High Performance Computing for Science and Engineering

3 October 2014

DIFFUSION – Random Walks and Finite Differences

DIFFUSION

OBSERVATIONS of DIFFUSION

- Soft rinks lose their fizz when CO_2 escapes
- Metabolites flow in and out of cells

Drugs diffuse out of clever encapsulating devices into the body

What is Brownian Motion ?

In 1827, while examining grains of pollen of the plant Clarkia pulchella suspended in water under a microscope, **Brown** observed minute particles, now known to be amyloplasts (starch organelles) and spherosomes (lipid organelles), ejected from the pollen grains, executing a **continuous jittery motion.**

He then observed the same motion in particles of inorganic matter, enabling him to **rule out the hypothesis that the effect was life-related**.

Although Brown did not provide a theory to explain the motion, and Jan Ingenhousz already had reported a similar effect using charcoal particles, in German and French publications of 1784 and 1785,[15] the phenomenon is now known as Brownian motion.

Source: Wikipedia

Brownian Motion

SOURCE: http://www.youtube.com/watch?v=LqVeBxtZbj0&feature=related

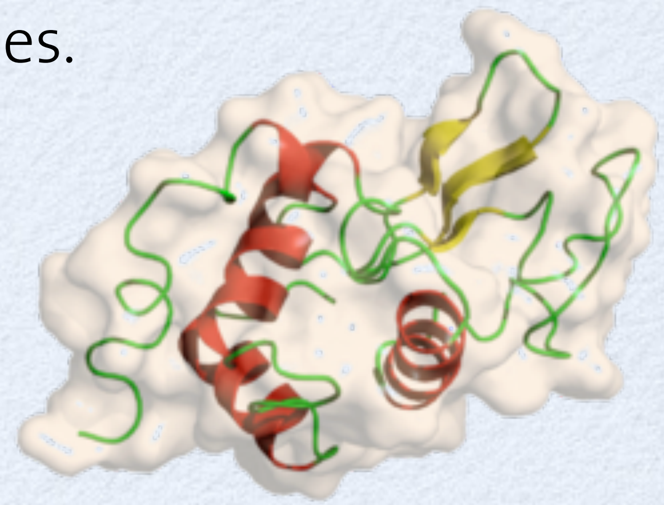
Enter Einstein !

A particle at absolute **temperature of T** has an **average Kinetic Energy** associated with movement in each of its axis of **kT/2.**

Einstein showed in 1905 that this is true irrespective of the size of the particles (Brownian motion)

$<m\,u_x^2> = kT/2$ (particle ensemble averaged over time)

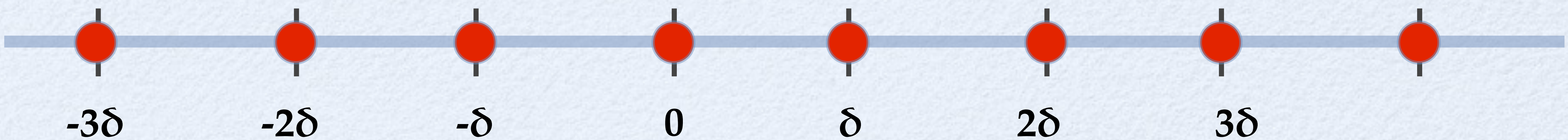
- **EXAMPLE : A molecule of the protein lysozyme**
- Molecular weight $1.4\ 10^4$ g - mass of one mole or $6*10^{23}$ molecules. So 1 molecule has mass $2.3*10^{-20}$ g
- with kT for T=27^o C is $4.14\ *10^{-14}$ g cm^2/sec
- we get $<u_x^2>^{1/2} = 13$ m/sec ~ 47 Km/h
- Molecule can cross the classroom in ~ 1 second
- But it does not ……



Brownian Motion : 2 Key issues

1. Motion is caused by the frequent **impacts** on the pollen grain of the continuously moving molecules of liquid in which it is suspended
2. Motion of these molecules is complicated so that its effect on the gain of pollen can be described only probabilistically in terms of exceedingly **frequent, statistically independent impacts**

A Stochastic Model of Diffusion: 1D Random Walk



ASSUMPTIONS/RULES :

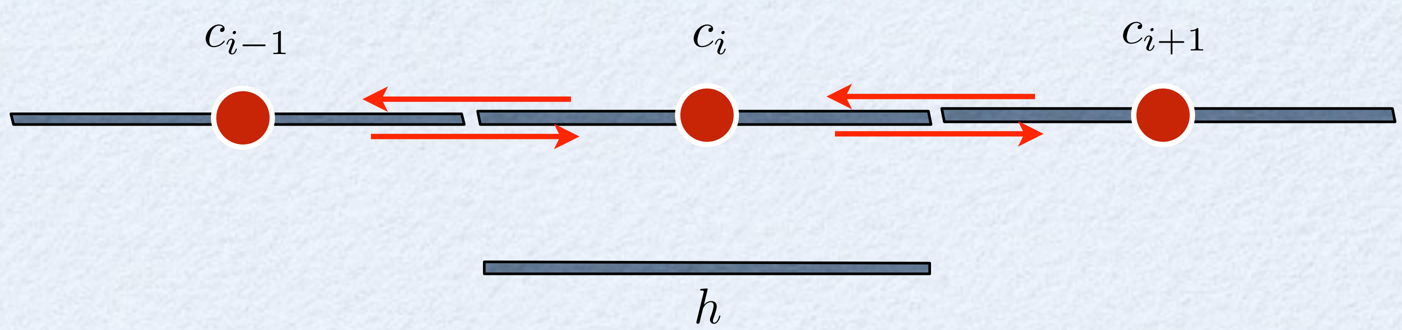
1. Each **particle s**teps to the left or to the right once every τ, moving with a velocity $\pm U$ a distance $\delta = \pm U\tau$ (τ, δ are constants - usually would depend on liquid, particle size, T)
2. The probability of going to the left or to the right is 1/2. Successive steps are independent. The walk is not biased
3. Each Particle moves independent of all other particles

CONSEQUENCES

1. Each Particle goes nowhere (on the average)

3. Root-Mean-Square displacement is proportional to square root of time.

Random Walk in 1D



- A species U, whose elements are labeled by an index i
- Particles start at the Center (t=0,x=0)

$$U_i \xrightarrow{k_{i,i+1}} U_{i+1} \qquad U_{i+1} \xrightarrow{k_{i+1,i}} U_i$$

$$U_i \xrightarrow{k_{i,i-1}} U_{i-1} \qquad U_{i-1} \xrightarrow{k_{i-1,i}} U_i$$

Uniform $\quad k_{i,j} = \frac{1}{2}$

1D Random Walk

According to rule 1 $\boxed{x_i(n) = x_i(n-1) \pm \delta}$

- Mean displacement of particles after the **n-th step**

$$
\begin{aligned}
< x(n) > &= \frac{1}{N} \sum_{i=0}^{N} x_i(n) \\
&= \frac{1}{N} \sum_{i=0}^{N} [x_i(n-1) \pm \delta] \\
&= \frac{1}{N} \sum_{i=0}^{N} x_i(n-1) \\
&=< x(n-1) > = \ \ldots \ =< x(0) > = \ 0
\end{aligned}
$$

Each Particle goes nowhere (on the average)

1D RW (continued)

How much do particles spread ?

$$x_i^2(n) = [x_i(n-1) \pm \delta]^2 = $$
$$= x_i^2(n-1) \pm 2\delta x_i(n-1) + \delta^2$$

- Mean square displacement of particles after the n-th step

$$< x^2(n) > = \frac{1}{N}\sum_{i=0}^{N} x_i^2(n)$$
$$= \frac{1}{N}\sum_{i=0}^{N} [x_i(n-1) \pm \delta]^2$$
$$= \frac{1}{N}\sum_{i=0}^{N} [x_i^2(n-1) \pm 2\delta x_i(n-1) + \delta^2]$$
$$=< x^2(n-1) > + \delta^2 \; =< x^2(n-2) > + 2\delta^2 = \dots$$
$$=< x^2(0) > + n\delta^2 \; = n\delta^2$$

- **Particle Spread** (mean square displacement)

$$\boxed{< x^2(n) > = \frac{t}{\tau}\delta^2 = \frac{\delta^2}{\tau} t}$$

1D RW

Define a diffusion coefficient : $D = \frac{\delta^2}{2\tau}$

$$< x^2 >= 2\,D\,t \;\; \rightarrow \;\; \sqrt{< x^2 >} = l = \sqrt{2Dt}$$

D: characterizes migration of particles of a given kind, in a given medium in a given temperature

e.g. : a small molecule in water in room temperature has D = 10-5 cm^2/sec

No such thing as diffusion velocity as displacement is proportional to square root of time.

Einstein

5. ***Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen;***
von A. Einstein.

