Partial differential equations

We shall study partial differential equations of the forms

$$\nabla^2 \psi = 0 \qquad \text{(Laplace equation)}$$

$$D \nabla^2 \rho = \frac{\partial \rho}{\partial t} \qquad \text{(Diffusion equation)}$$

$$\nabla^2 \psi - \frac{1}{u^2} \frac{\partial^2}{\partial t^2} \psi = 0 \,. \qquad \text{(Wave equation)}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r}\,) \psi = i\hbar \frac{\partial \psi}{\partial t} \qquad \text{(Schrödinger equation)}$$

Of course the diffusion and wave equations can be made more complicated with additional terms representing sources, but the basic ideas can already be described using the simplest variants.

Texts on mathematical methods of physics discuss the above equations for special geometries in which the equations can be reduced to several ordinary differential equations. Obviously if this is possible, it is probably the optimal way to proceed. However, we often encounter cases where the boundary curves or surfaces are not simple in any coordinate system, hence there is no better way to proceed than brute-force numerical solution using the most powerful computer available. The raison d'etre of this chapter is to describe methods for performing such calculations as expeditiously and simply as possible.

1. Laplace equation

Let us begin with the Laplace equation in two dimensions:

$$\nabla^2 \psi(x, y) \overset{df}{=} \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = 0 \,, \qquad (1)$$

where the boundary curve (which we shall imagine to be simple, smooth and closed) is described parametrically by

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} f(\tau) \\ g(\tau) \end{pmatrix}$$

and

$$\psi\Big(f(\tau), g(\tau)\Big) = \phi(\tau) \,.$$

Relaxation

A standard approach, the *relaxation method*, is simple and iterative—hence easy to program for automatic computers. The central idea is based on this mathematical fact: a function that satisfies Laplace's equation is approximated by its average. To make this more precise, let us average $\psi(x, y)$ over an area including the point (x_0 , y_0) :

$$\frac{1}{\Delta S}\iint_{\Delta S} dx\,dy\;\; \psi(x_0+x,\, y_0+y) \;\approx\; \psi(x_0 , y_0) \;+\; \nabla\psi(x_0 , y_0)\cdot\frac{1}{\Delta S}\iint_{\Delta S} dx\,dy\,\vec{x} \;+ \tag{2}$$

$$+\;\frac{\partial^2\psi}{\partial x_0\,\partial y_0}\;\frac{1}{\Delta S}\iint_{\Delta S} dx\,dy\,x\,y\;+$$

$$+\quad \nabla^2\,\psi\,\Big|_0\;\;\frac{1}{\Delta S}\iint_{\Delta S} dx\,dy\,\frac{1}{4}\left(x^2+y^2\right)+\;\ldots$$

Assuming the region, ΔS, over which we average is chosen symmetrically, the second and third terms on the right of Eq. 2 vanish by symmetry; the fourth term vanishes because the function ψ satisfies the Laplace equation. Clearly these remarks generalize to spaces of higher dimensionality than two.

