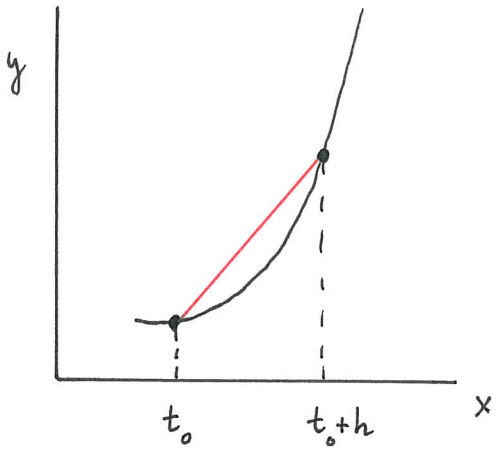
NUMERICAL METHODS
LECTURE 1



NUMERICAL APPROXIMATION TO DERIVATIVE RELIES ON SLOPE OF SECANT BETWEEN t_0 AND t_0+h

AS $h \to 0$ SLOPE OF SECANT APPROACHES SLOPE OF TANGENT

$$y'(t_0) \approx \frac{y(t_0+h) - y(t_0)}{h}$$

REWRITE $$y(t_0+h) \approx y(t_0) + h y'(t_0)$$

BASIS FOR EULER'S METHOD.

CONSIDER ODE

$$\frac{dx}{dt} = f(x,t) \qquad \text{WHERE} \quad x(0) = x_0$$

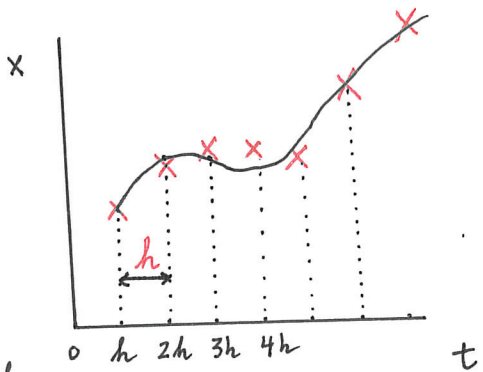
($t=0$)

INITIAL VALUE PROBLEM

> TASK: FIND $x(t)$ WHOSE DERIVATIVE IS EQUAL TO f EVALUATED AT $x(t)$

NUMERICAL APPROACH:

DON'T FIND $x(t)$ AT ALL VALUES OF t BUT AT DISCRETE VALUES OF t.



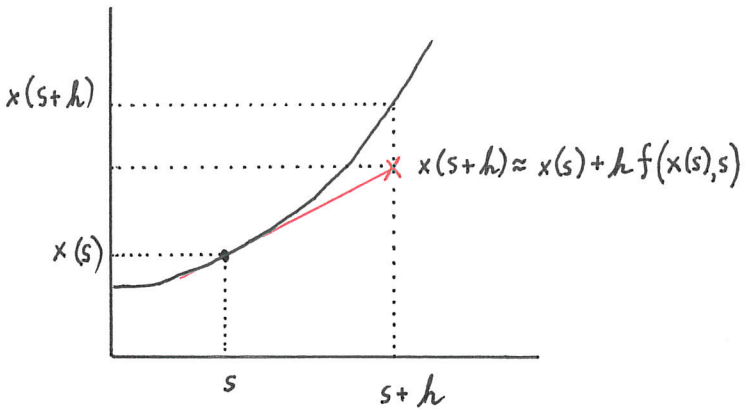
SIMPLEST CASE: EQUALLY SPACED VALUES OF t WITH STEPSIZE h.

LOOK FOR METHOD TO APPROXIMATE $x(t+h)$ GIVEN $x(t)$

THEN CAN APPLY METHOD REPEATEDLY TO FIND APPROXIMATIONS FOR $x(nh)$ FOR ANY n IF $x(0)$ SPECIFIED INITIALLY

EULER'S METHOD

THE ODE $$\frac{dx}{dt} = f(x,t)$$



IF KNOW x AT $t = s$

THEN USE IT TO COMPUTE

$$f(x(s), s)$$

WHICH ACCORDING TO ODE IS THE DERIVATIVE OF x AT $t = s$. THEN USE $f(x(s), s)$ TO COMPUTE $x(s+h)$ AT NEXT STEP:

$$\boxed{x(s+h) \approx x(s) + h\underbrace{f(x(s), s)}_{\left.\frac{dx}{dt}\right|_{t=s}}}$$

SAME AS KEEPING FIRST 2 TERMS IN TAYLOR EXPANSION

ASSUMING DERIVATIVE CHANGES LITTLE BETWEEN $t = s$ AND $t = s+h$ AND IMPORTANTLY USING VALUE OF DERIVATIVE AT BEGINNING OF STEP.

EULER METHOD "BY HAND"

APPROXIMATE SOLUTION OF

$$\frac{dx}{dt} = t - x^2$$ AT TIME $t = 2$

GIVEN $x(0) = 0 = x_0$

NO ANALYTIC SOLUTION; NUMERICAL SOLUTION ACCURATE TO 4 DECIMAL PLACES $x(2) = 1.1936$

TAKE $h = 1 \Rightarrow t_n = nh = n$

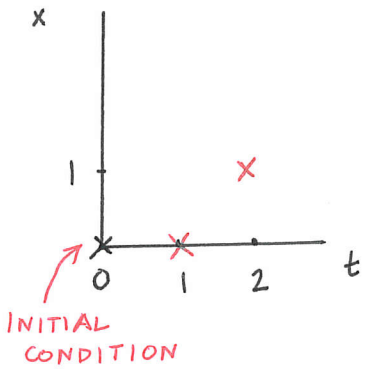
$x_n = x(t_n) = x(n)$

EULER METHOD :

$$x_{n+1} = x_n + h f(x_n, t_n)$$

$$= x_n + h(t_n - x_n^2)$$

$$x_{n+1} = x_n + (n - x_n^2)$$



$x_0 = 0$ GIVEN

$x_1 = x_0 + (0 - x_0^2) = 0$

$x_2 = x_1 + (1 - x_1^2) = 1$

so $x(2) = 1$

NOT SURPRISING THAT APPROXIMATION NOT VERY ACCURATE BC ASSUMING DERIVATIVE CONSTANT BETWEEN $t=0$ AND $t=1$, AND BETWEEN $t=1$ AND $t=2$

HOW CAN WE GET A BETTER APPROXIMATION?

HALVE THE STEPSIZE $h = 1/2 \Rightarrow t_n = \frac{n}{2}$, $x_n = x\left(\frac{n}{2}\right)$

EULER :

$$x_{n+1} = x_n + \frac{1}{2}\left(\frac{n}{2} - x_n^2\right)$$

HAD TO TAKE TWICE NUMBER OF STEPS TO GET TO SAME PLACE

$x_0 = 0$ GIVEN

$x_1 = x_0 + \frac{1}{2}(0 - x_0^2) = 0$

$x_2 = x_1 + \frac{1}{2}\left(\frac{1}{2} - x_1^2\right) = \frac{1}{4}$

$x_3 = x_2 + \frac{1}{2}\left(\frac{2}{2} - x_2^2\right) = \frac{1}{4} + \frac{1}{2}\left(1 - \frac{1}{16}\right) = \frac{23}{32}$

$x_4 = \ldots = \frac{834}{689} \simeq 1.2104$

BETTER APPROXIMATION BC ASSUMPTION THAT DERIVATIVE AT BEGINNING OF STEP IS SAME AS DERIVATIVE THROUGHOUT STEP BECOMES MORE ACCURATE WITH SMALLER STEP SIZE.

CAN WE GET A BETTER APPROXIMATION TO THE DERIVATIVE IN THE INTERVAL ?

