Computational Physics

Basic Equations of MHD

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{v}) = 0, \quad \frac{\partial(\rho\vec{v})}{\partial t} + \nabla\cdot\left[\rho\vec{v}\vec{v} - \vec{B}\vec{B} + P^*\right] = 0, \quad \frac{\partial E}{\partial t} + \nabla\cdot\left[\left[E+P^*\right]\vec{v} - \vec{B}(\vec{B}\cdot\vec{v})\right] = 0,$$

$$P^* = P + \frac{\vec{B}\cdot\vec{B}}{2} \qquad E = \frac{P}{\gamma-1} + \rho\frac{(\vec{v}\cdot\vec{v})}{2} + \frac{\vec{B}\cdot\vec{B}}{2}$$

What can a computer do? $+, -, \div, \times$

need to convert $\int, \frac{d}{dq}, \frac{\partial}{\partial q}, \vec{\nabla}, \vec{\nabla}\cdot, \vec{\nabla}\times \rightarrow +, -, \div, \times$

Basics → Bit yes/no, True/False, 0/1

Byte → 8 bits 8 yes or no

Single → 32 bits, 4 bytes → 7 digits $3.4\cdot10^{38}$

double → 64 bits 8 bytes → 15 digits $1.8\cdot10^{308}$

Example above $\rho, \vec{v}, \vec{B}, E, P$ → 9 Variables 36 and 72 bytes to store 1 grid points.

Problems are solved on grids

1D 512 array 36,864 bytes 1 time step, 36,864,000 bytes 1000 steps

2D ~ 18.9 giga bytes

3D ~ 9.7 Tera bytes

gridding, data storage important AMR

0 – 0 $\quad$ 1 – 1 (2^0) $\quad$ 2 – 10 (2^1+0) $\quad$ 3 – 11 (2^1+2^0) $\quad$ 8 – 1000 ($2^3+0+0+0$)

$125_{10} \to 1\cdot 10^2 + 2\cdot 10^1 + 5\cdot 10^0$

$125_2 \to 1111101 \to 2^6+2^5+2^4+2^3+2^2+0+2^0 = 64+32+16+8+4+0+1 = 125$

Fractions? $\frac{1}{3} \approx .01010101$

$0+\frac{1}{2^2}+0+\frac{1}{2^4}+0+\frac{1}{2^6}+0+\frac{1}{2^8} = \frac{1}{4}+\frac{1}{16}+\frac{1}{64}+\frac{1}{256} = .332031$ in Single

$\neq \frac{1}{3}$ rounding error. Only numbers of the form $\sum \frac{1}{2^n}$ are exact $\quad$ Error

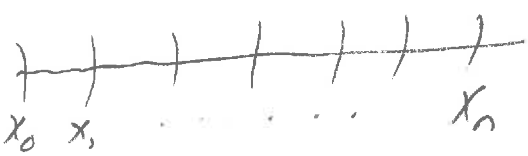
non integers are generally NOT exact.

Lets Start how to go from $\frac{dF}{dx}$ to $+, -, \div, \times$

$$\frac{dF}{dx} = \lim_{h\to 0} \frac{F(x+h)-F(x)}{h} \quad \text{also} \quad \frac{F(x)-F(x-h)}{h}$$

just Slope of Tangent line

define a 1D grid



define $F(x_i)$ on grid $\quad \frac{dF}{dx} \sim \frac{F(x+h)-F(x)}{h}$

where $h \neq 0$ $\quad$ clearly x_0 or x_n is lost

Pseudo code $\frac{F(x) - np.Roll(F(x), -1)}{h} \simeq \frac{dF}{dx}$

board example x^2 10 grid points

Code example $h\downarrow$ still ugly at 0, have to be careful here. Problem $\frac{dF}{dx}$ not equal $\frac{F(x+h) - F(x)}{h}$ if $h=0$

in computer, $h=0$ = problem

---

how to construct approximations and truncation error.

Start here. Taylor Expansions

$$F(x+h) = F(x) + \frac{\partial F}{\partial x} h + \frac{\partial^2 F}{\partial x^2}\frac{h^2}{2!} + \dots \frac{\partial F}{\partial x^n}\frac{h^n}{n!}$$

$h \longleftrightarrow \Delta x$

$$\underbrace{\frac{F(x+h) - F(x)}{h} = \frac{\partial F}{\partial x}}_{\text{approximation}} + \underbrace{F'' \frac{h}{2!} + \dots F^n \frac{h^{n-1}}{n!}}_{\text{Truncation error}}$$

Forward difference

$$F(x-h) = F(x) - F'(x)h + \frac{F''(x)h^2}{2!} - \frac{F'''(x)h^3}{3!} + \dots \frac{F^n(x)}{n!}(-h)^n$$

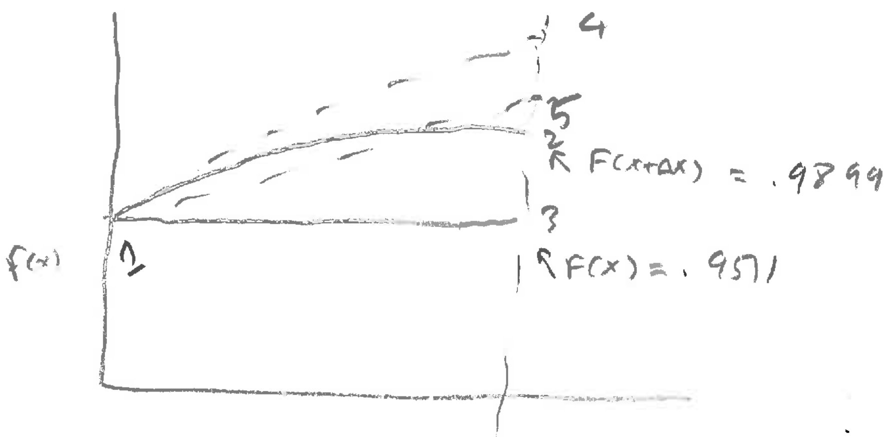
$$\frac{F(x) - F(x-h)}{h} = F'(x) - \frac{F''(x)h^2}{2!} + \frac{F'''(x)h^3}{3!} - \dots \frac{F^n(x)}{n!}(-h)^n$$

backward difference

Example $F(x) = \sin(2\pi x)$

$x = .2 \quad F(.2) = .9511$

$F(.22),\ \Delta x = .02 = .9899$



2 = $F(x+h)$ 3. $F(x)$ 4. $F(x) + F'(x)\Delta x$ .9899 .775% error

5 = $F(x) + F'(x)\Delta x + F''(x)\dfrac{\Delta x^2}{2}$ = .9824 = .01% error

Truncation error

$$\frac{dF}{dx} = \underbrace{\frac{F(x+h) - F(x)}{h}}_{\text{approximation}} - \underbrace{\frac{F''h}{2} - \frac{F'''}{6}\frac{h^2}{6} + \cdots}_{\text{Truncation error}}$$

There is ALWAYS error

Can we do better?

A $\quad F(x+\Delta x) = F(x) + F'\Delta x + \dfrac{F''\Delta x^2}{2} + F'''\dfrac{\Delta x^3}{3!} + \cdots F^n(x)\dfrac{\Delta x^n}{n!}$

B $\quad F(x-\Delta x) = F(x) - F'(x)\Delta x + F''\dfrac{(x)\Delta x^2}{2} - F'''\dfrac{(x)\Delta x^3}{3!} + \cdots F^n(x)\dfrac{(-\Delta x)^n}{n!}$

$A-B = 2F'\Delta x + O(\Delta x)^2$

error $\sim \Delta x^2$ not Δx

or $\quad \dfrac{F(x+\Delta x) - F(x-\Delta x)}{2\Delta x} = \dfrac{dF}{dx} + O(\Delta x^2)$ Truncation error

Central difference

Vs $\quad \dfrac{F(x+\Delta x) - F(x)}{\Delta x} = \dfrac{dF}{dx} + O(\Delta x)$ Truncation error

$\Delta x = .1$ FD BD .1 error CD $\sim (.1)^2$ error

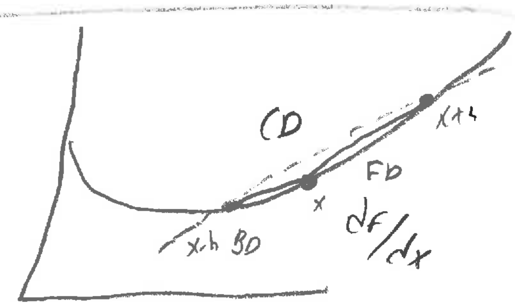
4th order $\quad F'(x) = \dfrac{-F(x+2h) + F(x+h) - 8F(x-h) + F(x-2h)}{12h}$ $+O(h)^4$ Truncation error

how to derive? Change $\Delta x \to 2\Delta x, 3\Delta x$ in A and B

add subtract

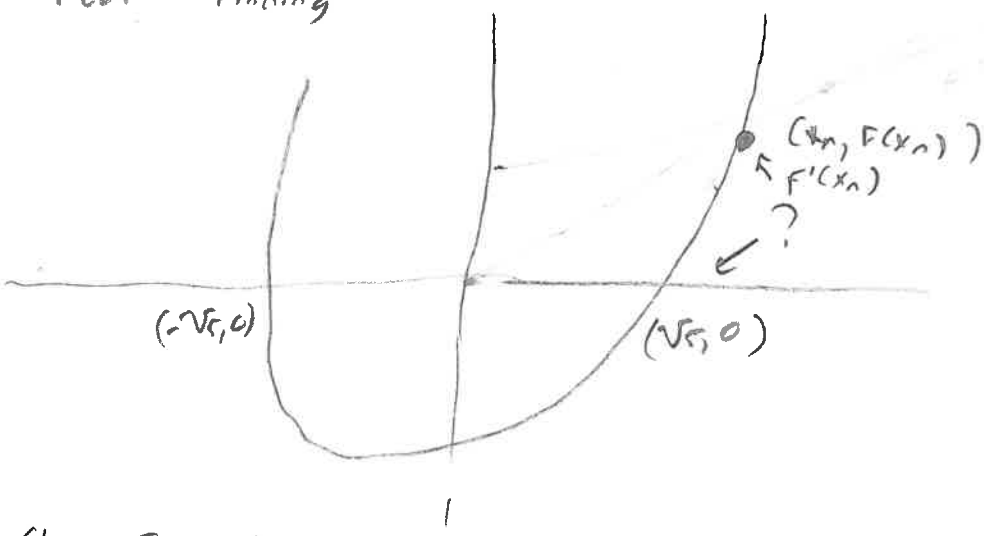
Segue Newton's Method

↓



$x^2 = 5$? how about $x^2 - 5 = 0$

root Finding



Point Slope Formula $y - y_1 = m(x - x_1)$ $m =$

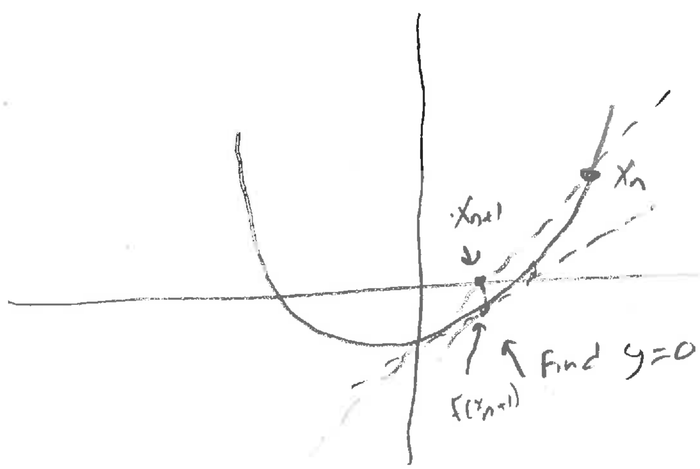
$y - F(x_n) = F'(x_n)(x - x_n)$

$y = F'(x_n)(x - x_n) + F(x_n)$

$F'(x_n)(\underset{\uparrow\, x_{n+1}}{x} - x_n) + F(x_n) = 0$

Solve $x_{n+1} = x_n - \dfrac{F(x_n)}{F'(x_n)}$

Iterate



guess root, The better the guess the Faster The convergence, $x^2=5 \rightarrow F(x)=x^2-5$ Answer = 2,23607

$x=\pm\sqrt{5}$ $\sqrt{4}<\sqrt{5}<\sqrt{9}$ Try 2,5 For x_n

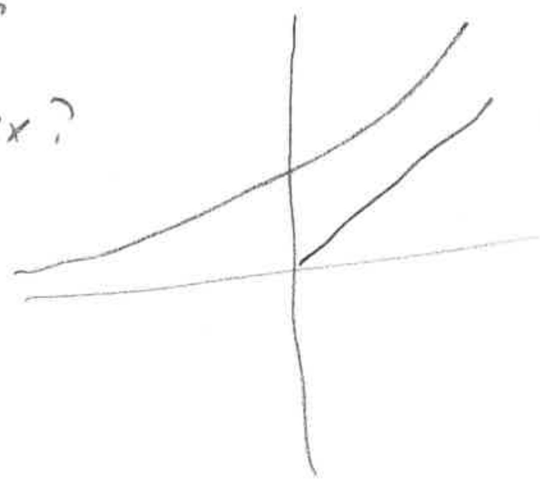
$$x_{n+1} = x_n - \frac{F(x_n)}{F'(x_n)} = x_n - \frac{(x_n^2-5)}{(2x_n)} = 2.5 - .25 = 2.25$$

$\frac{x_{n+1}}{real} = 1.00623$

$2.25 - .013889 = 2.23611 = x_{n+2}$ $\frac{x_{n+2}}{real} = 1.00002$

good enough

Pathological $\rightarrow$ $e^x=2x$?



no intersection

Next 2nd order derivatives, Partial derivatives, Vector Operations.

2nd order: 2 ways (infinite actually)

1: Treat $\frac{dF}{dx}$ as $g(x)$ and repeat or

Taylor Expansion again

$$F(x+\Delta x) \approx F(x) + F'(x)\Delta x + \frac{F''(x)(\Delta x)^2}{2} + \frac{F'''(x)(\Delta x)^3}{6} + \cdots$$

$$F(x-\Delta x) = F(x) - F'(x) + \frac{F''(x)(\Delta x)^2}{2} - \frac{F'''(x)(\Delta x)^2}{6} + \cdots$$

$$F(x+\Delta x) + F(x-\Delta x) \approx 2F(x) + F''(x)(\Delta x)^2 + \cdots$$

$$\boxed{\frac{F(x+\Delta x) + F(x-\Delta x) - 2F(x)}{\Delta x^2} \approx F''(x)}$$

Mixed Partial derivatives $\frac{\partial^2 F}{\partial x \partial y}$

Need a 2 D Grid!

Now $F = F(x,y)$

going to Switch Notation now For convenience
also, assume $\Delta x = \Delta y$ harder otherwise.