In dieser Arbeit soll gezeigt werden, daß nach der molekularkinetischen Theorie der Wärme in Flüssigkeiten suspendierte Körper von mikroskopisch sichtbarer Größe infolge der Molekularbewegung der Wärme Bewegungen von solcher Größe ausführen müssen, daß diese Bewegungen leicht mit dem Mikroskop nachgewiesen werden können. Es ist möglich, daß die hier zu behandelnden Bewegungen mit der sogenannten „Brownschen Molekularbewegung" identisch sind; die mir erreichbaren Angaben über letztere sind jedoch so ungenau, daß ich mir hierüber kein Urteil bilden konnte.

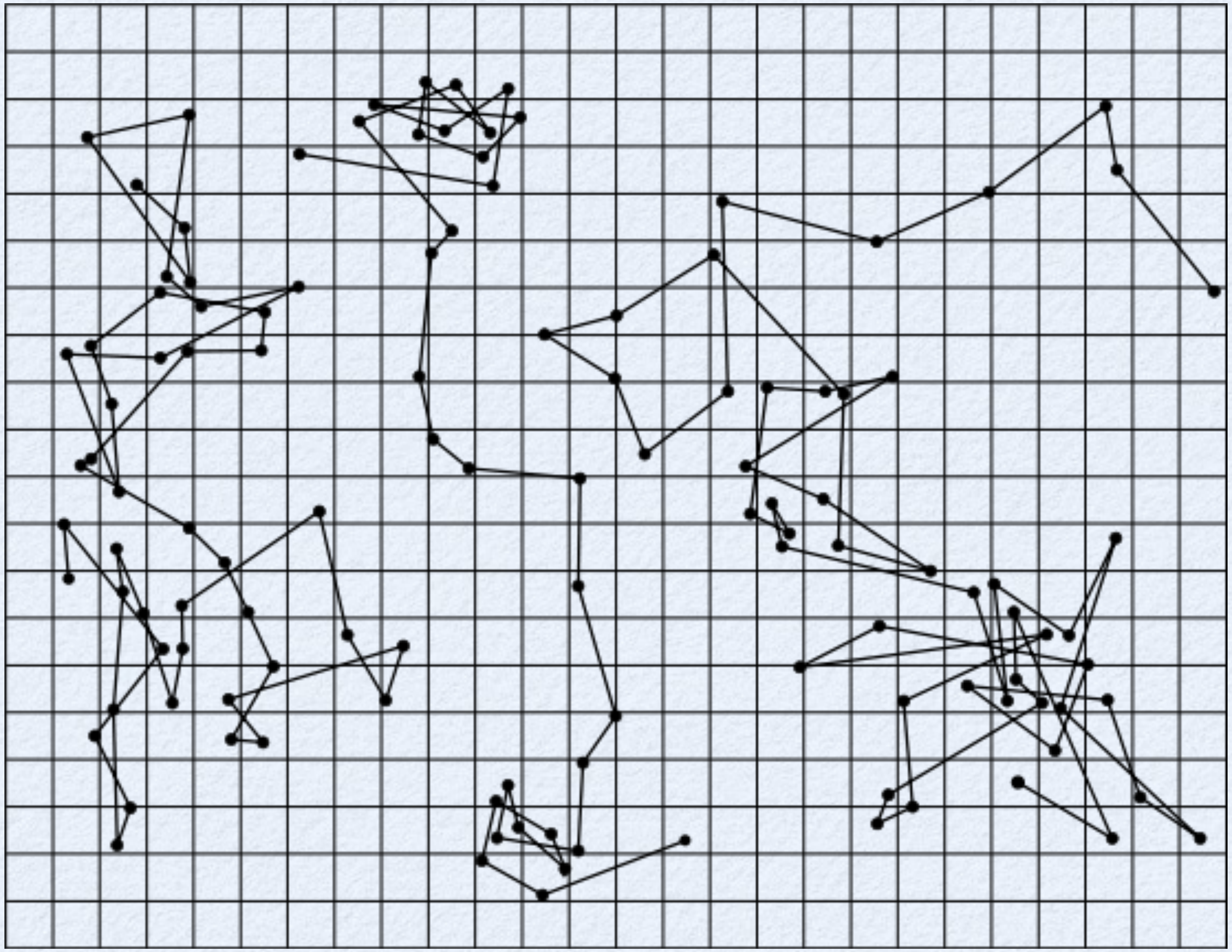
On the movement of small particles suspended in a stationary liquid demanded by the molecular-kinetic theory of heat

In this paper it will be shown that, according to the molecular- kinetic theory of heat, bodies of a microscopically visible size suspended in liquids must, as a result of thermal molecular motions, perform motions of such magnitudes that they can be easily observed with a microscope. It is possible that the motions to be discussed here are identical with so-called Brownian molecular motion; however, the data available to me on the latter are so imprecise that I could not form a judgment on the question...."

Nobel Prize 1926

Jean Perrin

Einstein's statement that thermal molecular motions should be easily observed under a microscope stimulated Jean Perrin to make quantitative measurements, culminating in his book The Atoms in 1909.



Reproduced from the book of Jean Baptiste Perrin, Les Atomes, three tracings of the motion of colloidal particles of radius 0.53 μm, as seen under the microscope, are displayed. Successive positions every 30 seconds are joined by straight line segments (the mesh size is 3.2 μm)

"I did not believe that it was possible to study the Brownian motion with such a precision."
Letter from Albert Einstein to Jean Perrin (1909).

...back to the Einstein paper

Assumption I

Es muß offenbar angenommen werden, daß jedes einzelne Teilchen eine Bewegung ausführe, welche unabhängig ist von der Bewegung aller anderen Teilchen; es werden auch die Bewegungen eines und desselben Teilchens in verschiedenen Zeitintervallen als voneinander unabhängige Vorgänge aufzufassen sein, solange wir diese Zeitintervalle nicht zu klein gewählt denken.

... each individual particle executes a motion which is independent of the motions of all other particles; it will also be considered that the movement of one and the same particle in different time intervals are independent processes, as long as these time intervals are not chosen too small.

Assumption II

Wir führen ein Zeitintervall τ in die Betrachtung ein, welches sehr klein sei gegen die beobachtbaren Zeitintervalle, aber doch so groß, daß die in zwei aufeinanderfolgenden Zeitintervallen τ von einem Teilchen ausgeführten Bewegungen als voneinander unabhängige Ereignisse aufzufassen sind.

We introduce a time interval t into consideration, which is very small compared to the observable time intervals, but nevertheless so large that in two successive time intervals t, the motions executed by the particle can be though of as events that are independent of each other.

...back to the Einstein paper, part 2

Let there be a total of **n** particles suspended in a liquid.

In a time interval t, the X-coordinates of the individual particles will increase by an amount **Δ**, where for each particle **Δ** has a different (positive or negative) value.

There will be a certain **frequency law** for **Δ**; the number **dn** of the particles which experience a shift which is between **Δ** and **Δ+dΔ** will be expressible by an equation of the form:

Seien nun in einer Flüssigkeit im ganzen n suspendierte Teilchen vorhanden. In einem Zeitintervall τ werden sich die X-Koordinaten der einzelnen Teilchen um Δ vergrößern, wobei Δ für jedes Teilchen einen anderen (positiven oder negativen) Wert hat. Es wird für Δ ein gewisses Häufigkeitsgesetz gelten; die Anzahl dn der Teilchen, welche in dem Zeitintervall τ eine Verschiebung erfahren, welche zwischen Δ und $\Delta + d\Delta$ liegt, wird durch eine Gleichung von der Form

$$\frac{dn}{n} = \phi(\Delta)\, d\Delta$$

φ is only different from zero for very small values of **Δ**, and satisfies the condition : **φ(Δ) = φ(-Δ)**

where: $\int_{-\infty}^{\infty} \phi(\Delta)\, d\Delta = 1$

...back to the Einstein paper, part 3

“We now investigate how the diffusion coefficient depends on φ*. We shall once more restrict ourselves to the case where the number* ν *of particles per unit volume depends only on x and t.*

Let **ν = *f(x,t)* be the number of particles per unit volume***. We compute the distribution of particle at the time t +* τ *from the distribution at time t. From the definition of the function* φ*(Δ) it is easy to find the number of particles which at time t+* τ *are found between two planes perpendicular to the x-axis and passing through points x and x + dx. One obtains*

$$f(x, t+\tau) dx = dx \int_{-\infty}^{\infty} f(x+\Delta, t)\phi(\Delta) d\Delta$$

But since t is very small we can set $f(x, t+\tau) \;=\; f(x,t) \;+\; \tau \frac{\partial f}{\partial t}$

Also develop f (x+Δ, t) in powers of Δ:

$$f(x+\Delta, t) \;=\; f(x,t) \;+\; \Delta \frac{\partial f(x,t)}{\partial x} \;+\; \frac{\Delta^2}{2!} \frac{\partial^2 f(x,t)}{\partial^2 x} \;+\; \ldots$$