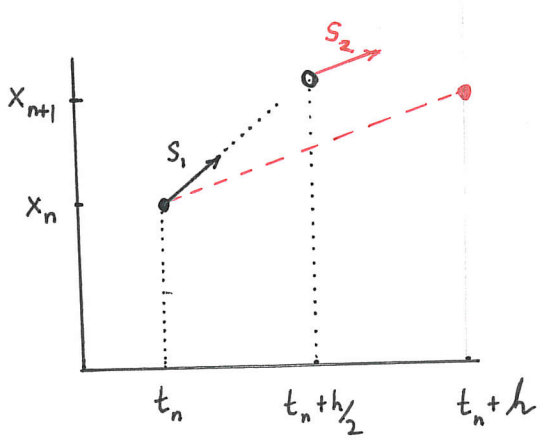
IDEA: EVALUATE f MORE THAN ONCE IN A STEP

MIDPOINT METHOD: EVALUTE f TWICE PER STEP

$$s_1 = f(x_n, t_n)$$

$$s_2 = f\left(x_n + \frac{h}{2} s_1, t_n + \frac{h}{2}\right)$$

$$x_{n+1} = x_n + h s_2$$



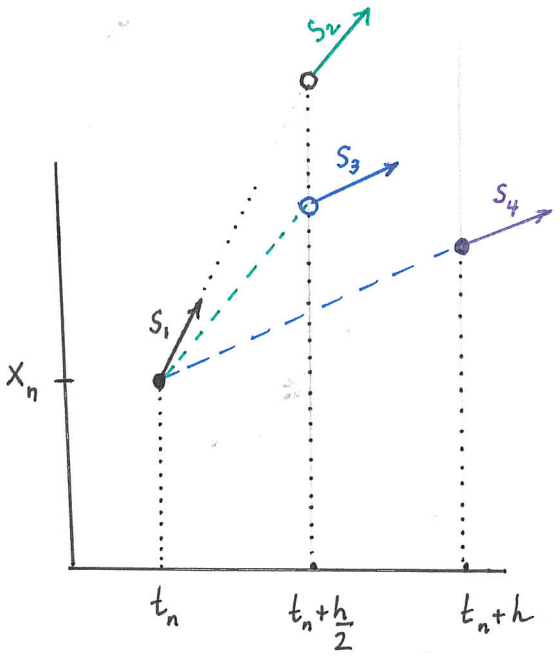
RUNGE KUTTA: EVALUATE f FOUR TIMES PER STEP

$$s_1 = f(x_n, t_n)$$

$$s_2 = f\left(x_n + \frac{h}{2} s_1, t_n + \frac{h}{2}\right)$$

$$s_3 = f\left(x_n + \frac{h}{2} s_2, t_n + \frac{h}{2}\right)$$

$$s_4 = f\left(x_n + h s_3, t_n + h\right)$$



$$x_{n+1} = x_n + \frac{h}{6}\left(s_1 + 2s_2 + 2s_3 + s_4\right)$$

CAN TAKE LARGER STEP THAN WITH EULER FOR SAME ACCURACY

ACCURACY

DETERMINING ACCURACY BY EXPERIMENT

FOR pTH ORDER ACCURATE SCHEME

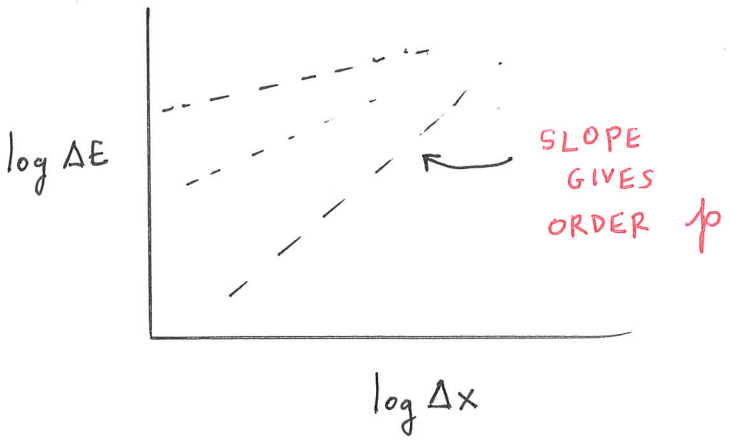
ERROR $\Delta E \sim (\Delta x)^p$

STEP SIZE

DIFFERENT WAYS TO QUANTIFY ERROR

$$\begin{cases} \Delta E = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(u_i - u^{exact}(x_i)\right)^2} \\ \Delta E = \frac{1}{N}\sum_{i=1}^{N}\left|u_i - u^{exact}(x_i)\right| \\ \Delta E = \max\left|u_i - u^{exact}(x_i)\right| \end{cases}$$

RUN SCHEME WITH A KNOWN SOLUTION (PREFERABLY AN ANALYTIC ONE) FOR A RANGE OF MESH SIZES Δx



- IF PROBLEM DOESN'T HAVE ANALYTIC SOLUTION, TAKE FINEST MESH IN A SET OF MESHES AND OBTAIN ΔE BY COMPARING SOLUTION ON COARSER MESH TO SOLUTION ON FINEST MESH.

HIGHER ORDER SCHEMES WILL CONVERGE TO CORRECT SOLUTION ON COARSER MESHES

RUNGE-KUTTA: 4th ORDER
MIDPOINT: 2nd ORDER
EULER: 1st ORDER

STABILITY

WHAT IF APPLY NUMERICAL METHOD OVER MANY, MANY STEPS.

EACH STEP INTRODUCES ERRORS

ROUND OFF ERROR: NUMERICAL ERROR INTRODUCED WHEN COMPUTER ROUNDS THE NUMBER TO SOME SIGNIFICANT FIGURE.

TRUNCATION ERROR: DEFINES WHAT'S BEING NEGLECTED IN APPROXIMATION TO DERIVATIVE

IS THE ERROR AMPLIFIED IN GOING FROM STEP $n \rightarrow n+1$, OR DOES IT DECREASE OR NOT GROW AT ALL?

CONSIDER $$\frac{du}{dt} = -\sigma u$$

WITH $u = u(0)$ AT $t = 0$

ANALYTIC SOLUTION $$u(t) = u(0)\, e^{-\sigma t}$$

IF DISCRETIZE IN TIME $t_n = n\,\Delta t$

ANALYTIC SOLUTION SATISFIES

$$u(t_{n+1}) = e^{-\sigma \Delta t}\, u(t_n)$$

$u(t_n)$: INITIAL CONDITION FOR NEXT TIME STEP WHICH IS Δt AWAY FROM t_n

NOW CONSIDER EULER SCHEME FOR ODE

$$\frac{u_{n+1} - u_n}{\Delta t} = \overbrace{-\sigma u_n}^{f(u,t)}$$

← EVALUATE AT BEGINNING OF TIME STEP

$$u_{n+1} = u_n - \sigma \Delta t\, u_n$$

AN EXPLICIT SCHEME: u_{n+1} DEPENDS ON u_n

$$u_{n+1} = \underbrace{(1 - \sigma \Delta t)}_{\text{AMPLIFICATION FACTOR} \equiv \lambda} u_n$$

IF INITIAL CONDITION IS u_0, SOLUTION AFTER "n" TIME STEPS IS

$$u_n = \lambda^n u_0$$

WHAT CONDITIONS SHOULD WE IMPOSE ON λ TO MAINTAIN STABILITY?

- WANT $\lambda \geq 0$ BC PHYSICAL SOLUTION FOR u_{n+1} IS POSITIVE SO NUMERICAL ONE SHOULD BE TOO

$$1 - \sigma \Delta t \geq 0 \quad \Rightarrow \quad \Delta t \leq \frac{1}{\sigma}$$

- MORE RELAXED STABILITY REQUIREMENT

$$|\lambda|^n < \mathcal{M}$$

WHERE $\mathcal{M}$ IS A POSITIVE, FINITE, REAL NUMBER

$$|\lambda| < \mathcal{M}^{1/n}$$

WHEN $n \to \infty$ $\Rightarrow$ $\boxed{|\lambda| < 1}$

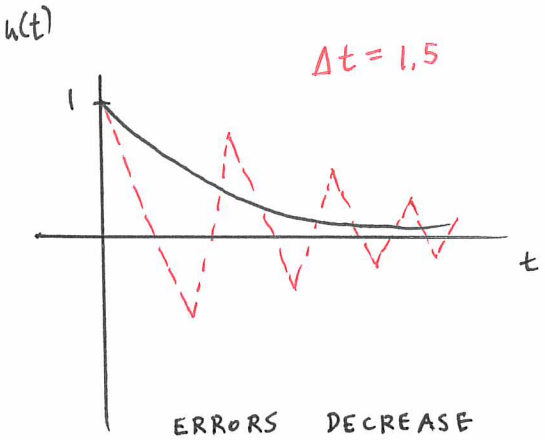
$$\rightarrow \quad 1 - \sigma \Delta t > -1$$

$$\therefore \quad \Delta t \leq \frac{2}{\sigma}$$

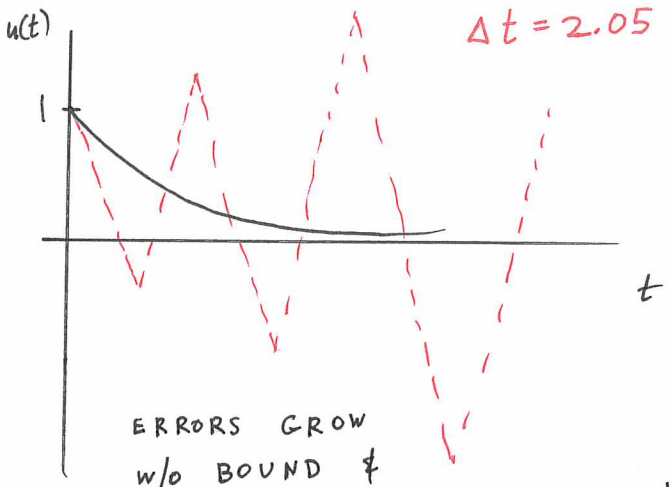
STABILITY REQUIREMENT RESTRICTS THE TIME STEP OF THE EXPLICIT SCHEME IF IT IS TO REMAIN STABLE