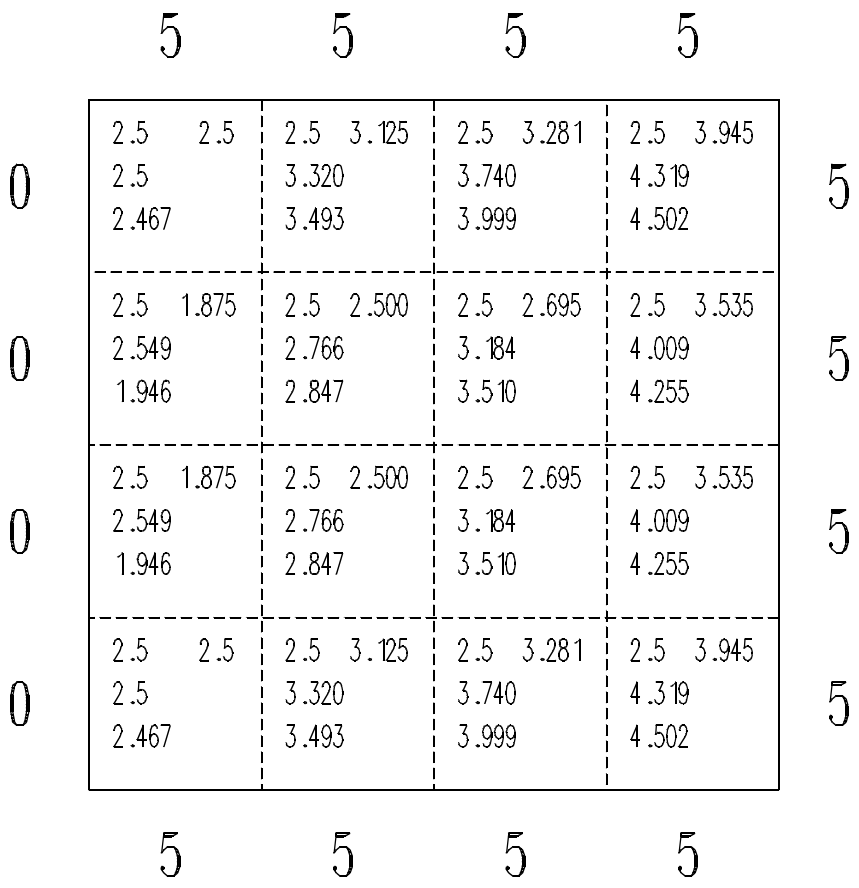
The relaxation method for solving a typical boundary value problem in potential theory (that is, Laplace's equation, with the value of ψ specified on a bounding curve or surface) thus consists of the following steps:

- choose a symmetric mesh to cover the region in which we desire a solution;
- fix the value of ψ at the mesh points corresponding to the boundary curve or surface;
- replace the value of ψ at every interior mesh point by the average of its nearest neighbors (chosen symmetrically);
- iterate until the process converges to the desired precision.

Certain tricks can (and should!) be used to speed up the relaxation process. First, any symmetries in the region of solution should be taken into account. Thus, for example, the reflection symmetry in the example on the next page halves the net computation time.

Second, the solution should be obtained first on a coarse mesh. The spacing between points can then be reduced systematically, with the previous solution serving as the initial guess for the next finer mesh.

On the following page is an example of the relaxation process in operation, solving Laplace's equation in a square region with the potential set to 5 on three sides and 0 on the fourth side of the square. We now see where the method derives its name: after sufficiently many iterations, an initial guess on the interior points *relaxes* to the true solution.



Analytic function theory

The virtue of relaxation is that it works in three dimensions as well as in two. However, strictly two-dimensional Laplace problems can be solved using the theory of functions of a complex variable. A complex function

$$f(z = x + iy) = u(x, y) + iv(x, y),$$

that is analytic within a boundary curve Γ satisifes the Cauchy-Riemann conditions

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}$$
$$\frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}$$

and hence both the real part, $u(x, y)$, and the imaginary part, $v(x, y)$, satisfy the two-dimensional Laplace equation,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 .$$

Suppose we are given that on the boundary Γ

$$u(s) \overset{df}{=} u\Big(x(s), y(s)\Big) ,$$

where we have parameterized Γ in terms of a real parameter s. If we can find an analytic function $w(z)$ that maps the interior of Γ into a region in the w-plane, bounded by a simpler curve[1]

$$C = w(\Gamma) ,$$

we need only find an analytic function that has the appropriate boundary value on C, and we have found the solution to our original Laplace equation. Often this can be done by inspection, although Cauchy's integral formula can be of assistance if the boundary has been mapped into a rectangular or circular region. This method has been so widely applied in the theory of irrotational fluid flow, electro- and magnetostatics that lists of typical conformal transformations have been compiled[2].