$i-1, j+1$	$i, j+1$	$i+1, j+1$	$F(x,y) = U(x,y)$
$i-1, j$	i, j	$i+1, j$	
$i-1, j-1$	$i, j-1$	$i+1, j-1$	

representations

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u}{\Delta x} \quad \text{Forward}$$

$$= \frac{u_{i,j} - u_{i-1,j}}{\Delta x} \quad \text{backward}$$

$$= \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta x}$$

$$\boxed{\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2}}$$

A $$u_{i+1,j} = u_{i,j} + (u')_{i,j}\,\Delta x + \frac{(u'')_{i,j}\,\Delta x^2}{2} + \cdots \frac{(u^n)_{i,j}(\Delta x^n)}{n!}$$

Note ${}'$ wrt x

B $$u_{i-1,j} = u_{i,j} - (u')_{i,j}\,\Delta x + (u'')_{i,j}\frac{(-\Delta x)^2}{2} + \cdots \frac{(u^n)_{i,j}(-\Delta x)^n}{n!}$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} + \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x + \left(\frac{\partial^3 u}{\partial x^2 \partial y}\right)_{i,j}\frac{(\Delta x)^2}{2} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \left(\frac{\partial u}{\partial y}\right)_{i,j} - \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x + \left(\frac{\partial^3 u}{\partial x^2 \partial y}\right)_{i,j}\frac{(\Delta x)^2}{2} + \cdots$$

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} - \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = 2\left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j}\Delta x$$

$$\frac{\overset{1}{\left(\frac{\partial u}{\partial y}\right)_{i+1,j}} - \overset{2}{\left(\frac{\partial u}{\partial y}\right)_{i-1,j}}}{2\Delta x} = \left(\frac{\partial^2 u}{\partial x \partial y}\right)_{i,j} + O(\Delta x^2)$$

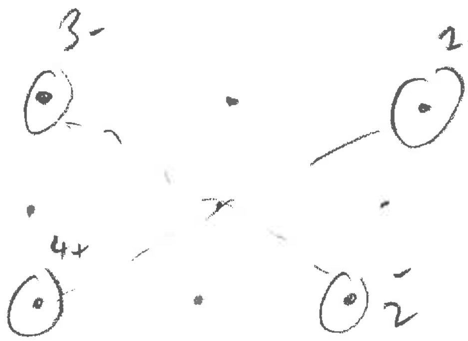
1 $\frac{\partial u}{\partial y}$ at $i+1$

use centered

$$\left(\frac{\partial u}{\partial y}\right)_{i+1,j} = \frac{u_{i+1,j+1} - u_{i+1,j-1}}{2\Delta y}$$

$$\frac{\partial u}{\partial y} \text{ at } i-1 = \left(\frac{\partial u}{\partial y}\right)_{i-1,j} = \frac{u_{i-1,j+1} - u_{i-1,j-1}}{2\Delta y}$$

$$\boxed{\text{So } \left(\frac{\partial^2 u}{\partial x, \partial y}\right)_{i,j} = \frac{\overset{1}{u_{i+1,j+1}} - u_{i+1,j-1} - u_{i-1,j+1} + \overset{4}{u_{i-1,j-1}}}{4\Delta x \Delta y} + O\left[(\Delta x)^2, (\Delta y)^2\right]}$$



$$\frac{(1+4) - (2+3)}{4\Delta x \Delta y}$$

We will return to the topic of mixed and 2nd order derivatives later. For now, you should be starting to see how we numerically compute

$\vec{\nabla} F$, $\nabla^2 F$, $\nabla \cdot \vec{A}$, $\vec{\nabla} \times \vec{A}$

Ex $\rightarrow$ $\vec{\nabla} \times \vec{A} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \partial_x & \partial_y & \partial_z \\ A_x & A_y & A_z \end{vmatrix}$ Ex $\vec{A} = A_x \hat{i} + A_y \hat{j}$

$\vec{\nabla} \times \vec{A} = \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \hat{k}$

$=$ np.gradient(A_y, dx)

$-$ np.gradient(A_x, dy)

We've come farther than you think!

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$ 1 D heat conduction

Time marching

FD good

BD/CD No good

$$\frac{\partial T}{\partial t} \sim \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \left(\frac{\partial^2 T}{\partial x^2}\right)_i^n \sim \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{(\Delta x)^2}$$

Solve

$$\frac{\partial T}{\partial t} - \alpha \frac{\partial^2 T}{\partial x^2} = 0 = \left[\frac{T_i^{n+1} - T_i^n}{\Delta t} - \alpha \frac{(T_{i+1}^n - 2T_i^n + T_{i-1}^n)}{(\Delta x)^2} \right]$$

Truncation error $\xrightarrow{+}$ $\left[-\left(\frac{\partial^2 T}{\partial t^2}\right)_i^n \frac{\Delta t}{2} + \alpha \left(\frac{\partial^4 T}{\partial x^4}\right)_i^n \frac{(\Delta x)^2}{12} + \dots \right]$ (11)

1st order in time 2nd order in space.

All you need is appending and a few loops.

LATER !!!

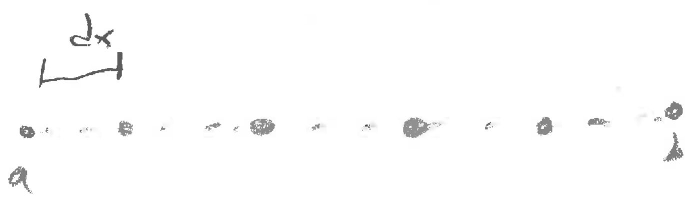
Integrals $\int F(x)\,dx$? No

$$\int_a^b F(x)\,dx, \quad \int_0^x F(x)\,dx = G(x), \quad \int_{-\infty}^{\infty} F(x)\,dx, \quad \int_c^d \int_{a(x)}^{b(x)} F(x,y)\,dx\,dy$$

Yes

Fundamentally

$$\lim_{dx \to 0} \sum F(x)\,dx = \int F(x)\,dx$$



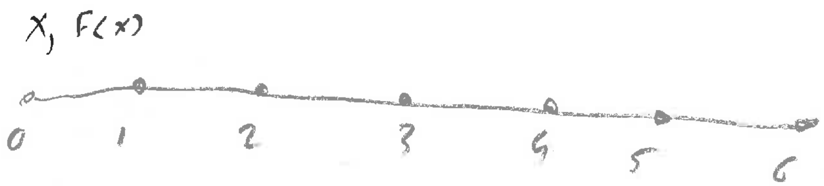
define $F(x) = x^2$

$$\int_0^1 x^2\,dx = \left.\frac{x^3}{3}\right|_0^1 = \frac{1}{3}$$

Let's do this by hand

With n = 10 1.9% accuracy. We can do better but later.

How about $G(x) = \int_0^x F(x)\,dx$?



num = 6

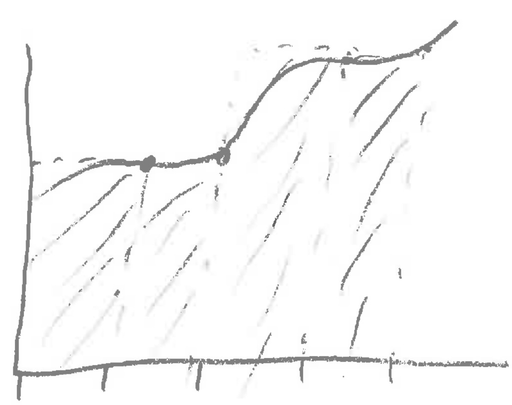
G(x):
```
out = np.zeros(len(x))
for i in range(0,num)
    out[i] = sum(F[0:i] * dx)
return out
```

iterate

Can we do better?

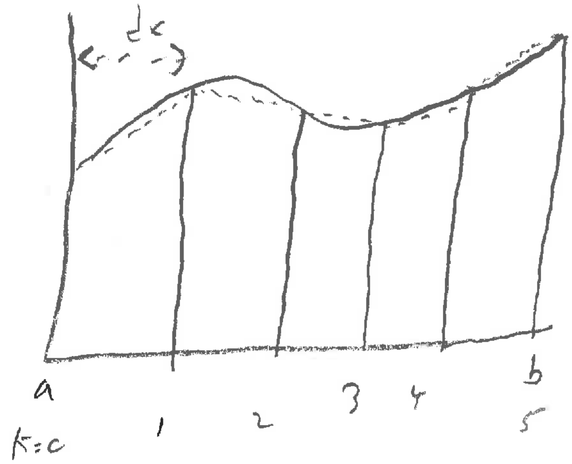
$\int \sim \sum F(x)\,dx$

Squares



(13)

Trapezoidal Rule



book example

$$A_k = \frac{1}{2} dx \left[F(a+(k-1)dx) + F(a+k\,dx) \right]$$

$N = 10 \quad k \in 1, 10$

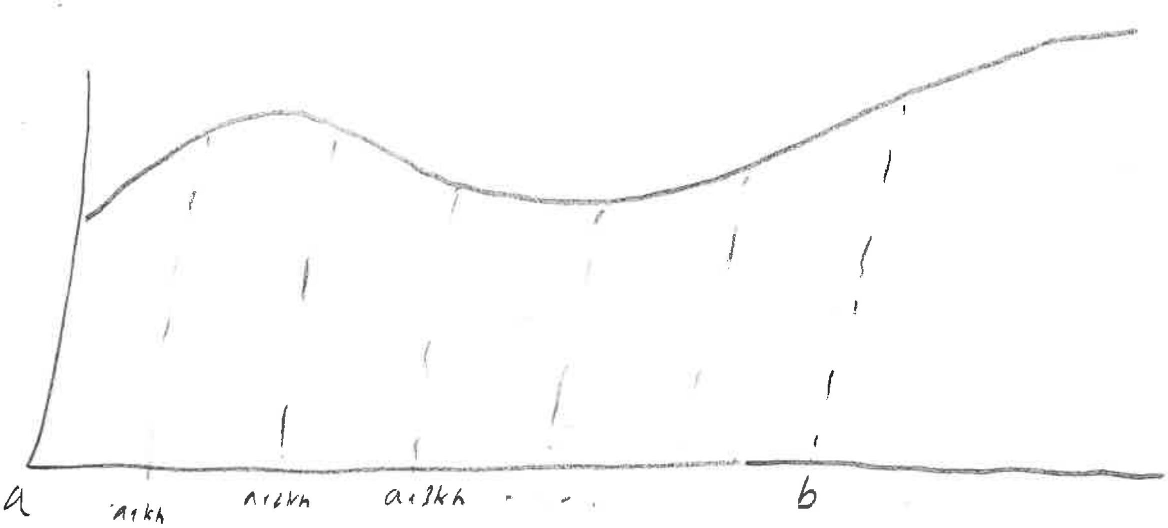
$$I(a,b) \simeq \sum_{k=1}^{N} \frac{1}{2} dx \sum_{k=1}^{N} F(a+(k-1)dx + F(a+k\,dx))$$

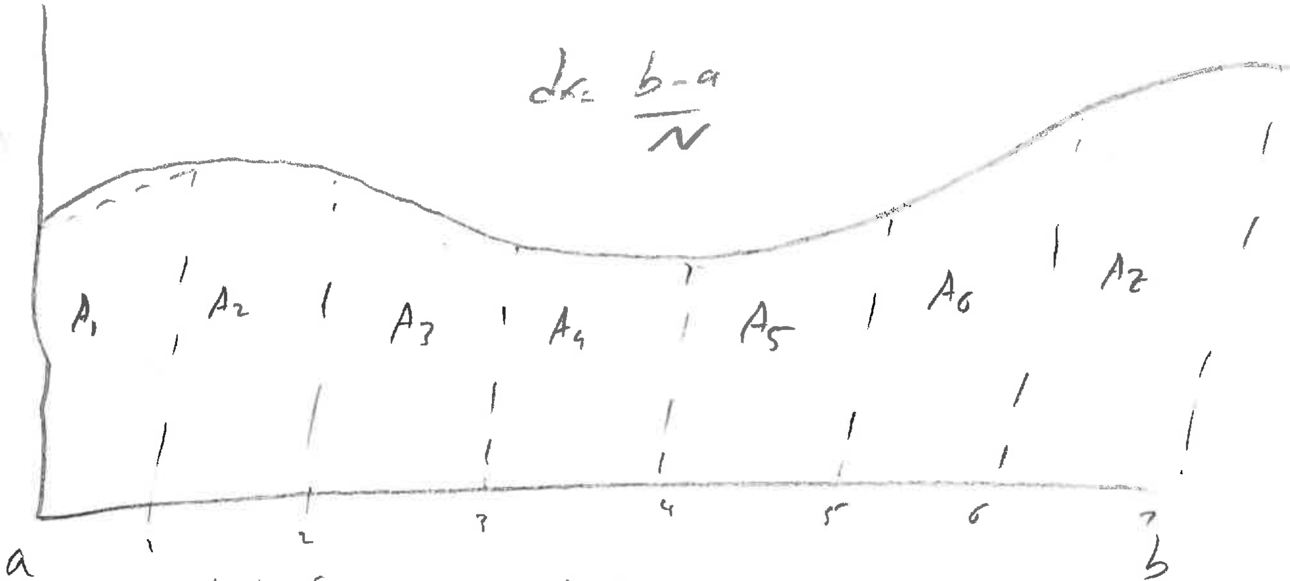
$$= \frac{1}{2} dx \left[F(a) + 2F(a+h) + 2F(a+2h) + \ldots\ldots \right]$$

$$= dx \left[\frac{1}{2} F(a) + \frac{1}{2} F(b) + \sum_{k=1}^{N-1} F(a+kh) \right]$$

How about $I(a,x)$?

Trickier, Let's be careful





$$A_1 = \frac{1}{2} dx \left(F(a) + F(a+dx) \right)$$

$$A_2 = \frac{1}{2} dx \left(F(a+dx) + F(a+2dx) \right)$$

$$A_3 = \frac{1}{2} dx \left(F(a+2dx) + F(a+3dx) \right)$$

$$A_7 = \frac{1}{2} dx \left(F(a+6dx) + F(b) \right)$$

$$I(a,x) = dx \left[\frac{1}{2} F(a) + \frac{1}{2} F(x) + \sum_{k=1}^{N-1} F(a+kdx) \right]$$

$$I(0) = \frac{1}{2} F(a)$$

$$I(1) = \frac{1}{2} (F(a) + F(a+dx))$$

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can be made with non constant dx

need IF statements

Next Simpson, Romberg integration, improper integrals, infinite limits ok

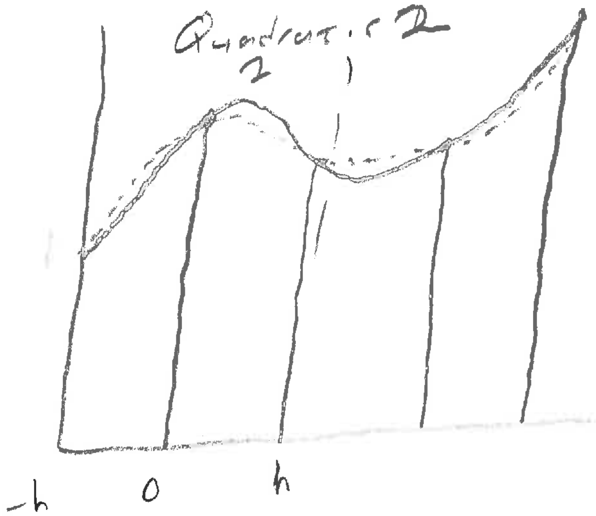
1 pt

2 pts

3?