CONDITIONAL STABILITY

EXAMPLE $\frac{du}{dt} = -u(t)$ $(\sigma = 1)$ with $u(0) = 1$



ERRORS DECREASE WITH TIME BC $\Delta t < 2$

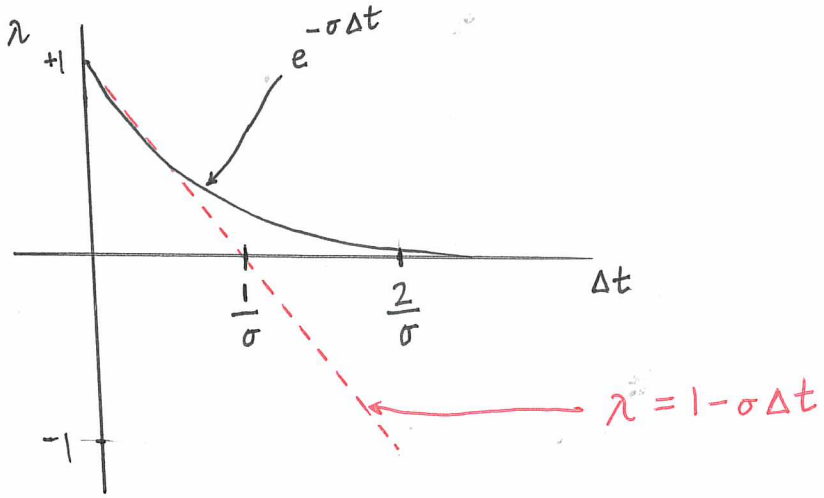


ERRORS GROW w/o BOUND & MASK TRUE SOLUTION BC $\Delta t > 2$

UNCONDITIONALLY UNSTABLE

CONDITIONAL STABILITY

CAN GAUGE QUALITY OF EULER METHOD BY COMPARING λ & $e^{-\sigma \Delta t}$



WHAT IF WE CONSIDER AN IMPLICIT SCHEME?

$$\frac{u_{n+1} - u_n}{\Delta t} = \overbrace{-\sigma u_{n+1}}^{f(u,t)}$$

← EVALUATE AT END OF TIME STEP

$$u_{n+1} + \sigma \Delta t\, u_{n+1} = u_n$$

$$u_{n+1} = \underbrace{\left(\frac{1}{1 + \sigma \Delta t}\right)}_{\text{AMPLIFICATION FACTOR} \equiv \lambda} u_n$$

$\lambda < 1$ FOR ALL NON-ZERO VALUES OF TIMESTEP : UNCONDITIONALLY STABLE

MULTIDIMENSIONAL EQUATIONS

EXAMPLE:

$$y_1' = -y_2$$

$$y_2' = 100 y_1 - 101 y_2$$

ORDER TWO HOMOGENEOUS LINEAR SYSTEM WITH CONSTANT COEFFICIENTS

$$\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -1 \\ 100 & -101 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}}_{\vec{y}}$$

$$\frac{d\vec{y}}{dx} = A\vec{y}$$

SOLVE BY FINDING EIGENVALUES & EIGENVECTORS OF A.

$$A\vec{v} = \lambda\vec{v}$$

$$\det(A - \lambda I) = 0 \leftarrow \text{2nd order polynomial for } \lambda_1, \lambda_2 \text{ \& can get corresponding EIGENVECTORS } \vec{v}_1, \vec{v}_2$$

CAN THEN CONSTRUCT A CHANGE OF BASIS MATRIX

$$R = \begin{pmatrix} \vdots & \vdots & & \vdots \\ v_1 & v_2 & \cdots & v_n \\ \vdots & \vdots & & \vdots \end{pmatrix} \leftarrow \text{COLUMNS ARE EIGENVECTORS}$$

$$A = R\Lambda R^{-1} \qquad \text{WHERE} \qquad \Lambda = \operatorname{diag}(\lambda_1, \lambda_2 \ldots \lambda_n)$$

$$\frac{d\vec{y}}{dx} = R\Lambda R^{-1}\vec{y}$$

MULTIPLY BY R^{-1} ON LEFT $\quad R^{-1}\frac{d\vec{y}}{dx} = \Lambda R^{-1}\vec{y}$

DEFINE $\vec{z} = R^{-1}\vec{y} \Rightarrow \frac{d\vec{z}}{dx} = \Lambda\vec{z}$

BUT Λ IS DIAGONAL SO HAVE DECOUPLED SYSTEM OF ODEs INTO n DECOUPLED EQUATIONS

$$\frac{dz_i}{dx} = \lambda_i z_i \Rightarrow z_i(x) = C_i e^{\lambda_i x}$$ (NO SUMMATION OVER i)

TRANSFORM BACK INTO ORIGINAL COORDINATES

$$\vec{y}(x) = R\vec{z}(x) = \sum_i C_i \vec{v}_i e^{\lambda_i x}$$

FOR $A = \begin{pmatrix} 0 & -1 \\ 100 & -101 \end{pmatrix}$

$$\det \begin{pmatrix} -\lambda & -1 \\ 100 & -101-\lambda \end{pmatrix} = 0 \Rightarrow \lambda^2 + 101\lambda + 100 = 0$$

$$\lambda_1 = -1$$

$$\lambda_2 = -100$$

$$y_1 = Ae^{-x} + Be^{-100x}$$

$$y_2 = Ce^{-x} + De^{-100x}$$

THE TERMS e^{-100x} ARE COMPLETELY NEGLIGIBLE WHEN IN DETERMINING THE VALUES OF y_1 & y_2 SOLVING EQUATIONS <u>ANALYTICALLY</u>.

WHAT IF SOLVE $\frac{d\vec{y}}{dx} = A\vec{y}$ BY (EXPLICIT) EULER METHOD?

$$\vec{y}_{n+1} = \vec{y}_n + \Delta x A \vec{y}_n$$

$$\vec{y}_{n+1} = (1 + \Delta x A)\vec{y}_n$$

$$\vec{y}_n = (1 + \Delta x A)^n \vec{y}_0$$

How do we find constraints on updating step Δx?

EXPAND $\vec{y}_0$ IN TERMS OF EIGENVECTORS

$$\vec{y}_0 = \sum \alpha_i \vec{v}_i$$

$$\vec{y}_n = \sum (1 + \Delta x A)^n \alpha_i v_i = \sum \alpha_i (1 + \Delta x \lambda_i)^n v_i$$

$$|(1 + \Delta x \lambda_i)| < 1 \quad \text{FOR STABILITY}$$

$$\lambda_1 = -1 \Rightarrow 1 - \Delta x > -1 \Rightarrow \Delta x < 2$$

$$\lambda_1 = -100 \Rightarrow 1 - 100\Delta x > -1 \Rightarrow \Delta x < \frac{1}{100}$$

HAVE TO SATISFY <u>BOTH</u> STABILITY CONDITIONS

<u>BC</u> OTHERWISE IF FIRST SOLUTION IS UNSTABLE, NO MATTER HOW LITTLE OF THAT SOLUTION WE START WITH IT WILL EVENTUALLY DOMINATE OUR RESULT.

STIFFNESS MEASURED BY RATIO $\dfrac{|\lambda_{max}|}{|\lambda_{min}|}$

IF RATIO IS LARGE, THE SYSTEM IS STIFF SO HARD TO INTEGRATE EXPLICITLY.

HOW CAN WE AVOID TAKING SMALL STEPS?

IMPLICIT METHOD

$$\frac{d\vec{y}}{dx} = A\vec{y}$$

$$\vec{y}_{n+1} = y_n + \Delta x A y_{n+1}$$

$$(I - \Delta x A) y_{n+1} = y_n$$

$$y_{n+1} = \frac{1}{(I - \Delta x A)} y_n$$

FOR NEGATIVE EIGENVALUES AMPLIFICATION FACTOR < 1

FOR ALL Δx BUT REQUIRES INVERSION OF A MATRIX

FOR LINEAR PROBLEM A SINGLE INVERSION IS SMALL COST COMPARED W GAIN OF BEING ABLE TO TAKE DECENT STEPS

IF COEFFICIENTS IN MATRIX VARY, THEN INVERSION MIGHT HAVE TO BE DONE EVERY STEP $\Rightarrow$ EXPENSIVE

SUMMARY OF ADVANTAGES & DISADVANTAGES OF EXPLICIT & IMPLICIT APPROACH

EXPLICIT APPROACH:

ADVANTAGE: SIMPLE TO SET UP & PROGRAM

DISADVANTAGE: IN SOME CASES STEPSIZE IS LIMITED BY STABILITY CONSTRAINTS; THIS CAN RESULT IN LONGER COMPUTER RUNNING TIMES TO MAKE CALCULATIONS OVER A GIVEN INTERVAL.

IMPLICIT APPROACH:

ADVANTAGE: STABILITY CAN BE MAINTAINED OVER MUCH LARGER VALUES OF STEPSIZE SO NEED FEWER TIMESTEPS TO COVER SAME INTERVAL.

