Classification of Partial Differential Equations.

- Parabolic Equation (Diffusion Eq.)
- Hyperbolic Equation (Advection Eq.)
- Elliptic Equation (Poisson Eq.)
  [Multi-Grid Method]

2nd Order Linear Partial Differential Equation

$$A\frac{\partial^2 f}{\partial x^2}+B\frac{\partial^2 f}{\partial x\partial y}+C\frac{\partial^2 f}{\partial y^2}+D\frac{\partial f}{\partial x}+E\frac{\partial f}{\partial y}+Ff+G=0$$

Elliptic	$B^2-4AC<0$
Parabolic	$B^2-4AC=0$
Hyperbolic	$B^2-4AC>0$

Characteristics of the partial differential equation is determined by the highest order derivative term.

Typical Equations

- **Elliptic Equation**
  Poisson Eq.
  (A = C = 1, B = 0)

$$\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y^2}=\rho$$

- **Parabolic Equation**
  Diffusion Eq.
  (A=κ, B = C = 0)

$$\frac{\partial f}{\partial t}=\kappa\frac{\partial^2 f}{\partial x^2}$$

- **Hyperbolic Equation**
  Wave Eq.
  (A = $-c^2$, B = 0, C = 1)

$$\frac{\partial^2 f}{\partial t^2}-c^2\frac{\partial^2 f}{\partial x^2}=0$$

Partial Differential Equation in space

・Boundary Problems (Boundary Conditions)

1D Poisson Eq. $\frac{d^2 f}{dx^2}=\rho=const \quad (0\le x\le 1)$

Boundary Condition : $f(0)=0, \quad f(1)=0$

2D Poisson Eq.

$$\frac{\partial^2 f}{\partial x^2}+\frac{\partial^2 f}{\partial y^2}=\rho=const \quad (x\in S)$$

Boundary Conditions : f is given at the surface - S

Differential Equation in time

- Initial Condition

Time goes in one way

Newton Eq. : $\dfrac{d^2\boldsymbol{r}}{dt^2} = \boldsymbol{F} \qquad (t_0 \le t \le t_1)$

Initial Condition: $\boldsymbol{r}(t_0) = \boldsymbol{r_0}\ , \quad \dot{\boldsymbol{r}}(t_0) = \dot{\boldsymbol{r}}_0$

: $\dfrac{d\boldsymbol{v}}{dt} = \boldsymbol{F}\ , \ \dfrac{d\boldsymbol{r}}{dt} = \boldsymbol{v} \qquad (t_0 \le t \le t_1)$

Initial Condition: $\boldsymbol{r}(t_0) = \boldsymbol{r_0}\ , \quad \boldsymbol{v}(t_0) = \boldsymbol{v_0}$

Partial Differential Equation in time and space

- Initial Boundary Problem

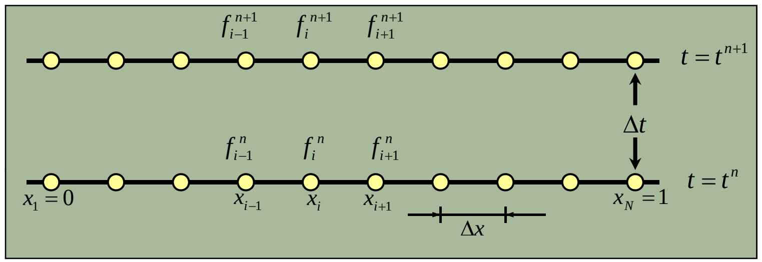
One-dimensional diffusion equation:

$$\frac{\partial f}{\partial t} = \kappa \frac{\partial^2 f}{\partial x^2} \qquad (0 \le x \le 1)$$