$\sum F(x)\,dx$  Trapezoid 

SIMPSON'S RULE



$$Ax^2+Bx+C = F(x)$$

$$F(h) = Ah^2+Bh+C$$

$$F(0) = C$$

$$F(-h) = Ah^2-Bh+C$$

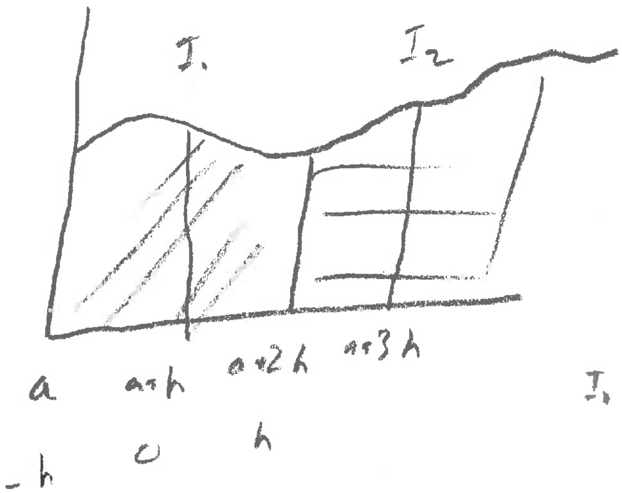
$$A = \frac{1}{h^2}\left[\frac{1}{2}F(-h) - F(0) + \frac{1}{2}F(h)\right],$$

$$B = \frac{1}{2h}\left[F(h) - F(-h)\right], \quad C = F(0)$$

$$\int_{-h}^{h}(Ax^2+Bx+C)\,dx = \frac{2}{3}Ah^3 + 2Ch = \frac{1}{3}h\left[F(-h) + 4F(0) + F(h)\right]$$

I(a,x) Start at x=a

↓



$$\frac{1}{3}h\left[(F(-h) + 4F(0) + F(h)\right]$$

$$\downarrow$$

$$I_1 = \frac{1}{3}h\left[F(a) + 4F(a+h) + F(a+2h)\right]$$

$$I_2 = \frac{1}{3}h\left[F(a+2h) + 4F(a+3h) + F(a+4h)\right]$$

$$+$$

$$I(a,x) = \frac{1}{3}h\left[F(a) + F(x) + 4\sum_{k=1}^{N/2} F(a+(2k-1)h) + 2\sum_{k=1}^{N/2-1} F(a+2kh)\right]$$

$$\text{or} = \frac{1}{3}h\left[F(a) + F(x) + 4\sum_{\substack{k\,\text{odd}\\ 1\ldots N-1}} F(a+kh) + 2\sum_{\substack{k\,\text{even}\\ 2\ldots N-2}} F(a+kh)\right]$$

Code I(a,x)

Note   even = a[2:num-1:2]   Then   4*sum(odd)
odd = a[1:num:2]   2*sum(even

MUCH Faster.

For loops suck

Integrals over infinite ranges

2 methods

Change of Variable

$$\int_a^{\infty} F(x)\,dx \qquad z = \frac{x-a}{1+x-a} \qquad x = \frac{z}{1-z} + a \qquad \frac{dx}{dz} = (1-z)^{-1} + z(1-z)^{-2}$$

$$= \frac{1}{(1-z)^2}$$

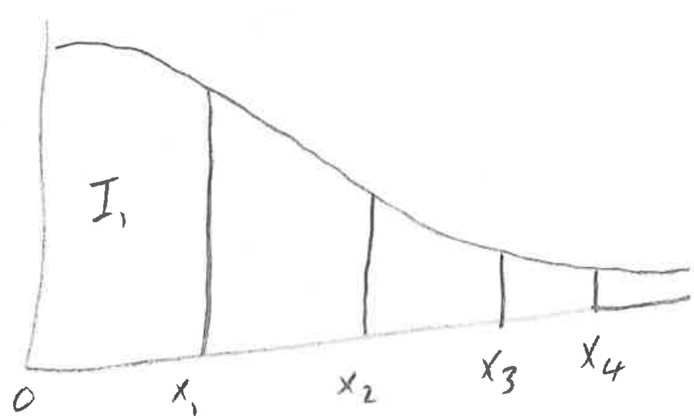
$$\int_0^1 \frac{1}{(1-z)^2} F\left(\frac{z}{1-z} + a\right) dz$$

$$\int_{-\infty}^{a} F(x)\,dx \rightarrow \quad z \rightarrow -z$$

$$\int_{-\infty}^{\infty} F(x)\,dx \qquad x = \frac{z}{1-z^2} \quad dx = \frac{1+z^2}{(1-z^2)^2}\,dz \rightarrow \int_{-1}^{1} \frac{1+z^2}{(1-z^2)^2} F\left(\frac{z}{1-z^2}\right) dz$$

or

graphically



$$I_1 = \int_0^{x_1} F(x)\,dx \qquad I_2 = \int_{x_1}^{x_2} F(x)\,dx \qquad I_3 = \int_{x_2}^{x_3} F(x)\,dx \quad \cdots$$

Compute I_1, I_2 is $I_1 + I_2 \sim I_1$ Stop

if not Compute I_3 is $I_1 + I_2 + I_3 \sim I_1 + I_2$ Stop

if not Compute I_4 is $I_1 + I_2 + I_3 + I_4 \sim I_1 + I_2 + I_3$ Stop

While loop...

Multiple integrals

LATER MONTE CARLO

I've skipped adaptive, Romberg, and Gaussian Quadrature. Time permitting - - - -

ODES

Differential Equations

Easy Start 2nd order $\vec{F} = m\vec{a}$ using Forward Euler

$$\frac{\vec{F}}{m} = \frac{d^2\vec{r}}{dt^2} = \frac{d\vec{v}}{dt} \qquad \text{Let } \vec{F} = 0\hat{i} + (-g)\hat{j} \qquad g = 9.8\,\frac{m}{s^2}$$

Simple
$$\vec{r}(T) = (x_0 + V_{x0}T)\hat{i} + (y_0 + V_{y0}T - \tfrac{1}{2}gT^2)\hat{j}$$
$$\vec{V}(T) = V_{x0}\hat{i} + (V_{y0} - gT)\hat{j}$$

Now numerically

$$\frac{d\vec{v}}{dT} = 0\hat{i} - \frac{g}{m}\hat{j} \qquad \text{remember } \frac{F(x+h) - F(x)}{h} = \frac{dF}{dx}$$

How about $\lim_{\Delta T \to 0} \frac{V(T+\Delta T) - V(T)}{\Delta T} = \frac{dV}{dT}$

or $\frac{\vec{V}(T+\Delta T) - \vec{V}(T)}{\Delta T} = 0\hat{i} - \frac{g}{m}\hat{j}$ 2 equations

The 1st is trivial $V_x(T) = V_{x0}$ $X(T) = X_0 + V_{x0}T$

The second? $V_y(T+\Delta T) - V_y(T) = -\frac{g}{m}\Delta T$ Skip Subscript

$$\underbrace{V_y(T_0 + \Delta T)}_{V(T_1)} = V(T_0) \underbrace{- \frac{g}{m}\Delta T}_{\Delta V} \qquad V(T_1) = V(T_0) + \Delta V$$

$$V(T_2) = V(T_1) - \frac{g}{m}\Delta T, \quad V(T_3) = V(T_2) - \frac{g\Delta T}{m}$$

got it? Code it! use np.append

how about $X(T)$?

$$\frac{dx}{dT} = V(T)$$

$$\frac{\Delta y}{\Delta T} = V(T) \qquad y(T_0+\Delta T) = \overbrace{y(T_0) + V(T_0)\Delta T}^{y(T_1)}$$

$$\text{or} \quad y(T_0) + \left[\frac{V(T_0) + V(T_1)}{2}\right]\Delta T$$

$$y(T_1+\Delta T) = y(T_1) + \quad \text{better} \quad \overline{V(T)}$$

$T_0 \to T_1 \quad T_1 \to T_2$

How to pick ΔT?

Harder

$$\frac{d\vec{V}}{dT} = \frac{1}{2}\frac{\rho}{m} v^2 C_d A \, \hat{v} - \frac{g}{m}\hat{j} = -bv^2\hat{v} - \frac{g}{m}\hat{j} \qquad b = \frac{1}{2m}\rho C_d A$$

$\hat{i}, \hat{j}$

$$-bv^2\hat{v}? \qquad -b\,(V_x^2+V_y^2)\,\frac{(V_x\hat{i} + V_y\hat{j})}{\sqrt{V_x^2+V_y^2}}$$

$$\frac{d\vec{V}}{dT} = -b\left(\sqrt{V_x^2+V_y^2}\right)V_x\hat{i} - \left(b\,(V_x^2+V_y^2)^{1/2}V_y + \frac{g}{m}\right)\hat{j}$$

$$V_x(T+\Delta T) = V_x(T) - b\,(V_x^2+V_y^2)^{1/2}V_x\,\Delta T$$

$$V_y(T+\Delta T) = V_y(T) - \left[b(V_x^2+V_y^2)V_y + \frac{g}{m}\right]\Delta T$$

$$y(T+\Delta T) = y(T) + \overline{V_y(T)}\,\Delta T$$

$$x(T+\Delta T) = x(T) + \overline{V_x(T)}\,\Delta T$$

need x_0, y_0, V_{x0}, V_{y0}

Harder

$$\frac{\partial\,\text{Temp}}{\partial t} = \alpha\frac{\partial^2 T}{\partial x^2} \qquad T = T(x,t)$$

$$\vec{F} = m\frac{d\vec{v}}{dT} \qquad \vec{F} = \underbrace{-\frac{1}{2}\rho C_d A}_{b \text{ if } \rho = \text{constant}} V^2\hat{v} - g\hat{j}$$

$$V^2\hat{v} = \frac{(V_x^2 + V_y^2)(V_x\hat{i} + V_y\hat{j})}{\sqrt{V_x^2+V_y^2}} = \sqrt{V_x^2+V_y^2}\,(V_x\hat{i} + V_y\hat{j})$$

$X_0 = 0 \qquad y_0 = 4346\,m$

$V_{x0} = 250\frac{m}{s} \qquad V_{y0} = 0\frac{m}{s}$

Stop at $y = 0$

Speed at $y=0$ no drag, drag, exponentially stratified atmosphere

X vs y

$$\frac{d\vec{V}}{dT} = \left(\frac{dV_x}{dT}\hat{i} + \frac{dV_y}{dT}\hat{j}\right)\frac{1}{m}$$

Stratification Not clear

$$\frac{dV_x}{dT}\hat{i} = \left(-\frac{1}{2}\frac{\rho C_d A}{m}\sqrt{V_x^2+V_y^2}\right)V_x\hat{i}$$

$$\frac{dV_y}{dT}\hat{j} = -\left[\left(\frac{1}{2}\frac{\rho C_d A}{m}\sqrt{V_x^2+V_y^2}\right)V_y + g\right]\hat{j}$$

$\rho(y) = \rho_0 e^{-\frac{kT}{mg}y}$ $\quad H^{-1}$

$k = 1.38\cdot10^{-23}\,J\cdot K^{-1}$

$T = 8250\,m$

$g = 9.8$

M = mean molecular mas

$\rho(y) = \rho_0 e^{-\frac{y}{H}}$

$H \approx 8250\,m \qquad \rho_0 = 1.225\frac{kg}{m^3}$

$V(T_i+\Delta T) = V(T_i) + \frac{F}{m}(\vec{V}(T_i), y(T_i))\,\Delta T$

Time marching not Space

V_{x_0} [ ]

↓

V_{x_1} [ ]

↓

" "

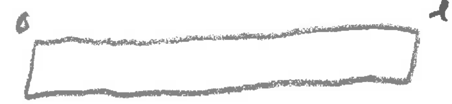
$\Delta T = ?$ $y_F = \frac{1}{2} g T^2$ $T = .1$ $\Delta x = 5\,cm$ good enough

$\Delta y_{total} = 270\ m \sim 5500$ Steps For No drag how many does it take

$\frac{dx}{dT} = V$ $X(T_i+\Delta T) = x_i + V_i\,\Delta T$

Check $mg = \frac{1}{2}\rho C_d A V^2$ $V_T = \left(\frac{2mg}{\rho C_D A}\right)^{1/2}$ $m = 75$ $C = .5$ $A = .1$ $V \sim 155\,\frac{m}{s}$

Let $T = \sum C_n e^{i(kx - \omega t)}$ 1D



$\frac{\partial T}{\partial t} = -i\omega T$ $\alpha \frac{\partial^2 T}{\partial x^2} = -\alpha k^2 T$ So $i\omega = \alpha k^2$

Now $\frac{\omega}{k} = -i\alpha k$ dispersion relation $\frac{\omega}{k}$ = Phase Velocity

$\frac{d\omega}{dk} = -2i\alpha k \neq \frac{\omega}{k}$ = group Velocity dispersive

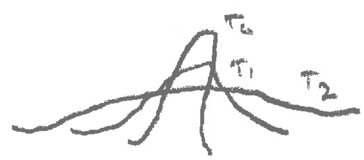
Sound $\omega = k C_s^2$ ← Sound speed $\frac{d\omega}{dk} = \frac{\omega}{k}$ non-dispersive

How to Solve?

$T(x,t) = \sum C_n e^{i(kx + i\alpha k^2 t)}$ $k = \frac{2\pi}{\lambda}$ $\omega = 2\pi\nu$

$T(x,t) = \sum C_n e^{ikx} e^{-\alpha k^2 t}$ decays with time

Shorter waves = faster decay



Solution? IC's, BC's 1 IC $\frac{\partial T}{\partial t}$ 2 BC $\frac{\partial^2 T}{\partial x^2}$

1 initial shape $T(x,0) = g(x)$ Starting Shape

2 $T(0,t) = 0 \rightarrow \sum [a_n \cos(k\cdot 0) + b_n \sin(k\cdot 0)] e^{-\alpha k^2 t} = 0$

$a_n = 0$

3. $T(l,t) = 0 \rightarrow \sum b_n \sin(k\cdot l) e^{-\alpha k^2 t} = 0$

So $\sin(kl) = 0$ or $kl = n\pi$

Now $T(x,t) = \sum b_n \sin\left(\frac{n\pi x}{l}\right) e^{-\alpha k^2 t}$

just need b_n get from $g(x)$ and Fourier's "Trick"

Properly Normalized $A\,\text{SIN}\left(\frac{n\pi x}{\ell}\right)$ Form a complete orthonormal set,

$$F(x) = \sum b_n A\,\text{SIN}\left(\frac{n\pi x}{\ell}\right), \quad \int_0^{\ell} A^2\,\text{SIN}\left(\frac{n\pi x}{\ell}\right)\text{SIN}\left(\frac{m\pi x}{\ell}\right)dx = \delta_{mn}$$

$$\delta_{mn} = \begin{cases} 1 & m=n \\ 0 & m\neq n \end{cases}$$ Think $\hat{i}, \hat{j}, \hat{k}$ Example

$A = ?$ $$\int_0^{\ell} A^2\,\text{SIN}^2\left(\frac{n\pi x}{\ell}\right)dx = 1$$

$$A^2\int_0^{\ell} \text{SIN}^2(kx)\,dx = 1$$

Let $u = \frac{n\pi x}{\ell} = kx$

$du = k\,dx$

$x=0 \quad u=0 \qquad x=\ell \quad u=n\pi$

$$\frac{A^2}{k}\int_0^{n\pi} \text{SIN}^2(u)\,du = 1 \qquad \frac{A^2}{k}\int_0^{n\pi}\left(\frac{1}{2} - \cancel{\frac{\cos(2u)}{2}}\right)du = 1$$

0

$$\frac{A^2}{k}\left.\frac{u}{2}\right|_0^{n\pi} = \frac{n\pi}{2}\cdot\frac{A^2\ell}{n\pi} = 1 \qquad A = \sqrt{\frac{2}{\ell}}$$

