PDEs and the Green's Function

Hariharan Senthilkumar

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Abstract

This paper will cover PDEs extensively and delve into physical applications and representations of PDEs, such as transport, waves, vibration, and diffusion. We walk through and derive the underlying theorems that govern PDEs, and we give special focus to the physical applications in things like the heat and wave equations. We will also talk about boundary problems and how they tie the Green's function and PDEs together. All information, images, ideas, proofs, structure, and so on come directly from the sources cited below, especially Strauss. The whole paper is based completely on these textbooks, with additional commentary and analysis provided by the author.

1 Notation

Let us go over some commonly used notation in this paper. We will cover this extensively later on, but it is still important to define it up top for consistency. This is all notation in three dimensions, but similar notation will be used for two dimensions and one dimension:

$$\text{grad} f = \nabla f = \text{vector}(f_x, f_y, f_z)$$

$$\text{div } \mathbf{F} = \nabla \cdot \mathbf{F} = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z},$$

$$\Delta u = \text{div grad } u = \nabla \cdot \nabla u = u_{xx} + u_{yy} + u_{zz},$$

$$|\nabla u|^2 = |\text{grad } u|^2 = u_x^2 + u_y^2 + u_z^2,$$

where $\mathbf{F} = (F_1, F_2, F_3)$ is a vector field. In this paper, we rely completely on Strauss's notation and ideas, so we write the Laplacian $\nabla \cdot \nabla$ as Δ, not ∇^2. Also, we write the derivatives by subscripts, so

$$\frac{\partial u}{\partial x} = u_x, \frac{\partial u}{\partial y} = u_y, ...$$

2 PDEs: General

[1] [4] In ordinary differential equations (ODEs), the function depends on a single variable, but in PDEs we focus on multiple independent variables $x, y, z, ...$ PDEs also have a dependent variable (which is the unknown function of the aforementioned independent variables) that we write as $u(x, y, z, ...)$.

Definition 2.1. In a PDE, the independent variables, the dependent variable, and the partial derivatives are all related. Using the variables we listed above, a PDE can be written as:

$$F(x, y, u(x, y), u_x(x, y), u_y(x, y)) = F(x, y, u, u_x, u_y) = 0$$

PDE solutions are usually written as a function $u(x, y, z, ...)$ such that it satisfies the equation above, or at least in some region of the $x, y, z, ...$ variables. "Solving" a PDE is not isolating u on one side of the equation, but rather it is about finding a function that makes the PDE valid across some domain, because locality does matter since some solutions may not exist globally.

There are many different types of PDEs, such as linear and non-linear. We define linearity as the following:

Definition 2.2. For an equation like $\mathscr{L}u = 0$, we call $\mathscr{L}$ the operator. This means that if we have some function v, $\mathscr{L}v$ is a new function. An example of this is $\mathscr{L} = \frac{\partial}{\partial x}$ where $\mathscr{L}$ is an operator that takes v into v_x. Another example is the PDE $u_x + yu_y = 0$, where the operator $\mathscr{L}$ is $\mathscr{L} = \frac{\partial}{\partial x} + \frac{y\partial}{\partial y}$. We can therefore define linearity as:

$$\mathscr{L}(u + v) = \mathscr{L}u + \mathscr{L}v, \mathscr{L}(cu) = c\mathscr{L}u$$

for any function u and v and any constant c. Whenever the above equations are true, $\mathscr{L}$ is called a linear operator.

Example. The equation $\mathscr{L}u = 0$ is linear if $\mathscr{L}$ is a linear operator.

There are also other types of linearity, like homogeneous and inhomogeneous linear equations.

Example. $\mathscr{L}u = 0$ is a homogenous linear equation if $\mathscr{L}$ is a linear operator. $\mathscr{L}u = g$ is an inhomogeneous linear equation when $g \neq 0$.

This is important because a homogeneous equation $\mathscr{L}(u) = 0$ has the property that the set of all solutions forms a vector space, meaning that all linear combinations of solutions are solutions. For inhomogeneous equations $\mathscr{L}u = g$, the solution space contains a particular solution along with the general solution to the homogeneous equation. This decomposition is important to solving boundary value problems and using Green's functions.

In linear PDEs, if we have some equation $\mathscr{L}u = 0$ where u and v are solutions, $u + v$ is also a solution. If $u_1, u_2, u_3, ..., u_n$ are all solutions for the equation, then so is any linear combination

$$c_1u_1(x) + c_2u_2(x) + c_3u_3(x) + ... + c_nu_n(x) = \sum_{j=1}^{n} c_ju_j(x) \text{ where } c_j \text{ are constants.}$$

This makes sense when we look at the definition of a linear operator, since if $\mathscr{L}$ is linear, then $\mathscr{L}(u + v) = \mathscr{L}u + \mathscr{L}v$ and $\mathscr{L}(cu) = c\mathscr{L}u$. So, if each u_j satisfies $\mathscr{L}u_j = 0$, then $\mathscr{L}(\sum c_ju_j) = \sum c_j\mathscr{L}u_j = 0$. This is also known as the superposition principle.

Linearity also tells us that the sum of an inhomogeneous and homogeneous solution results in an inhomogeneous function. Suppose that u_p solves $\mathscr{L}u = g$ and u_h solves $\mathscr{L}u = 0$. Then,

$\mathscr{L}(u_p + u_h) = \mathscr{L}u_p + \mathscr{L}u_h = g + 0 = g$, meaning that the sum is still a solution to the inhomogeneous equation. This shows why we only need to find one particular solution and add the general homogeneous solution to it so that we can get all possible solutions.

Before we continue and explore the more physical aspects of PDEs, we have to spend more time with linear equations, starting with first-order linear equations. The simplest solution to a PDE is $\frac{\partial u}{\partial x} = 0$ where $u = u(x, y)$ and the general solution is $u = f(y)$ where y is any one-variable function. This is because the equation says that u does not vary with x, which means that all variation has to be in the y-direction. This means that u is constant along horizontal lines in the xy-plane. Any function $f(y)$ fits because $\partial f(y)\partial x = 0$ regardless of f's form. This is why $u = f(y)$ gives us the general solution.

