

Everything you Never Wanted to Know about Finite Difference Methods for Solving Partial Differential Equations

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These notes discuss using finite differences to solve physical problems that are expressed using partial differential equations (PDEs). If a PDE cannot be solved analytically, then we approximate the solution by solving it numerically. Finite difference methods are just one way to approximate the solution of PDEs that are *linear*. The solutions are motivated by examples; the PDEs are linear equations. Nonlinear PDEs require different approximation techniques.

Just like the solution to an integral is a family of functions¹, the solution to a PDE is also a family of functions.

To obtain a unique solution to the PDE we can constrain the solution by specifying the *boundary conditions* of the region. and then use these (fixed) boundary values to determine the values of the interior region. These constraints, usually defined as functions, are called the *Dirichlet boundary conditions*.

1 An elliptic partial-differential equation

The Poisson equation is an example of an elliptic partial-differential equation.

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2}(x, y) + \frac{\partial^2 u}{\partial y^2}(x, y) = f(x, y)$$

It is called *elliptic* because of its similarity to the equation for an ellipse: $\frac{x^2}{a^2} + \frac{y^2}{b^2} = r$.

This type of PDE is used to describe time-independent physical problems, such as the steady-state distribution of heat (as temperature) in a plane region.

We want to find the solution to this PDE: the function $u(x, y)$, which denotes the temperature at position (x, y) in the plane; x and y have *physical units*.

If the function $f(x, y) \neq 0$ at x, y , then this positions is a heat source (or sink). When $f(x, y) = 0$ for all interior positions, it means that the interior has no heat sources or sinks:

¹Recall taking integrals: you learned that you had to add a parameter c to the result, called the *constant of integration*. This result represents a *family* of solutions. You make the solution *unique* by substituting a value for c .

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2}(x, y) + \frac{\partial^2 u}{\partial y^2}(x, y) = 0$$

This is called Laplace's equation, and commonly is denoted $\nabla^2 = 0$.

1.1 Physical Problem

Consider a thin metal square plate with dimensions 0.5 meters by 0.5 meters. Two adjacent boundaries are held at a constant 0 deg C. The heat on the other two boundaries increases linearly from 0 deg C to 100 deg C. We want to know what the temperature is at each point when the temperature of the metal has reached steady-state,

2 A parabolic partial-differential equation

A (one-dimensional) parabolic PDE of the form

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

and is used in the study of gas diffusion and often referred to as the *diffusion equation*.

It is called *parabolic* because of its similarity to the parabolic equation: $y = ax^2$ (or, $y - ax^2 = 0$).

If we again use heat as an example, solution to this equation is the function $u(x, t)$, where $u(x, t)$ is the temperature of x at time t .

2.1 Physical Problem

Consider a rod of length l that is perfectly insulated. We want to examine the flow of heat along the rod over time.

The two ends of the rod are held at 0 deg C. We denote heat as temperature, and seek the solution to the equation $u(x, t)$: the temperature of x at time $t > 0$.

3 A hyperbolic partial-differential equation

The one-dimensional *wave equation* is an example of a hyperbolic PDE:

$$\alpha^2 \frac{\partial^2 u}{\partial x^2}(x, t) = \frac{\partial^2 u}{\partial t^2}(x, t)$$

Again, note the similarity to the equation for a hyperbola: $\frac{x^2}{a^2} - \frac{y^2}{b^2} = r$.

3.1 Physical Problem

An elastic string is stretched between two horizontal supports that are separated by length l . The PDE defines vertical displacement of the string at time t . (We are assuming that when we “pluck” the string, it *only* vibrates in one direction.)

4 Finite Differences

We approximate the solution to $u(x, y)$ (and also $u(x, t)$) by only looking at the values at only particular points in the problem space. This is done by constructing a grid. Each point $g_{i,j}$ on the grid (implemented as a 2-dimensional array) represents the approximation of $u(x_i, y_j)$ (and also $u(x_i, t_j)$).

4.1 Elliptic PDEs and Central Differences Method

Using the example elliptic PDE problem:

We seek a solution to

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2}(x, y) + \frac{\partial^2 u}{\partial y^2}(x, y) = f(x, y)$$

where, $a < x < b$, $c < y < d$, and boundary values are defined by some function $g(x, y)$, over all ordered pairs (x, y) that denote the borders.