DISADVANTAGE: (1) MORE COMPLICATED TO SET UP & PROGRAM (2) MASSIVE MATRIX INVERSION MIGHT BE REQUIRED PER TIME STEP, SO COMPUTER TIME PER STEP MIGHT BE LARGER THAN IN EXPLICIT APPROACH (3) SINCE CAN TAKE LARGE STEPS, TRUNCATION ERROR IS LARGE SO USING IMPLICIT METHOD TO FOLLOW EXACT TRANSIENTS MAY NOT BE AS ACCURATE AS EXPLICIT METHOD. BUT IF ONLY CARE ABOUT STEADY STATE, TIME INACCURACY MIGHT BE LESS IMPORTANT.

HIGHER ORDER ODEs

REDUCING ODE OF ORDER N TO SYSTEM OF N LINEAR ODEs

AN ODE OF ORDER N CAN BE REDUCED TO A SET OF N SIMULTANEOUS COUPLED FIRST ORDER EQUATIONS INVOLVING N DEPENDENT VARIABLES

EXAMPLE HARMONIC OSCILLATOR

$$\ddot{x} + x = 0$$

$$\vec{y} = \begin{pmatrix} x \\ \dot{x} \end{pmatrix} \quad \Rightarrow \quad \frac{d\vec{y}}{dt} = \frac{d}{dt}\begin{pmatrix} x \\ \dot{x} \end{pmatrix} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{M}\begin{pmatrix} x \\ \dot{x} \end{pmatrix}$$

WHAT IS THE STABILITY CONDITION ON Δt WHEN SOLVING WITH EULER METHOD?

$$\frac{d\vec{y}}{dt} = M\vec{y}$$

$$y_{n+1} = (1 + M\Delta t)\, y_n$$

$$y_n = (1 + M\Delta t)^n\, y_0$$

EXPAND $\vec{y}_0$ IN TERMS OF EIGENVECTORS $\vec{v}_i$

$$y_0 = \sum_{i=1}^{N} \alpha_i \vec{v}_i \quad \Rightarrow \quad y_n = \sum_i \underbrace{(1 + \Delta t \lambda_i)^n}_{\text{AMPLIFICATION FACTOR}} \alpha_i \vec{v}_i$$

$$M = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \det(M - \lambda I) = 0$$

$$\det\begin{pmatrix} -\lambda & 1 \\ -1 & -\lambda \end{pmatrix} = 0 \quad \Rightarrow \quad \lambda^2 + 1 = 0$$

$$\lambda = \pm i$$

IF $|(1 + \Delta t \lambda_i)| > 1$ THEN UNSTABLE

$$\lambda = \pm i \qquad |1 \pm i\Delta t| = \sqrt{1^2 + (\Delta t)^2} > 1$$

FOR ALL Δt UNSTABLE

CLASSIFICATION OF PARTIAL DIFFERENTIAL EQUATIONS

THREE CLASSES: HYPERBOLIC
PARABOLIC
ELLIPTIC

METHODS OF SOLVING DIFFERENT PDEs ARE DIFFERENT

HOW TO CLASSIFY SECOND ORDER PDEs

WRITE GENERAL LINEAR SECOND ORDER PDE GOVERNING ψ AS FUNCTION OF INDEPENDENT VARIABLES x

$$\sum_{i,j} c_{ij} \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \psi + \sum_i c_i \frac{\partial}{\partial x_i} \psi + c\psi = \text{CONSTANT}$$

CONSIDER THE COEFFICIENTS c_{ij} & REGARD THEM AS DEFINING A SURFACE IN THE MULTIDIMENSIONAL SPACE VIA QUADRATIC ASSOCIATED WITH THEM

$$\sum_{i,j} c_{ij} x_i x_j + \sum c_i x_i = \text{constant}$$

COMPARE TO GENERAL EQUATION FOR CONIC SECTION IN CARTESIAN COORDINATES

$$ax^2 + bxy + cy^2 + dx + ey + f = 0$$

$b^2 - 4ac > 0$	HYPERBOLIC
$b^2 - 4ac = 0$	PARABOLIC
$b^2 - 4ac < 0$	ELLIPTIC

EX 1 LAPLACE'S EQUATION

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

$$x^2 + y^2 = \text{const}$$

COMPARE TO $ax^2 + bxy + cy^2 + dx + ey + f = 0$

$a = 1 \quad b = 0 \quad c = 1$

$b^2 - 4ac = -4$ so ELLIPTICAL PDE

NEGATIVE (GRAVITATION, ELECTROSTATICS)

EX 2 SECOND ORDER WAVE EQUATION

$$\frac{\partial^2 u}{\partial t^2} = c_s^2 \frac{\partial^2 u}{\partial x^2}$$

$$t^2 - c_s^2 x^2 = \text{const}$$

$a = 1 \quad b = 0 \quad c = -c_s^2$

$b^2 - 4ac = -4(-c_s^2)$ POSITIVE so HYPERBOLIC PDE

(INFO PROPAGATES AS WAVES
e.g WATER WAVES, SOUND WAVES, EM RADIATION)

EX 3 ONE DIMENSIONAL HEAT CONDUCTION EQUATION

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

$$t - \alpha x^2 = \text{const}$$

$a = -\alpha \quad b = 0 \quad c = 0$

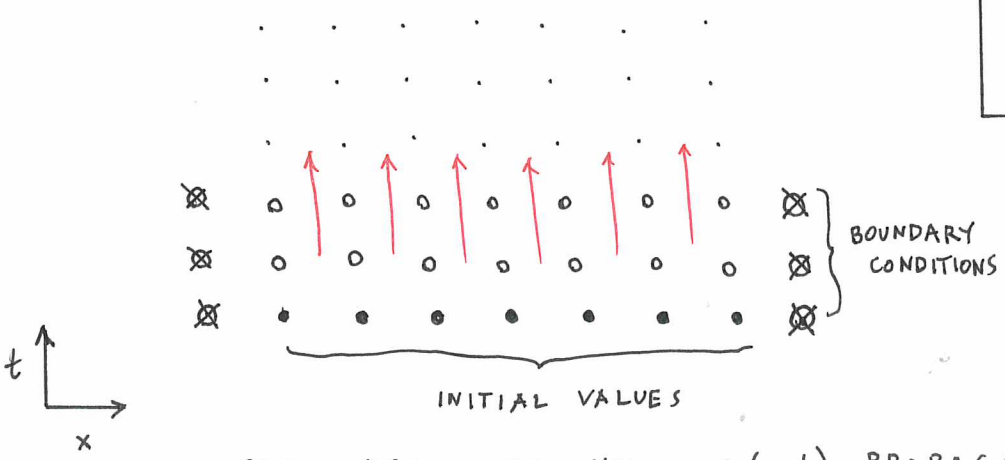
$b^2 - 4ac = 0$ so PARABOLIC

(INFO TRAVELS AS DIFFUSIVE PROCESSES
e.g. HEAT TRANSFER, DIFFUSION OF PHOTONS OUT OF SUN

ESSENTIAL DISTINCTION BETWEEN 3 TYPES OF PDEs FROM COMPUTATIONAL POINT OF VIEW . . .

HYPERBOLIC (e.g. WAVE EQU) AND PARABOLIC (e.g. DIFFUSION EQU) ARE INITIAL VALUE PROBLEMS

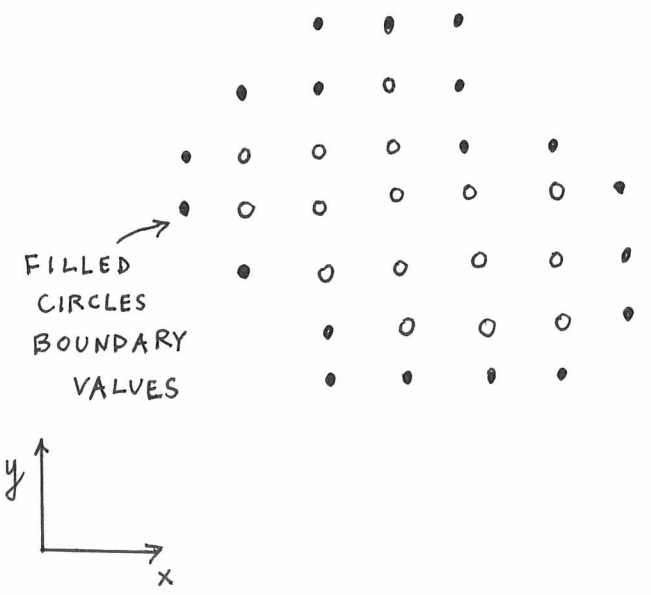
A TIME EVOLUTION PROBLEM



- PDE DESCRIBES HOW $u(x,t)$ PROPAGATES.
- ONLY ONE OR A FEW PREVIOUS ROWS NEED TO BE MAINTAINED IN MEMORY.
- INITIAL VALUES FOR $u(x,t)$ GIVEN IN ONE TIME SLICE
- ADVANCE SOLUTION IN TIME COMPUTING SUCCESSIVE ROWS OF OPEN DOTS