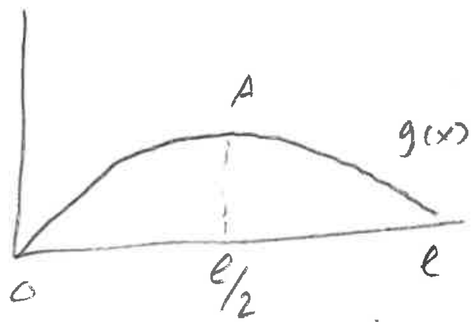
$b_n = ?$ $$g(x) \cong \sum b_n\,\text{SIN}\left(\frac{n\pi x}{\ell}\right)$$

$$\int g(x)\,\text{SIN}\left(\frac{m\pi x}{\ell}\right)dx = \int \sum b_n \underbrace{\text{SIN}\left(\frac{n\pi x}{\ell}\right)\text{SIN}\left(\frac{m\pi x}{\ell}\right)}_{\frac{\ell\cdot\delta_{mn}}{2}}dx$$

$$\frac{\ell b_n}{2} = \int_0^{\ell} g(x)\, \mathrm{SIN}\left(\frac{m\pi x}{\ell}\right) dx$$

$$b_n = \frac{2}{\ell}\int_0^{\ell} g(x)\, \mathrm{SIN}\left(\frac{m\pi x}{\ell}\right) dx$$

Concrete Example



$$ax^2 + bx + c = g(x)$$

$$a(0)^2 + b(0) + c = 0$$

$$c = 0 \quad \underline{1}$$

$$a\ell^2 + b\ell = 0$$

$$a\ell + b = 0 \qquad a = -\frac{b}{\ell} \quad \underline{2}$$

$$-\frac{b}{\ell}\left(\frac{\ell^2}{4}\right) + b\frac{\ell}{2} = A$$

$$-\frac{b\ell}{4} + \frac{b\ell}{2} = A$$

$$\frac{b\ell}{4} = A \qquad b = \frac{4A}{\ell} \quad \underline{3}$$

$$g(x) = -\frac{4A}{\ell^2}x^2 + \frac{4A}{\ell}x$$

Let $A = 1$ $\ell = 1$ $g(x) = -4x^2 + 4x$

$$b_n = 2\int_0^1 (-4x^2 + 4x)\, \mathrm{SIN}\left(\frac{m\pi x}{1}\right) dx$$

$$b_n = 2\left[\underbrace{\frac{8}{m^3\pi^3} - \frac{8\cos(m\pi)}{m^3\pi^3}}_{\substack{0 \text{ if } m = 0,2,4,\ldots \\ 16 \text{ if } m = 1,3,5\ldots}} - \frac{4m\pi\, \mathrm{SIN}(m\pi)}{m^3\pi^3}\right] \quad m = 0,1,2,3\ldots$$

↑ always zero

$$T(x,\tau) = 2\cdot\sum_{m \text{ odd}} \frac{16}{m^3\pi^3} \sin\left(\frac{m\pi x}{\ell}\right) e^{-\alpha k^2 \tau}$$

huh? α? $\alpha k^2 \tau$ is dimensionless

So α has units $\frac{s}{m^2}$ or diffusion rate per meter

when $\tau = \frac{1}{\alpha k^2}$ $e^{-\alpha k^2 \tau} = e^{-1}$ $\tau_0 = \frac{1}{\alpha k^2}$ e folding time

Maybe computer time

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \qquad \frac{T_j^{n+1 \leftarrow \text{time}} - T_j^n}{\Delta \tau} = \alpha\left[\frac{T_{j+1}^n - 2T_j^n + T_{j-1}^n}{(\Delta x)^2}\right]$$

T_j ↖ space

1st order FD ↙ 2nd order CD ↙

$$T_j^{n+1} = T_j(\tau + \Delta\tau) \qquad T_j^{n+1} = T_j^n + \frac{\alpha\Delta\tau}{(\Delta x)^2}\left[T_{j+1}^n - 2T_j^n + T_{j-1}^n\right] + O(\Delta\tau) + O(\;)$$

$\Delta\tau = ?$ Look at amplification factor $\frac{\epsilon_j^{n+1}}{\epsilon_j^n} = G$

A = analytic solution, D = exact solution of difference error

N = Numerical solution from a computer with finite accuracy

Discretization error = A − D

Round off error = ϵ = N − D

N = D + ϵ Exact + Round off error

We are Solving N Let $u \to N = D + \epsilon$ and $j \to i$

$$\frac{D_i^{n+1} + \epsilon_i^{n+1} - D_i^n - \epsilon_i^n}{k\Delta T} = \frac{D_{i+1}^n + \epsilon_{i+1}^n - 2D_i^n - 2\epsilon_i^n + D_{i-1}^n + \epsilon_{i-1}^n}{(\Delta x)^2}$$

by definition $\dfrac{D_i^{n+1} - D_i^n}{k\Delta T} = \dfrac{D_{i+1}^n - 2D_i^n + D_{i-1}^n}{(\Delta x)^2}$

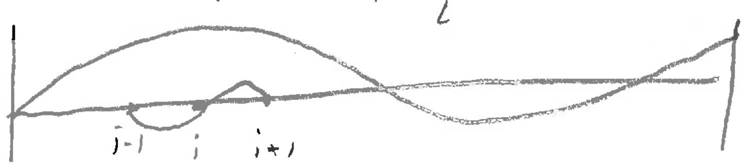
We are left with $\dfrac{\epsilon_i^{n+1} - \epsilon_i^n}{k\Delta T} = \dfrac{\epsilon_{i+1}^n - 2\epsilon_i^n + \epsilon_{i-1}^n}{(\Delta x)^2}$

Want $\left|\dfrac{\epsilon_i^{n+1}}{\epsilon_i}\right| = |G| \leq 1$ or error grows!!

$\epsilon(x) = \sum_m A_m e^{ik_m x}$ $k_m = \left(\frac{2\pi}{\ell}\right) m$ $m = 1, 2, 3$

$\lambda_{max} = L$ $k_1 = \frac{2\pi}{L} \cdot 1$

$m \uparrow \lambda \downarrow$



0 $\lambda_{min} = 2\Delta x$ L

↖ minimum resolvable mode

if N+1 gridpoints N intervals $\Delta x = \frac{L}{N}$

$\lambda_{min} = \frac{2L}{N}$ For a grid with N+1 pts

$k_{min} = \dfrac{2\pi}{\lambda_{min}} = \dfrac{2\pi}{2L/N} = \underline{\dfrac{2\pi}{L}\dfrac{N}{2}}$ So $\epsilon(x) = \sum_{m=1}^{N/2} A_m e^{ik_m x}$

$$\epsilon(x,T) = \sum_{m=1}^{N/2} A_m(T) e^{ik_m x} = \sum_{m=1}^{N/2} e^{aT} e^{ik_m x}$$

Lets assume $\epsilon(x,T) = e^{aT} e^{ikx}$ just one wave

1: Then
$$\frac{\overbrace{e^{a(T+\Delta T)} e^{ikx}}^{\epsilon_i^{n+1}} - \overbrace{e^{aT} e^{ikx}}^{\epsilon_i^{n}}}{k\Delta T} = \frac{\overbrace{e^{aT} e^{ik(x+\Delta x)}}^{\epsilon_{i+1}^{n}} - \overbrace{2e^{aT} e^{ikx}}^{\epsilon_i^{n}} + \overbrace{e^{aT} e^{ik(x-\Delta x)}}^{\epsilon_{i-1}^{n}}}{(\Delta x)^2}$$

2: divide by $e^{aT} e^{ikx}$

3: $$\frac{e^{a\Delta T} - 1}{k\Delta T} = \frac{e^{ik\Delta x} - 2 + e^{-ik\Delta x}}{(\Delta x)^2}$$

4: $$e^{a\Delta T} = 1 + \frac{k\Delta T}{(\Delta x)^2}\left(e^{ik\Delta x} + e^{-ik\Delta x} - 2\right)$$ " $\frac{e^{ikx} + e^{-ikx}}{2} = \cos(x)$ "

5: $$e^{a\Delta T} = 1 + \frac{2k\Delta T}{(\Delta x^2)}\left(\cos(k\Delta x) - 1\right)$$ " $\sin^2\left(\frac{kx}{2}\right) = \frac{1-\cos(kx)}{2}$

6: $$e^{a\Delta T} = 1 - \frac{4k\Delta T}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)$$

7: $$\frac{\epsilon_i^{n+1}}{\epsilon_i} = \frac{e^{a(T+\Delta T)} e^{ikx}}{e^{aT} e^{ikx}} = e^{a\Delta T} = G$$

8: Need $$\left|\frac{\epsilon_i^{n+1}}{\epsilon_i}\right| = \left|e^{a\Delta T}\right| = \left|1 - \frac{4k\Delta T}{(\Delta x)^2}\sin^2\left(\frac{k\Delta x}{2}\right)\right| \leq 1$$

or $$1 - \frac{4k\Delta T}{(\Delta x)^2} \sin^2\left(\frac{k\Delta x}{2}\right) \le 1$$

$\uparrow$ always positive — always True

and

$$1 - \frac{4k\Delta T}{(\Delta x)^2} \sin^2\left(\frac{k\Delta x}{2}\right) \ge -1$$ multiply by (-1)

So $$\frac{4k\Delta T}{(\Delta x)^2} \sin^2\left(\frac{k\Delta x}{2}\right) - 1 \le 1$$

From which $$\frac{4k\Delta T}{(\Delta x)^2} \sin^2\left(\frac{k\Delta x}{2}\right) \le 2$$

or $$\frac{k\Delta T}{(\Delta x)^2} \underbrace{\sin^2\left(\frac{k\Delta x}{2}\right)}_{max=1} \le \frac{1}{2}$$

So $$\frac{k\Delta T}{(\Delta x)^2} \le \frac{1}{2}$$

or $$\Delta T \le \frac{(\Delta x)^2}{2k}$$

Δx, k Set ΔT $\quad$ $\Delta x \downarrow$ $\Delta T \downarrow$ $\quad$ $k \uparrow$ $\Delta T \downarrow$

generically, if a equation deals with wave propagation $\Delta T \leq C_{Fl} \dfrac{\Delta x}{V_{max}}$ $C_{Fe} \sim .5 \sim .8$

again $$\frac{\partial T}{\partial t} - \alpha\frac{\partial^2 T}{\partial x^2} = \left|\frac{T_j^{n+1} - T_j^n}{\Delta t} - \frac{\alpha(T_{j+1}^n - 2T_j^n + T_{j-1}^n)}{(\Delta x)^2}\right| +$$

difference equation

$$\left[-\left(\frac{\partial^2 T}{\partial t^2}\right)_j^n \frac{\Delta t}{2} + \alpha\left(\frac{\partial^4 T}{\partial x^4}\frac{(\Delta x)^2}{12}\right) + \cdots\right]$$

Truncation error

Can we do better? Segue

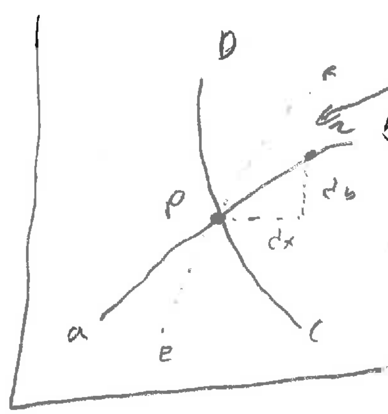
Classes of PDEs and impacts on computation

Quasi linear PDES

System $$a_1\frac{\partial u}{\partial x} + b_1\frac{\partial u}{\partial y} + c_1\frac{\partial v}{\partial x} + d_1\frac{\partial v}{\partial y} = f_1(x, y, u, v)$$
$$a_2\frac{\partial u}{\partial x} + b_2\frac{\partial u}{\partial x} + c_2\frac{\partial v}{\partial x} + d_2\frac{\partial v}{\partial y} = f_2(x, y, u, v)$$

$a_1, a_2, b_1, b_2, c_1, c_2, d_1, d_2$ may be functions of $x, y, u,$ and v

at any point in XY u, v take on unique values and their first and second derivatives are finite.



Characteristic curve

Lines where $\frac{\partial u}{\partial x \text{ or } dy}$, $\frac{\partial v}{\partial x \text{ or } dy}$ are indeterminate and maybe discontinuous.

WHAT? You just said . . . .

Now $$du = \frac{\partial u}{\partial x}dx + \frac{\partial u}{\partial y}dy \qquad dv = \frac{\partial v}{\partial x}dx + \frac{\partial v}{\partial y}dy$$

$$\begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \begin{bmatrix} \partial u/\partial x \\ \partial u/\partial y \\ \partial v/\partial x \\ \partial v/\partial y \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ du \\ dv \end{bmatrix}$$

How do we get our unique $\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}, \frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}$?

$[A]x = b$

$\frac{\partial u}{\partial x}$ 1st

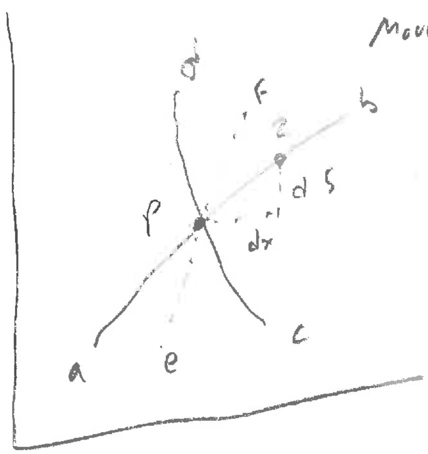
$$[A] = \begin{bmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{bmatrix} \qquad [B] = \begin{bmatrix} F_1 & b_1 & c_1 & d_1 \\ F_2 & b_2 & c_2 & d_2 \\ du & dy & 0 & 0 \\ dv & 0 & dx & dy \end{bmatrix}$$

Cramers Rule

$$\frac{\partial u}{\partial x} = \frac{|B|}{|A|}$$

$$x_i = \frac{\det[A_i]}{\det[A]}$$

D_i = matrix formed by replacing i-th column of A with vector b



Move along a-b from p-2

$dx = x_2 - x_p \quad dy = y_2 - y_p$
$du = u_2 - u_p \quad dv = v_2 - v_p$

$\frac{\partial u}{\partial x} \to$ unique value

do the same along c-d

Same Value has to be direction shouldn't matter

What if we move along ef and $\det[A] = 0$

So $\frac{\partial u}{\partial x}, \ldots$ don't exist? These are characteristic curves. Lines are indeterminate $|A| = 0$

What are they?