Initial Condition: $f(x,0) = f_0(x) \qquad (0 \le x \le 1)$

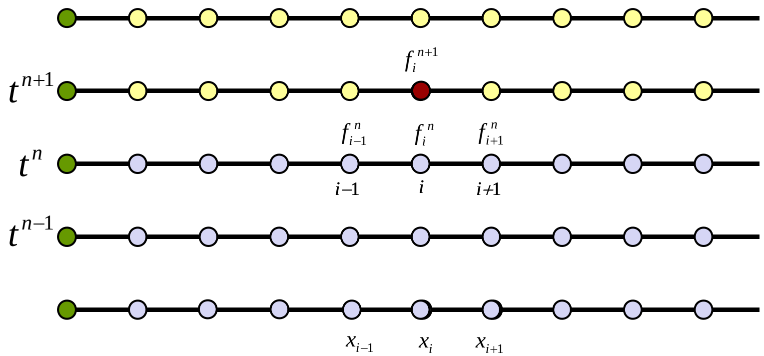
Boundary Condition: $f(0,t) = 0\ , \quad f(1,t) = 0$

Discretization in time and space (Notation)



$f(x_i, t^n) = f_i^n$ $\quad f(x_i + \Delta x,\ t^n + \Delta t) = f_{i+1}^{n+1}$

Time and Space Cone for Information travel



Introduction to finite Difference Method

Finite Difference Approximation

Differential operators are replaced by finite difference expressions

Derivation of finite difference expressions

$$\frac{\partial f}{\partial x} \rightarrow \frac{f_{i+1} - f_i}{\Delta x}$$

Forward Difference

Taylor Expansion Series

$$f(x_i + \Delta x) = f(x_i) + \left.\frac{\partial f}{\partial x}\right|_{x=x_i} \Delta x + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} \Delta x^2 + \frac{1}{6}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^3 + \cdots$$

$$\frac{f_{i+1} - f_i}{\Delta x} = \left.\frac{\partial f}{\partial x}\right|_{x=x_i} + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} \Delta x + \frac{1}{6}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^2 + \cdots$$

$$= \left.\frac{\partial f}{\partial x}\right|_{x=x_i} + O(\Delta x) \qquad (1)$$

The accuracy of the finite difference is the first order of Δx .

Backward Difference

Taylor Expansion Series

$$f(x_i - \Delta x) = f(x_i) - \left.\frac{\partial f}{\partial x}\right|_{x=x_i} \Delta x + \frac{1}{2}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} \Delta x^2 - \frac{1}{6}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^3 + \cdots$$

$$\frac{f_i - f_{i-1}}{\Delta x} = \left.\frac{\partial f}{\partial x}\right|_{x=x_i} - \frac{1}{2}\left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} \Delta x + \frac{1}{6}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^2 + \cdots$$

$$= \left.\frac{\partial f}{\partial x}\right|_{x=x_i} + O(\Delta x) \qquad (2)$$

The accuracy of the finite difference is the first order of Δx .

Central Difference

Subtracting (2) from (1) ,

$$f(x_i + \Delta x) = f(x_i - \Delta x) + 2\left.\frac{\partial f}{\partial x}\right|_{x=x_i} \Delta x + \frac{1}{3}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^3 + \cdots$$

$$\frac{f_{i+1} - f_{i-1}}{2\Delta x} = \left.\frac{\partial f}{\partial x}\right|_{x=x_i} + \frac{1}{6}\left.\frac{\partial^3 f}{\partial x^3}\right|_{x=x_i} \Delta x^2 + \cdots$$