ELLIPTIC (e.g. POISSON, LAPLACE) PDEs ARE BOUNDARY VALUE PROBLEMS

A STATIC SOLUTION PROBLEM

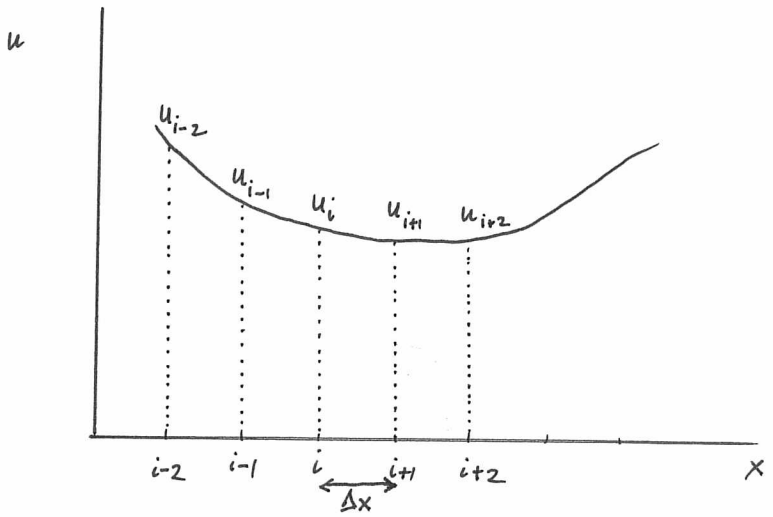


WANT TO FIND A SINGLE "STATIC" FUNCTION THAT SATISFIES PDE WITHIN SOME (x,y) REGION

BOUNDARY CONDITIONS SPECIFIED & ITERATIVE PROCESS IS EMPLOYED TO FIND VALUES AT ALL INTERNAL POINTS.

ALL GRID POINTS MUST BE MAINTAINED IN MEMORY.

HOW TO APPROXIMATE PDE ON A MESH WITH FINITE DIFFERENCE APPROXIMATION



SUPPOSE WANT TO FIGURE OUT DERIVATIVE AT $x = x_i$

$$\frac{du}{dx} = \lim_{\Delta x \to 0} \frac{u(x+\Delta x) - u(x)}{\Delta x}$$

HOW ARE YOU GOING TO GET COMPUTER TO DO IT?

$$\left.\frac{du}{dx}\right|_{x=x_i} \approx \frac{u(x_i+\Delta x) - u(x_i)}{\Delta x} = \frac{u_{i+1} - u_i}{\Delta x}$$

FORWARD EULER APPROXIMATION

$$\left.\frac{du}{dx}\right|_{x=x_i} \approx \frac{u(x_i) - u(x_i-\Delta x)}{\Delta x} = \frac{u_i - u_{i-1}}{\Delta x}$$

BACKWARD EULER

$$\left.\frac{du}{dx}\right|_{x=x_i} \approx \frac{u(x_i+\Delta x) - u(x_i-\Delta x)}{2\Delta x} = \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

CENTERED DIFFERENCE

ALL THESE DEFINITIONS ARE EQUIVALENT IN THE CONTINUUM LIMIT BUT LEAD TO DIFFERENT APPROXIMATIONS IN THE DISCRETE CASE.

IS THERE A WAY TO QUANTIFY THE ERROR COMMITTED IN THE DIFFERENT FINITE DIFFERENCE APPROXIMATIONS (FDAs) OF THE FIRST DERIVATIVE? TAYLOR SERIES

FIND TRUNCATION ERROR FOR FORWARD DIFFERENCE APPROXIMATION

$$\frac{u_{i+1}-u_i}{\Delta x} = \frac{1}{\Delta x}\left[\underbrace{u_i + u_x(0)\Delta x + \frac{1}{2!}u_{xx}(0)\Delta x^2 + \frac{1}{3!}u_{xxx}(0)\Delta x^3 + \ldots}_{u_{i+1}} - u_i \right]$$

($u_x(0) = \left.\frac{du}{dx}\right|_{x=x_i}$, $u_{xx}(0) = \left.\frac{d^2u}{dx^2}\right|_{x=x_i}$)

$$= \underbrace{u_x(0)}_{\text{THIS IS WHAT WE'RE GETTING AN APPROXIMATION TO}} + \frac{1}{2!}u_{xx}(0)\Delta x + \frac{1}{3!}u_{xxx}(0)\Delta x^2 + \ldots$$

$$\left.\frac{du}{dx}\right|_{x=i} = u_x(0) = \underbrace{\frac{u_{i+1}-u_i}{\Delta x}}_{\text{FINITE DIFFERENCE APPROXIMATION}} \underbrace{- \frac{1}{2!}\left.\frac{d^2u}{dx^2}\right|_{x=x_i}\Delta x - \frac{1}{3!}\left.\frac{d^3u}{dx^3}\right|_{x=x_i}\Delta x^2}_{\text{TRUNCATION ERROR}}$$

$O(\Delta x)$ ← LOWEST ORDER TERM IN TRUNCATION ERROR INVOLVES Δx TO FIRST ORDER SO THE APPROXIMATION IS "FIRST ORDER ACCURATE"

EXTENSION TO PARTIAL DERIVATIVE

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \underbrace{\frac{u_{i+1,j}-u_{i,j}}{\Delta x}}_{\text{FDA}} \underbrace{- \frac{1}{2!}\left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j}\Delta x - \frac{1}{3!}\left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j}\Delta x^2}_{O(\Delta x)\ \text{TRUNCATION ERROR}}$$

FIND TRUNCATION ERROR FOR CENTERED DIFFERENCE APPROXIMATION

$$\left.\frac{du}{dx}\right|_{x=x_i} \sim \frac{u_{i+1} - u_{i-1}}{2\Delta x}$$

$$u_{i+1} = u_i + u_x(0)\,\Delta x + \frac{1}{2!}u_{xx}(0)\,\Delta x^2 + \frac{1}{3!}u_{xxx}(0)\,\Delta x^3 + \frac{1}{4!}u_{xxxx}(0)\,\Delta x^4 + \dots$$

$$u_i = u(0)$$

$$u_{i-1} = u_i - u_x(0)\,\Delta x + \frac{1}{2!}u_{xx}(0)\,\Delta x^2 - \frac{1}{3!}u_{xxx}(0)\,\Delta x^3 + \frac{1}{4!}u_{xxxx}(0)\,\Delta x^4 + \dots$$

SO $$u_{i+1} - u_{i-1} = 2u_x(0)\,\Delta x + \frac{1}{3}u_{xxx}(0)\,\Delta x^3 + \frac{2}{5!}u_{xxxxx}(0)\,\Delta x^5 + \dots$$

SOLVE FOR $u_x(0)$

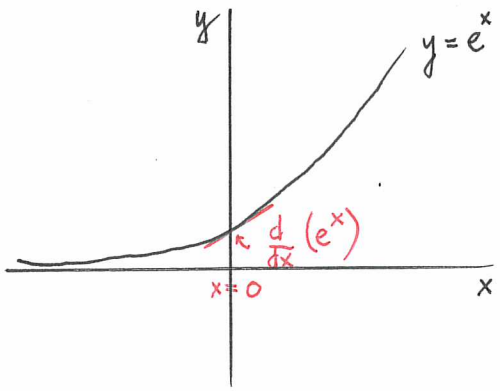
$$\left.\frac{du}{dx}\right|_{x=x_i} \equiv u_x(0) = \underbrace{\frac{u_{i+1} - u_{i-1}}{2\Delta x}}_{\text{FDA}} \underbrace{- \frac{1}{6}u_{xxx}(0)\,\Delta x^2}_{O(\Delta x^2)\ \text{TRUNCATION ERROR}} + \dots$$

FINITE DIFFERENCE APPROXIMATION TO $\frac{d}{dx}(e^x)$ AT $x = 0$

	$\frac{u_{i+1}-u_i}{\Delta x}$	$\frac{u_i - u_{i-1}}{\Delta x}$	$\frac{u_{i+1} - u_{i-1}}{2\Delta x}$
Δx	FORWARD	BACKWARD	CENTERED
1.0	1.718	0.632	1.175
0.1	1.05	0.95	1.00167
0.01	1.005	0.995	1.0000167
0.001	1.0005	0.9995	1.000000167

ERRORS DECREASE LINEARLY WITH Δx

ERRORS DECREASE QUADRATICALLY WITH Δx



WHAT IF WANT 4TH ORDER TRUNCATION ERROR TO 1st ORDER DERIVATIVE?