Diffusion

Recall: $f(x,t+\tau)dx = dx\int_{-\infty}^{\infty} f(x+\Delta,t)\phi(\Delta)d\Delta$

with the expansions becomes:

$$f + \frac{\partial f}{\partial t}\tau \;=\; f(x,t)\int_{-\infty}^{\infty}\phi(\Delta)d\Delta \;+\; \Delta\frac{\partial f(x,t)}{\partial x}\int_{-\infty}^{\infty}\Delta\phi(\Delta)d\Delta \;+\; \frac{\partial^2 f(x,t)}{\partial x^2}\int_{-\infty}^{\infty}\frac{\Delta^2}{2!}\phi(\Delta)d\Delta \;+\; \dots$$

Based on the assumptions we have made for $\phi(\Delta)$ odd terms cancel

setting: $\frac{1}{\tau}\int_{-\infty}^{\infty}\frac{\Delta^2}{2}\phi(\Delta)d\Delta = D$

and keeping only the first and third term of the rhs we obtain

$$\boxed{\frac{\partial f}{\partial t} \;=\; D\frac{\partial^2 f}{\partial x^2}}$$

DIFFUSION: Gradients are eliminated (Fick's law)

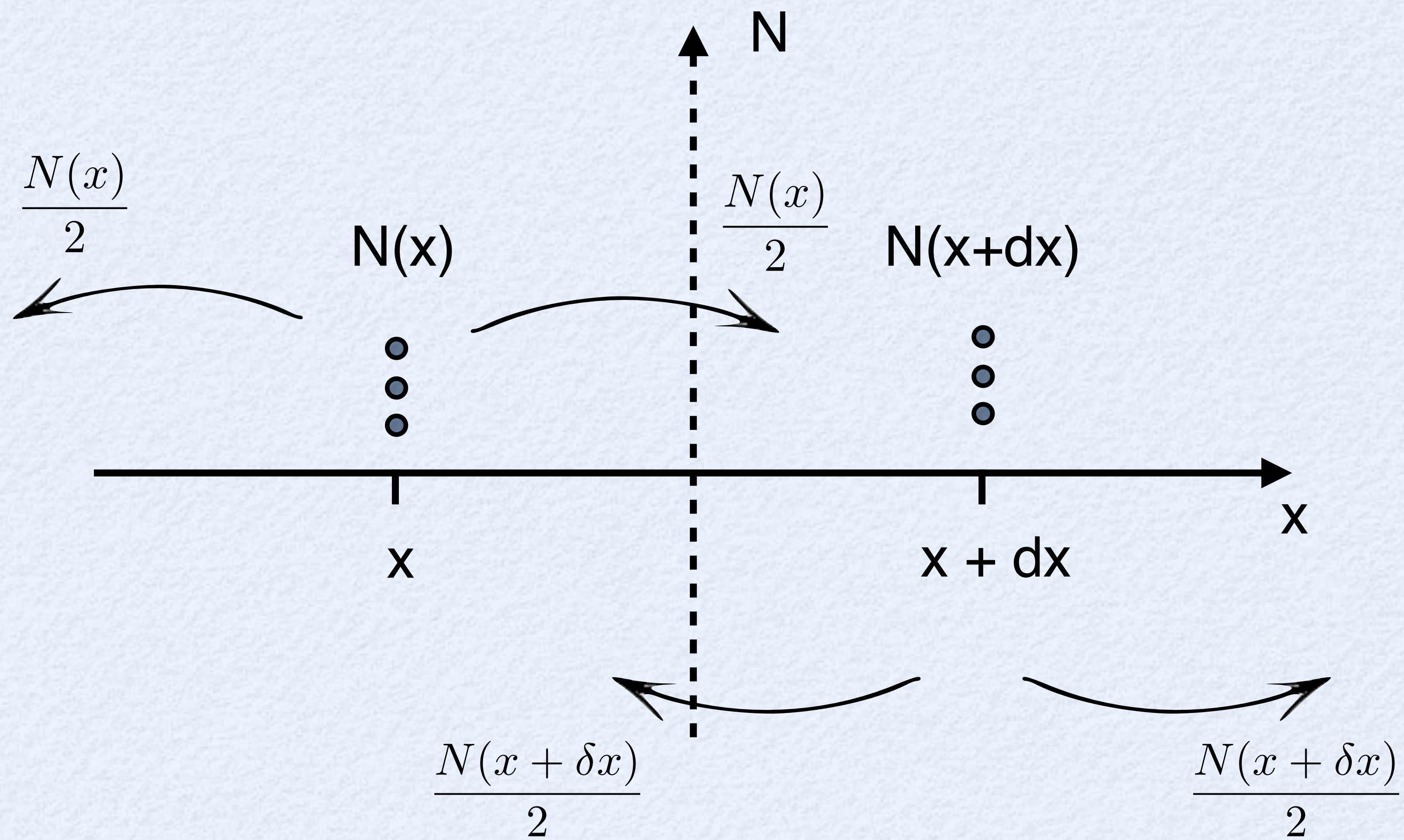
Why do particles move from higher to lower concentrations ?

How does a particle know which direction is downhill ? After all its particle moves independently and randomly.

Reversibility: According to Newton's law the motion of one particle is fully time-reversible and random. Yet when particles move together, they move in a particular direction

Fick's 1st Law

Let **N(x)** the initial **number of particles** at each point on the x-axis



How many particles move in an unit of time across the unit area from point x to point $x + \delta x$? What is the net flux (J_x) in the direction x?

Fick's 1st Law

At time $t + \delta t$ **half** of the particles will cross to the right of x and the other half to the left. The net number crossing to the **right** will be

$$\frac{N(x)}{2} - \frac{N(x+\delta x)}{2} \tag{1.2}$$

To get the flux we divide by area and time interval δt

$$J_x = -\frac{1}{2}\left[N(x+\delta x) - N(x)\right] \cdot \frac{1}{A\delta t} \tag{1.3}$$

Multiply by $\frac{\delta x^2}{\delta x^2}$ to get

$$J_x = -\frac{\delta x^2}{2\delta t} \cdot \frac{1}{\delta x}\left[\frac{N(x+\delta x)}{A \cdot \delta x} - \frac{N(x)}{A \cdot \delta x}\right] \tag{1.4}$$

Fick's 1st Law

We define the quantity $\frac{\delta x^2}{2\delta t} = D$ as the diffusion coefficient and

$$\frac{N(x)}{A \cdot \delta x} = c(x)$$

as the concentration (number of particles per unit volume).

$$J_x = -D\frac{1}{\delta x}[c(x+\delta x) - c(x)] = -D\frac{\partial c}{\partial x}.$$

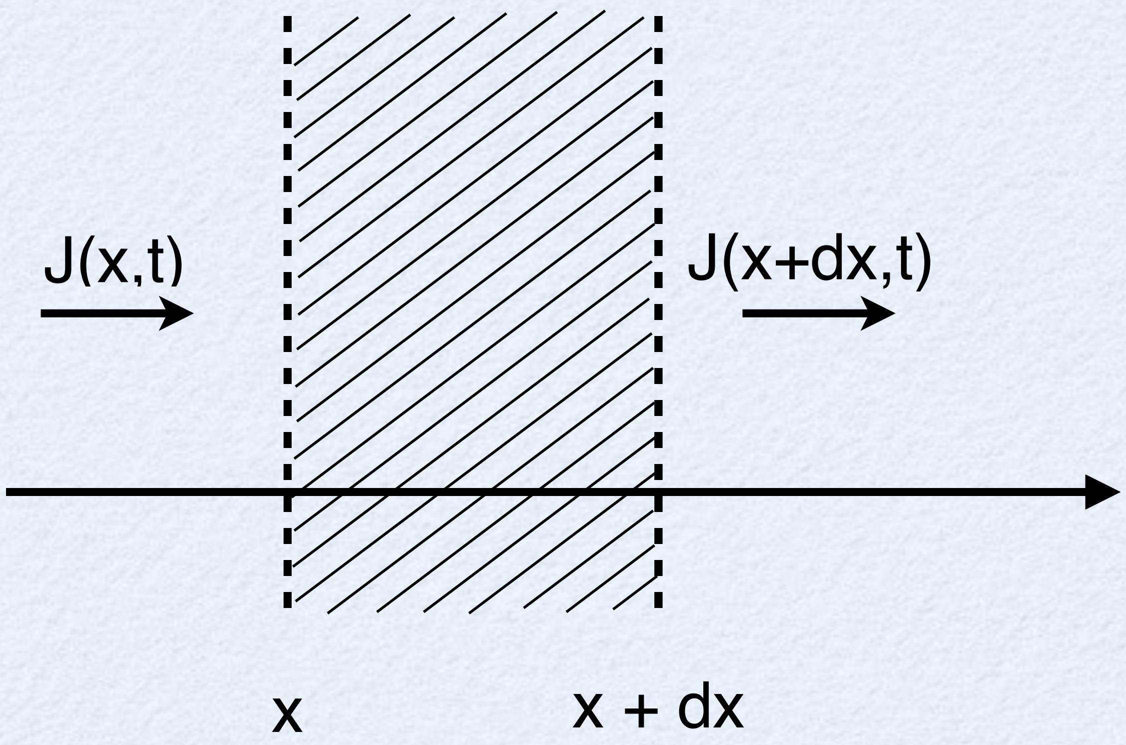
Then with $\delta x \to 0$ we obtain the **Fick's first law:**.