$$= \left.\frac{\partial f}{\partial x}\right|_{x=x_i} + O(\Delta x^2)$$

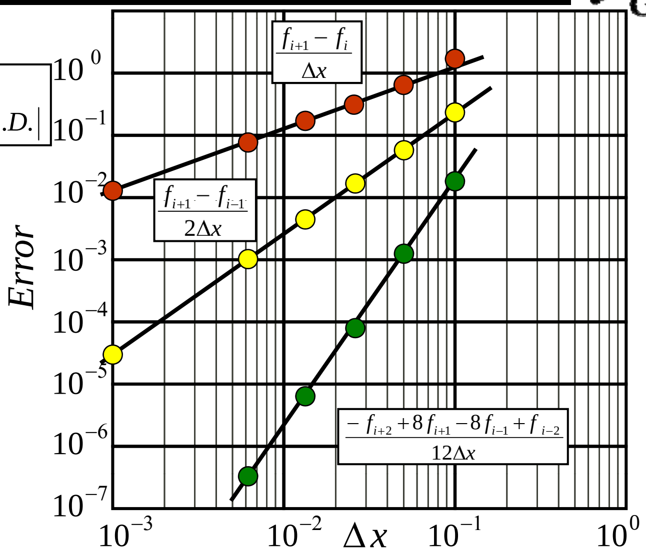
The accuracy of the finite difference is the second order of Δx .

Accuracy of Finite Difference Expressions

$$Error = \left| k_x \cos k_x x_i - F.D. \right|$$

$$k_x = 2\pi$$

$$f_i = \sin k_x x_i$$



Source Code

Typical Finite Difference Expressions for 1st-order derivative

$$\frac{\partial f}{\partial x} = \frac{f_{i+1} - f_i}{\Delta x} \qquad (\Delta x)$$

$$\frac{\partial f}{\partial x} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} \qquad (\Delta x^2)$$

$$\frac{\partial f}{\partial x} = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2\Delta x} \qquad (\Delta x^2)$$

$$\frac{\partial f}{\partial x} = \frac{-f_{i+2} + 6f_{i+1} - 3f_i - 2f_{i-1}}{6\Delta x} \qquad (\Delta x^3)$$

$$\frac{\partial f}{\partial x} = \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12\Delta x} \qquad (\Delta x^4)$$

Finite Difference for 2nd-order derivative

By adding (1) to (2) ,

$$f(x_i + \Delta x) + f(x_i - \Delta x) = 2f(x_i) + \left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} \Delta x^2 + \frac{1}{12}\left.\frac{\partial^4 f}{\partial x^4}\right|_{x=x_i} \Delta x^4 + \cdots$$

$$\frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} = \left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} + \frac{1}{12}\left.\frac{\partial^4 f}{\partial x^4}\right|_{x=x_i} \Delta x^2 + \cdots$$

$$= \left.\frac{\partial^2 f}{\partial x^2}\right|_{x=x_i} + O(\Delta x^2)$$

The accuracy of the finite difference is the second order of Δx .

Typical Finite Difference Expressions for 2nd-order derivative

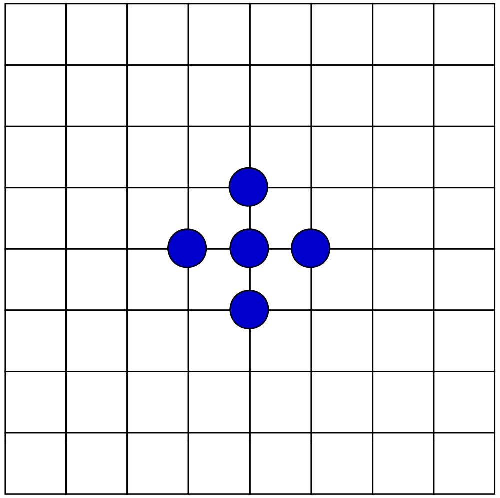
$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+2} - 2f_{i-1} + f_i}{\Delta x^2} \qquad (\Delta x)$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \qquad (\Delta x^2)$$

$$\frac{\partial^2 f}{\partial x^2} = \frac{-f_{i+2} + 16f_{i+1} - 30f_i + 16f_{i-1} - f_{i-2}}{12\Delta x^2} \qquad (\Delta x^4)$$