$u = y^2 - y$ and $u = e^y \cos(y)$ are examples of possible solutions. The solutions don't depend on x which means that they are constant on the lines where y is constant on the xy plane. Let us also explore various solving methods for these type of equations.

Example. Solve $au_x + bu_y = 0$ where a, b are constants where both are not 0.

Geometric Method The left side of the equation in the example is a directional derivative of u in the direction of the vector $V = (a, b) = a\mathbf{i} + b\mathbf{j}$, which always has to be 0. The directional derivative in direction V is defined as $D_V u = au_x + bu_y$. This means that the PDE states that $D_v u = 0$ so u does not change when we move alone the V direction. Therefore, the level sets of u have to be orthogonal to V, so we now want to describe these level sets explicitly.

From this, we can determine the following: We can also say that:

1. $u(x, y)$ has to be constant in the direction of V
2. The vector $(b, -a)$ is orthogonal to V.
3. The lines that are parallel to V have the equations $bx - ay =$ constant, which are called characteristic lines.

Given this, we can say that the solution is a constant on a characteristic line, which means that $u(x, y)$ depends on $bx - ay$ alone, so the solution is $u(x, y) = f(bx - ay)$ where f is any function of one variable. This is the general solution. Any differentiable function f of $bx - ay$ will satisfy the PDE because $u_x = f'(bx - ay) \cdot b$ and $u_y = f'(bx - ay) \cdot (-a)$ so $au_x + bu_y = abf' - abf' = 0$. This shows that any such f satisfies the equation.

Coordinate Method Let us change the variables to $x' = ax + by$ and $y' = bx - ay$. This change of variables is important because it aligns one of the new axes with vector $V = (a, b)$ which is the direction where the directional derivative vanishes. More specifically, we choose x' because moving along it corresponds to moving along the V direction, while y' is chosen to be orthogonal to x', which shows the invariant direction. This makes the PDE simpler because we expect the solution to be constant along x', making the directional derivative easier to express these coordinates.

Then, we can replace the x and y derivatives by x' and y' derivatives. Using chain rule, we can say the following:

$$u_x = \frac{\partial u}{\partial x} = \frac{\partial u}{\partial x'}\frac{\partial x'}{\partial x} + \frac{\partial u}{\partial y'}\frac{\partial y'}{\partial x} = au_{x'} + bu_{y'}$$

Here, we apply the multivariable chain rule. We compute how u changes with respect to x with the intermediate variables x' and y'. Since $x' = ax + by$, we have $\frac{\partial x'}{\partial x} = a$ and something similar for y'. This step changes the original derivatives into the rotated coordinate frame.

$$u_y = \frac{\partial u}{\partial y} = \frac{\partial u}{\partial y'}\frac{\partial y'}{\partial y} + \frac{\partial u}{\partial x'}\frac{\partial x'}{\partial y} = bu_{x'} - au_{y'}$$

As before, the partial derivatives of x' and y' with respect to y give us

$$\frac{\partial x'}{\partial y} = b \text{ and } \frac{\partial y'}{\partial y} = -a$$

which tell us the coefficients in the chain rule. By doing this, we express the original gradient in terms of the new rotated coordinates.

Therefore

$$au_x + bu_y = a(au_{x'} + bu_{y'}) + b(bu_{x'} - au_{y'}) = u_{x'}(a^2 + b^2).$$

By substituting the expressions for u_x and u_y and grouping the terms, we see that the combination $au_x + bu_y$ becomes a scalar multiple of $u_{x'}$. The cross-terms that have $u_{y'}$ cancel out perfectly because of our choices of x' and y'. This is why we are doing the coordinate change, to diagonalize the operator into a simple derivative with respect to one variable.

Since $a^2 + b^2 \neq 0$, the equation becomes $u_{x'} = 0$ in the new variables. The nonzero condition is necessary because it makes sure that $(a, b) \neq (0, 0)$ which in turn makes sure that this is true change of coordinates. Since $u_{x'} = 0$ we can see that u is constant in the $x'-$direction which is what we could expect from the geometric method. We have rotated the coordinate system so that the direction of constancy aligns with one axis.

This means that the solution is $u = f(y') = f(bx - ay)$ where f is an arbitrary function of one variable, so we got the same answer as before.

3 Waves and Diffusion

[1] [3] Now, we will explore the basics of flows, vibrations, and diffusion. For context, PDEs have historically been very closely tied with physics and because of this a lot of PDE problems are fundamentally physical problems. Let us explore these types of problems.

3.1 Simple Transport

Say that there is water flowing at a constant rate c in a pipe with a fixed cross section in the positive x direction, and there is a pollutant in the water. Let $u(x, t)$ be the concentration in grams/centimeter at time t. This means that $u_t + cu_x = 0$.

We can derive this equation by recognizing that the amount of pollutant (in grams) in the interval $[0, b]$ at time t is

$$M = \int_0^b u(x, t)\, dx.$$

This integral defines the total mass of pollutant in the interval at a given time. Since the concentration is in grams per centimeter, integrating over a length gives total grams.

This mass should be conserved as the pollutant moves, assuming there's no source, sink, or diffusion.

At some later time $t+h$ the same pollutant molecules have moved right by $c \cdot h$ centimeters, which means that

$$M = \int_0^b u(x,t)\ dx = \int_{ch}^{b+ch} u(x,t+h)\ dx.$$

Instead of computing the mass at time $t+h$ in $[0,b]$ we calculate the mass in $[ch, b+ch]$. We do this because the fluid shifts each pollutant particle to the right by ch. The conservation of mass means that the content that was originally in $[0,b]$ is now exactly in $[ch, b+ch]$.

When we differential with respect to b, we get

$$u(b,t) = u(b+ch, t+h).$$

By differentiating both sides with respect to b, we treat the integral's upper limit as variable, which means that the concentration at position b and time t is equal to the concentration at position $b+ch$ and a later time $t+h$.