Another way to approach the two-dimensional Laplace equation using complex variable methods is based on the Cauchy integral representation of an analytic function: if $f(z)$ is analytic within and continuous on a simple closed curve Γ, then for any interior point z,

$$f(z) = u + iv = \frac{1}{2\pi i} \int_{\Gamma} dt \, \frac{f(t)}{t - z} .$$

Suppose we parametrically represent the curve as

$$t(s) = t_1(s) + i t_2(s)$$

where the real parameter s runs from a to b and $t(a) = t(b)$; then we may write

$$u(x, y) = \int_a^b ds \Big[K(s \mid x, y)\, v(s) + L(s \mid x, y)\, u(s) \Big]$$

$$v(x, y) = \int_a^b ds \Big[K(s \mid x, y)\, u(s) - L(s \mid x, y)\, v(s) \Big]$$

where in an obvious notation, $u(s) \equiv u\Big(t_1(s), t_2(s)\Big)$ is the value of the solution of the Laplace equation on the boundary. The functions K and L are just

$$K(s \mid x, y) + iL(s \mid x, y) \overset{df}{=} \frac{1}{2\pi} \frac{dt}{ds} \frac{1}{t(s) - x - iy} .$$

The problem with this way of writing the solution is that the function $v(s)$—that is, the imaginary part of $f(z)$ on the boundary—must be known before we can compute $u(x, y)$ in the interior. To construct this function, however, we need only solve a 1-dimensional integral equation:

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1. ...in an obvious notation
2. see, *e.g.*, H. Kober, *Dictionary of conformal representations* (Dover Publications, Dover Publications, New York, 1952). For examples of conformal transformation methods, also see William R. Smythe, *Static and dynamic electricity*, 3d ed. (McGraw-Hill, New York, 1968).

$$v(r) = \int_a^b ds \left[\kappa(s \mid r)\, u(s) - \lambda(s \mid r)\, v(s) \right]$$

where

$$\kappa(s \mid r) = K\Big(s \mid t_1(r), t_2(r)\Big) = \frac{1}{2\pi} \mathrm{Re}\left(\frac{\dot{t}(s)}{t(s) - t(r)} \right)$$

and

$$\lambda(s \mid r) = L\Big(s \mid t_1(r), t_2(r)\Big) = \frac{1}{2\pi} \mathrm{Im}\left(\frac{\dot{t}(s)}{t(s) - t(r)} \right),$$

where $\dot{t}(s) = dt/ds$. We must solve the integral equation

$$v(r) = \int_a^b ds \Big(\kappa(s \mid r)\, u(s) - \lambda(s \mid r)\, v(s) \Big) \ ;$$

although it might seem as though $\lambda(s \mid r)$ becomes infinite like $(s - r)^{-1}$ as $s \to r$ in the integral, in fact the integral equation is non-singular since $\lim_{s \to r} |\lambda(s \mid r)| < \infty$. In formal terms we have

$$v + \lambda v = \kappa u \ ,$$

whose formal solution is

$$v = (1 + \lambda)^{-1} \kappa\, u \ .$$

We now look at the computational complexity of this method of solution. In practical terms we evaluate (numerically) a 1-dimensional integral for each point in the interior where we want to know $u(x, y)$. Thus we replace the integrals by sums

$$u(x, y) = \int_a^b ds \Big[K(s \mid x, y)\, v(s) + L(s \mid x, y)\, u(s) \Big]$$

$$\approx \sum_{k=1}^{N} w_k \Big[K(s_k \mid x, y)\, v(s_k) + L(s_k \mid x, y)\, u(s_k) \Big] \ ;$$

therefore we need to know the boundary values $u(s)$ and $v(s)$ at the points $\{s_k\}\Big|_1^K$. If we replace the integral in the 1-dimensional integral equation by the same quadrature formula, we obtain K linear algebraic equations for the values $v(s_k)$, which we can solve by standard methods. To obtain the solution at N^2 points in the interior will then require time proportional to

$$\tfrac{1}{3} K^3 + K N^2 \ ,$$

which may be considered an order N^2 or an N^3 algorithm, depending on whether K is much smaller than, or comparable to, N. This is clearly an example where it might be helpful to employ Gaussian quadrature, since we can get high accuracy with a much smaller number of points than would be required by a Newton-Cotes formula.

On the other hand, if we set up mesh points; replace the differential operators with difference operators, let the values of $u(x, y)$ at the interior points be the unknowns and the values at boundary points be inhomogeneous terms, we obtain a *sparse* system of N^2 equations that can be solved in N^2 time. This method of direct solution is discussed below in the context of the Poisson equation.