Solve $\begin{vmatrix} a_1 & b_1 & c_1 & d_1 \\ a_2 & b_2 & c_2 & d_2 \\ dx & dy & 0 & 0 \\ 0 & 0 & dx & dy \end{vmatrix} = 0$

1 $(a_1c_2 - a_2c_1)(dy)^2 - (a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)dx\,dy + (b_1d_2 - b_2d_1)(dx)^2 = 0$

2 divide $\frac{1}{dx^2}$ $(a_1c_2 - a_2c_1)\left(\frac{dy}{dx}\right)^2 - (a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)\frac{dy}{dx} + (b_1d_2 - b_2d_1) = 0$

3. Let $a = (a_1c_2 - a_2c_1)$ $b = -(a_1d_2 - a_2d_1 + b_1c_2 - b_2c_1)$ $c = (b_1d_2 - b_2d_1)$

Now $a\left(\frac{dy}{dx}\right)^2 + b\left(\frac{dy}{dx}\right) + c = 0$

$\frac{dy}{dx} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ $D = b^2 - 4ac$

System is

if $D > 0$ 2 real characteristic curves hyperbolic

$D = 0$ 0 characteristics parabolic

$D < 0$ 2 imaginary characteristics elliptic

Comes from analytic geometry $ax^2 + bxy + cy^2 + dx + ey + f = 0$

$b^2 - 4ac > 0$ Conic is a hyperbola

$b^2 - 4ac = 0$ conic is a parabola

$b^2 - 4ac < 0$ Conic is an ellipse

Now if only $|A| = 0$ $\frac{\partial u}{\partial v} \to \infty$ No No

want indeterminate set $|B| = 0$ also

Expansion leads to an ordinary differential equation

which only holds along characteristic curve

$|B| = 0 \rightarrow$ compatibility equation ID along characteristics. Widely used for inviscid, supersonic flows

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much easier if $f_1, f_2 = 0$

Then $w = \begin{Bmatrix} u \\ v \end{Bmatrix}$ $\begin{pmatrix} a_1 & c_1 \\ a_2 & c_2 \end{pmatrix}\left(\frac{\partial w}{\partial x}\right) + \begin{pmatrix} b_1 & d_1 \\ b_2 & d_2 \end{pmatrix}\left(\frac{\partial w}{\partial y}\right) = 0$

$$[K]\frac{\partial w}{\partial x} + M\frac{\partial w}{\partial y} = 0$$

$$\frac{\partial w}{\partial x} + \underbrace{[K]^{-1}[M]}_{[N]}\frac{\partial w}{\partial y} = 0$$

real eigenvalues for $[N] \rightarrow$ hyperbolic

complex $\rightarrow$ elliptic

Ex $\quad (1-M_\infty^2)\frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} = 0$

$$\frac{\partial u'}{\partial y} - \frac{\partial v'}{\partial x} = 0$$

$$\underbrace{\begin{bmatrix} 1-M_\infty^2 & 0 \\ 0 & -1 \end{bmatrix}}_{[K]}\frac{\partial w}{\partial x} + \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{[M]}\frac{\partial w}{\partial y} = 0$$

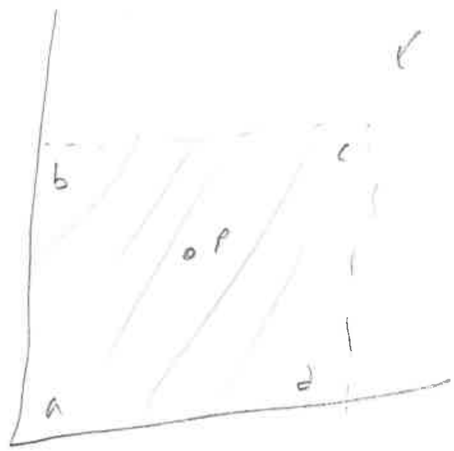
$$[N] = \begin{bmatrix} 0 & \frac{1}{1-M_\infty^2} \\ -1 & 0 \end{bmatrix} \qquad \lambda = \pm\sqrt{\frac{1}{M_\infty^2 - 1}}$$

$M_\infty > 1$ hyperbolic $\quad M_\infty < 1$ elliptic

Elliptic $\nabla^2 \phi = 0$ imaginary characteristics

No regions of influence or domains of dependence

Pure boundary value problems.



Generally Steady State Solutions

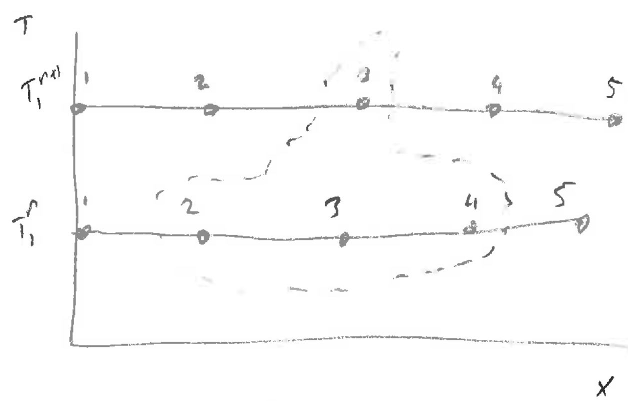
P immediately influences whole region

Not good For marching

We'll solve this later

Back to heat Conduction **Implicit**!

Explicit



↑ Time marching

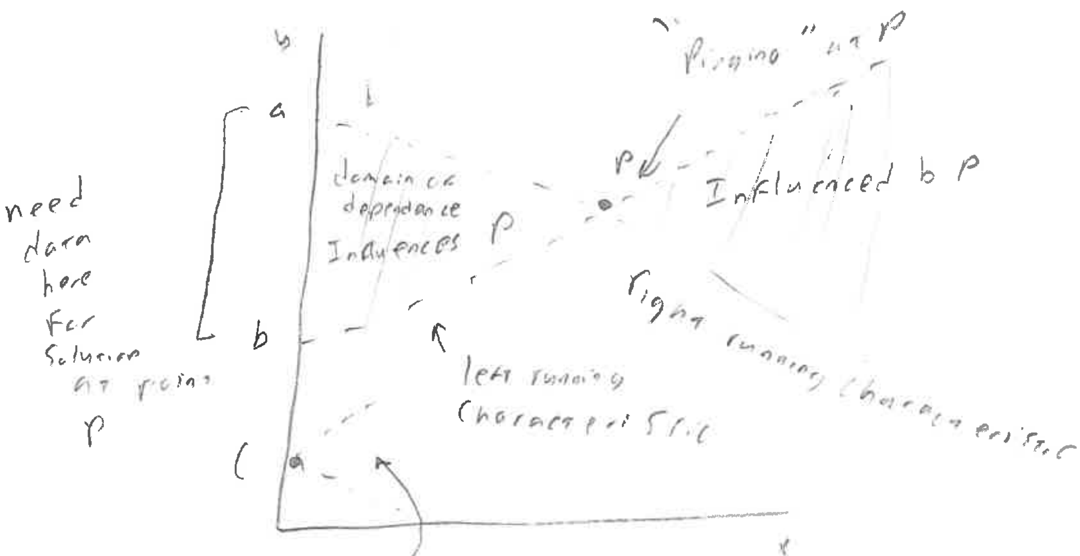
$$T_i^{n+1} = T_i^n + \frac{\alpha \Delta t}{(\Delta x)^2}\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$$

$$T_3^{n+1} = T_3^n + \frac{\alpha \Delta t}{(\Delta x)^2}\left(T_4^n - 2T_3^n + T_2^n\right)$$

Solve explicitly 1 unknown time

So what? Affect what and how solution can be known

Hyperbolic 2 characteristics

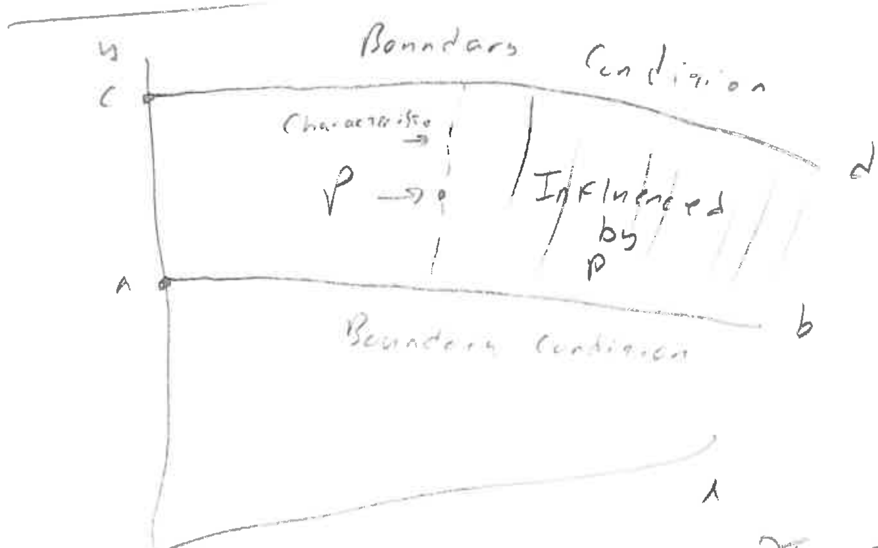


Influenced by C

Ex Inviscid Flow

Good for time marching

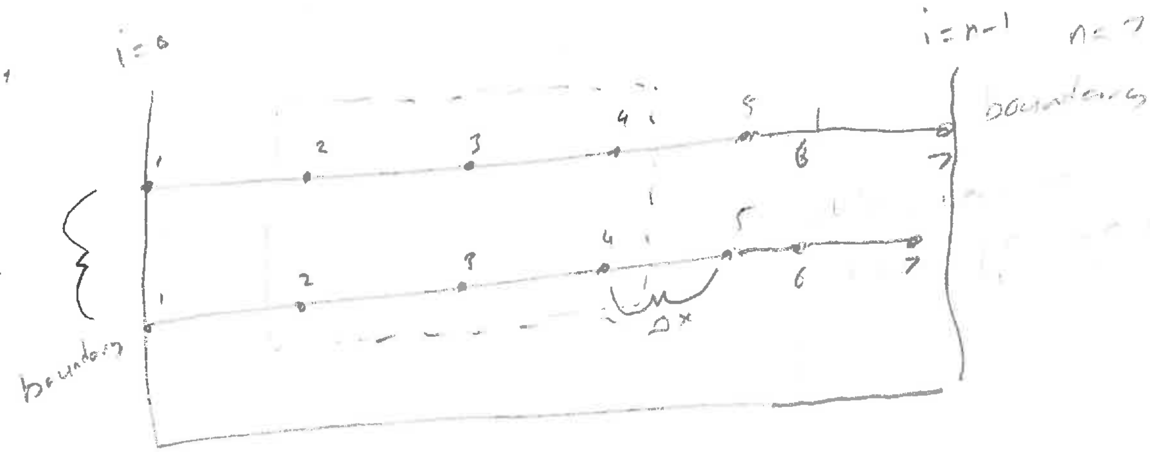
Parabolic 1 characteristic



Good for time marching

Ex heat Conduction $\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$

How about



$$\frac{T_i^{n+1} - T_i^n}{\Delta \tau} = \alpha \frac{\frac{1}{2}\left[T_{i+1}^{n+1} + T_{i+1}^{n}\right] + \frac{1}{2}\left[-2T_i^{n+1} - 2T_i^n\right] + \frac{1}{2}\left[T_{i-1}^{n+1} + T_{i-1}^{n}\right]}{(\Delta x)^2}$$

Crank-Nicolson

good for Parabolic equations

rearrange

$$\boxed{\frac{\alpha \Delta \tau}{2(\Delta x)^2} T_{i-1}^{n+1} - \left[1 + \frac{\alpha \Delta \tau}{(\Delta x)^2}\right] T_i^{n+1} + \frac{\alpha \Delta \tau}{2(\Delta x)^2} T_{i+1}^{n+1} = -T_i^n - \frac{\alpha \Delta \tau}{2(\Delta x)^2}\left[T_{i+1}^n - 2T_i^n + T_{i-1}^n\right]}$$

Let $A = \frac{\alpha \Delta \tau}{2(\Delta x)^2}$ $\quad B = \left(1 + \frac{\alpha \Delta \tau}{(\Delta x)^2}\right)$ $\quad k_i = -T_i^n - \frac{\alpha \Delta \tau}{2(\Delta x)^2}\left[T_{i+1}^n - 2T_i^n + T_{i-1}^n\right]$

Then $A T_{i-1}^{n+1} - B T_i^{n+1} + A T_{i+1}^{n+1} = k_i$

At grid point 2 $\quad \underbrace{A T_1 - B T_2 + A T_3}_{\text{not known}} = \underset{\uparrow \text{ known}}{k_2}$ dropped superscript

but T_1 is known → boundary condition

So $\quad -BT_2 + AT_3 = \underbrace{k_2 - AT_1}_{k_2'}$

$-BT_2 + AT_3 = k_2'$

At grid point 3: $AT_2 - BT_3 + AT_4 = k_3$

At grid point 4: $AT_3 - BT_4 + AT_5 = k_4$

At grid point 5: $AT_4 - BT_5 + AT_6 = k_5$

At grid point 6: $AT_5 - BT_6 + AT_7 = k_6$

but T_7 is known so $AT_5 - BT_6 = k_6 - AT_7 = k_6'$

Matrix Equation

$$\begin{bmatrix} -B & A & 0 & 0 & 0 \\ A & -B & A & 0 & 0 \\ 0 & A & -B & A & 0 \\ 0 & 0 & A & -B & A \\ 0 & 0 & 0 & A & -B \end{bmatrix} \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \\ T_6 \end{bmatrix} = \begin{bmatrix} k_2' \\ k_3 \\ k_4 \\ k_5 \\ k_6' \end{bmatrix}$$

Seems more complicated

why use?

$\Delta T \rightarrow$ can be large

implicit is

unconditionally stable

Tri diagonal

Thomas' algorithm

generally, implicit is only good for steady states

otherwise if time marching solution is to be correct

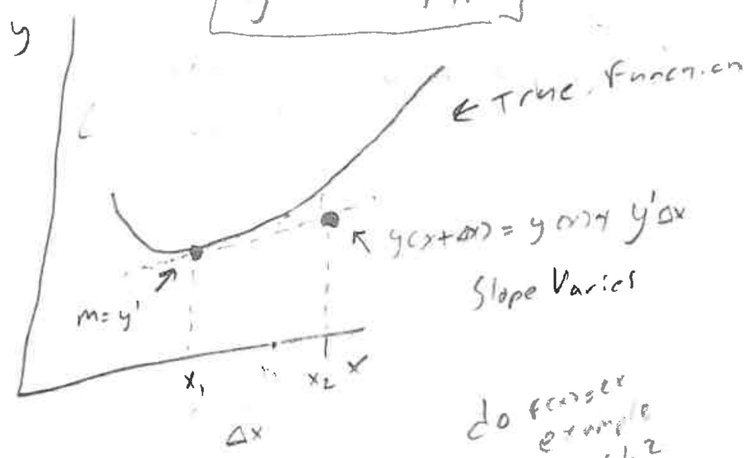
Truncation error dominates

Back To ODES

$$\frac{dx}{dt} = \frac{(x(t+\Delta t) - x(t))}{\Delta t} = F(t)$$ derivative constant across Δt?