GO BACK TO 2ND ORDER SCHEME

$$\frac{u_{i+1} - u_{i-1}}{2\Delta x} = u_x(0) + \frac{1}{6} u_{xxx}(0)\Delta x^2 + \frac{1}{5!} u_{xxxxx}(0)\Delta x^4 + \cdots$$

REPLACE Δx BY $2\Delta x$

$$\frac{u_{i+2} - u_{i-2}}{4\Delta x} = u_x(0) + \frac{1}{6} u_{xxx}(0) 4(\Delta x)^2 + \frac{1}{5!} u_{xxxxx}(0) 2^4 \Delta x^4 + \cdots$$

MULTIPLY TOP EQUATION BY 4 & SUBTRACT IT FROM 2ND EQU.

$$\frac{u_{i+2} - u_{i-2}}{4\Delta x} - \frac{2u_{i+1} - 2u_{i-1}}{\Delta x} = u_x(0) - 4u_x(0) + \frac{1}{5!} u_{xxxxx}(0) 2^4 \Delta x^4 - \frac{4}{5!} u_{xxxxx}(0)\Delta x^4 + \cdots$$

SOLVE FOR $u_x(0)$

$$\left.\frac{du}{dx}\right|_{x=x_i} = u_x(0) = \underbrace{\frac{-u_{i+2} + u_{i-2} + 8u_{i+1} - 8u_{i-1}}{12\Delta x}}_{\text{FDA}} + \underbrace{\frac{1}{30} u_{xxxxx}(0)\Delta x^4 + \cdots}_{O(\Delta x^4)\ \text{TRUNCATION ERROR}}$$

STENCIL WIDTH & ORDER OF ACCURACY

$$\left.\frac{du}{dx}\right|_{x=x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \frac{1}{6} u_{xxx}(0)\Delta x^2$$

3 POINT STENCIL $\{u_{i-1}, u_i, u_{i+1}\}$

$$\left.\frac{du}{dx}\right|_{x=x_i} = \frac{-u_{i+2} + u_{i-2} + 8u_{i+1} - 8u_{i-1}}{12\Delta x} + \frac{1}{30} u_{xxxxx}(0)\Delta x^4$$

5 POINT STENCIL $\{u_{i-2}, u_{i-1}, u_i, u_{i+1}, u_{i+2}\}$

MORE ACCURATE REPRESENTATION $\longrightarrow$ LARGER STENCIL

FINITE DIFFERENCE APPROXIMATIONS TO PARTIAL DIFFERENTIAL EQUATIONS

ONE-DIMENSIONAL HEAT CONDUCTION EQUATION WITH CONSTANT (+ POSITIVE) CONDUCTION COEFFICIENT "σ"

$$\boxed{\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}}$$

FOR UNIFORM 1D MESH WITH ZONES OF SIZE Δx & TIMESTEP Δt

TIME

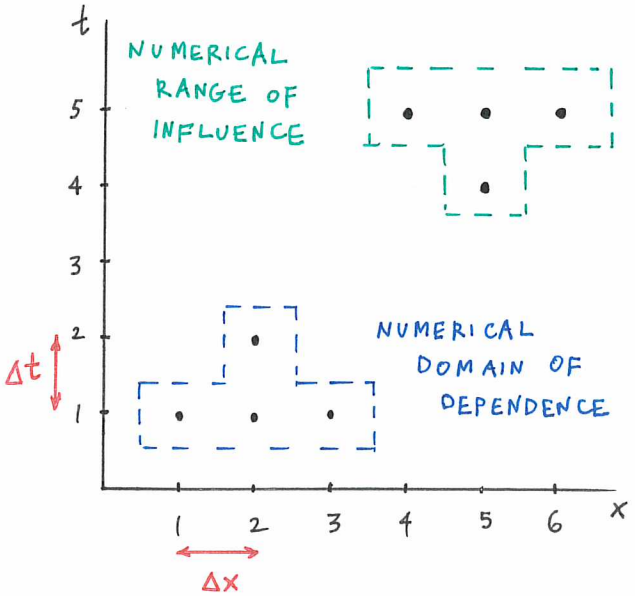
SPACE

$$\underbrace{\frac{u_i^{n+1} - u_i^n}{\Delta t}}_{\text{FORWARD DIFFERENCE IN TIME } O(\Delta t)} = \sigma \underbrace{\left[\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \right]}_{O(\Delta x^2) \text{ FDA TO } \left.\frac{\partial^2 u}{\partial x^2}\right|_{x=x_i}}$$

EXPLICIT FORM

DIFFERENT ORDER OF ACCURACY IN SPACE & TIME.

STENCIL FOR SCHEME



NUMERICAL DOMAIN OF DEPENDENCE

u_i^{n+1} AT TIME $t^{n+1} = t^n + \Delta t$

DEPENDS ON $\{u_{i-1}^n, u_i^n, u_{i+1}^n\}$

AT TIME t^n

NUMERICAL RANGE OF INFLUENCE

A PERTURBATION TO u_i^n AT TIME t^n WILL ONLY INFLUENCE

$\{u_{i+1}^{n+1}, u_i^{n+1}, u_{i-1}^{n+1}\}$

DOES THE FDA HAVE THE SAME DOMAIN OF DEPENDENCE & RANGE OF INFLUENCE AS PDE?

REARRANGE FDA FOR 1D HEAT CONDUCTION EQV.

$$u_i^{n+1} = u_i^n + \frac{\sigma \Delta t}{(\Delta x)^2}\left[u_{i+1}^n - 2u_i^n + u_{i-1}^n \right]$$

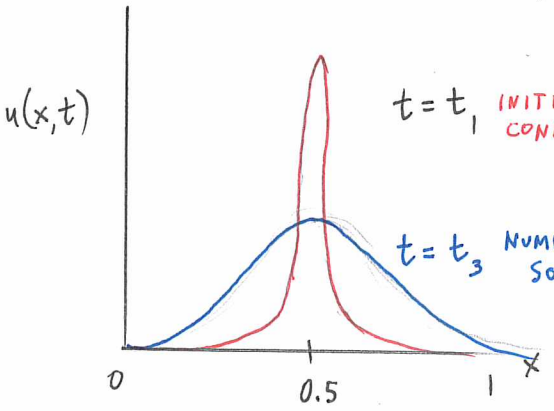
CONSIDER ITS ACCURACY...

LOOK AT DIFFUSION OF INFINITELY THIN & INFINITELY HIGH SPIKE

$0 \leq x \leq 1$

SINGULAR SO ADVANCE ANALYTICAL SOLUTION TO t_1

$$u(x,0) = \delta(x - 0.5)$$



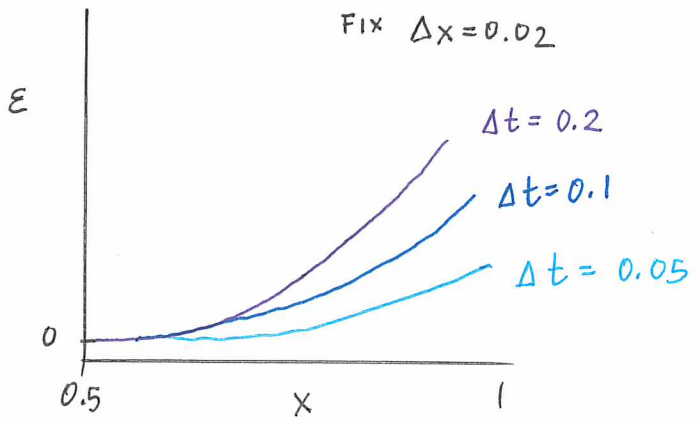
BOUNDARY CONDITION $u(0,t) = u(1,t) = 0$ AT ALL TIMES

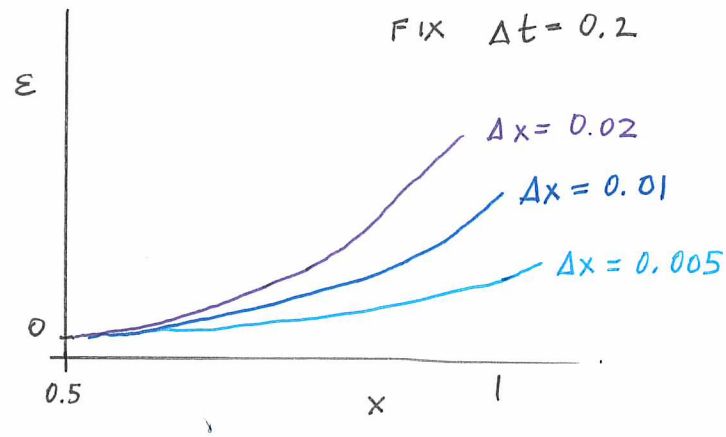
ANALYTICAL SOLUTION

$$w(x,t) = 2\sum_{n=1}^{\infty} \sin\left(\frac{\pi n}{2}\right) \sin(\pi n x) \exp(-\pi^2 n^2 \sigma t)$$

DEFINE ERROR

$$\varepsilon(t) = \text{MAX} \frac{|u(x,t) - w(x,t)|}{w(x,t)}$$





IMPOSSIBLE TO GET ARBITRARILY HIGH ACCURACY WHILE KEEPING Δt CONSTANT & DECREASING Δx (OR KEEPING Δx CONSTANT WHILE DECREASING Δt).