Choose integers n and m so that the interval $[a, b]$ is partitioned into h equal parts, and interval $[c, d]$ is partitioned into k equal parts. h corresponds to a non-infinitesimal δx , so the smaller the $h(k)$ the better the approximation. (And similarly for k and δy .)

$$x_i = a + ih, 0 \leq i \leq n$$

$$y_j = c + jk, 0 \leq j \leq m$$

(From a programming point of view, i is an index, and x_i is a distance.)

The Taylor series expansion in the variable x about x_i , with just the first term gives the central-difference formula

$$\frac{\partial^2 u}{\partial x^2}(x_i, y_j) = \frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{h^2}$$

and for the variable y about y_j ,

$$\frac{\partial^2 u}{\partial y^2}(x_i, y_j) = \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1}))}{k^2}$$

Using these central difference formulas, the Poisson equation at the points (x_i, y_j) becomes:

$$\frac{u(x_{i+1}, y_j) - 2u(x_i, y_j) + u(x_{i-1}, y_j)}{h^2} + \frac{u(x_i, y_{j+1}) - 2u(x_i, y_j) + u(x_i, y_{j-1}))}{k^2} = f(x_i, y_j)$$

Using this Central Difference formula to calculate every inner grid point $g_{i,j}$, ($1 \leq i \leq n - 1$ and $1 \leq j \leq m - 1$) (which approximates the function $u(x_i, y_j)$) results in the Central Difference Method:

$$2 \left[\left(\frac{h}{k} \right)^2 + 1 \right] g_{i,j} - (g_{i+1,j} + g_{i-1,j}) - \left(\frac{h}{k} \right)^2 (g_{i,j+1} + g_{i,j-1}) = -h^2 f(x_i, y_j)$$

where $g_{i,j}$ is computed for every inner grid cell $1 \leq i \leq n - 1$, $1 \leq j \leq m - 1$. Hence $g_{i,j}$ approximates the function $u(x_i, y_j)$.

(In the Central Differences Figure, $\lambda = h^2/k^2$) If $h = k = 1$ and $f(x, y) = 0$ for all internal grid cells, the formula for $g_{i,j}$ simplifies to:

$$g_{i,j} = \frac{g_{i,j+1} + g_{i,j-1} + g_{i+1,j} + g_{i-1,j}}{4}$$

The truncation error of the Central Difference Method is $O(h^2 + k^2)$.

4.2 Parabolic PDEs: Forward-Difference and Backward-Difference Methods

The Taylor series expansion in t about t_j , with just the first term is the formula

$$\frac{\partial u}{\partial t}(x_i, t_j) = \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{k}$$

and in x about x_i is

$$\frac{\partial^2 u}{\partial x^2}(x, t) = \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j))}{h^2}$$

The resulting difference formula is

$$\frac{g_{i,j+1} - g_{i,j}}{k} - \alpha^2 \frac{g_{i+1,j} - 2g_{i,j} + g_{i-1,j}}{h^2} = 0$$

where $g_{i,j}$ approximates $u(x_i, t_j)$.

Solving for $g_{i,j+1}$ gives

$$g_{i,j+1} = \left(1 - \frac{2\alpha^2 k}{h^2}\right) g_{i,j} + \alpha^2 \left(\frac{k}{h^2}\right) (g_{i+1,j} + g_{i-1,j})$$

This is known as the Forward Difference method. The initial conditions must be defined for all x at $t = 0$. The Forward Difference method is conditionally stable only when h and k are chosen so that $\alpha^2 \frac{k}{h^2} \leq \frac{1}{2}$

The Backward-Difference method is unconditionally stable. We use, instead, the backward-difference formula for $\frac{\partial u}{\partial t}$:

$$\frac{\partial u}{\partial t}(x_i, t_j) = \frac{u(x_i, t_j) - u(x_i, t_{j-1})}{k}$$

By substitution, we get

$$\frac{g_{i,j} - g_{i,j-1}}{k} - \alpha^2 \frac{g_{i+1,j} - 2g_{i,j} + g_{i-1,j}}{h^2} = 0$$

and the difference equation becomes ($\lambda = \alpha^2(k/h^2)$)

$$g_{i,j-1} = (1 + 2\lambda)g_{i+1,j} - \lambda g_{i+1,j} - \lambda g_{i,j-1}$$

Unfortunately for us, it cannot be solved explicitly with an iterative algorithm.