No

$$\boxed{y' = F(x_i, y_i)}$$



do easier example $x(1,2$

$$y' = \frac{y(x+\Delta x) - y(x)}{\Delta x} = F(x,y)$$

$$y(x+\Delta x) = y(x) + F(x,y)\Delta x$$

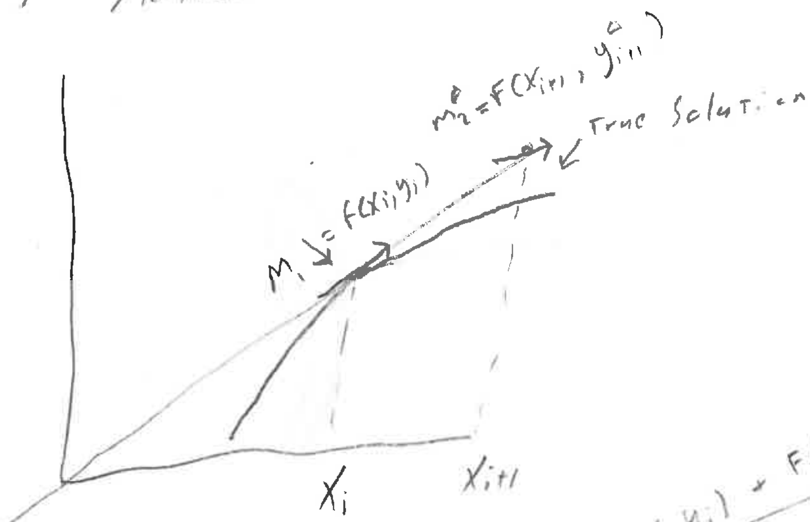
remember $y(x) = \int_0^x F(x)dx$

Integrator Time

Heun's Method

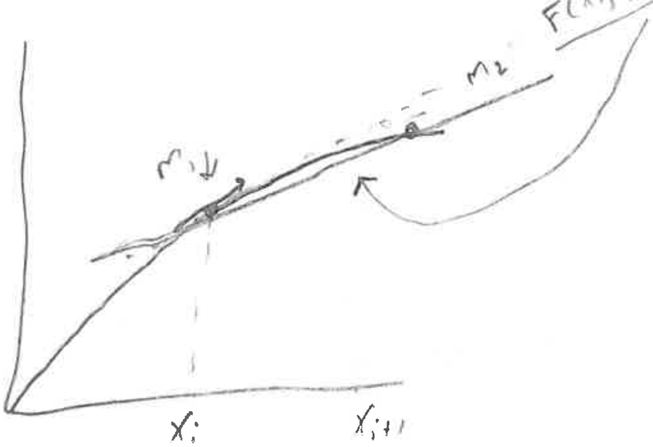
Predictor corrector

Predictor



$$\frac{F(x_i, y_i) + F(x_{i+1}, y_{i+1}^0)}{2} = \frac{m_1 + m_2}{2}$$

Corrector



Now

Predictor $Y^{0}_{i+1} = y_i + F(x_i, y_i)\,\Delta x$

Corrector $Y_{i+1} = y_i + \left(\dfrac{F(x_i, y_i) + F(x_{i+1}, y^{c}_{i+1})}{2}\right)\Delta x$

---

just x $\quad Y_{i+1} = y_i + \left(F(x_i) + F(x_{i+1})\right)\frac{h}{2}$ midpoint method

---

Runge Kutta Schemes → Integration schemes

$y_{i+1} = y_i + \phi(x_i, y_i, h)\,h$

$\phi = a_1 k_1 + a_2 k_2 + \dots a_n k_n$ → increment function

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + p_2 h,\ y_i + q_{11} k_1 h)$

$k_3 = F(x_i + p_2 h,\ y_i + q_{21} k_1 h + q_{22} k_2 h)$

$k_n = F(x_i + p_{n-1} h,\ y_i + q_{n-1,1} k_1 h + q_{n-1,2} k_2 h + \dots\ q_{n-1,n-1} k_{n-1} h)$

essentially a multislope evaluation with weights.

2nd order

$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2)h$

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + p_1 h,\ y_i + q_{11} k_1 h)$

$a_1 + a_2 = 1 \qquad a_2 p_1 = \frac{1}{2} \qquad a_2 q_{11} = \frac{1}{2}$

Derivation

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2) h$$

$$k_1 = F(x_i, y_i) \quad k_2 = F(x_i + p_1 h, y_i + q_{11} k_1 h)$$

$$y_{i+1} \approx y_i + \underset{\substack{\uparrow \\ y_i' = \frac{dy}{dx}}}{F(x_i, y_i)} h + \frac{F'(x_i, y_i) h^2}{2!} \quad \text{2nd order approximation}$$

$$F'(x_i, y_i) = \frac{\partial F(x,y)}{\partial x} + \frac{\partial F(x,y)}{\partial y} \frac{dy}{dx}$$

$$\boxed{y_{i+1} = y_i + F(x_i, y_i) h + \left(\frac{\partial F}{\partial x} + \frac{\partial F}{\partial y} \frac{dy}{dx} \right) \frac{h^2}{2!}} \quad A$$

now $\quad g(x+r, y+s) = g(x,y) + r\frac{\partial g}{\partial x} + s\frac{\partial g}{\partial y} + \cdots\cdots$

or $\quad k_2 = F(x_i + p_1 h, y_i + q_{11} k_1 h) = \underbrace{F(x_i, y_i) + p_1 h \frac{\partial F}{\partial x} + q_{11} k_1 h \frac{\partial F}{\partial y}}_{k_2} + O(h^2)$

So $\quad y_{i+1} = y_i + a_1 F(x_i, y_i) h + a_2 F(x_i, y_i) h + a_2 p_1 \frac{\partial F}{\partial x} h^2 + a_2 q_{11} F(x_i, y_i) \frac{\partial F}{\partial y} h^2 \ldots$

$$= y_i + (a_1 + a_2) F(x_i, y_i) h + \left[a_2 p_1 \frac{\partial F}{\partial x} + a_2 q_{11} F(x_i, y_i) \frac{\partial F}{\partial y} \right] h^2 + O(h^3)$$

compare to A

$$a_1 + a_2 = 1 \qquad a_2 p_1 = \frac{1}{2} \qquad a_2 q_{11} = \frac{1}{2}$$

if $\quad a_2$ known

$$a_1 = 1 - a_2$$

$$p_1 = q_{11} = \frac{1}{2a_2}$$

$\boxed{a_2 = \frac{1}{2}}$, $\underline{y_{i+1} = y_i + (\frac{1}{2}k_1 + \frac{1}{2}k_2)h}$ $a_1 = \frac{1}{2}$ $p_1 = q_{11} = 1$

$k_1 = F(x_i, y_i)$ Heun's Method

$k_2 = F(x_i + h, y_i + k_2 h)$

$\boxed{a_2 = 1}$ $a_1 = 0$, $p_1 = q_{11} = \frac{1}{2}$

$\underline{y_{i+1} = y_i + k_2 h}$

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + \frac{h}{2}, y_i + \frac{1}{2}k_1 h)$

Ralston's Method $\boxed{a_2 = \frac{2}{3}}$ minimum Truncation error

$y_{i+1} = y_i + (\frac{1}{3}k_1 + \frac{2}{3}k_2)h$

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + \frac{3}{4}h, y_i + \frac{3}{4}k_1 h)$

Lets Compare For $-2x^3 + 12x^2 - 20x + 8.5 = F(x,y) = \frac{dy}{dx}$

Third order

$y_{i+1} = y_i + \frac{1}{6}(k_1 + 4k_2 + k_3)h$

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$

$k_3 = F(x_i + h, y_i - k_1 h + 2k_2 h)$

4th order

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$$

$k_1 = F(x_i, y_i)$

$k_2 = F(x_i + \frac{1}{2}h, \; y_i + \frac{1}{2}k_1 h)$

$k_3 = F(x_i + \frac{1}{2}h, \; y_i + \frac{1}{2}k_2 h)$

$k_4 = F(x_i + h, \; y_i + k_3 h)$

---

ok we've just been doing more sophisticated integrals, lets get real.

$$\frac{dx}{dT} = -x(T)^3 + \sin(T)$$

def F(T, x)
return $-x^3 + \sin(T)$

$a = 0$, $b = 10$, $N = 100$, $h = \frac{b-a}{N}$

```
Tpoints = arange(a, b, h)
xpoints = []
x = 0.0
for T in Tpoints
    xpoints.append(x)
    k1 = h· F(T, x)
    k2 = h· F(T+½h, x+.5*k1)
    k3 = h· F(T+½h, x+½k2)
    k4 = h· F(T+h, x+k3)
    x += (k1 + 2(k2+k3) + k4)/6
```

Coupled Systems ?

$m\dfrac{dV}{dT} = -kx$ $\qquad \ddot{x} + \dfrac{k}{m}x = 0$ $\qquad x(t) = A\cos(\omega T) + B\sin(\omega T)$

$\dot{x}(0) = 1 \qquad x(0) = 1$

$\dfrac{dV}{dT} = -\dfrac{k}{m}x \qquad \dfrac{dy_2}{dT} = -\dfrac{k}{m}y_1$

$\dot{x}(T) = -A\omega\sin(\omega T) + B\omega\cos(\omega T)$

$V = \dfrac{dx}{dT} \qquad y_2 = \dfrac{dy_1}{dT}$

$A = 1 \qquad B = 1$

$\dfrac{dy_1}{dT} = y_2, \quad \dfrac{dy_2}{dT} = -\dfrac{k}{m}y_1$

$\underline{F(x) = -wx}$

$V_1 = F(x)$

$X_1 = V$

$V_2 = F(x + \frac{h \cdot X_1}{2})$

$X_2 = (V + \frac{h \cdot V_1}{2})$

$V_3 = F(x + \frac{h \cdot X_2}{2})$

$X_3 = (V + \frac{h \cdot V_2}{2})$

$V_4 = F(x + h \cdot X_3)$

$X_4 = (V + h \cdot V_3)$

$V_n = V + (V_1 + 2V_2 + 2V_3 + V_4) \cdot \frac{h}{6}$

$X_n = X + (X_1 + 2X_2 + 2X_3 + X_4) \cdot \frac{h}{6}$

So $\int F(x)\,dx$, $\dfrac{dx}{dT} = F(x,T)$, $\underbrace{\dfrac{dV}{dT} = F(x,T) \quad \dfrac{dx}{dT} = V}_{\text{Second order}}$

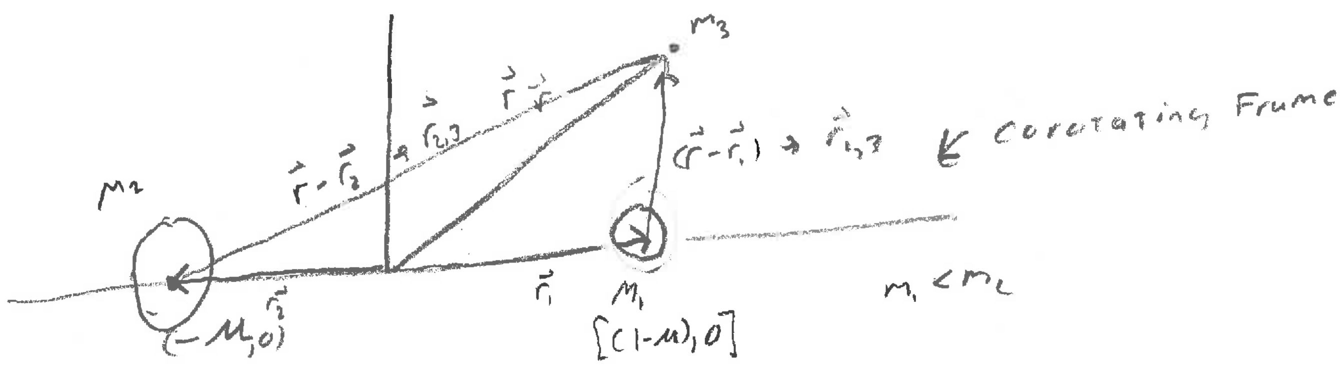
handy ?

There's much more

Let's look at error in the SHO case,

$m_2 > m_1 >> m_3$

essentially



Let $M_1 = \mu \quad M_2 = 1-\mu \quad \dfrac{M_1}{M_1+M_2} = M_1$

Show Wikipedia page on Lagrange points

and $|\vec{r}_1| + |\vec{r}_2| = 1 \quad |\vec{r}_2 - \vec{r}_1| = 1$

$\vec{r}_1 = (1-\mu)\hat{x} \quad r_2 = -\mu\hat{x}$

So $\vec{r} - \vec{r}_1 = \vec{r} - (1-\mu)\hat{x} = \vec{r}_{1,3} \qquad |\vec{r}_{1,3}|^2 = (x-1+\mu)^2 + y^2$

$\vec{r} - \vec{r}_2 = \vec{r} + \mu\hat{x} = \vec{r}_{2,3} \qquad |\vec{r}_{2,3}|^2 = (x+\mu)^2 + y^2$

$$\vec{F}_3 = -\frac{G M_1 m_3}{|\vec{r}-\vec{r}_1|^3}(\vec{r}-\vec{r}_1) - \frac{G M_2 m_3 (\vec{r}-\vec{r}_2)}{|\vec{r}-\vec{r}_2|^3}$$

$$\vec{F}_3 = \frac{-G M_1 m_3 \vec{r}_{1,3}}{((x-1+\mu)^2+y^2)^{3/2}} - \frac{G M_2 m_3}{((x+\mu)^2+y^2)^{3/2}}\vec{r}_{2,3}$$

] rotating

Need to add centrifugal $a = \dfrac{v^2}{r} = \dfrac{(r\omega)^2}{r} = \omega^2 r = \omega^2 x\hat{x} + \omega^2 y\hat{y}$

and coriolis $= 2\dot{y}\hat{x} - 2\dot{x}\hat{x}$

(44)

recalling $\frac{G(M_1+M_2)}{|r_{12}|^3} = \omega$ keplers law

$$\ddot{x} = 2\dot{y} + x - \frac{\mu}{|r_{1,3}|^3}(x-1+\mu) - \frac{(1-\mu)}{|r_{2,3}|^3}(x+\mu)$$

$$\ddot{y} = -2\dot{x} + y - \frac{(1-\mu)y}{|r_{2,3}|^3} - \frac{\mu y}{|r_{1,3}|^3} = -2\dot{x} + y\left(1 - \frac{\mu}{|r_{1,3}|^3} - \frac{(1-\mu)}{|r_{2,3}|^3}\right)$$

huh?

call $\dot{x}_2 = \ddot{x}$ $\quad x_2 = \dot{x}_1$ $\quad \vec{a} = F(x, y, r_{2,3}, r_{1,3}, v_x, v_y) = \frac{dv}{d\tau}$

$\dot{y}_2 = \ddot{y}$ $\quad y_2 = \dot{y}_1$ $\quad \vec{v} = \frac{d\vec{r}}{d\tau}$

$\vec{a}$ $\quad V$

ok? $x_0, y_0, v_{x0}, v_{y0} = (\vec{r}_0, \vec{v}_0)$

$$\boxed{\begin{aligned} k\vec{r}1 &= \vec{V}_0 \Delta T \\ k\vec{V}1 &= a(\vec{r}_0, \vec{v}_0, r_{1,3}, r_{2,3}) \end{aligned}}$$

$$k\vec{r}2 = \left(\vec{V}_0 + \vec{a}(\vec{r}_0, \vec{v}_0, r_{13}, r_{23})\frac{\Delta T}{2}\right)\Delta T = \left(\vec{V}_0 + \frac{k\vec{V}1}{2}\right)\Delta T$$

$$k\vec{v}2 = a\left(\vec{r}_0 + \frac{\vec{V}_0 \Delta T}{2}, \vec{V}_0 + a(\vec{r}_0, \vec{v}_0, r_{13}, r_{12})\frac{\Delta T}{2}\right)\Delta T = a\left(\vec{r}_0 + \frac{k\vec{r}1}{2}, \vec{V}_0 + \frac{k\vec{v}2}{2}\right)\Delta T$$

ok euler

$$\ddot{x} = 2\dot{y} + x - \frac{\mu}{|r_{1,3}|^3}(x-1+\mu) - \frac{(1-\mu)}{|r_{2,3}|^3}(x+\mu)$$

$$\ddot{y} = -2\dot{x} + y\left(1 - \frac{\mu}{|r_{1,3}|^3} - \frac{(1-\mu)}{|r_{2,3}|^3}\right)$$

$$\vec{a} = \ddot{x}\hat{i} + \ddot{y}\hat{j} = F(\vec{r}, \vec{v}, |r_{1,3}|, |r_{2,3}|)$$

$$\boxed{\begin{aligned} \overrightarrow{kr1} &= \vec{V}_0 \Delta T \\ k\vec{V}1 &= \vec{a}(\vec{r}_0, \vec{V}_0, |r_{1,3}|, |r_{2,3}|)\Delta T \end{aligned}}$$ euler step

$$\overrightarrow{kr2} = \left[\vec{r}_0 + a(\vec{r}_0, \vec{V}_0, |r_{1,3}|, |r_{2,3}|)\frac{\Delta T}{2}\right]\Delta T = \left(\vec{V}_0 + \frac{k\overrightarrow{V1}}{2}\right)\Delta T$$

$$k\vec{v}2 = \left[a\left(\vec{r}_0 + \frac{\vec{V}_0\Delta T}{2}, \vec{V}_0 + \vec{a}(\vec{r}_0, V_0, r_{13}, r_{23})\frac{\Delta T}{2}\right)\right]\Delta T = \left(a\left(\vec{r}_0 + \frac{k\overrightarrow{r2}}{2}, \vec{V}_0 + \frac{k\overrightarrow{V1}}{2}, r_{13}, r_{23}\right)\right)$$