Δt AND Δx MUST DECREASE SIMULTANEOUSLY TO GET CONVERGENCE TO ANALYTICAL SOLUTION.

FOR LINEAR SYSTEMS WITH WELL POSED INITIAL & BOUNDARY CONDITIONS **STABILITY** IS A NECESSARY & SUFFICIENT CONDITION FOR **CONVERGENCE** TO THE PHYSICAL SOLUTION OF THE PDE.

INTRO TO VON-NEUMANN STABILITY ANALYSIS

AGAIN CONSIDER LINEAR HEAT CONDUCTION EQU. IN 1 DIMENSION

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2}$$

WHERE σ IS A POSITIVE, CONSTANT COEFFICIENT

EVENLY SPACED GRID IN SPACE & TIME

$$x_j = j\Delta x$$

$$t^{n+1} = t^n + \Delta t$$

WE FOUND

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

FDA FOR LINEAR 1D HEAT CONDUCTION EQUATION

WHERE

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

FOR VON-NEUMANN STABILITY ANALYSIS **ASSUME DOMAIN IS INFINITE** (BCs ARE RARELY CAUSE OF PROBLEM SO IGNORE THEM)

DIFFERENCE EQUATION IS LINEAR.
DECOMPOSE IT INTO SEPARATE FOURIER MODES.

$$u_j^n = U_k^n e^{ikx_j}$$

$$u_{j+1}^n = U_k^n e^{ikx_j + ik\Delta x}$$

$$u_{j-1}^n = U_k^n e^{ikx_j - ik\Delta x}$$

$$u_j^{n+1} = U_k^{n+1} e^{ikx_j}$$

AMPLITUDE HAS A TIME DEPENDENCE

SUBSTITUTE INTO FDA

$$U_k^{n+1} e^{ikx_j} = U_k^n e^{ikx_j} + \mu\left(U_k^n e^{ikx_j + ik\Delta x} - 2U_k^n e^{ikx_j} + U_k^n e^{ikx_j - ik\Delta x} \right)$$

ELIMINATE COMMON FACTOR e^{ikx_j}

$$U_k^{n+1} = U_k^n \left[1 + \mu\left(e^{ik\Delta x} - 2 + e^{-ik\Delta x} \right) \right]$$

$$= U_k^n \left[1 + 2\mu\left(\cos(k\Delta x) - 1 \right) \right]$$

$$= U_k^n \left[1 - 2\mu\left(1 - \cos(k\Delta x) \right) \right]$$

use $\sin^2 a = \frac{1}{2}(1 - \cos 2a)$

$$U_k^{n+1} = U_k^n \left[1 - 4\mu \sin^2\left(\frac{k\Delta x}{2} \right) \right]$$

AMPLIFICATION FACTOR FOR FDA

$$\lambda_{FDA}(k) \equiv \frac{U_k^{n+1}}{U_k^n} = 1 - 4\mu \sin^2\left(\frac{k\Delta x}{2} \right)$$

NOTE "k" DEPENDENCE OF AMPLIFICATION FACTOR

AMPLIFICATION FACTOR FOR PDE

$$\lambda_{PDE}(k) = e^{-\sigma k^2 \Delta t} = e^{-(k\Delta x)^2 \left[\frac{\sigma \Delta t}{\Delta x^2} \right]} = e^{-\mu (k\Delta x)^2} \Rightarrow \left| \lambda_{PDE}(k) \right| \le 1$$

FOR ALL k

DIFFERENTIAL EQU. DICTATES THAT u DECREASES WITH TIME THROUGH DISSIPATION. WE WANT NUMERICAL METHOD TO PRESERVE THIS PROPERTY.

WANT $\left| \lambda_{FDA}(k) \right| \le 1$ FOR ALL k

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

IF $1 - 4\mu \sin^2\left(\frac{k\Delta x}{2} \right) > 0$ THEN STABILITY REQUIRES $1 - 4\mu \sin^2\left(\frac{k\Delta x}{2} \right) \le 1 \rightarrow \mu \ge 0$

IF $1 - 4\mu \sin^2\left(\frac{k\Delta x}{2} \right) < 0$ THEN STABILITY REQUIRES $-1 + 4\mu \sin^2\left(\frac{k\Delta x}{2} \right) \le 1$

$$\Rightarrow \mu \sin^2\left(\frac{k\Delta x}{2} \right) \le \frac{1}{2}$$

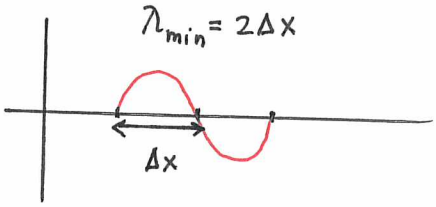
$$\rightarrow \mu \le 1/2$$

NOTE: IF $k\Delta x$ IS SMALL THEN $\mu \sin^2\left(\frac{k\Delta x}{2}\right)$ IS SMALL

AND UNPROBLEMATIC.

WE'RE MOST WORRIED ABOUT $k\Delta x$ THAT MAKES

$$\sin^2\left(\frac{k\Delta x}{2}\right) \sim 1$$



SMALLEST WAVE LENGTH THAT CAN BE REPRESENTED ON GRID

$$\Rightarrow k_{max} = \frac{2\pi}{\lambda_{min}} = \frac{2\pi}{2\Delta x} = \frac{\pi}{\Delta x}$$

$$\sin^2\left(\frac{k_{max}\Delta x}{2}\right) = \sin^2\left(\frac{\pi}{2}\right) = 1$$

SO IF WANT SMALLEST WAVELENGTH MODES TO BE STABLE NEED $\boxed{\mu \leq \frac{1}{2}}$

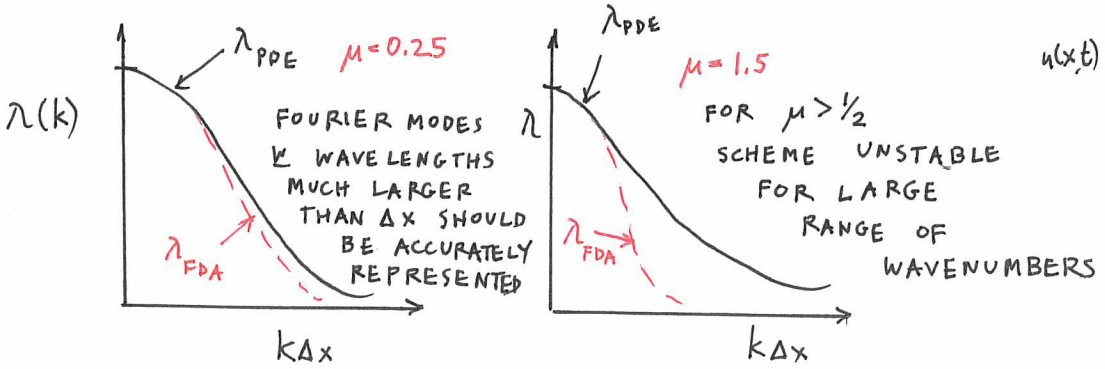
RECALL $\mu = \frac{\sigma \Delta t}{\Delta x^2}$

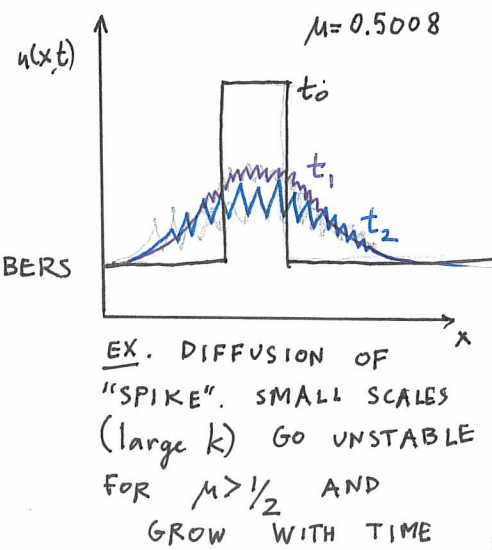
$$\Rightarrow \boxed{\Delta t \leq \frac{\Delta x^2}{2\sigma}}$$

STABILITY CONDITION FOR LINEAR 1D HEAT CONDUCTION ~~EQ.~~ TIME EXPLICIT SCHEME

$\frac{\Delta x^2}{\sigma}$ IS CHARACTERISTIC DIFFUSION TIME

So STABILITY CONDITION ENFORCES THAT COMPUTED DIFFUSION IS SLOWER THAN PHYSICAL DIFFUSION ACROSS ONE ZONE.





EX. DIFFUSION OF "SPIKE". SMALL SCALES (large k) GO UNSTABLE FOR $\mu > 1/2$ AND GROW WITH TIME

TIME EXPLICIT TREATMENT REQUIRED

$$\Delta t \sim (\Delta x)^2$$

SO AS MESH IS REFINED, TIMESTEP CAN BECOME UNACCEPTABLY SMALL.