$$\boxed{J_x = -D\frac{\partial c}{\partial x}}$$

Fick's 2nd Law

Conservation of mass (total number of particles conserved). Over time δt

- $J_x A \delta t$ particles enter at x
- $J_x(x + \delta x) A \delta t$ particles leave at $x + \delta x$



Fick's 2nd Law

If particles are neither increased or destroyed then we have a change as

$$\frac{1}{\delta t}[c(t+\delta t)-c(t)]\cdot A\delta x = -\frac{1}{\delta t}[J_x(x+\delta x)-J_x(x)]\cdot A\delta t \quad (1.8$$

$$= -\frac{1}{\delta x}[J_x(x+\delta x)-J_x(x)] \quad (1.9$$

Fick's 2nd Law

Note. $c = \ldots$

$\ldots$ Temperature $\rightarrow$ Heat Transfer (Fourier Law)

$\ldots$ Pollutant concentration $\rightarrow$ Coastal Engineering

$\ldots$ Probability distribution $\rightarrow$ Statistical Mechanics

$\ldots$ Price of an option (Black-Scholes) $\rightarrow$ Financial Engineering

Diffusion on an Infinite Bar

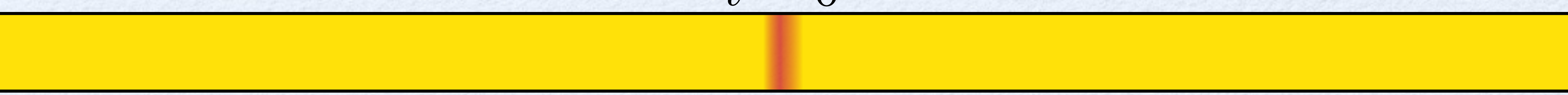
Example 1. Source of heat applied to an infinite bar.
Let

- $t = 0, \; T = Q\delta(x)$
- $x = \pm\infty, \; T = 0 \; \forall t$

for

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2} \tag{1.13}$$

$t = 0$



$t > 0$

Diffusion on an Infinite Bar

Take Fourier Transform:

$$\hat{T}(k,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} T(x,t)e^{-ikx}\,dx \tag{1.14}$$

$$\frac{\partial \hat{T}}{\partial t} = -Dk^2\hat{T} \;\Rightarrow\; \hat{T} = A(k)e^{-Dk^2 t} \tag{1.15}$$

$$t = 0 \;\Rightarrow\; \hat{T} = \frac{Q}{2\pi} \quad \text{(from the initial condition)} \tag{1.16}$$

$$\hat{T} = \frac{Q}{2\pi}e^{-Dk^2 t} \tag{1.17}$$

Invert:

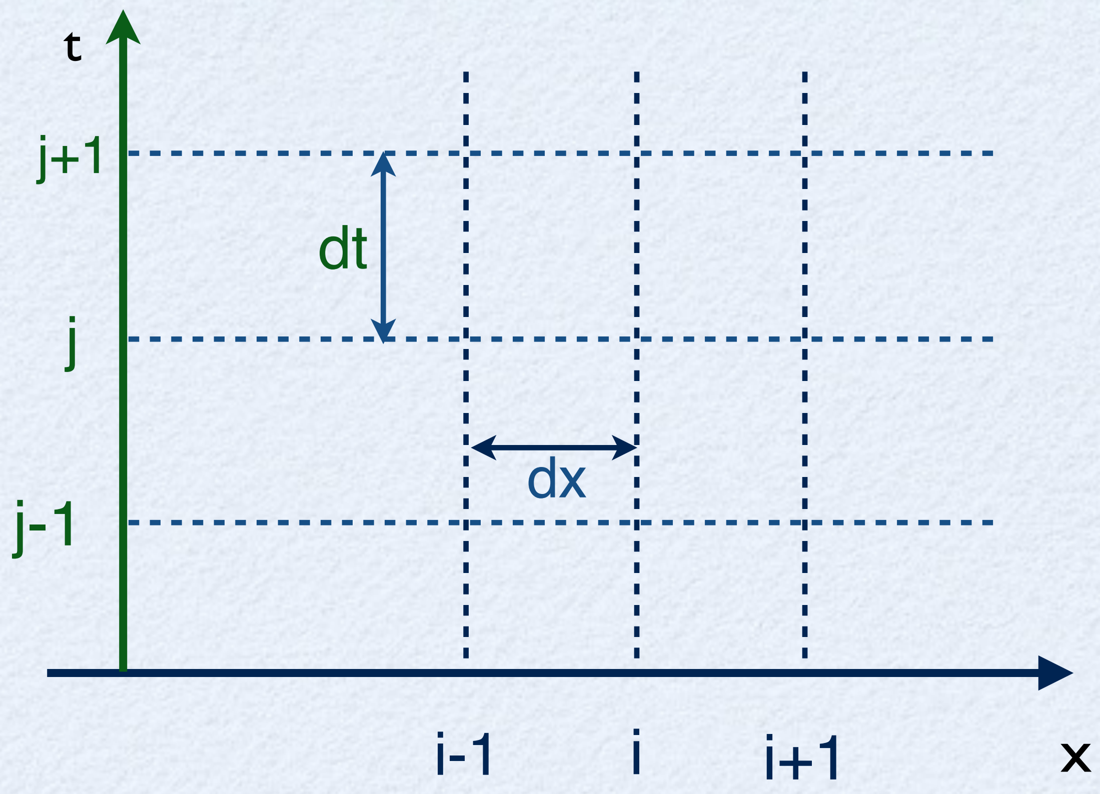
$$\boxed{T = \frac{Q}{2\pi}\int_{-\infty}^{\infty} e^{ikx}e^{-Dk^2 t}\,dk = \frac{Q}{\sqrt{4\pi Dt}}\cdot e^{-\frac{x^2}{4Dt}}} \tag{1.18}$$

Diffusing YET Conserved

Note. $\boxed{\int T(x,t)\, dx = Q \ \forall t}$ (property that must be conserved). This follows from the equation as

$$\int_{-\infty}^{\infty} \frac{\partial T}{\partial t}\, dx = D\left[\frac{\partial T}{\partial x}\right]_{-\infty}^{\infty} = 0 \quad (T \to 0 \text{ as } x \to \infty) \tag{1.19}$$

DIFFUSION AND FINITE DIFFERENCES



Notation: $u(x_i, t_j) = u_{ij}$

Finite difference approximations for a function $y(x)$

$$y(x) = y_i + (x - x_i)y_i' + \frac{(x - x_i)^2}{2}y_i'' + \frac{(x - x_i)^3}{6}y_i''' + \text{h.o.t.} \tag{1.20}$$

Finite Differences: Taylor Series

Now we look for $y(x)$ around (x_i) i.e.

$$y_{i-1} = y_i - \delta x y_i' + \frac{\delta x^2}{2} y_i'' - \frac{\delta x^3}{6} y_i''' + \text{h.o.t.} \tag{1.21}$$

$$y_{i+1} = y_i + \delta x y_i' + \frac{\delta x^2}{2} y_i'' + \frac{\delta x^3}{6} y_i''' + \text{h.o.t.} \tag{1.22}$$

FD – 1st Derivative

How about the first derivative?

- Central difference

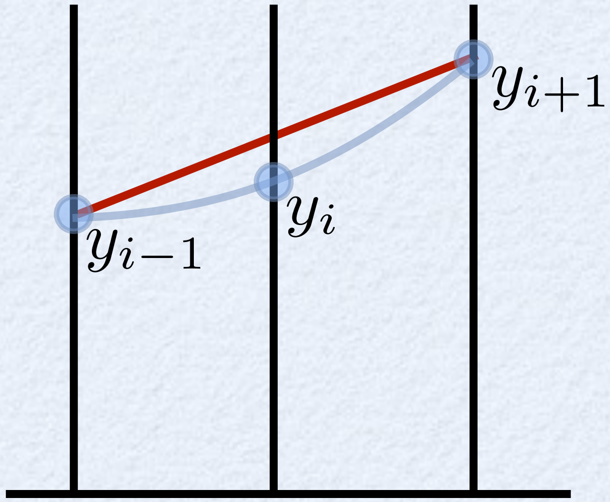
$$y_i' \cong \frac{y_{i+1} - y_{i-1}}{2\delta x} - \underbrace{\frac{\delta x^2}{6} y_i'''}_{\text{error}} \tag{1.25}$$