So $k\vec{v}2 = a\left(\vec{r}_0 + \frac{k\overrightarrow{r2}}{2}, \vec{V}_0 + \frac{k\overrightarrow{V1}}{2}, r_{12}, r_{13}\right)\Delta T$

$$\boxed{\begin{aligned} \overrightarrow{kr3} &= \left(\vec{V}_0 + \frac{k\overrightarrow{V2}}{2}\right)\Delta T \\ k\overrightarrow{V3} &= a\left(\vec{r}_0 + \frac{k\overrightarrow{r2}}{2}, \vec{V}_0 + \frac{k\overrightarrow{V2}}{2}, r_{13}, r_{23}\right)\Delta T \end{aligned}}$$

$$\boxed{\begin{aligned} \overrightarrow{kr4} &= \left(\vec{V}_0 + k\overrightarrow{V3}\right)\Delta T \\ k\vec{V}4 &= a\left(\vec{r}_0 + k\overrightarrow{r3}, \vec{V}_0 + k\overrightarrow{V3}, r_{13}, r_{23}\right)\Delta T \end{aligned}}$$

$$\vec{r}_n = \vec{r}_0 + \frac{1}{6} \vec{kr1} + \frac{1}{3} \vec{kr_2} + \frac{1}{3} k\vec{r3} + \frac{1}{6} k\vec{r4}$$

$$\vec{V}_n = \vec{V}_0 + \frac{1}{6} k\vec{V1} + \frac{1}{3} k\vec{V2} + \frac{1}{3} k\vec{V3} + \frac{1}{6} kV4$$

Switched a bit by putting ΔT into

k's

Also, 1 swindle. What was it?

$r_{1,3}$, $r_{2,3}$ really need to be updated

k1	r_{13} (x, y)	r_{23} ( )	
k2	r_{13} $\left(x + \frac{kx_1}{2}, y + \frac{ky_1}{2}\right)$	r_{23} ...	
k_3	r_{13} $\left(x + \frac{kx_2}{2}, y + \frac{ky_2}{2}\right)$	r_{23} ...	
k_4	r_{13} $(x + kx_3, y + ky_3)$	r_{23} ...	

Outline

define

```
rad13(x, y, u)
    return sqrt((x-1+u)^2 + y^2)

rad23(x, y, u)
    return sqrt((x+u)^2 + y^2))

xddot
yddot      see example code
```

$$\vec{X}_n = \vec{X}_0 + \frac{1}{6} kX1 + \frac{1}{3} kX_2 + \frac{1}{3} kX3 + \frac{1}{6} k\vec{X}4$$

$$\vec{V}_n = \vec{V}_0 + \frac{1}{6} kv1 + \frac{1}{3} kv2 + \frac{1}{3} kv3 + \frac{1}{6} kv4$$

$|r_1| + |r_2| = 1, \quad |r_2 - r_1| = 1, \quad m_1 + m_2 = 1,$

$\vec{r}_1 = 1-\mu$	$m_1 = \mu$
$\vec{r}_2 = -\mu$	$m_2 = 1-\mu$

$$\mu = \frac{m_1}{m_1 + m_2} = m_1$$

Ex $\mu = .2$ $\quad m_1 = .2$ $\quad r_1 = .8$

$m_2 = .8$ $\quad r_2 = -.2$ $\qquad m_2 \; \cdots \; m_1$

$$r_1^2 = (x - 1 + \mu)^2 + y^2$$

$$r_2^2 = (x + \mu)^2 + y^2$$

Now $G = 1$, $w = 1$ $\quad \ddot{\vec{r}} - w\vec{r} - 2w\dot{\vec{v}} = \frac{-\mu}{r_1^3}(\vec{r} - \vec{r}_1) - \frac{(1-\mu)}{r_2^3}(\vec{r} - \vec{r}_2)$

$$\ddot{X} - \vec{r} - 2\vec{V} = \frac{-\mu}{r_1^3}$$

Example

$\vec{a} = F(\vec{x}, \vec{v})$

$\vec{v} = \vec{a}\,dT$ (1st order)

$\vec{x} = \vec{v}\,dT$ (1st order) $\rightarrow$ Euler Not Energy Conserving

$a_x = F(v_y, x, \mu, r_1, r_2)$

$a_y = F(v_x, y, \mu, r_1, r_2)$

Better

$x_0, y_0, v_{x0}, v_{y0} = (\vec{x}_0, \vec{v}_0)$

$$k\vec{x}1 = \vec{v}_0 \Delta T$$

$$k\vec{v}1 = a(\vec{x}_0, \vec{v}_0)\Delta T$$

$$k\vec{x}2 = \left(\vec{v}_0 + \frac{a(\vec{x}_0, \vec{v}_0)\Delta T}{2}\right)\Delta T = \left(\vec{v}_0 + \frac{k\vec{v}1}{2}\right)\Delta T$$

$$k\vec{v}2 = \left(a\left(\vec{x}_0 + \frac{\vec{v}_0\Delta T}{2}, \vec{v}_0 + \frac{a(\vec{x}_0, \vec{v}_0)\Delta T}{2}\right)\right)\Delta T = a\left(\vec{x}_0 + \frac{k\vec{x}1}{2}, \vec{v}_0 + \frac{k\vec{v}1}{2}\right)\Delta T$$

$$k\vec{x}3 = \left(\vec{v}_0 + \frac{k\vec{v}2}{2}\right)\Delta T$$

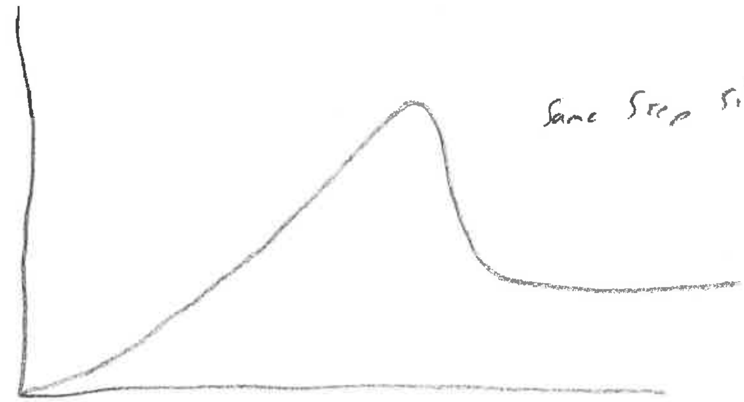
$$k\vec{v}3 = a\left(\vec{x}_0 + \frac{k\vec{x}2}{2}, \vec{v}_0 + \frac{k\vec{v}2}{2}\right)\Delta T$$

$$k\vec{x}4 = \left(\vec{v}_0 + k\vec{v}3\right)\Delta T$$

$$k\vec{v}4 = a\left(\vec{x}_0 + k\vec{x}3, \vec{v}_0 + k\vec{v}3\right)\Delta T$$

$\vec{x}$

Variable Step Size RK4



Let h change

1. Pick error allowed (ϵ)

   Ex $\epsilon = .001$ per $T=1$

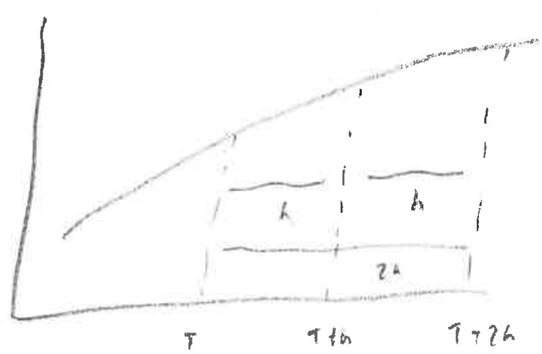
   Then $\epsilon_{Total} = .01$ For $T \in [0,10]$

2. Compare error To ϵ

3. Change h

Pick an h, Small, For 2yr orbit $h \sim 1$ hour

1st



do: 2 individual Steps with h 4th order accurate error is 5th order or $\sim Ch^5$ where C is a constant we don't know

Then $X(T+2h) = X_1 + 2Ch^5$

First estimate

do: 1 step with step size $2h$

Then $x(t+2h) = x_2 + c(2h)^5 = x_2 + 32ch^5$

↑ second estimate ↑ error

Now $x_1 - x_2 = 30ch^5$

Now $\epsilon = ch^5 = \dfrac{(x_1 - x_2)}{30}$

desired $\longrightarrow \epsilon' = ch'^5$

↑ target h

$$\epsilon' = ch'^5 = ch^5\left(\frac{h'}{h}\right)^5 = \frac{1}{30}(x_1 - x_2)\left(\frac{h'}{h}\right)^5$$

Pick a target accuracy δ s.t.

$$\delta = \frac{\frac{1}{30}|x_1 - x_2|\left(\frac{h'}{h}\right)^5}{h'} \quad \text{error per desired timestep}$$

↑ you pick

Then $h' = h\left(\dfrac{30h\delta}{|x_1 - x_2|}\right)^{1/4} = h\rho^{1/4}$

$\rho = \dfrac{30(h\delta)}{|x_1 - x_2|}$ ← target accuracy

ratio $\dfrac{(h\delta) \leftarrow \text{target}}{\text{actual accuracy}}$

Method. 1: Take 2 successive RK4 steps to calculate x_1

2: Take 1 step at $2h$ to calculate x_2

3: calculate ρ

a: if $\rho > 1$ fine, calculate new $h' = h\rho^{1/4}$ for next timestep
move to $x(t+2h)$ with larger step

b: if $\rho < 1$ bad, not accurate enough
calculate $h' = h\rho^{1/4}$, reduce step, try again

So either accept, move to $X(T+2h)$, increase h

or reduce h, keep trying

Cons → 3 RK4 steps per implementation

Pros → usually faster, better accuracy

really need a safety factor.

if h increases limit the increase by maximum

of 2h

2D? $\epsilon_x = \frac{1}{30}(x_1 - x_2)$ $\quad \epsilon_y = \frac{1}{30}(y_1 - y_2)$

$\frac{1}{30}|x_1 - x_2| \longrightarrow \sqrt{\epsilon_x^2 + \epsilon_y^2}$

Making RK4 order h^6?

recall 2 step

$X(T+2h) = x_1 + 2ch^5 + O(h^6)$

$ch^5 = \frac{1}{30}(x_1 - x_2)$

So $X(T+2h) = x_1 + \frac{1}{15}(x_1 - x_2) + O(h^6)$

1 → do above with caveats that $\rho > 1$

Then $X(T+2h) = x_1 + \frac{1}{15}(x_1 - x_2)$

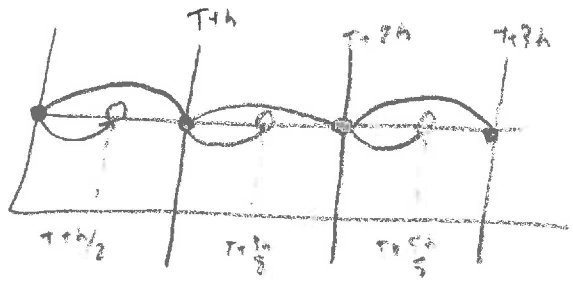
I could make this more annoying

6th order, flexible adaptive, stiff solver etc.

just use odeint

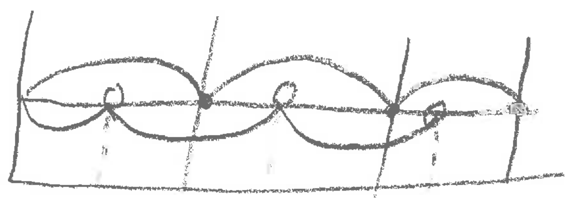
For energy and momentum conserving problems it gets easier

RK4



use midpoint to calculate endpoint
midpoint calculated at beginning of each

Leapfrog



midpoint calculated from midpoint

$x(T+\frac{1}{2}h) = x(T) + \frac{1}{2} h F(x,T)$ $\qquad F(x,T) = \frac{dx}{dT}$

Euler

$$x(T+h) = x(T) + hF\left(T+\tfrac{1}{2}h,\ x(T+\tfrac{1}{2}h)\right) + O(h^2)$$

$$x(T+\tfrac{3}{2}h) = x(T+\tfrac{1}{2}h) + hF\left(T+h,\ x(T+h)\right)$$

$$x(T+2h) = x(T+h) + hF\left(T+\tfrac{3}{2}h,\ x(T+\tfrac{3}{2}h)\right)$$

$$\vec{r}(T+h) = \vec{r}(T) + hF\left(T+\tfrac{1}{2}h,\ \vec{r}(T+\tfrac{1}{2}h)\right)$$

$$\vec{r}(T+\tfrac{3}{2}h) = \vec{r}(T+\tfrac{1}{2}h) + hF\left(T+h,\ \vec{r}(T+h)\right)$$

Why? Time reversible, conserves energy and momentum

Verlet Method

Verlet Method

$\vec{F} = m\vec{a}$ $\quad \frac{dx}{dt} = v \quad \frac{dv}{dt} = F(x,t)$

let $\vec{r} = (x, v)$

$$\frac{d\vec{r}}{dt} = F(r, t)$$

know $x(t)$, $v(t+\frac{1}{2}h)$

$x(t+h) = x(t) + h\,v(t+\frac{1}{2}h)$

$v(t+\frac{3}{2}h) = v(t+\frac{1}{2}h) + h\,F(t+h, x(t+h))$

iterate

works for $x(v)$, $v(x)$ $\rightarrow$ gravity, springs

hmm what if we want $E = PE + KE$?

need $v(t+h)$ not $v(t+\frac{?}{2}h)$

Single backward Euler step

$v(t+\frac{1}{2}h) = v(t+h) - \frac{1}{2}h\,F(t+h, x(t+h))$

$$\boxed{v(t+h) = v(t+\frac{1}{2}h) + \frac{1}{2}h\,F(t+h, x(t+h))}$$

given $x(t)$, $v(t)$

once

$$\frac{d^2\vec{r}}{dt^2} = F(\vec{r}, t) \rightarrow v(t+\tfrac{1}{2}h) = v(t) + \tfrac{1}{2}h\,F(t, r(t))$$

iterate

$r(t+h) = r(t) + h\,v(t+\frac{1}{2}h)$

$k = h\,F(t+h, r(t+h))$

$v(t+h) = v(t+\frac{1}{2}h) + \frac{1}{2}k$

$v(t+\frac{3}{2}h) = v(t+\frac{1}{2}h) + k$

Why? Time reversal and energy conservation.