We then differentiate with respect to h and by setting $h=0$ we get

$$0 = cu_x(b,t) + u_t(b,t).$$

The right-hand side, $u(b+ch, t+h)$ is a function of h and we differentiate it using multivariable chain rule. By evaluating at $h=0$, we return the instantaneous rate of change at position b, and the resulting PDE is $u_t + cu_x = 0$.

The equation means that the rate of change u_t of concentration is proportional to the gradient u_x, and we assume diffusion to be negligible. When we solve the equation, we find the concentration is a function of $(x-ct)$ only. This is because the general solution of $u_t + cu_x = 0$ is any function in the form $u(x,t) = f(x-ct)$. This can easily be seen using the characteristic methods where each characteristic curve satisfies $\frac{dx}{dt} = c$ and along these curves u remains constant.

This means that the substance moves right at a fixed speed c, which means that each individual particle moves right at that same speed c. The solution is constant along lines $x = ct + \text{constant}$, so the pollutant shifts to the right with velocity c.

3.2 Vibrating String

Say that we have a string, like a guitar or violin string, that is either a flexible, elastic homogenous string or a string that undergoes small transverse vibrations. At some time t, the string may look like the one in Figure 1.

Say that $u(x,t)$ is the displacement from the equilibrium at time t and position x. The tension is directed tangentially along the string since the tension is tangentially directed along the string, as seen in Figure 2. Let us call $T(x,t)$ the magnitude of the tension vector and let ρ be the density of the string (the density being constant since the string is homogenous). We will use Newton's law on the part of the string between two arbitrary points x_0 and x_1. The slope at x_1 is $u_x(x_1,t)$, and Newton's law $F=ma$ in its longitudinal (x) and transverse (u) components is

$$\text{Longitudinal: } \frac{T}{\sqrt{1+u_x^2}}\Big|_{x_0}^{x_1} = 0$$

$$\text{Transverse: } \frac{Tu_x}{\sqrt{1+u_x^2}}\Big|_{x_0}^{x_1} = \int_{x_0}^{x_1} \rho u_{tt} dx$$

The right hand sides of the above equations are the product of the mass components that are integrated over the string. Since we are assuming that there is no longitudinal motion, the motion here is entirely transverse.

Now, let us assume that $|u_x|$ is very small. If we look at the Taylor expansion of $\sqrt{1+u_x^2}$, we get

$$\sqrt{1+u_x^2} = 1 + \frac{1}{2}u_x^2 + \cdots$$

where the dots are the higher powers of u_x. We can drop u_x^2 and all higher powers because if u_x is very small, then these higher powers must be even smaller. This means that we can replace $\sqrt{1+u_x^2}$ with 1.

After replacing the value with 1, the first equation tells us that T is constant along the string. If we differentiate the transverse equation above (assuming that T is independent of both t and x), then we get $(Tu_x)_x = \rho u_{tt}$. Rewritten, that is $u_{tt} = c^2 u_{xx}$ where $c = \sqrt{\frac{T}{\rho}}$, where c is the wave speed, and the speed depends on the tension T and the mass density ρ. This is also known as the wave equation.

Now, it is important to note that this is not an extremely rigorous derivation, but our goal here is to understand why this equation works and it's many, many useful applications. There are at least three variations to the wave equation we found above that help us in different conditions.

If there is a significant air resistance factor r, then there is an extra proportional term to the speed u_t, so we can rewrite the equation as

$$u_{tt} - c^2 u_x x + r u_t = 0 \text{ where } r > 0.$$

This is because the term ru_t represents a resistive force, like air drag, which lessens kinetic energy. This equation is a damped wave equation which shows decaying oscillations rather than constant waves.

If there is a transverse elastic force (like in a coiled spring), there is an extra proportional term to the displacement u, resulting in the equation

$$u_{tt} - c^2 u_{xx} + ku = 0 \text{ where k¿0.}$$

This is because the term ku is a Hookean restoring force which leads to solutions that have standing waves or harmonic motion.

If there is an external force applied, there is an extra term which results in the equation:

$$u_{tt} - c^2 u_{xx} = f(x,t)$$

, making the equation inhomogeneous. This is because $f(x,t)$ introduces energy into a system and affects nonhomogeneous behavior.

Figure 1. Example: vibrating string

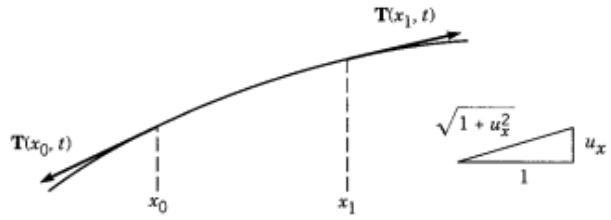

Figure 2. Force of tension directed tangentially along the string

3.3 Vibrating Drumhead

A drumhead is an elastic, flexible, homogenous two-dimensional string. It appears as a membrane stretched across a frame, as seen in Figure 3.

Say that this membrane lies in the xy plane where $u(x, y, t)$ is the vertical displacement and there is no horizontal movement. The horizontal components of Newton's law gives us the constant tension T. Say that D is any domain in the xy plane, like a circle or rectangle. Using reasoning similar to the vibrating string, and defining the boundary curve as ∂D, we can say that the vertical component approximately gives:

$$F = \int_{\partial D} T \frac{\partial u}{\partial n} ds = \int \int_D \rho u_{tt} \, dx \, dy = ma.$$

In the above equation, the left side is net vertical force on the boundary ∂D integrated using the tension T and the normal derivative $\frac{\partial u}{\partial n}$. The normal derivative $\frac{\partial d}{\partial n} = n \cdot \nabla u$ is the directional derivative in the outward normal direction where n is the unit outward normal vector on ∂D. Using Green's theorem, we can rewrite this as

$$\int \int_D \nabla \cdot (T \nabla u) \, dx \, dy = \int \int_D \rho u_{tt} \, dx \, dy.$$

Using the divergence theorem changes the boundary integral into an area integral over D by converting the tension forces into Laplacian expressions.