- Backward difference

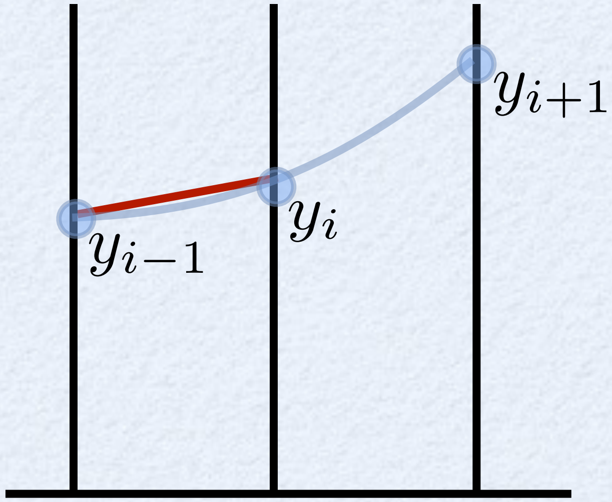
$$y_i' \cong \frac{y_i - y_{i-1}}{\delta x} + \frac{\delta x}{2} y_i'' \tag{1.26}$$

- Forward difference

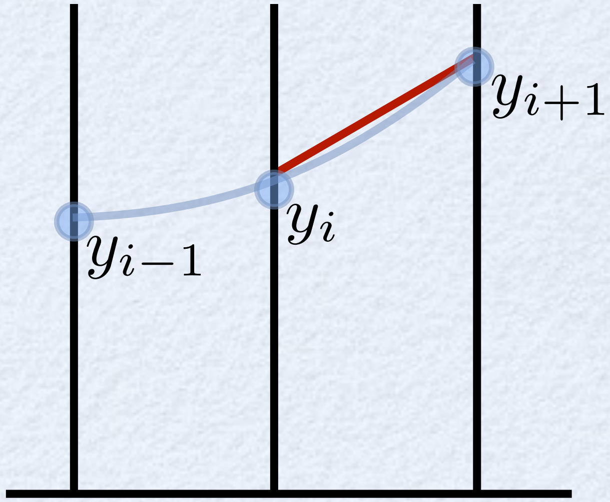
$$y_i' \cong \frac{y_{i+1} - y_i}{\delta x} - \frac{\delta x}{2} y_i'' \tag{1.27}$$



Central difference



Backward difference



Forward difference

1D Diffusion – EXPLICIT FD

Applying Finite Differences to the diffusion equation we get:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{\partial x^2}$$
$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{\delta t}$$
$$\Rightarrow u_{i,j+1} = u_{i,j} + \frac{\nu \delta t}{\delta x^2}(u_{i+1,j} + u_{i-1,j} - 2u_{i,j})$$

where ν is diffusion coefficient.

Diffusion in 1D – IMPLICIT FD

Discretization with finite differences and implicit Euler

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j+1} + u_{i-1,j+1} - 2u_{i,j+1}}{\delta x^2}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{\delta t}$$

$$\Rightarrow u_{i,j+1} = u_{i,j} + \nu \frac{\delta t}{\delta x^2}\left(u_{i+1,j+1} + u_{i-1,j+1} - 2u_{i,j+1}\right)$$

Does it work ? I. von Neumann Stability Analysis

Periodic BC + PDEs with linear, constant coefficients + uniformly spaced grids (limitation!

Key concert in von Neumann analysis:

assume solution in the form:

$$u_j^{(n)} = \rho^n e^{ikx_j}.$$

(

von Neumann Stability Analysis

With $x_{j+1} = x_j + \delta x$ and $x_{j-1} = x_j - \delta x$ we get

$$\rho = 1 + \frac{\nu \delta t}{\delta x^2}\left[2\cos(k\delta x) - 2\right]$$

For stability we must have that $\mid \rho \mid \leq 1$, otherwise solutions grow unbounded.

von Neumann Stability Analysis

$-1 \le 1 + \frac{2\nu\delta t}{\delta x^2}[\cos(k\delta x) - 1]$ can be expressed as

$$2\frac{\nu\delta t}{\delta x^2}[\cos(k\delta x) - 1] \ge -2$$

$$\Rightarrow \delta t \le \frac{\delta x^2}{\nu[1 - \cos(k\delta x)]}$$

Worst case: $\cos(k\delta x) = -1$. So the time step is limited to

$$\boxed{\delta t \le \frac{\delta x^2}{2\nu}}$$

$\Rightarrow$ time step proportional to mesh squared. <- EXPENSIVE

von Neumann Stability Analysis

Summary The von Neumann analysis is an analytical technique that is applied to the full (space-time) discretization of the PDE.
It works when space-dependent terms are eliminated after substituting the wave form. E.g. if $\nu = \nu(x)$ von Neumann would not work.

Tipp Using $\nu(x)|_{max}$ and/or smallest δx would give also some good estimates.

HOW does it work ? The Modified Equation

From central difference approximations we have

$$\frac{\phi_{j+1}^{n} - 2\phi_{j}^{n} + \phi_{j-1}^{n}}{h^2} \approx \frac{\partial^2 \phi_j^n}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4 \phi_j^n}{\partial x^4} \qquad \text{for space}$$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\delta t} \approx \frac{\partial \phi_j^n}{\partial t} + \frac{\partial t}{2}\frac{\partial^2 \phi_j^n}{\partial t^2} \qquad \text{for time}$$

Modified Equation

So applying the finite difference scheme to diffusion equation:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\delta t} = \nu \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{h^2} \tag{1.44}$$

is equivalent to solving the following PDE

$$\frac{\partial \phi}{\partial t} = \nu \frac{\partial^2 \phi}{\partial x^2} \underbrace{- \frac{\delta t}{2} \frac{\partial^2 \phi}{\partial t^2} + \frac{\nu h^2}{12} \frac{\partial^4 \phi}{\partial x^4}}_{(*)} \tag{1.45}$$

Modified Equation

So the truncation term is

$$\boxed{\epsilon \approx \left(\frac{\nu h^2}{12} - \nu^2 \frac{\delta t}{2}\right) \frac{\partial^4 \phi}{\partial x^4}} \tag{1.47}$$

and the error is zero for

$$\nu \delta t = \frac{h^2}{6}. \tag{1.48}$$

When such a choice is made, the method becomes second order in space.

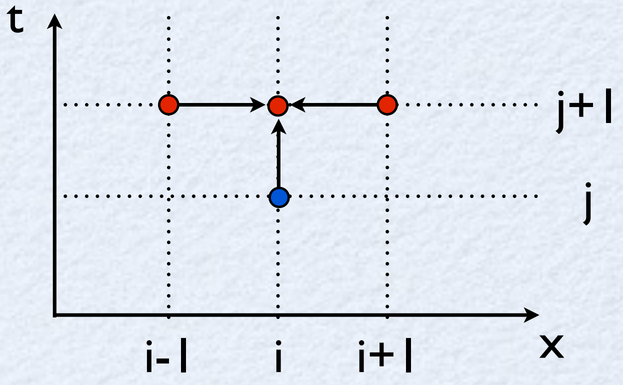
The above scheme is **consistent** i.e., that the discrete equation is equal to the continuum equation in the limit $\delta t \to 0$ & $h \to 0$.

Diffusion in 1D: Solving with FD

Discretization with finite differences and **implicit** Euler

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i+1,j+1} + u_{i-1,j+1} - 2u_{i,j+1}}{\delta x^2}$$

$$\frac{\partial u}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{\delta t}$$



Diffusion in 1D – IMPLICIT FD scheme

Solve a linear system with an nxn matrix

$$\begin{pmatrix} u_{0,j} \\ \vdots \\ u_{i,j} \\ \vdots \\ u_{n,j} \end{pmatrix} = \begin{pmatrix} 1+2\nu\frac{\delta t}{\delta x^2} & -\nu\frac{\delta t}{\delta x^2} & 0 & \cdots & 0 \\ -\nu\frac{\delta t}{\delta x^2} & 1+2\nu\frac{\delta t}{\delta x^2} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1+2\nu\frac{\delta t}{\delta x^2} & -\nu\frac{\delta t}{\delta x^2} \\ 0 & \cdots & 0 & -\nu\frac{\delta t}{\delta x^2} & 1+2\nu\frac{\delta t}{\delta x^2} \end{pmatrix} \begin{pmatrix} u_{0,j+1} \\ \vdots \\ u_{i,j+1} \\ \vdots \\ u_{n,j+1} \end{pmatrix}$$

Assuming 0-dirichlet boundary conditions

Gaussian elimination requires **O(n^3) operations**

Tridiagonal systems

We look now into solving a linear system $Ax = v$

when A is a **tridiagonal** matrix:

$$A = \begin{pmatrix} b_0 & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ a_1 & b_1 & c_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & a_2 & b_2 & c_2 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & a_{n-2} & b_{n-2} & c_{n-2} \\ 0 & 0 & 0 & 0 & \cdots & 0 & a_{n-1} & b_{n-1} \end{pmatrix}$$

Solved very efficiently using the Tridiagonal Matrix algorithm known as **Thomas algorithm** - a special case of Gaussian elimination

Thomas algorithm

We first eliminate the sub-diagonal elements α_i and obtain a new system $Ax' = v'$

$$A' = \begin{pmatrix} b'_0 & c_0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & b'_1 & c_1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & b'_2 & c_2 & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & b'_{n-2} & c_{n-2} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & b'_{n-1} \end{pmatrix}, v' = \begin{pmatrix} v'_0 \\ v'_1 \\ v'_2 \\ \vdots \\ v'_{n-2} \\ v'_{n-1} \end{pmatrix},$$

$$\boxed{\begin{aligned} b'_i &= b_i - c_{i-1}\frac{a_i}{b'_{i-1}}, \; i = 1..n-1 \\ v'_i &= v_i - v_{i-1}\frac{a_i}{b'_{i-1}}, \; i = 1..n-1 \end{aligned}}$$

Thomas algorithm

The new system can be easily solved as follows:

$$\boxed{\begin{aligned} x_{n-1} &= \frac{v'_{n-1}}{b'_{n-1}} \\ x_i &= \frac{1}{b'_i}\left(v'_i - c_i x_{i+1}\right), \; i = (n-2)\,..\,0 \end{aligned}}$$

The solution can be obtained in O(n) operations

Gaussian elimination requires O(n^3) operations

Diffusion: The Crank-Nicholson Method

John Crank
1916-Oct. 3, 2006

Phyllis Nicolson
1917-1968

“His work with Phyllis Nicolson, a near contemporary of his as a student at Manchester University, on the numerical solution of the heat equation sprang from a method for solving this problem which had been proposed by LF Richardson in 1910.