Let's let $h \to -h$

$$x(T-h) = x(T) - h\,F(T-\tfrac{1}{2}h,\ x(T-\tfrac{1}{2}h))$$

$$x(T-\tfrac{3}{2}h) = x(T-\tfrac{1}{2}h) - h\,(F(T-h,\ x(T-h))$$

$T \to T+\frac{3}{2}h$

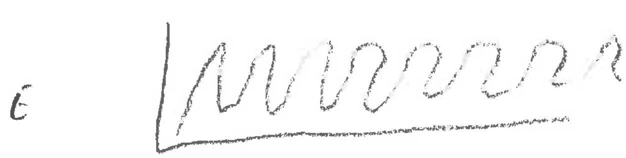
$$x(T+\tfrac{1}{2}h) = x(T+\tfrac{3}{2}h) - h\,F(T+h,\ x(T+h))$$

$$x(T) = x(T+h) - h\,F(T+\tfrac{1}{2}h,\ x(T+\tfrac{1}{2}h))$$

which is exactly the same as going forward with $h \to -h$. So you can start at the end and "retrace" the solution back to the start. This is NOT the case for replacing $h \to -h$ in a RK scheme.

Ex $\frac{d\theta}{dT} = \omega \qquad \frac{d\omega}{dT} = -\frac{g}{\ell}\sin\theta$

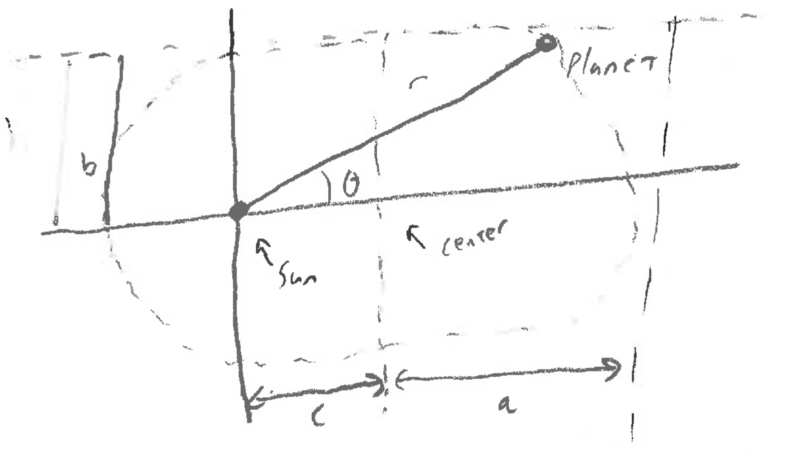
RK2 energy builds (or decays)



leapfrog

good for periodic systems springs, orbits, etc

2 Body



$b = \sqrt{a^2 - c^2}$

$$r(\theta) = \frac{a(1-e^2)}{1-\epsilon\cos(\theta)} \qquad e = \text{eccentricity}$$

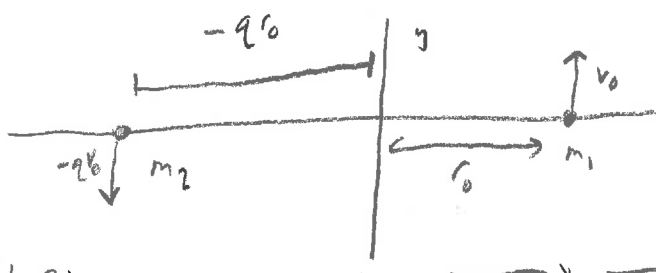
$$\frac{1}{2} r^2 \frac{d\theta}{d\tau} = \frac{\pi a^2 (1-e^2)^{1/2}}{\tau} \qquad \tau^2 = \frac{4\pi^2 a^3}{G(m_1+m_2)}$$

Pick $d\tau \sim \frac{\tau}{1000}$

$$\vec{r}_{cm} = \frac{m_1\vec{r}_1 + m_2\vec{r}_2}{m_1+m_2} = 0 \qquad \vec{V}_{cm} = \frac{m_1\vec{V}_1 + m_2\vec{V}_2}{m_1+m_2} = 0$$

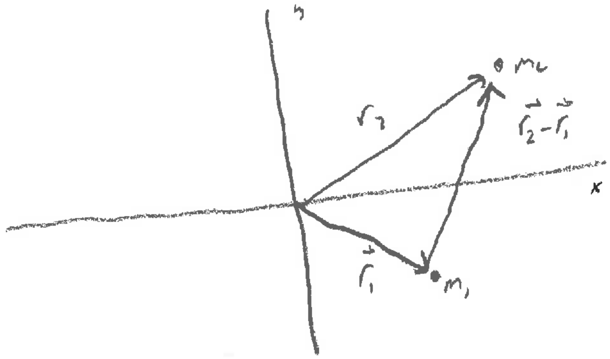
$X_1(0) = r_0 \quad y_1(0) = 0 \quad x_2(0) = -qr_0 \quad y_2(0) = 0 \qquad q = \frac{m_1}{m_2}$

$V_{x_1}(0) = 0 \quad V_{y_1}(0) = V_0 \quad V_{x_2}(0) = 0 \quad V_{y_2}(0) = -qV_0$



$$r_0 = \left(\frac{1-e}{1+q}\right)a \qquad V_0 = \frac{1}{1+q}\left(\sqrt{\frac{1+e}{1-e}}\right)\sqrt{\frac{G(m_1+m_2)}{a}}$$

2 body orbit → has exact solution



$$\vec{F}_1 = \frac{G m_1 m_2}{|\vec{r}_{12}^{\,2}|} \frac{(\vec{r}_2 - \vec{r}_1)}{|\vec{r}_{12}|} = -\vec{F}_2$$

$$\vec{a}_1 = \frac{\vec{F}_1}{m_1} \qquad \vec{a}_2 = \frac{\vec{F}_2}{m_2}$$

$$\frac{d\vec{r}_1}{dt} = \vec{V}_1 \quad \frac{d\vec{r}_2}{dt} = \vec{V}_2 \quad \frac{d\vec{V}_1}{dt} = \vec{a}_1 = \frac{\vec{F}_1}{m_1} \quad \frac{d\vec{V}_2}{dt} = \frac{\vec{F}_2}{m_2}$$ 8 ODES

need $\vec{r}_1(0)$, $\vec{r}_2(0)$, $\vec{V}_1(0)$, $\vec{V}_2(0)$

$$\frac{dx_1}{dt} = V_{x1} \quad \frac{dy_1}{dt} = V_{y1} \quad \frac{dx_2}{dt} = V_{x2} \quad \frac{dy_2}{dt} = V_{y2}$$

$$\frac{dV_{x1}}{dt} = \frac{G m_2}{|r_{12}|^2}\left(\frac{x_2 - x_1}{|r_{12}|}\right) \quad \frac{dV_{y1}}{dt} = \frac{G m_2}{|r_{12}|^2}\left(\frac{y_2 - y_1}{|r_{12}|}\right)$$

$$\frac{dV_{x2}}{dt} = \frac{G m_1}{|r_{12}|^2}\left(\frac{x_1 - x_2}{|r_{12}|}\right) \quad \frac{dV_{y2}}{dt} = \frac{G m_1}{|r_{12}|^2}\left(\frac{y_1 - y_2}{|r_{12}|}\right)$$

ElectroStatics

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \qquad \epsilon_0 = 8.85 \cdot 10^{-12} \frac{C^2}{Nm^2}$$

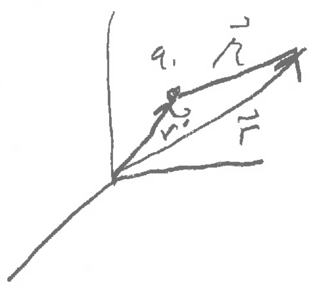
$\rho =$ charge density

Integral Solution

$$\vec{E}(r) = \frac{1}{4\pi\epsilon_0} \int \frac{\hat{\mathscr{r}}}{\mathscr{r}^2} \rho(r') \, d\tau'$$

3D

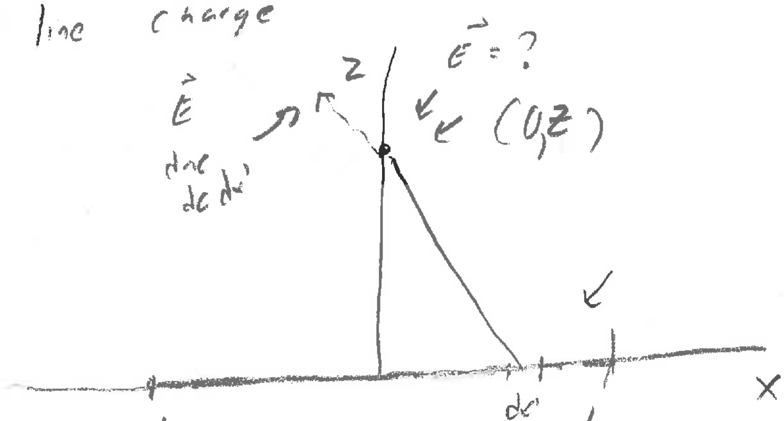
volume element
$dx\,dy\,dz$
$r\,d\phi\,dr\,dz$
$r^2 \sin\theta \, dr\,d\phi\,d\theta$



$$\vec{r}' + \vec{\mathscr{r}} = \vec{r}$$

$\vec{\mathscr{r}} = \vec{r} - \vec{r}' \rightarrow$ Field Location − charge location

Ex line charge



$$d\vec{E}(x, z) = \frac{1}{4\pi\epsilon_0} \int_{-L}^{L} \frac{\lambda(r')\,\hat{\mathscr{r}}}{\mathscr{r}^2} \, d\ell'$$

$\lambda =$ constant $\quad \vec{r} = 0\hat{i} + z\hat{j} \quad \vec{r}' = x\hat{i} + \hat{j}$

$$\hat{\mathscr{r}} = \frac{-x\hat{i} + z\hat{j}}{\sqrt{x^2+z^2}} \quad \mathscr{r}^2 = \left(\sqrt{x^2+z^2}\right)^2 = x^2+z^2 \quad (55)$$

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \int_{-L}^{L} \frac{\lambda(-x\hat{i} + z\hat{j})}{(x^2+z^2)\sqrt{x^2+z^2}}\, dx$$

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \int_{-L}^{L} \frac{-\lambda x\hat{i} + \lambda z\hat{j}}{(x^2+z^2)^{3/2}}\, dx$$

$$E(x,z)\,\hat{i} = 0$$

$$E(x,z)\,\hat{j} = \frac{\lambda z}{z^2\sqrt{z^2+x^2}} \cdot \frac{1}{4\pi\epsilon_0} \Bigg|_{-L}^{L}$$

$$\vec{E} = \frac{1}{4\pi\epsilon_0} \frac{2\lambda L}{z\sqrt{z^2+L^2}}\,\hat{j}$$

For $z \ll L$ $\vec{E} \simeq \frac{1}{4\pi\epsilon_0} \frac{2\lambda}{z}$

Another Way

$\vec{E} = -\nabla V$ Field = - gradient potential

$\vec{\nabla}\cdot\vec{E} = \frac{\rho}{\epsilon_0}$ $\vec{\nabla}\cdot\vec{\nabla}V = \nabla^2 V = \frac{\rho}{\epsilon_0}$

Poisson's Equation

Let's Start

With no charge but potentials specified

on the boundaries

$$\vec{\nabla}\cdot\vec{\nabla} V = \nabla^2 V = 0 \rightarrow \nabla\cdot\vec{E} = 0$$

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

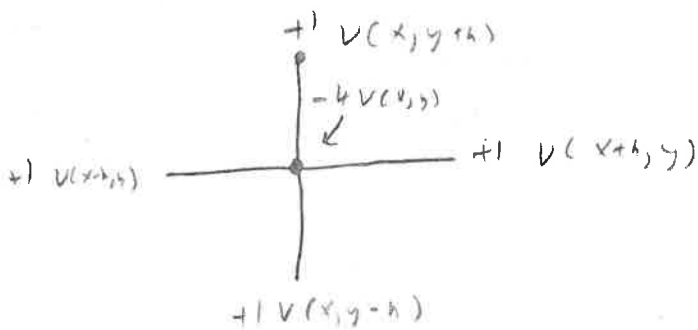
relaxition Method

$$\frac{\partial^2 V}{\partial x^2} = \frac{V(x+h,y) + V(x-h,y) - 2V(x,y)}{h^2}$$

$$\frac{\partial^2 V}{\partial y^2} = \frac{V(x,y+h) + V(x,y-h) - 2V(x,y)}{h^2}$$

Same size h_c d_x, d_y can EASILY change

$$\text{So} \quad \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = \frac{V(x+h,y) + V(x-h,y) + V(x,y+h) + V(x,y-h) - 4V(x,y)}{h^2}$$



geometric average

$$V(x,y) = \text{ by } \nabla^2 V = 0$$

$$\text{So} \quad V(x,y) = \left[V(x+h,y) + V(x-h,y) + V(x,y+h) + V(x,y-h)\right]\cdot\frac{1}{4}$$

For $\nabla^2 V = 0$ $h \to$ not important

$\nabla^2 V = \frac{\rho}{\epsilon_0}$ Same but add $\frac{\rho h^2}{4\epsilon_0}$

So what?

Specify $\rho(i,j)$ add $\frac{\rho(i,j)h^2}{4\epsilon_0}$ if zero Laplace

1. Specify $V(i,j)$ at the boundaries and zero everywhere else

2. Calculate $V'(x,y) = \frac{1}{4}\left[V(x+h,y) + V(x-h,y) + V(x,y+h) + V(x,y-h)\right] + \frac{\rho(i,j)h^2}{4\epsilon_0}$

3. Compare $V'(x,y)$ to $V(x,y)$
   a.) Set a tolerance ϵ, $1e^{-6}$ is ok
   b.) compare error $= \frac{\left|\Sigma V(x,y) - \Sigma V'(x,y)\right|}{N_x N_y}$ = error / gridpoint
   c.) if error $< \epsilon$ Stop
   D.) if error $> \epsilon$ $V(x,y) \to V'(x,y)$ go to 2

$\vec{E}$? $\vec{E} = -\vec{\nabla} V \to$ no gradient time

Slow   100x100 ~ 10 minutes

Enter overrelaxation   Trick #1

$\phi(x,y) + \Delta\phi(x,y) = \phi'(x,y)$

$\Delta\phi(x,y) = \phi'(x,y) - \phi(x,y)$ Put in

$\phi_w(x,y) = \phi(x,y) + (1+w)\,\Delta\phi(x,y)$

overrelaxed

$w \in (0,1)$ algebra happens

$$\phi_w(x,y) = \left(\frac{1+w}{4}\right)\left[\phi(x+h,y) + \phi(x-h,y) + \phi(x,y+h) + \phi(x,y-h)\right] - w\,\phi(x,y)$$

Gauss-Seidel → Never calculate arrays Twice

New   Monte Carlo

Random # generator $x' = (ax+c) \bmod m$ linear congruential

Pick a, c, m

1. NOT RANDOM!! Correlation only, not good for physics
2. Always > 0
3. a, c, m matter → if c, m even, all even or odd.
4. initial value is the "seed"

Look up numpy.random

(5-9)

generating on interval [a, b]

(b-a) * np.random.rand(10) + a

b = 1   a = -1

Example

Want repeatability → np.random.seed(#)

Example

Radioactive decay

$N(t) = N(0)\, 2^{-t/\tau}$ τ = half life

Fraction not decayed = $\dfrac{N(t)}{N(0)} = 2^{-t/\tau}$

Fraction decayed = $1 - 2^{-t/\tau}$

$^{208}Tl \rightarrow {}^{208}Pb$ τ = 3.053 minutes

Thelium   lead

Example