Since D is arbitrary, we can use the second vanishing theorem to see that $\rho u_{tt} = \nabla \cdot (T \nabla u)$ and since T is constant, we get:

$$u_{tt} = c^2 \nabla \cdot (\nabla u) \equiv c^2 (u_{xx} + u_{yy})$$

. The reasoning behind these steps is that if two integrands agree over all regions D, the functions have to be equal almost everywhere. Since T is constant and pulls out of divergence, we know that $\nabla \cdot (T \nabla u) = T(\Delta u)$.

In the above equation, which we call the two-dimensional wave equation, $c = \sqrt{\frac{T}{\rho}}$ like in the wave equation before and $\nabla \cdot (\nabla u) =$ div grad u $= u_{xx} + u_{yy}$ is the two-dimensional Laplacian.

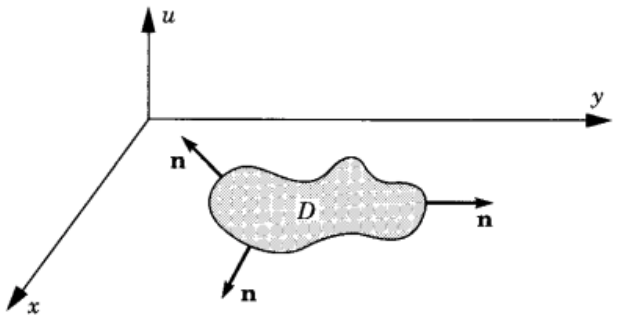

Figure 3. The two-dimensional string: a "drumhead"

Looking at both the one-dimensional and two-dimensional wave equations, the pattern seems clear enough for us to write a three-dimensional wave equation:

$$u_{tt} = c^2(u_{xx} + u_{yy} + u_{zz}).$$

The operator

$$\mathscr{L} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial}{\partial z^2}$$

is the three-dimensions nsional Laplacian operator which we typically write as Δ.

3.4 Diffusion

Given a motionless liquid filling a straight pipe and some chemical like a dye, diffusing through the liquid, we can define simple diffusion using the following logic:

The dye moves from regions of high concentration to low concentration, and the rate of this motion is proportional to the concentration gradient; this is known as the Fick's law of diffusion. If $u(x,t)$ is the concentration of the dye at position x and time t, then in the part of the pipe that spans from x_0 to x_1, the mass of the dye is written as:

$$M(t) = \int_{x_0}^{x_1} u(x,t)\ dx \rightarrow \frac{dM}{dt} = \int_{x_0}^{x_1} u_t(x,t)\ dx.$$

This integral sets up the conservation law because the total amount of dye in a specific part of the pipe is the integral of concentration. By taking the time derivative of the integral this allows us to find the local rate of change u_t.

The mass in this part of the pipe doesn't change unless the liquid flows in and out of the ends. Using Fick's law:

$\frac{dM}{dt}$ = flows into$-$flows out = $ku_x(x_1,t) - ku_x(x_0,t)$ where k is the constant of proportionality.

Fick's law tells us that the diffusive flux at any point is $-ku_x$, but since we are calculating the net flux into the interval, we write it as a difference of flux terms at the boundaries.

We equate the two expressions for $\frac{dM}{dt}$, one from conservation of mass and the other from Fick's Law:

$$\int_{x_0}^{x_1} u_t(x,t)\ dx = ku_x(x_1,t) - ku_x(x_0,t).$$

We differentiate both sides with respect to the upper endpoint x_1, changing the integral equation into a local pointwise differential equation. We assume that the interval $[x_0, x_1]$ is arbitrary which allows the differentiation to be valid everywhere. Using the Fundamental Theorem of Calculus, we get $u_t = ku_{xx}$.

This is known as the diffusion equation. The equation $u_t = ku_{xx}$ tells us how concentration changes under pure diffusion. The second derivative u_{xx} represents the curvature of the concentration graph where positive curvature means the function is concave up. In three dimensions, we write

$$\int\int\int_D ut\ dx\ dy\ dz = \int\int_{\partial D} k(\mathbf{n}\cdot\nabla u)\ dS,$$

where D is any solid domain and ∂D is its bounding surface.

The left-hand side of this equation is the total rate of change of dye in the volume D. The right hand-side of the equation is the total net flux into D which we calculate by integrating the normal component of $-k\nabla u$ over the boundary.

Using the divergence theorem and the arbitrary nature of D we can write the three-dimensional diffusion equation as

$$u_t = k(u_{xx} + u_{yy} + u_{zz} = k\Delta u.$$

The divergence theorem changes the boundary integral into a volume integral $\nabla\cdot(k\nabla u)$. Since D is arbitrary, the equality has to hold pointwise, which yields the PDE. The term Δu is the Laplacian which tells us about the spatial curvature of u in all directions.

If there is an external source of the dye or if k can change and is not constant, we get the inhomogeneous equation

$$u_t = \nabla\cdot(k\nabla u) + f(x,t).$$

This generalized e uation is very useful because it lets us describe many physical concepts like heat, brownian motion, and more.

3.5 Heat Flow

Say that $u(x,y,z,t)$ is the temperature and say that $H(t)$ is the amount of heat contained in a region D. We can say that

$$H(t) = \int\int\int_D c\rho u\ dx\ dy\ dz$$

where c is the specific heat of the material and ρ is the density. As aforementioned, $u(x,y,z,t)$ is the scalar temperature field, and we also know that $c\rho u$ is the heat per unit volume for each point. Multiplying by $c\rho$ converts temperature to energy, and the integral gives the total thermal energy stored in D.

The change in heat is

$$\frac{dH}{dt} = \int\int\int_D c\rho u_t \, dx \, dy \, dz.$$

We get this by applying Leibniz's rule to the integral with respect to time. Since c and ρ are constant, the derivative goes inside the integral and acts solely on u, giving u_t.