Richardson's method yielded a numerical solution which was very easy to compute, but which was numerically unstable — and thus useless. The instability was not recognised until lengthy numerical computations were carried out by Crank, Nicolson, and others. Crank and Nicolson devised a method which is numerically stable and which turned out to be so fundamental and useful that it is a cornerstone of every discussion of the numerical solution of partial differential equations.

Since its inception, it has been used routinely in computer codes, with applications ranging from **options pricing and oceanography to pattern formation and petrology.”**

SOURCE: http://www.telegraph.co.uk/news/obituaries/1533100/Professor-John-Crank.html

The Crank-Nicolson Method

John Crank
1916-Oct. 3, 2006

Phyllis Nicolson
1917-1968

We have seen that the best way to solve stiff problems in ODEs is through implicit integrators. PDE results in systems of **N-ODEs**. This may be prohibitively expensive in 2D and 3D. It would require inverting large systems of equations $\Rightarrow$ multistep methods prohibitively expensive $\Rightarrow$ use simpler methods.

Trapezoidal rule for time advancement of semi-discretized diffusion equation:

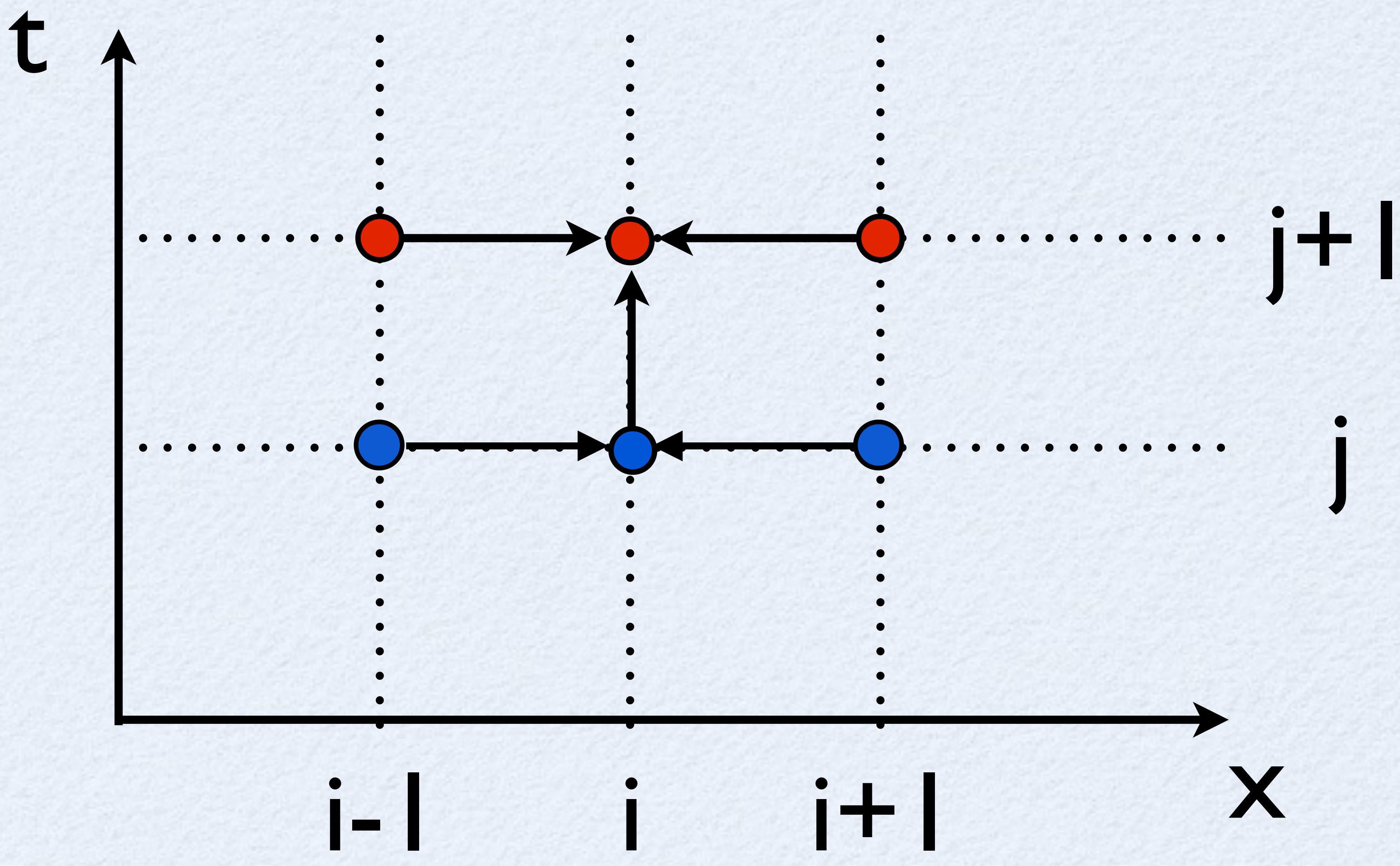
$$\frac{d\phi_j}{dt} = \frac{\nu}{h^2}(\phi_{j+1} - 2\phi_j + \phi_{j-1}),\ j = 1, 2, \ldots, N \tag{1.49}$$

we get

$$\phi_j^{n+1} - \phi_j^n = \frac{\nu \delta t}{2h^2}[(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n) + (\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1})] \tag{1.50}$$

for $j = 1, 2, \ldots, N$.

The Crank-Nicolson Method – IMPLICIT FD scheme



The Crank-Nicolson Method

Set $\alpha = \frac{\nu \delta t}{h^2}$:

$$-\alpha\phi_{j-1}^{n+1} + 2(1+\alpha)\phi_j^{n+1} - \alpha\phi_{j+1}^{n+1} = \alpha\phi_{j-1}^{n} + 2(1-\alpha)\phi_j^{n} + \alpha\phi_{j+1}^{n} \tag{1.51}$$

$$\Rightarrow \boxed{A\phi^{(n+1)} = A'\phi^{(n)}} \tag{1.52}$$

We solve with

$$A = \mathrm{Tr}[-\alpha, 2(1+\alpha), -\alpha] \tag{1.53}$$

$$A' = \mathrm{Tr}[\alpha, 2(1-\alpha), \alpha] \tag{1.54}$$

The system is tridiagonal so the system of equations will be solved in $\mathcal{O}(n)$ operations. We have Cost(CN)$\approx$ 2$\cdot$Cost(Euler). However, CN is an implicit method, and thus it is unconditionally stable.

Note. CN is the method of choice for 1D , in higher dimensions it is expensive.

Modified Equation for CN

Trapezoidal rule is second order with respect to time $t_n + \frac{\partial t}{2} = t_{n+\frac{1}{2}}$, so we make Taylor series expansion around $(x_j, t_{n+\frac{1}{2}})$.
Use already known results for central differences

$$\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{h^2} \approx \frac{\partial^2 \phi^n}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4 \phi_j^n}{\partial x^4} \tag{1.55}$$

$$\frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{h^2} \approx \frac{\partial^2 \phi^{n+1}}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4 \phi_j^{n+1}}{\partial x^4} \tag{1.56}$$

$$\frac{\phi_j^{n+1} - \phi_j^n}{\delta t} \approx \frac{\partial \phi_j^{n+\frac{1}{2}}}{\partial t} + \frac{\delta t^2}{24}\frac{\partial^3 \phi^{n+\frac{1}{2}}}{\partial t^3} \tag{1.57}$$

Modified Equation for CN

We can show:

$$\frac{\psi^{n+1} + \psi^{n}}{2} = \psi^{n+\frac{1}{2}} + \frac{\delta t^2}{8}\frac{\partial^2 \psi^{n+\frac{1}{2}}}{\partial t^2}$$

So applying this to the spatial derivatives we find that the modified equation is:

$$\begin{aligned}\frac{\partial \phi}{\partial t} - \nu\frac{\partial^2 \phi}{\partial x^2} &= -\frac{\delta t^2}{24}\frac{\partial^3 \phi}{\partial t^3} + \nu\left(\frac{\delta t^2}{8}\frac{\partial^2}{\partial t^2}\frac{\partial^2}{\partial x^2} + \frac{h^2}{12}\frac{\partial^4}{\partial x^4}\right)\phi \\ &= \boxed{\frac{\nu}{12}\left(\nu^2 \delta t^2 \frac{\partial^6 \phi}{\partial x^6} + h^2 \frac{\partial^4 \phi}{\partial x^4}\right)}\end{aligned}$$

where we used the heat equation to eliminate t.