2. Poisson equation

If the coefficient functions in the diffusion, wave or Schrödinger equations are independent of time[3], the substitution

$$\psi(\vec{r}, t) = \phi(\vec{r})\, e^{i\omega t}$$

leads to the Poisson equation:

$$\nabla^2 \phi + k^2 \phi = 0 . \qquad (3)$$

There are several good methods for treating Eq. 3. The first is the variational, or Rayleigh-Ritz method, based on the fact that Eq. 3 can be derived by varying the functional

$$\Lambda(\{\phi\}) \overset{df}{=} \frac{\int d\vec{r}\, \nabla\phi \cdot \nabla\phi}{\int \vec{dr}\, \phi^2}$$

subject to the condition that the variation, $\delta\phi$, vanishes on the boundary (curve or surface) of the region of interest.

A typical question we might want to answer is "What values of k^2—that is, the eigenvalues—are consistent with the given boundary conditions?" The variational method replaces the exact solution ϕ by a *trial function* χ that contains adjustable parameters. Since the eigenvalue represents a minimum (or at least a stationary point) of the functional Λ we compute $\Lambda(\{\chi\})$ and minimize with respect to the parameters. To make this more specific, consider the lowest frequency of a stretched string with fixed endpoints. The equation we want to solve is

$$\frac{d^2\phi}{dx^2} + \frac{\omega^2}{u^2}\phi = 0$$

and the variational principle states

$$\omega^2 \le u^2 \frac{\int_0^L dx \left(\frac{d\phi}{dx}\right)^2}{\int_0^L dx\, \phi^2} .$$

3. ...also there must be no source terms.

Suppose we choose the trial function to be $\chi(x) = x\,(L-x)$—this satisfies the boundary conditions and is simple to compute with. (In fact this function has no additional parameters that we can vary.) The result is the estimate

$$\omega^2 \le u^2 \frac{\int_0^L dx\,(L-2x)^2}{\int_0^L dx\,x^2\,(L-x)^2} = 10\frac{u^2}{L^2}.$$

Since the exact eigenvalue is $\pi^2\,u^2/L^2$, this simple bound is seen to be accurate to about 1.3%.

Next suppose we try the function

$$\chi_2(x) = x(L-x) + \alpha\,x(L-x)(L-2x)$$

where α is an undetermined parameter. The value of the resulting functional is

$$\Lambda(\{\chi_2\}) = \frac{10 + 276\alpha^2}{1 + \alpha^2/7}\,\frac{u^2}{L^2}$$

This is minimized by $\alpha = 0$. We leave it as an exercise to explain why this particular trial function produces the same result as the simpler one, and to suggest a better trial function with a zero or zeros within the interval.

As a second example, consider a circular uniform drumhead clamped at the rim. Again the transverse displacement obeys a wave equation, which—upon separating out the time dependence—yields the Poisson equation in two dimensions:

$$\nabla^2\phi + \frac{\omega^2}{u^2}\phi = 0.$$

We know the exact solution corresponding to the lowest frequency is $J_0(kr)$ where

$$\frac{\omega R}{u} = 2.40482..$$

is the first zero of J_0. However, let us try a trial function

$$\chi(r,\theta) = \cos\left(\frac{\pi r}{2R}\right)$$

and evaluate the functional $\Lambda(\{\chi\})$. We see that, after removing the dimensional quantities we are left with

$$\omega^2 \le \frac{u^2}{R^2}\,\frac{\int_0^1 dr\,r\left(\chi'(r)\right)^2}{\int_0^1 dr\,r\left(\chi(r)\right)^2} = \frac{u^2}{R^2}\left(\frac{\pi}{2}\right)^2 \frac{\int_0^{\pi/2} dx\,x\sin^2 x}{\int_0^{\pi/2} dx\,x\cos^2 x} = \frac{u^2}{R^2}\left(\frac{\pi}{2}\right)^2 \frac{\pi^2+4}{\pi^2-4} = (2.4146\ldots)^2$$

—again a rather good estimate.