Fourier's law tells us that the heat flux vector $\overrightarrow{q} = -\kappa\nabla u$ where $\kappa > 0$ is thermal conductivity. The negative sign makes sure that the heat flows from higher to lower temperatures, and since there are no internal sources/sinks, heat can only leave D through its boundary.

This means that the change of heat energy in D corresponds to a heat flux across the boundary, meaning that

$$\frac{dH}{dt} = \int\int_{\partial D} \kappa(\mathbf{n} \cdot \nabla u) \, dS,$$

where κ is the heat conductivity (a proportionality constant). The boundary integra; represents the total heat flux leaving D. The term $n \cdot \nabla u$ is the normal derivative of temperature across the surface, and $\kappa(n \cdot \nabla u)$ is the flux magnitude per unit area.

Using the divergence theorem, we have

$$\int\int\int_D c\rho \frac{\partial u}{\partial t} \, dx \, dy \, dz = \int\int\int_D \nabla \cdot (\kappa \nabla u) \, dx \, dy \, dz.$$

The divergence theorem changes the surface integral; of the normal component into a volume integral of the divergence. As we have said before, D is arbitrary and the integrals over the same volume are equal, and this implies that the integrands must be equal pointwise.

From the above equation, we have the heat equation:

$$c\rho \frac{\partial u}{\partial t} = \nabla \cdot (\kappa \nabla u).$$

This is the general form of the heat equation, and it states that the rate of change in temperature at any point is equal to the divergence of the heat flux vector. If κ is constant, this becomes $u_t = \frac{\kappa}{c\rho}\Delta u$ which is the standard diffusion equation.

3.6 Stationary Waves and Diffusion

In the four previous examples, the physical state is not affected by time, so $u_t = u_t t = 0$. This means that both the wave and diffusion equations reduce to

$$\Delta u = u_{xx} + u_{yy} + u_{zz} = 0.$$

We call this the Laplace equation, and its solutions are called harmonic functions. This happens when the system has reached equilibrium, meaning that no energy/heat is entering or leaving, and nothing changes with time. The wave and diffusion equations simplify into Laplace's equation when the time derivatives are gone, as seen above.

Consider a constantly heated object that was heated in an oven. The heat is likely not evenly spaced out throughout the object, but the object will eventually reach an equilibrium. This is a harmonic function $u(x, y, z)$.

3.7 Hydrogen Atom

Suppose that we have an electron moving around a proton, where the electron has a mass of m, a charge of e, and h is Plank's constant divided by 2π. Say that the coordinate origins (x, y, z) be at the proton and say that $r = (x^2 + y^2 + z^2)^{1/2}$ is the spherical coordinate. The motion of the electron is given by a wave function $u(x, y, z, t)$ that satisfies Schrödinger equation:

$$ihu_t = \frac{h^2}{2m}\Delta u + \frac{e^2}{r}u$$

in $-\infty < x, y, z < \infty$. Note that u is complex-valued. The left-hand side of the above equation represents the Hamiltonian acting on the wave function U. The Laplacian tells us about the kinetic energy and the $\frac{e^2}{r}$ term represents the Coulomb potential due to the proton.

We are also supposed to have

$$\int\int\int |u|^2 \, dx \, dy \, dz = 1 \text{ the integral over all space.}$$

This is a normalization that makes sure that the total probability of finding an electron somewhere in space is 1. In quantum mechanics, $|u|^2$ is a representation of the probability density function.

We call the coefficient function $\frac{e^2}{r}$ the potential; for any single electron atom, like a helium ion, e^2 is replaced with Ze^2 where Z is the atomic number. The potential represents the attractive force between the negatively charged electron and the positively charged nucleus and the term Z scales the nuclear charge, strengthening the attractive potential for heavier atoms.

Quantum mechanics tells us that a wave function $u(x, y, z, t)$ is a possible state of an electron because we cannot measure quantities. If D is any region in the xyz space:

$$\int\int\int_D |u|^2 \, dx \, dy \, dz.$$

This expression represents the probability of finding an electron in region D at some time t. Note that the integrand $|u|^2$ must be real and nonnegative. This integral tells us the likelihood that a measurement of the particle's position at time t lies in D.

We can calculate the expected z coordinate of the electron's position at time t with the integral

$$\int\int\int z|u(x, y, z, t)|^2 \, dx \, dy \, dz.$$

This is the mean of the z position with respect to the probability distribution $|u|^2$ and similar formulas exist for the x and y coordinates.

The expected z coordinate of the electron's momentum, where $\overline{u}$ is the complex conjugate of u, is

$$\int\int\int -ih\frac{\partial u}{\partial z}(x, y, z, t) \cdot \overline{u}(x, y, z, t) \, dx \, dy \, dz.$$

This expression comes from the momentum operator $\hat{p_z} = -ih\frac{\partial}{\partial z}$.

The other observable values can be found by operators A that act on functions. We can calculate the expected value of the observable A as

$$\int\int\int Au(x,y,z,t)\cdot\overline{u}(x,y,z,t)\ dx\ dy\ dz.$$

This is the general formula for the expected observable and it is represented by the operator A. The inner product $\langle Au,u\rangle$ represents the mean of the measurement outcome of A when the system is in the state u.

The position is given by the operator $Au=\mathbf{x}u$ where $\mathbf{x}=x\mathbf{i}+y\mathbf{j}+z\mathbf{k}$ and the momentum is given by the operator $Au=-ih\nabla u$. In many types of particles, the wave function u depends on time t and the coordinates of all the particles, meaning that the wave function is a function of many variables. Therefore, the Schrödinger equation becomes

$$ihu_t=\sum_{i=1}^{n}\frac{h^2}{2m_i}(u_{x_ix_i}+u_{y_iy_i}+u_{z_iz_i})+V(x_1,...,z_n)u$$

for n particles where the potential function V depends on all $3n$ coordinates.

The above equation is known as the many-body Schrödinger equation. Every particle has a Laplacian scaled by its mass, known as the kinetic term, and all the particles interact through the potential V.