Modified Equation for CN

This method is second order accurate and as $h \to 0$ and $\delta t \to 0$ we recover the original PDE $\Rightarrow$ convergence. Convergence $\Rightarrow$ Numerics $\xrightarrow[\delta t \to 0]{h \to 0}$ Exact

Note on the timestep: The ratio of the two error terms in (1.59) are $\frac{\nu^2 \delta t^2}{h^2} \sim h'^2$.
This length scale must be some fraction of the computational region, say $\frac{L}{2} = \frac{Nh}{2}$.

$$\Rightarrow \frac{\nu^2 \delta t^2}{h^2} \sim \frac{N^2 h^2}{4} \Rightarrow \frac{\nu \delta t}{h} \sim \frac{Nh}{2} \Rightarrow \frac{\nu \delta t}{h^2} \sim \frac{N}{2} \qquad \Rightarrow \delta t \sim \frac{N}{2} \frac{h^2}{\nu} \text{ (very generous)} \tag{1.60}$$

Note. CN is the method of choice for 1D but it is somewhat difficult to extend to more than one dimension.

Fourier Analysis of CN

We do a Von Neumann Stability Analysis for the Crank-Nicholson method.
Assume a solution: $\phi_j^n = \phi^n e^{ikx_j}$ and substitute it into (1.50) to obtain

$$\rho = \frac{\phi^{n+1}}{\phi^n} = \frac{(1-2\alpha) + 2\alpha \cdot \cos(k\delta x)}{(1+2\alpha) - 2\alpha \cdot \cos(k\delta x)}. \tag{1.61}$$

ρ is always < 1 and $\rho_{\min} = \frac{1-4\alpha}{1+4\alpha}$ for $k\delta x = \pi$.
As $\alpha > 0$ the value is never smaller than -1, so the method is unconditionally stable.
Recall that $\alpha = \frac{\nu \delta t}{h^2}$.

2D Diffusion and Finite Differences

Given equation

$$\frac{\partial \phi}{\partial t} = \nu \left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} \right) = \nu \nabla^2 \phi$$

Using central differences for the spatial derivatives we obtain

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{\partial^2 \phi}{\partial x_1^2} \approx \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{h_1^2} = \left. \frac{\delta^2 \phi}{\delta x_1^2} \right|_{i,j}$$

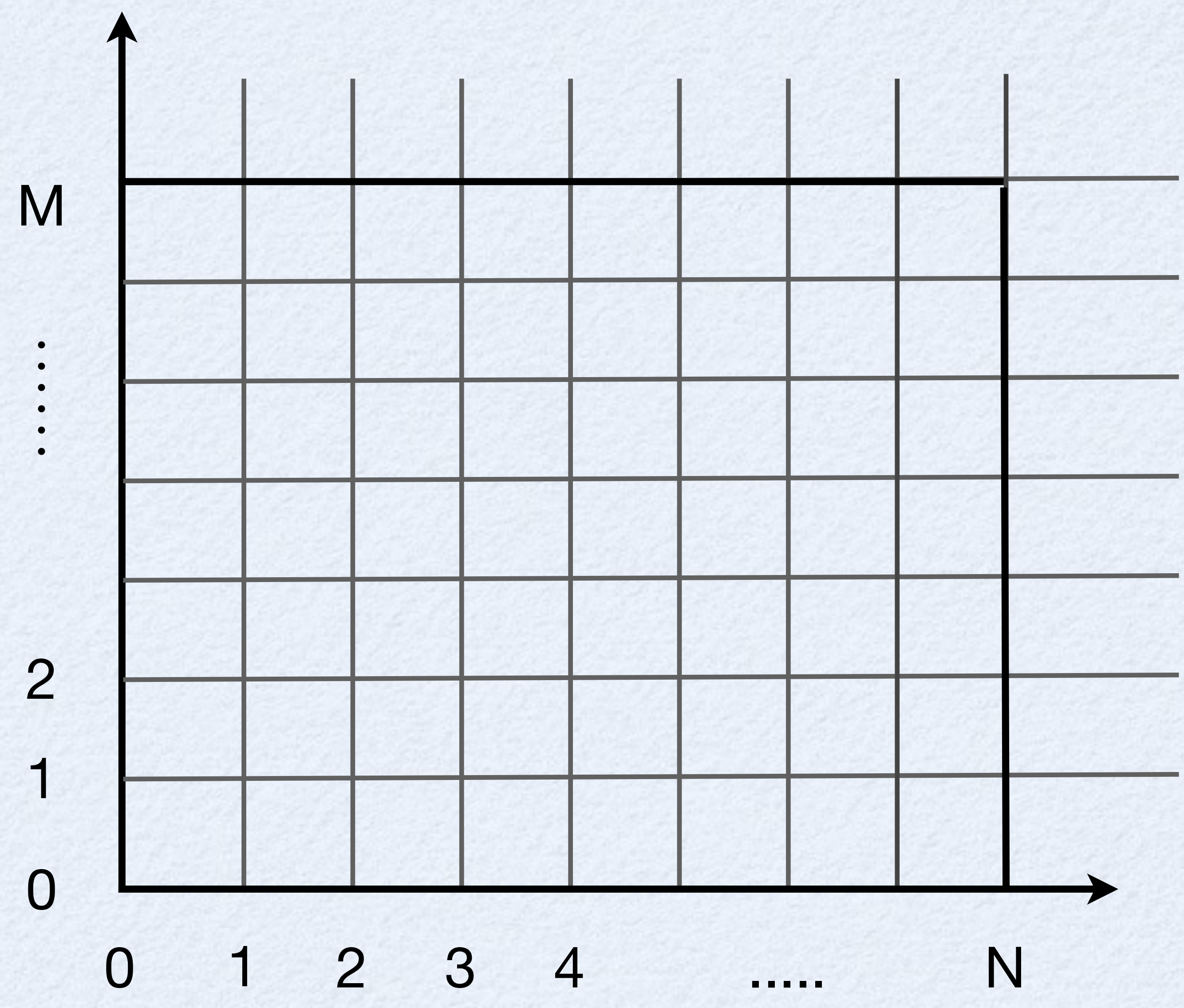
$$\frac{\partial^2 \phi}{\partial y^2} = \frac{\partial^2 \phi}{\partial x_2^2} \approx \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{h_2^2} = \left. \frac{\delta^2 \phi}{\delta x_2^2} \right|_{i,j}$$

$$\Rightarrow \frac{\partial \phi}{\partial t} = \nu \left(\frac{\delta^2 \phi}{\delta x_1^2} + \frac{\delta^2 \phi}{\delta x_2^2} \right)$$

$$\phi = (\phi_{1,1}, \phi_{1,2}, \ldots, \phi_{1,M}, \phi_{2,1}, \ldots, \phi_{N,M})^T$$

2D Diffusion and Finite Differences

Leftmost elements in space → topmost elements in vector
M interior points in x_2 and N interior points in x_1 and rectangular region.



2D Diffusion and Finite Differences

So the matrix of size $MN \times MN$ becomes

$$\begin{bmatrix}
-2\left(\frac{1}{h_1^2}+\frac{1}{h_2^2}\right) & h_2^{-2} & 0 & \cdots & 0 & h_1^{-2} & 0 & 0 & \cdots \\
h_2^{-2} & -2\left(\frac{1}{h_1^2}+\frac{1}{h_2^2}\right) & h_2^{-2} & \cdots & 0 & 0 & h_1^{-2} & 0 & \cdots \\
0 & h_2^{-2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \ddots & & & & & & \\
0 & 0 & \ddots & & & & & & \\
h_1^{-2} & 0 & & & & & & & \\
0 & h_1^{-2} & & & & & & & \\
0 & 0 & & & & & & & \\
\cdots & \cdots & & & & & & &
\end{bmatrix} \tag{1.67}$$

Only five diagonals of this $MN \times MN$-matrix contain non-zero elements. Two of the diagonals are very far from the main diagonal $\rightarrow$ **block-tridiagonal matrix**.

Gauss Elimination $\sim NM^3$
Hence the cost per grid point for 2D would have been more than M^2 more expensive that in 1D (M^4 in 3D).