The moral of the story: check first for stability before using Forward Differences.

5 Hyperbolic PDEs and 5-star Difference Equation

The difference equation for

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

subject to the initial conditions

$$u(0, t) = u(l, t) = 0, t > 0 \text{ (boundary values held constant),}$$

$$u(x, 0) = f(x), 0 \leq x \leq l \text{ (initial temperature),}$$

$$\frac{\partial u}{\partial t}(x, 0) = g(x), 0 \leq x \leq l \text{ (initial rate of change)}$$

$$\frac{g_{i,j+1} - 2g_{i,j} + g_{i,j-1}}{k^2} - \alpha^2 \frac{g_{i+1,j} - 2g_{i,j} + g_{i-1,j}}{h^2} = 0$$

where $\lambda = \alpha k/h$.

Solving for $g_{i,j+1}$ gives us

$$g_{i,j+1} = 2(1 - \lambda^2)g_{i,j} + \lambda^2(g_{i+1,j} + g_{i-1,j}) - g_{i,j-1}$$

which requires two previous time steps; and so the initial conditions requires values not just for $t = 0$ but also for $t = 1$.

But the values at $t = 1$ is not a border value! To make a long story short, we use the difference equation

$$g_{i,1} = (1 - \lambda^2)f(x_i) + \frac{\lambda^2}{2}f(x_{i+1}) + \frac{\lambda^2}{2}f(x_{i-1}) + kg(x_i)$$

for $g_{i,1}, 1 \leq i \leq m - 1$ and hope for the best.

6 Solving Laplace's equation

6.1 Jacobi Iteration

Jacobi iteration uses the values from the previous iteration $l - 1$ to compute the value at the current iteration l .

(We assume $h = k = 1$ and $\nabla^2 = 0$.)

$$(g_{i,j})^l = 0.25 [(g_{i-1,j})^{l-1} + (g_{i+1,j})^{l-1} + (g_{i,j-1})^{l-1} + (g_{i,j+1})^{l-1}]$$

Jacobi iteration is an inherently data-parallel algorithm.