Game

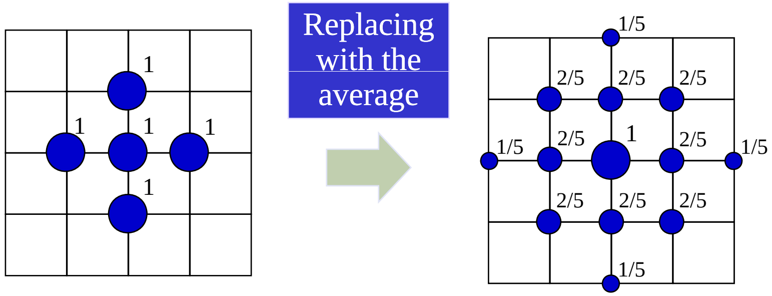
Rule: get a new value by replacing the average about surroundings



Initial

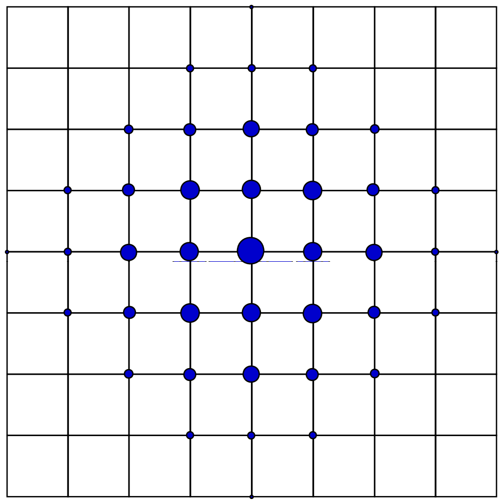
Game

Rule: get a new value by replacing the average about surroundings

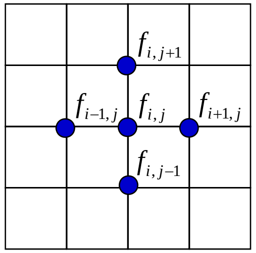


Game

Rule: get a new value by replacing the average about surroundings



Game



***i* : grid index in the *x*-direction**

***j* : grid index in the *y*-direction**

This average process is

$$f^*_{i,j} = \frac{f_{i,j} + f_{i+1,j} + f_{i-1,j} + f_{i,j+1} + f_{i,j-1}}{5}$$

Game

$$f_{i,j}^{n+1} = \frac{f_{i,j}^{n} + f_{i+1,j}^{n} + f_{i-1,j}^{n} + f_{i,j+1}^{n} + f_{i,j-1}^{n}}{5}$$

n : present value

n+1 : the value after average

By subtracting $f_{i,j}$ from both side

$$f_{i,j}^{n+1} - f_{i,j}^{n} = \frac{f_{i+1,j}^{n} - 2f_{i,j}^{n} + f_{i-1,j}^{n} + f_{i,j+1}^{n} - 2f_{i,j}^{n} + f_{i,j-1}^{n}}{5}$$

Game

When we regard $\Delta t = 1.0,\ \Delta x = \Delta y = 1.0,\ \kappa = 1/5,$

$$\frac{f_{i,j}^{n+1} - f_{i,j}^{n}}{\Delta t} = \kappa \frac{f_{i+1,j}^{n} - 2f_{i,j}^{n} + f_{i-1,j}^{n}}{\Delta x^2} + \kappa \frac{f_{i,j+1}^{n} - 2f_{i,j}^{n} + f_{i,j-1}^{n}}{\Delta y^2}$$

2-dimendional diffusion equation

$$\frac{\partial f}{\partial t} = \kappa \left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} \right)$$

Parabolic Equation

1-dimeisional diffusion eq.

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2}$$

κ : diffusion coefficient

Image of diffusion equation: spreading distribution with fading out.