Peaceman-Rachford Methods

Key Ideas :

- Treat one direction **implicitly** (small matrix) and the other **explicitly** (small time step). Methods of this kind are ***conditionally unstable.***
- **Reverse Roles** for the directions **at each half time step**. The method is ***unconditionally stable*** over the whole step.

Peaceman-Rachford: Alternating Direction Implicit

Step 1 x_1 direction: Backward Euler
x_2 direction: Explicit Euler

$$\phi_{i,j}^{n+\frac{1}{2}} = \phi_{i,j}^{n} + \frac{\nu \delta t}{2}\left[\frac{\delta^2 \phi_{i,j}^{n+\frac{1}{2}}}{\delta x_1^2} + \frac{\delta^2 \phi_{i,j}^{n}}{\delta x_2^2}\right] \tag{1.77}$$

Step 2 x_1 direction: Explicit Euler
x_2 direction: Backward Euler

$$\phi_{i,j}^{n+1} = \phi_{i,j}^{n+\frac{1}{2}} + \frac{\nu \delta t}{2}\left[\frac{\delta^2 \phi_{i,j}^{n+\frac{1}{2}}}{\delta x_1^2} + \frac{\delta^2 \phi_{i,j}^{n+1}}{\delta x_2^2}\right] \tag{1.78}$$

- Each step is second order in space, first order in time and conditionally stable.
- The full method is second order in space and time and unconditionally stable.

Peaceman-Rachford (ADI)

We can add the previous two equations to obtain

$$\phi_{i,j}^{n+1} - \phi_{i,j}^{n} = \nu \delta t \left[\frac{\delta^2 \phi_{i,j}^{n+\frac{1}{2}}}{\delta x_1^2} + \frac{1}{2} \left(\frac{\delta^2 \phi_{i,j}^{n}}{\delta x_2^2} + \frac{\delta^2 \phi_{i,j}^{n+1}}{\delta x_2^2} \right) \right] \tag{1.79}$$

which shows that the overall method is equivalent to treating x_1 by the midpoint rule and x_2 by the trapezoidal rule. Both methods are second order accurate for the time integration.

Diffusion in 3D

Since events in x, y and z direction happen independently, the diffusion equation in three dimensions is:

$$\boxed{\frac{\partial c}{\partial t} = D\left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2}\right)} \tag{1.12}$$

FFTs + PDEs

EXAMPLE 1 : COLLOCATION for Non-linear Advection

Non-Linear Advection $$\frac{\partial u}{\partial t} + c(x)\frac{\partial u}{\partial x} = 0$$ with periodic boundary conditions and the initial condition u(x,0) = q(x)

COLLOCATION METHODS :

$$u(x_j) = \sum_{k=0}^{N-1} u_k \, C_k \, (x_j), \quad j = 0, \ldots, N-1$$

LEAPFROG TIME INTEGRATION :

$$u_j^{n+1} = u_j^n - 2\,\delta t\, c(x_j) \sum_{k=0}^{N-1} u_k^n \, C_{k,x} \, (x_j), \quad j = 0, \ldots, N-1$$

Much more accurate than a 3 point FD but much more expensive -~ O(N**2) per time step

EXAMPLE 1 : COLLOCATION for Non-linear Advection

ENTER THE FOURIER TRANSFORM

$$\frac{\partial u}{\partial t} + c(x)\frac{\partial u}{\partial x} = 0$$

with periodic boundary conditions and the initial condition u(x,0) = q(x)

COLLOCATION METHODS : Compute the derivative via Fourier Transforms

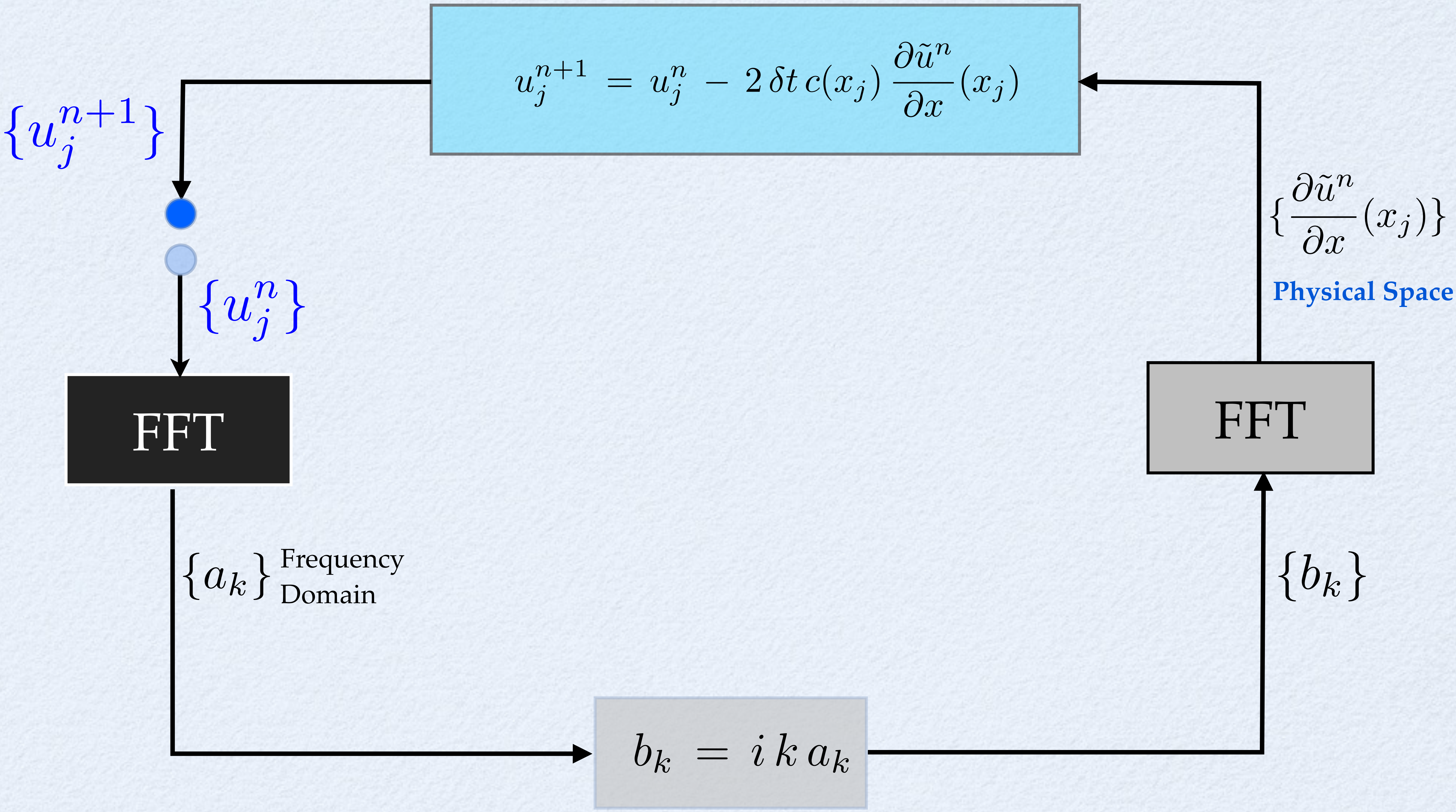
$$\frac{\partial \tilde{u}}{\partial x} = \sum_{k=-\infty}^{\infty} ik\,\hat{u}_k\,e^{ikx}$$

LEAPFROG TIME INTEGRATION + FOURIER SERIES:

$$u_j^{n+1} = u_j^n - 2\,\delta t\,c(x_j)\,\frac{\partial \tilde{u}^n}{\partial x}(x_j), \quad j = 0,\ldots,N-1$$

Much more accurate than a 3 point FD and NOT more expensive -~ O(N) per time step

Leapfrog/Pseudospectral Method for Non-linear Advection



Example 2: the Diffusion Equation

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

periodic boundary conditions

Finite Differences : IMPLICIT in time/Central in Space

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

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

$$i = 1, 2, \ldots M - 1 \text{ and } j = 1, 2, \ldots N - 1$$

System for $(N-1) \times (M-1)$ unknowns:
often too large to solve directly with linear algebra solvers

FFTs for Diffusion Eq. with PBCs

$$\frac{\partial\phi}{\partial t} = \nu\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right)$$ periodic boundary conditions

Assuming ϕ periodic:

(1) Represent ϕ using a two dimensional Fourier Series - get $\hat{\phi}$
(2) form the second derivatives of ϕ by multiplying $\hat{\phi}$ by $-k_1^2$ and $-k_2^2$
(3) Discretize Implicitly in time

Results in an algebraic equation for $\hat{\phi}^{n+1}$:

$$(1 + \nu\delta t(k_1^2 + k_2^2)\hat{\phi}^{n+1}_{k_1,k_2} = \hat{\phi}^{n}_{k_1,k_2}$$

(4) Solve for $\hat{\phi}^{n+1}$
(5) Take the inverse Fourier transform to get ϕ^{n+1}

Leapfrog/Pseudospectral Method for Diffusion