4 Boundary Problems

[1] PDEs usually have many solutions, and we try to find out a single solution by using additional conditions to narrow down the possible solutions. These conditions are usually either initial or boundary conditions. An initial condition tells us about the physical state at some time t_0.

For the diffusion equation, for some given function $\phi(x)=\phi(x,y,z)$, an initial condition is

$$u(\mathbf{x},t_0)=\phi(\mathbf{x}).$$

$\phi(x)$ is the initial concentration for the diffusing substance, the initial temperature for heat flow, and the initial condition for the Schrödinger equation.

For the wave equation, there are two initial conditions where $\phi(x)$ is the initial position and $\psi(x)$ is the initial velocity:

$$u(\mathbf{x},t_0)=\phi(\mathbf{x}),\ \frac{\partial u}{\partial t}(\mathbf{x},t_0)=\psi(\mathbf{x}).$$

In every problem we looked at in the previous subsection, there is a domain D where the PDE is valid. In the vibrating string, D is the interval $0<x<1$ so D's boundary has only the two points $x=0$ and $x=l$. In the drumhead, the domain is a plane and its boundary is a closed curve. For a diffusing substance, D is a container holding the liquid meaning that its boundary is a surface such that $S=\partial D$. For the hydrogen atom the domain is all space so there is not any boundary.

There are three major boundary condition types, where a is a function of x,y,z, and t:

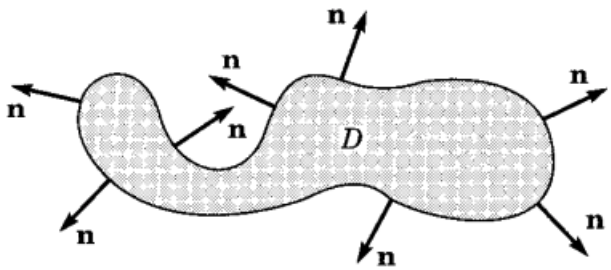

Figure 4. The unit normal vector pointing outward from D.

1. (D) u is specified, known as the Dirichlet condition.
2. (N) $\frac{\partial u}{\partial n}$ is specified, known as the Neumann condition.
3. (R) $\frac{\partial u}{\partial n} + au$ is specified, known as the Robin condition.

Each of these conditions hold for all t and for $\mathbf{x} = (x, y, z)$ in ∂D. We write $(D), (N), (R)$ as equations, like when we write (N) as $\frac{\partial u}{\partial n} = g(\mathbf{x}, t)$ where g is a function that is called the boundary datum.

These boundary conditions are called homogeneous if the function $g(\mathbf{x}, t)$ equals 0, and if not, they are called inhomogeneous. As we have been doing, we call $\mathbf{n} = (n_1, n_2, n_3)$ the unit normal vector on ∂D which point outward from D, as seen in Figure 4. $\frac{\partial u}{\partial n} \equiv \mathbf{n} \cdot \nabla u$ is the directional derivative of u in the outward normal direction.

In one-dimensional problems where D is an interval $0 < x < 1$ then the boundary has just two endpoints, and these boundary conditions appear as:

$$\text{(D) } u(0, t) = g(t) \text{ and } u(l, t) = h(t)$$

$$\text{(N) } \frac{\partial u}{\partial x}(0, t) = g(t) \text{ and } \frac{\partial u}{\partial x}(1, t) = h(t)$$

There are similar conditions for the Robin condition. Now, let us explore some examples of these boundary conditions.

The Vibrating String: If a string is held steady at both ends, we have homogeneous Dirichlet conditions $u(0, t) = u(l, t) = 0$. If the string were free and could move transversely with no resistance, then there would be no tension T at the end, so $u_x = 0$; this is known as the Neumann condition. If the end of the string was free to move along a tack but was attached to a coiled spring that pulls its back to equilibrium, then the Robin condition would be correct. If the string's end was moved in a particular way, there would be an inhomogeneous Dirichlet condition at the end.

Diffusion: If there is a diffusing substance in a container D so that nothing can escape or enter, then we know that the concentration gradient in the normal direction disappears by Fick's law. This means that $\frac{\partial u}{\partial n} = 0$ on $S = \partial D$; this is the Neumann condition. If we make the container porous so that any escaped substance immediately vanishes, then we write $u = 0$ on S.

Heat: We describe heat conduction with the diffusion equation $u(\mathbf{x}, t)$. If we have an insulated object D and heat is flowing through D, then no heat crosses the boundary and

we have the Neumann condition $\frac{\partial u}{\partial n} = 0$. If D is immersed in a large pool of a specified temperature $g(t)$ and there is perfect thermal conduction, then we would have the Dirichlet condition $u = g(t)$ on ∂D.

Say that we have a uniform rod that is insulated along the length $0 \leq x \leq 1$ where the end at $x = l$ is submerged in $g(t)$. If heat exchanges at the end and in the pool of temperature in accordance with Newton's Law of Cooling, then

$$\frac{\partial u}{\partial x}(l,t) = -a[u(l,t) - g(t)], a > 0.$$

This is an inhomogeneous Robin condition.

Sound: Small disturbances in the air can be described by linearized equations, which are

$$\frac{\partial v}{\partial t} + \frac{c_0^2}{\rho_0}\text{grad } \rho = 0$$
$$\frac{\partial \rho}{\partial t} + \rho_0 \text{ div } \mathbf{v} = 0$$

where ρ_0 is density and c_0 is speed of sound in still air.

Say that the curl of v is 0, meaning that there are no eddies in sound and $\mathbf{v}$ is irrotational. From this, we can conclude that ρ and and all components of $\mathbf{v}$ satisfy the wave equation

$$\frac{\partial^2 \mathbf{v}}{\partial t^2} = c_0^2 \Delta \mathbf{v} \text{ and } \frac{\partial^2 \rho}{\partial t^2} = c_0^2 \Delta \rho.$$

In a different system, like some room D with sound-insulated walls, the air molecules can only move parallel to the boundary, so no sound can travel in a normal direction to the boundary. This means that $\mathbf{v} \cdot \mathbf{n} = 0$ on ∂D. We know that there is a function ψ such that $\mathbf{v} = \text{grad } \psi$. The function also satisfies the wave equation

$$\frac{\partial^2 \psi}{\partial t^2} = c_0^2 \Delta \psi$$

where the boundary condition is $-\mathbf{v} \cdot \mathbf{n} = \mathbf{n} \cdot \text{grad } \psi = 0$.