6.2 Gauss-Seidel Iteration

If Jacobi is executed sequentially over the grid, i.e.,

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for (int i = 0; i < n; i++)
  for (int j = 0; j < m; j++)
    g[i][j] = ... ;
```

we see that, in iteration l , at $g[i][j]$ we have already computed the values for $g[i-1][j]^l$ and $g[i][j-1]^l$. The values computed in iteration l are “better” than those computed in iteration $l - 1$. Gauss-Seidel uses the “best” values:

$$(GS_{i,j})^l = (g_{i,j})^l = 0.25 [(g_{i-1,j})^l + (g_{i,j-1})^l + (g_{i+1,j})^{l-1} + (g_{i,j+1})^{l-1}]$$

Consequently Gauss-Seidel converges faster. And if it converges faster, it is a good guess that there is less error propagation than with Jacobi.

Gauss-Seidel is an inherently sequential algorithm since it relies on the fact that certain neighboring cells have values. This means we can't use it *as is* for a parallel implementation. Instead we need to use red-black tiling, which works great.

6.3 Gauss-Seidel with SOR Iteration

SOR (Successive Over-Relaxation) takes Gauss-Seidel one step further. The idea is that since the value $g_{i,j}$ in iteration l is better than value $g_{i,j}$ in iteration $l - 1$, give additional weight to the value in iteration l . It's basically a *weighted average*. Notice, also, that SOR actually uses $g_{i,j}^l$; just plain Gauss-Seidel doesn't.

Taking $(GS_{i,j})^l$ from the previous equation,

$$(g_{i,j})^l = \omega(GS_{i,j})^l + (1 - \omega)(g_{i,j})^{l-1}$$

$0 < \omega < 1$ is the relaxation parameter. Typical values for ω range between $0.6 \dots 0.8$.

(You will also see $1 < \omega < 2$, in which case the typical range is $1.25 \dots 1.80$, and often ω is 1.25. In this case you multiply the $l - 1$ value by $(2 - \omega)$ and divide the result by 2).

(For the above central differences we assume $h = k = 1$ and $\nabla^2 = 0$.)

7 Central Differences Iterative Solution

- Choose TOLERANCE
 - Choose n, m ; compute h, k .
