(0)}.$$

The amplification factor in this case satisfies $|(1 - 2\mu \sin^2 \frac{1}{2}\alpha\delta x)/(1 + 2\mu \sin^2 \frac{1}{2}\alpha\delta x)| < 1$ for all values of μ, α and β, so the method is unconditionally stable. The practical implication is that the step-size in time, δt, may be chosen independently of the spatial step-size δx: both may be chosen on the grounds of truncation error alone and we are not hampered by stability requirements.