Higher eigenvalues and eigenfunctions

We have seen above how to obtain variational upper bounds for the lowest eigenvalue of a Hermitian operator[4]. Suppose we want estimates of higher eigenvalues and their corresponding eigenfunctions: it is easy to see that the appropriate procedure is to find the lowest variational eigenfunction, then choose functions from a space orthogonal to that function. This will yield estimates of the higher eigenvalues. (However, it is easy to see that the functional Λ no longer represents an upper bound to the next eigenvalue since the trial function may contain an admixture of the true lowest eigenstate.)

Precision of variational estimates

Another point that is worth making here is that the eigenvalue obtained by the Rayleigh-Ritz method is always relatively more accurate than the corresponding eigenfunction ϕ. That is, it is easy to show that if $||\chi - \phi|| < \varepsilon$, then $|\omega - \omega_{exact}| < \text{const} \times \varepsilon^2$. The proof may be found in Mathews and Walker, or in Goertzel and Tralli.

Variational lower bounds

Suppose A is a Hermitian, positive operator (the operator $-\nabla^2$ fits these criteria). Then it is straightforward to show that if the second and higher eigenvalues are well-separated from the lowest one,

$$\delta - \overline{\omega}^4 \geq \left(\omega_{exact}^2 - \overline{\omega}^2\right)^2,$$

where

$$\frac{\overline{\omega}^2}{u^2} = \Lambda(\{\chi\})$$

as before, and

$$\delta(\{\chi\}) = u^4 \frac{(A\chi, A\chi)}{(\chi, \chi)}.$$

This yields the lower bound

$$\omega_{exact}^2 \geq \overline{\omega}^2 - \sqrt{\delta - \overline{\omega}^4}$$

to the eigenvalue. To illustrate this we consider once again the circular drumhead. With the trial function

$$\chi(r) = 1 - \frac{r^2}{R^2}$$

we find $\delta = 48\, u^4/R^4$, $\overline{\omega}^2 = 6\, u^2/R^2$, hence with the above choice of trial function,

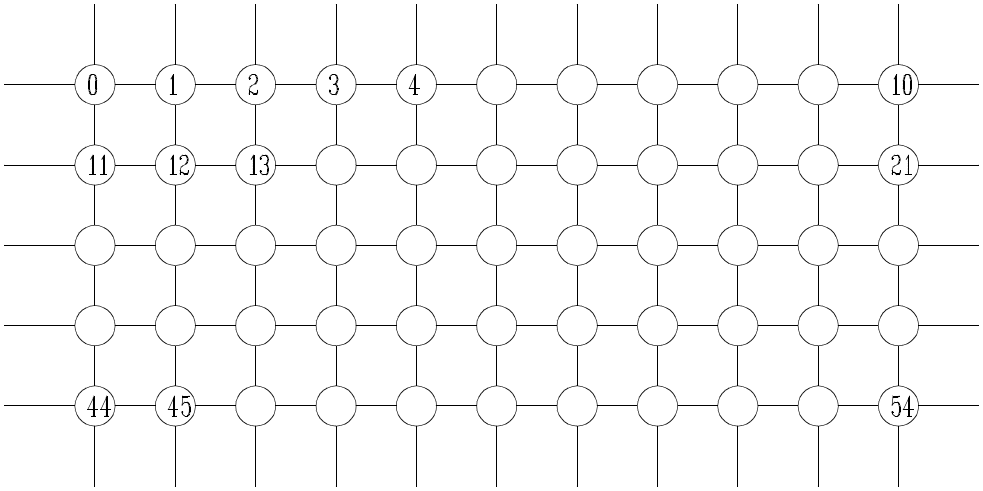
4. This method is sometimes called the Rayleigh-Ritz procedure after its inventors.

$$2.4494\ldots > \omega_{exact} R/u > 1.5924\ldots$$

Indeed the lower bound is not terribly good, but it *is* a lower bound.