→ Increasing entropy

Particle Collision Process from the microscopic view

Thermal Conduction :	Electron Collision
Viscousity:	Ion Collision
Nuclear Reactor :	Neutron Collision

1-dimensional

Diffusion Equation

$$\frac{\partial \phi}{\partial t} = \kappa \frac{\partial^2 \phi}{\partial x^2}$$

κ : diffusion coefficient

Applying the forward finite difference to the time derivative term and the center finite difference to the spatial difference,

$$\frac{\phi_j^{n+1} - \phi_j^{n}}{\Delta t} = \kappa \frac{\phi_{j+1}^{n} - 2\phi_j^{n} + \phi_{j-1}^{n}}{\Delta x^2}$$

We can reduce to

$$\phi_j^{n+1} = \phi_j^{n} + \mu\left(\phi_{j+1}^{n} - 2\phi_j^{n} + \phi_{j-1}^{n}\right)$$

where $\mu = \frac{\kappa \Delta t}{\Delta x^2}$

Sample Program 1

```
#include "xwin.h"
#define   N   101

int  main() {

     double f[N],  fn[N],  x[N],  mu = 0.25;
     int    j,  icnt = 0;

     while(icnt < 100) {
            for(j=1; j < N-1; j++) {
                fn[j] = f[j] + mu*(f[j+1] - 2.0*f[j] + f[j-1]);
            }
            for(j=0; j < N; j++) f[j] = fn[j];     /* updating */
     }
}
```

Source Code

Stability Analysis (1/3)

von Neumann's Method

Assuming the perturbation $\phi_j^n = \delta\phi^n \mathrm{e}^{ik\cdot j\Delta x}$

Where the notation *i* is the imaginary, *k* is the wave number, *j* is grid index, *j*Δ*x* is the grid position.

Substituting into $\phi_j^{n+1} = \phi_j^n + \mu\left(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n\right)$

$$\delta\phi^{n+1} e^{ik\cdot j\Delta x} = \delta\phi^n e^{ik\cdot j\Delta x} + \mu\left(\delta\phi^n e^{ik\cdot(j+1)\Delta x} - 2\delta\phi^n e^{ik\cdot j\Delta x} + \delta\phi^n e^{ik\cdot(j-1)\Delta x}\right)$$

Stability Analysis (2/3)

***n*+1 step／*n* step : amplitude ratio**

$$\delta\phi_j^{n+1} / \delta\phi_j^n = 1 + \mu\left(e^{-ik\Delta x} - 2 + e^{ik\Delta x}\right)$$
$$= 1 - 2\mu(1 - \cos k\Delta x)$$

$$\cos k\Delta x = \frac{e^{ik\Delta x} + e^{-ik\Delta x}}{2}$$

$\left|\delta\phi^{n+1} / \delta\phi^n\right| < 1$ **: The amplitude of the perturbation decrease in time.**

→ **The calculation is stable.**

Stability Analysis (3/3)

Amplitude ratio: $\delta\phi_j^{n+1} / \delta\phi_j^n = 1 - 2\mu(1 - \cos k\Delta x)$

$\mu < 0$:	unstable,
$0 < \mu < 1/2$:	stable
$1/2 < \mu$:	unstable depending on the value k

We consider only the case of $0 < \kappa$,

$$\mu < \frac{1}{2} \quad \Rightarrow \quad \Delta t < \frac{1}{2}\frac{\Delta x^2}{\kappa}$$

We have to choose Δt satisfying the condition, but Δt should be decrease propotionally to Δx^2 with decrease of Δx.

2-dimendional
Diffusion Equation

$$\frac{\partial f}{\partial t} = \kappa\left(\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}\right)$$

Forward Difference in time $O(\Delta t)$

Central Difference in space $O(\Delta x^2)$

$$\frac{f_{i,j}^{n+1} - f_{i,j}^{n}}{\Delta t} = \kappa\frac{f_{i+1,j}^{n} - 2f_{i,j}^{n} + f_{i-1,j}^{n}}{\Delta x^2} + \kappa\frac{f_{i,j+1}^{n} - 2f_{i,j}^{n} + f_{i,j-1}^{n}}{\Delta y^2}$$

Source Code