When we have an open window in room D, the atmospheric pressure is constant. The pressure, which we call P, is proportional to the density ρ, so ρ is constant at the window, which in turn means that ρ satisfies the Dirichlet boundary condition $\rho = \rho_0$.

When we have a soft wall, like a membrane stretched across an open window, the pressure difference $P - P_0$ across the membrane is proportional to the normal velocity $\mathbf{v} \cdot \mathbf{n}$. We write this as $P - P_0 = Z\mathbf{v} \cdot \mathbf{n}$ where Z is the acoustic impedance of the wall.

$P - P_0$ is therefore proportional to $\rho - \rho_0$ for small disturbances, so the linearized equations that we listed at the beginning of the "Sound" subsection satisfy the boundary condition $\mathbf{v} \cdot \mathbf{n} = a(\rho - \rho_0)$.

5 Green's Functions

[1] [2] Now that we have covered PDEs and the mathematical basis that we need to properly understand Green's functions

5.1 Green's Identities

To understand Green's functions, we need to consider Green's identities and their applications. Let us start with Green's first identity, which we can derive by applying the one-dimensional product rule in all three directions to get

$$(vu_x)_x = v_x u_x + vu_{xx}, (vu_y)_y = v_y u_y + vu_{yy}, (vu_z)_z = v_z u_z + vu_{zz}.$$

By summing everything up, we get

$$\nabla \cdot (v\nabla u) = \nabla v \cdot \nabla u + v\nabla u.$$

We now use the identity for the divergence of the product of a scalar and a vector field:

$$\nabla \cdot (v\nabla u) = (\nabla v) \cdot (\nabla u) + v(\nabla \cdot \nabla u) = \nabla v \cdot \nabla u + v\Delta u,$$

where $\Delta u = \nabla \cdot \nabla u = u_{xx} + u_{yy} + u_{zz}$ is the Laplacian. This holds pointwise for any scalar functions u and v that have continuous derivatives.

By integrating both sides of the identity above over a domain $D \subset \mathbb{R}^3$, we get

$$\int_D \nabla \cdot (v\nabla x) d\mathbf{x} = \int_{\partial D} v(\nabla u \cdot \mathbf{n}) dS = \int_{\partial D} v\frac{\partial u}{\partial n} dS,$$

where $\mathbf{n}$ is the outward unit normal to the boundary surface ∂D and dS is the surface element. We can plug this back into the earlier equation to get:

Theorem 5.1.

$$\int_{\partial D} v\frac{\partial u}{\partial n} dS = \int_D \nabla v \cdot \nabla u d\mathbf{x} + \int_D v\Delta u d\mathbf{x}.$$

We call this Green's first identity, and it is valid across any function pair u and v and across any solid region D.

We can derive Green's second identity by applying the first identity to (u, v) and (v, u). From the first identity, we know two things:

$$\int_{\partial D} v\frac{\partial u}{\partial n} dS = \int_D \nabla u \cdot \nabla v d\mathbf{x} + \int_D v\Delta u d\mathbf{x}.$$

$$\int_{\partial D} u\frac{\partial v}{\partial n} dS = \int_D \nabla u \cdot \nabla v d\mathbf{x} + \int_D u\Delta v d\mathbf{x}.$$

Theorem 5.2. *Green's second identity is*

$$\int\int\int_D (u\Delta v - v\Delta u) d\mathbf{x} = \int\int_{\partial D} (u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}) dS.$$

By subtracting the two equations above, the $\int_D \nabla u \cdot \nabla v$ terms cancel out, so we now have

$$\int_{\partial D} u\frac{\partial v}{\partial n} dS - \int_{\partial D} v\frac{\partial u}{\partial n} dS = \int_D u\Delta v d\mathbf{x} - \int_D v\Delta u d\mathbf{x}.$$

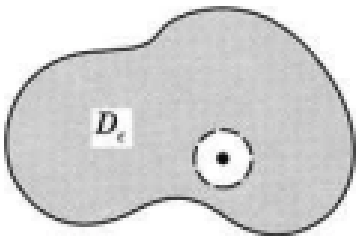

Figure 5. Region D_ϵ with the sphere cut out of it

We can rewrite this as

$$\int_D (u\Delta v - v\Delta u)d\mathbf{x} = \int_{\partial D} (u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n})dS.$$

We call this Green's second identity.

Now that we know Green's two identities, we also need to understand Green's Representation Theorem to be able to properly define what a Green's function is.

Theorem 5.3. *The representation theorem formula can represent any harmonic function as an integral over the boundary. If $\Delta u = 0$ in D, then*

$$u(\mathbf{x}_0) = \int\int_{\partial D} [-u(\mathbf{x})\frac{\partial}{\partial n}(\frac{1}{|\mathbf{x}-\mathbf{x}_0|}\frac{\partial u}{\partial n})]\frac{dS}{4\pi}.$$

Proof: The representation formula we see above is a specific case of Green's second identity where $v(\mathbf{x}) = (-4\pi|\mathbf{x}-\mathbf{x}_0|)^{-1}$. When we do this, we can see that the right side of this specific case of the second identity lines up with the right side of the representation theorem, but the left side clearly does not.