3. Direct numerical techniques

The Laplace equation, for example, can be tackled by more direct means than relaxation. If we imagine the points on a solution grid (in, say, two dimensions) are labelled sequentially as shown below, then if we replace the second derivatives by second differences,



$$\nabla^2\psi = 0$$

$$\Rightarrow \quad \psi(x+h, y) - 2\psi(x, y) + \psi(x-h, y) + \psi(x, y+h) - 2\psi(x, y) + \psi(x, y-h) = 0$$

we have, *e.g.*,

$$\psi_{12} + \psi_{14} + \psi_2 + \psi_{24} - 4\psi_{13} = 0\,.$$

The system of (inhomogeneous) linear equations we derive (one for each point in the grid) turns out to be quite sparse and simple—only the nearest neighbors in the grid interact with any given point. Therefore determining the solution at N interior points requires much less than $O\left(N^3\right)$ time to solve: in fact, it can be obtained in $O(N)$ time.

A similar treatment applies to the Poisson equation, as well as the time-independent Schroedinger equation.

4. Direct techniques for the wave equation

Recently Cole[5] has proposed a new differencing scheme for solving the wave equation, that permits coarser meshes for a given precision, thereby reducing considerably the computational effort of a given problem. Consider the wave equation in one spatial dimension:

$$\frac{\partial^2\psi}{\partial t^2} - v^2(x)\frac{\partial^2\psi}{\partial x^2} = 0$$

The usual technique for solving such equations replaces the partial derivatives by second differences, exactly as with the Laplace equation:

$$\Delta_t^2\,\psi - \left(\frac{\Delta t}{\Delta x}\right)^2 v^2(x)\,\Delta_x^2\,\psi = 0\,.$$

We then integrate forward in time *via*

$$\psi(t+\Delta t, x) = 2\psi(t, x) - \psi(t-\Delta t, x) + \left(\frac{\Delta t}{\Delta x}\right)^2 v^2(x)\,\Delta_x^2\,\psi(t, x)\,.$$

It is clear from this scheme that the initial solution, $\psi(t=0, x)$, and the initial time derivative, $\partial_t\,\psi(t=0, x)$, must be known[6] for all x.

The scheme advocated by Cole is based on a modified difference operator

$$\bar{\Delta}_x\,\psi(t, x) \overset{df}{=} \psi(t, x+\beta\Delta x) - \psi(t, x-(1-\beta)\Delta x)$$

and a correction function $s(x, \Delta x, \ldots)$ such that

$$\frac{\partial\psi}{\partial x} \approx \frac{\bar{\Delta}_x\,\psi}{s(x, \Delta x, \ldots)}\,.$$

For example, if ψ were a solution of the 1-dimensional wave equation corresponding to wave number k, we could choose s to give the exact partial derivative. That is, let $\psi = e^{ikx}$ and choose $\beta = \frac{1}{2}$; then

$$\partial_x\,e^{ikx} = ik\,e^{ikx} = \frac{e^{ikx}}{s}\left(e^{ik\Delta x/2} - e^{-ik\Delta x/2}\right)$$

or

$$s = \frac{2}{k}\sin\left(\frac{k\Delta x}{2}\right).$$

To apply this idea to the wave equation we also express the time derivative as a non-standard finite difference and write

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5. James B. Cole, *Computers in Physics* **11** (1997) 287; *ibid*. **12** (1998) 82.
6. If we are working with two or three spatial dimensions the initial data are specified on a surface or volume (hypersurface).

$$\psi(t+\Delta t, x) = 2\psi(t, x) - \psi(t-\Delta t, x) + u^2(x)\,\bar{\Delta}_x^2\,\psi(t, x)$$

where

$$u(x) = \frac{\sin(\omega\Delta t/2)}{\sin(k(x)\,\Delta x/2)}\,v(x)$$

and

$$k(x) = \frac{\omega}{v(x)}\,.$$

This approximation is exact in a regime of fixed ω and constant $v(x)$; in practice, when the solution is a superposition of frequencies with a limited bandwidth, and when $v(x)$ varies reasonably slowly, it is far more accurate than the standard scheme, for a given mesh size.