 - Compute $\lambda = (h^2/k^2)$
 - Compute $\mu = 2(1 + \lambda)$
2. Initialize the border points with the boundary values; initialize the inner points to 0.
3. Perform either: Jacobi (see 6.1), Gauss-Seidel (see 6.2) or Gauss-Seidel with SOR (see 6.3) iteration using the appropriate differences equation.
4. If this is a steady-state problem, iterate until, for $a < i < b, c < j < d$

$$|(g_{i,j}^l) - (g_{i,j}^{l-1})| \leq TOLERANCE$$

Otherwise, iterate until $t == t_{end}$.

8 Annotated Bibliography

Most of these are “old” books that I’ve accumulated over the years. One thing I’ve found about old books is that they give warm-and-folksy explanations with lots of pictures.

C. Ray Wylie and Louis CV. Barrett. Advanced Engineering Mathematics. 5th Ed. McGraw-Hill NY 1982. *This text was used by the engineering students in GE’s Advanced Engineering Course.*

L. Hopf. Introduction to the Differential Equations of Physics. Dover Publications. 1948. *It’s a Dover book. What more needs to be said?*

Hugh Hildreth Skilling. Fundamentals of Electric Waves. John Wiley & Sons. 1942. *Yup, an oldie that I got years ago at a library book sale. It's one of my warm-and-fuzzy books. It gives such a wonderful explanation of pdes, and you realize that basically everything can be thought of in terms of electricity.*

Probably any numerical analysis or numerical methods book that discusses finite differences.

The following figures graphically depict the various difference methods. Multiply each value by the formula inside the square (should a formula exist).

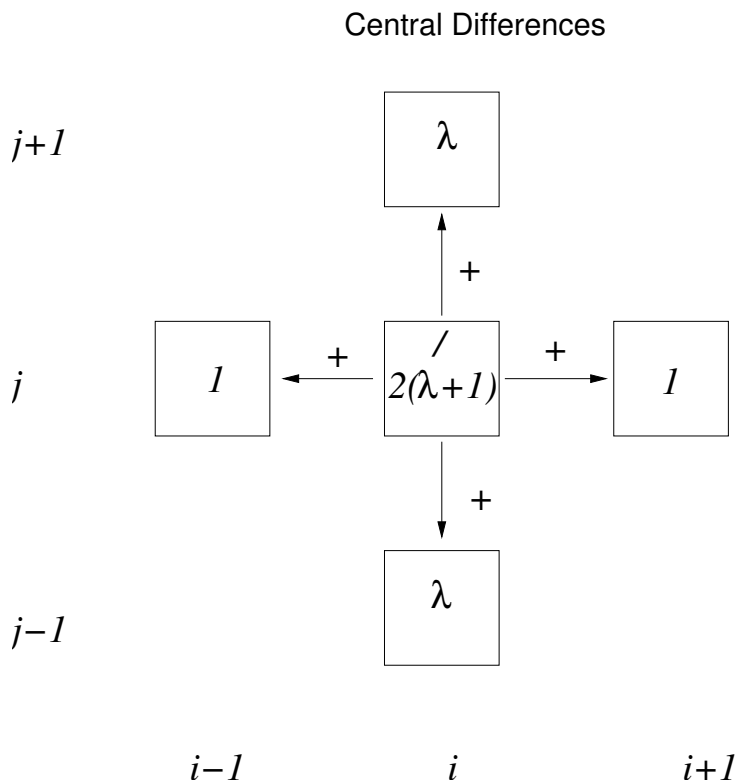


Figure 1: Central Differences Method for Two-Dimensional Elliptic PDE

Forward Differences

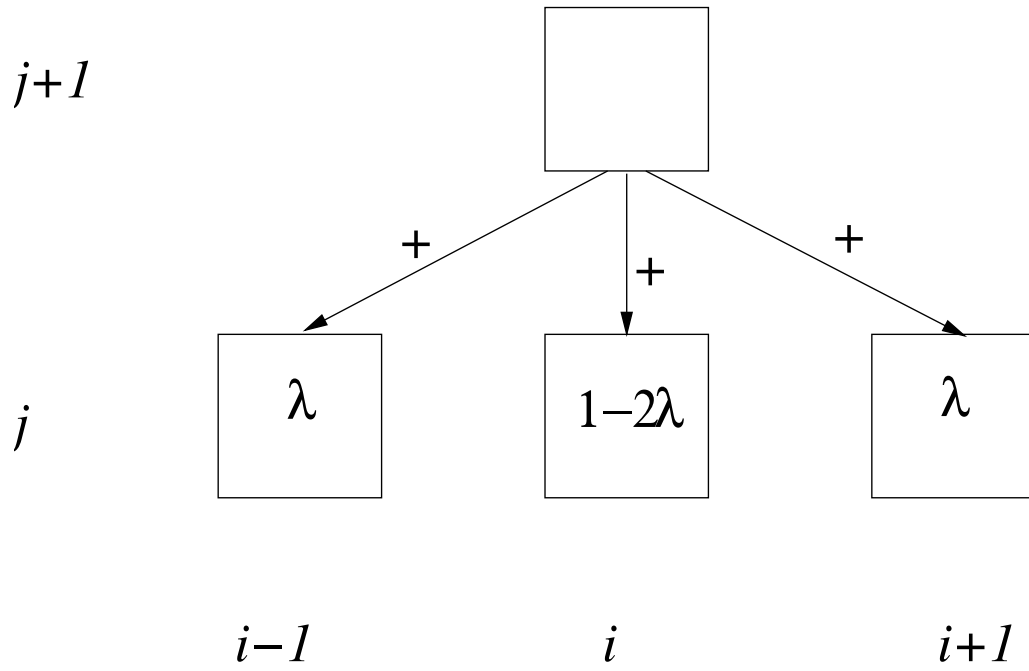


Figure 2: Forward Differences Method for One-Dimensional Parabolic PDE

Higher-Order Differences

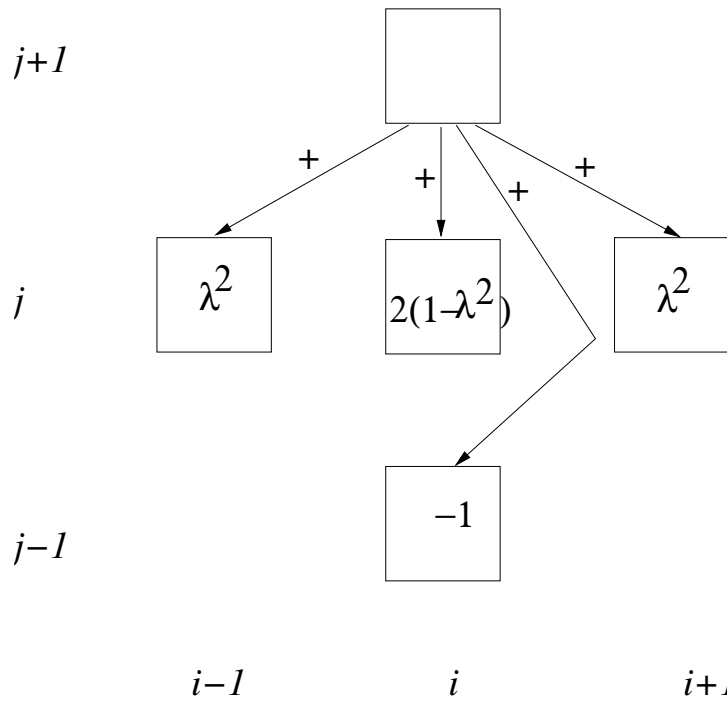


Figure 3: Higher-Order Differences Method for One-Dimensional Hyperbolic PDE