To fix this, we use the fact that the function $v(\mathbf{x})$ us infinite at point $\mathbf{x}_0$. This means that we cannot use Green's second identity on the whole domain D, so imagine we cut out a small ball around $\mathbf{x}_0$. Say that D_ϵ, the region D, has a sphere with center $\mathbf{x}_0$ and radius ϵ cut out of it, as seen in Figure 5. Say that $\mathbf{x}_0$ is the origin, which in turn means that $v(\mathbf{x}) = -\frac{1}{4\pi r}$ where $r = \sqrt{x^2+y^2+z^2} = |\mathbf{x}|$. When we write Green's second identity with the $v(\mathbf{x})$ we specified earlier combined with the fact that $\Delta u = 0 = \Delta v$ in D_ϵ, we have

$$-\int\int_{\partial D_\epsilon} [u\cdot\frac{\partial}{\partial n}(\frac{1}{r}) - \frac{\partial u}{\partial n}\cdot\frac{1}{r}]dS = 0.$$

However, ∂D_ϵ has two parts, the boundary ∂D and the sphere $r = \epsilon$. On the sphere, $\frac{\partial}{\partial n} = -\frac{\partial}{\partial r}$, meaning that the integral splits into two:

$$-\int\int_{\partial D} [u\cdot\frac{\partial}{\partial n}(\frac{1}{r}) - \frac{\partial u}{\partial n}\cdot\frac{1}{r}]dS = -\int\int_{r=\epsilon} [u\cdot\frac{\partial}{\partial r}(\frac{1}{r}) - \frac{\partial u}{\partial r}\cdot\frac{1}{r}]dS.$$

The equation above works for any small $\epsilon > 0$. We can use Green's representation theorem if the right side of the above equation approaches $4\pi u(\mathbf{0})$ as $\epsilon \to 0$. On the sphere's surface, we have

$$\frac{\partial}{\partial r}(\frac{1}{r}) = -\frac{1}{r^2} = -\frac{1}{\epsilon^2}.$$

This means that

$$\frac{1}{\epsilon^2}\int\int_{r=\epsilon} u dS + \frac{1}{\epsilon}\int\int_{r=\epsilon} \frac{\partial u}{\partial r} dS = 4\pi\overline{u} + 4\pi\epsilon\overline{\frac{\partial u}{\partial r}},$$

where $\overline{u}$ is the average value of $u(\mathbf{x})$ on the sphere $|\mathbf{x}| = r = \epsilon$ and $\overline{\frac{\partial u}{\partial r}}$ is the average value of $\frac{\partial u}{\partial n}$ on this sphere.

As ϵ approaches 0, the equation above becomes

$$4\pi u(\mathbf{0}) + 4\pi \cdot 0 \cdot \frac{\partial u}{\partial r}(\mathbf{0}) = 4\pi u(\mathbf{0}).$$

This is because u is continuous and $\frac{\partial u}{\partial r}$ is bounded, so the equation where we split the integral into two pieces now is the same formula as the representation theorem, on both sides,therefore completing the proof. □

5.2 Theorems and Exploration

Now that we have the basis to fully understand and explore Greens' functions, let us look at how we can use Green's functions to analyze the Dirichlet problem. When we looked at the representation theorem, we used the function $v(\mathbf{x}) = (-4\pi|\mathbf{x} - \mathbf{x}_0|)^{-1}$. This function has two important properties, the fact that it is harmonic except at x_0 and the fact that it has a singularity there. We will try to get rid of one of the terms in the representation theorem formula because the resulting function is the Green's function for D.

Definition 5.4. Green's function $G(\mathbf{x})$ for the operator $-\Delta$ and the domain D at point $\mathbf{x}_0 \in D$ is a function for $\mathbf{x} \in D$ such that it satisfies the following conditions:

- $G(\mathbf{x})$ has continuous second derivatives and $\Delta G = 0$ in D except when $\mathbf{x} = \mathbf{x}_0$
- $G(\mathbf{x}) = 0$ for $x \in \partial D$
- $$G(\mathbf{x}) + \frac{1}{4\pi|\mathbf{x} - \mathbf{x}_0|}$$

  is finite at $\mathbf{x}_0$ and it is harmonic at $\mathbf{x}_0$ there are continuous second derivatives everywhere.

We write the Green's function as $G(\mathbf{x}, \mathbf{x}_0)$.

With this definition, here is an important theorem that we can prove using our new knowledge.

Theorem 5.5. *Given some $G(\mathbf{x}, \mathbf{x}_0)$, the solution for the Dirichlet problem is*

$$u(\mathbf{x}_0) = \int\int_{\partial D} u(\mathbf{x}) \frac{\partial G(\mathbf{x}, \mathbf{x}_0)}{\partial n} dS.$$

Proof: We can write the representation formula as

$$u(\mathbf{x}_0) = \int\int_{\partial D} (u\frac{\partial v}{\partial n} - \frac{\partial u}{\partial n}v)dS,$$

where $v(\mathbf{x} = -(4\pi|\mathbf{x}-\mathbf{x_0}|)^{-1}$. By writing $G(\mathbf{x}, \mathbf{x_0}) = v(\mathbf{x}) + H(\mathbf{x})$, we can see that $H(\mathbf{x})$ is a harmonic function across D using the conditions from the definition of the Green's function.

By applying Green's second identity to $u(\mathbf{x})$ and $H(\mathbf{x})$, we get

$$\int\int_{\partial D} (u\frac{\partial H}{\partial n} - \frac{\partial u}{\partial n}H)dS = 0.$$

Adding the two equations of our proof from above, we get

$$u(\mathbf{x}_0) = \int\int_{D} (u\frac{\partial G}{\partial n} - \frac{\partial u}{\partial n}G)dS.$$

But according to the second condition in the definition of the Green's function, G disappears on ∂D, so the last term is gone and we are left with

$$u(\mathbf{x}_0) = \int\int_{\partial D} u(\mathbf{x})\frac{\partial G(\mathbf{x}, \mathbf{x}_0)}{\partial n}dS.$$

□

6 Conclusion and Acknowledgements

There are obviously many, many more applications of the Green's function and PDEs both in mathematics and in real life. We have explored how PDEs affect physical phenomena like waves and diffusion, and we have also seen how they can be used to model mathematical spaces as well. Green's function alone has innumerable uses that are essential to our understanding of physics and many other fields. I would like to thank Simon Rubinstein-Salzedo and Serkan Salik for all the advice they have given me, without which I could not have written this paper.

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