5. Monte Carlo methods

If we can devise a random process whose distribution is the solution of the equation we are interested in, then an approximate solution can be obtained by simulating the random process. For example, the diffusion equation (heat equation)

$$\frac{\partial\rho}{\partial t} = D\,\nabla^2\,\rho$$

can be derived from particles engaging in a random walk. Thus by following the behavior of many such particles we can determine the function $\rho(\vec{x}, t)$ corresponding to a particular set of boundary or initial conditions. Terms involving first derivatives can be simulated by external forces; similarly terms involving sources or sinks are simulated by a probability for a particle to be born or to die.

6. Integral equation techniques

Some partial differential equations can be transformed into integral equations: consider, for example, the time-independent Schroedinger equation,

$$\left[\nabla^2 + k^2 - U(\vec{r}\,)\right]\psi(\vec{r}\,) = 0\,, \qquad (4)$$

for positive energies, $k^2 > 0$. We cannot solve the problem until we know the volume containing the system (for example, it might be a box of peculiar shape, or it might be infinite 3-dimensional space) as well as the boundary condition (*e.g.* the solution vanishes at the walls of the box, or it might contain, asymptotically, only outgoing radial waves appropriate to a scattering problem).

The object is to express the solution in terms of the solutions of the problem for which there is no potential $U(\vec{r}\,)$: suppose we know how to solve

$$\left(\nabla^2 + k^2\right)G(\vec{r}, \vec{r}\,') = \delta^{(3)}(\vec{r} - \vec{r}\,')\,; \qquad (5)$$

then, left-multiplying Eq. 5 by $\psi(\vec{r})$, and Eq. 4 by $G(\vec{r},\vec{r}')$ we may subtract the two to find

$$\psi(\vec{r})\,\delta^{(3)}(\vec{r}-\vec{r}') =$$

$$= \psi(\vec{r})\,\nabla^2 G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\,\nabla^2\psi(\vec{r}) + G(\vec{r},\vec{r}')\,U(\vec{r})\,\psi(\vec{r})$$

$$\equiv \nabla\cdot\left[\psi(\vec{r})\,\nabla G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\,\nabla\psi(\vec{r})\right] + G(\vec{r},\vec{r}')\,U(\vec{r})\,\psi(\vec{r})\,.$$

Then integrating over $\vec{r}$ (and interchanging the labels $\vec{r}$ and $\vec{r}'$) we obtain

$$\psi(\vec{r}) = \iiint_V G(\vec{r},\vec{r}')\,U(\vec{r}')\,\psi(\vec{r}')\,d\vec{r}' \qquad (6)$$

$$+ \iint_S \left[\psi(\vec{r}')\,\nabla G(\vec{r},\vec{r}') - G(\vec{r},\vec{r}')\,\nabla\psi(\vec{r}')\right]\cdot d\vec{S}'$$

where S is the surface bounding the solution volume V. Assuming we may impose either of the boundary conditions

$$\psi(\vec{r})\Big|_S = 0$$

or

$$\hat{n}\cdot\nabla\psi(\vec{r})\Big|_S = 0$$

we may drop the surface integral in Eq. 6 to obtain

$$\psi(\vec{r}) = \chi(\vec{r}) + \iiint_V G(\vec{r},\vec{r}')\,U(\vec{r}')\,\psi(\vec{r}')\,d\vec{r}' \qquad (7)$$

where we have added an appropriate solution $\chi(\vec{r})$ of the homogeneous differential equation to ensure that the solution of Eq. 7 reduces to that of the homogeneous equation in the absence of the potential U.

The key to being able to solve Eq. 7 by replacing it with a finite set of linear equations lies in the character of the potential, $U(\vec{r})$. If it is sufficiently well-behaved as $r\to 0$ and $r\to\infty$, the *kernel* $G(\vec{r},\vec{r}')\,U(\vec{r}')$ is a *compact* linear operator[7]. If it belongs to that class of operators, it is guaranteed that if we take more points to represent the numerical integral, the solution of the corresponding algebraic equations approaches the solution of the integral equation as closely as we would like. That is, the more time and money we spend, the better the approximation.

7. Basically, a compact operator can be approximated by a finite matrix, such that as the rank of the matrix is increased, the approximation becomes better.