CAN AVOID CONSTRAINT ON TIMESTEP BY GOING TO IMPLICIT SCHEME

INSTEAD OF $\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \left[\dfrac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{(\Delta x)^2} \right]$ EXPLICIT

EVALUATE R.H.S. AT t^{n+1}

$$\star \quad \boxed{\dfrac{u_j^{n+1} - u_j^n}{\Delta t} = \sigma \left[\dfrac{u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}}{(\Delta x)^2} \right]}$$ IMPLICIT SCHEME

HAVE ONE EQUATION FOR 3 UNKNOWNS: $\left(u_{j-1}^{n+1}, u_j^{n+1}, u_{j+1}^{n+1} \right)$

NICE THING ABOUT IMPLICIT SCHEME:

$$U_k^{n+1} = \frac{1}{1 + 4\mu \sin^2\left(\frac{k\Delta x}{2}\right)} U_k^n$$

≤ 1 FOR ALL k

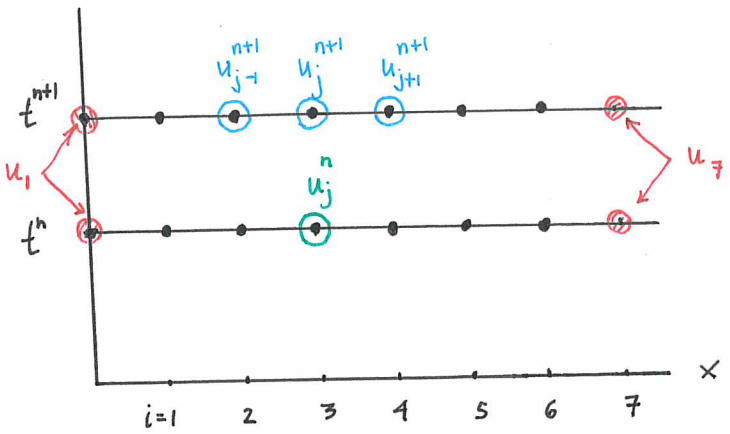
UNCONDITIONALLY STABLE!

NO CONSTRAINT ON TIMESTEP

BUT TO SOLVE FOR UNKNOWNS HAVE TO WRITE ★ EQU. ABOVE AT ALL INTERIOR GRID POINTS TO GET A SYSTEM OF ALGEBRAIC EQUATIONS FOR WHICH ALL u_j^{n+1} CAN BE SOLVED SIMULTANEOUSLY.

REWRITE ★ PUTTING ALL UNKNOWNS ON L.H.S. AND KNOWNS ON R.H.S.

$$\underbrace{\frac{\sigma \Delta t}{\Delta x^2}}_{A} u_{j-1}^{n+1} - \underbrace{\left(1 + 2\sigma \frac{\Delta t}{(\Delta x)^2}\right)}_{B} u_j^{n+1} + \underbrace{\frac{\sigma \Delta t}{\Delta x^2}}_{A} u_{j+1}^{n+1} = \underbrace{-u_j^n}_{K_j}$$



BOUNDARY CONDITIONS AT $i=1$ AND $i=7$

$$u(1,t) = u_1$$
$$u(7,t) = u_7$$

$$A u_{j-1}^{n+1} - B u_j^{n+1} + A u_{j+1}^{n+1} = K_j$$

AT GRID PT. 2: $j=2$ $\quad A u_1^{n+1} - B u_2^{n+1} + A u_3^{n+1} = K_2$

u_1 GIVEN BY B.C.s SO MOVE u_1 TERM TO R.H.S.

$$\Rightarrow -B u_2^{n+1} + A u_3^{n+1} = K_2 - A u_1^{n+1}$$

AT GRID PT. 3: $j=3$ $\quad A u_2^{n+1} - B u_3^{n+1} + A u_4^{n+1} = K_3$

AT GRID PT. 4: $j=4$ $\quad A u_3^{n+1} - B u_4^{n+1} + A u_5^{n+1} = K_4$

ETC.

VECTOR FOR u_j^{n+1} VALUES

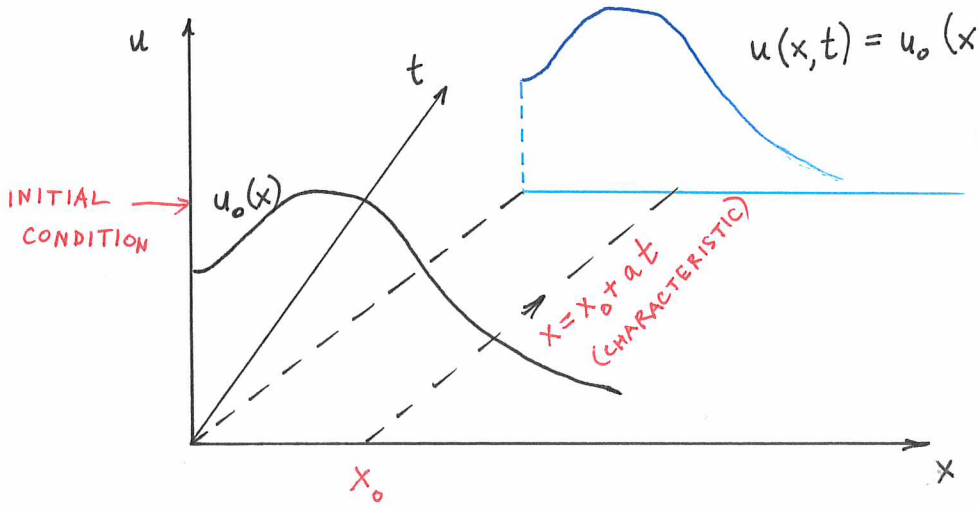
$$\begin{pmatrix} -B & A & 0 & 0 & 0 \\ A & -B & A & 0 & 0 \\ 0 & A & -B & A & 0 \\ 0 & 0 & A & -B & A \\ 0 & 0 & 0 & A & -B \end{pmatrix} \begin{pmatrix} u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{pmatrix} = \begin{pmatrix} K_2 - A u_1 \\ K_3 \\ K_4 \\ K_5 \\ K_6 - A u_7 \end{pmatrix}$$

TRIDIAGONAL MATRIX TO INVERT

LET'S NOW CONSIDER HYPERBOLIC PDE

LINEAR SCALAR ADVECTION EQUATION

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \qquad \text{WHERE} \quad a > 0$$



GIVEN $u_0(x)$ AT $t=0$, TO GET SOLUTION AT LATER TIME, SLIDE THE ORIGINAL PROFILE TO THE RIGHT ALONG THE X-AXIS WITH A SPEED "a".

THE 1D SOLUTION PROPAGATES AS A SHAPE PRESERVING WAVE BC THE CHARACTERISTICS ARE STRAIGHT LINES IN SPACE - TIME.

FOR FINITE DIFFERENCE APPROXIMATION, START WITH MOST NAIVE DISCRETIZATION

$$\underbrace{\frac{u_j^{n+1} - u_j^n}{\Delta t}}_{O(\Delta t)} = -a \underbrace{\left[\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right]}_{O(\Delta x^2)}$$

AN EXPLICIT SCHEME

(FTCS = FORWARD TIME CENTERED SPACE)

REARRANGE

$$u_j^{n+1} = u_j^n - \frac{\mu}{2}\left\{u_{j+1}^n - u_{j-1}^n\right\} \qquad \text{WHERE} \quad \mu \equiv \frac{a\Delta t}{\Delta x}$$

PERFORM VON-NEUMANN STABILITY ANALYSIS (e.g. $u_j^n = U_k^n e^{ikj}$ etc) TO FIND

$$\lambda_{FDA}(k) = \frac{U_k^{n+1}}{U_k^n} = 1 - i\mu\sin(k\Delta x) \quad \Rightarrow \quad |\lambda_{FDA}(k)| = 1 + \mu^2 \sin^2 k\Delta x$$

SO $|\lambda_{FDA}(k)| > 1$ FOR ALL WAVENUMBERS k!

METHOD SEEMS REASONABLE BUT IS UNCONDITIONALLY UNSTABLE!

HOW CAN YOU CURE THE INSTABILITY?

LAX-FRIEDRICHS SCHEME

REPLACE u_j^n TERM IN TIME DERIVATIVE BY ITS AVERAGE

$$u_j^n \longrightarrow \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)$$

$$\frac{u_j^{n+1} - \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)}{\Delta t} = -a\left[\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right]$$

REARRANGE

$$u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{a\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right)$$

let $\mu = \dfrac{a\Delta t}{\Delta x}$

PERFORM VON-NEUMANN STABILITY ANALYSIS TO FIND

$$\lambda_{FDA}(k) = \frac{U_k^{n+1}}{U_k^n} = \cos(k\Delta x) - i\mu \sin(k\Delta x)$$

$$|\lambda_{FDA}(k)| = \cos^2(k\Delta x) + \mu^2 \sin^2(k\Delta x)$$

$$= \cos^2(k\Delta x) + \mu^2 \sin^2(k\Delta x) + \sin^2(k\Delta x) - \sin^2(k\Delta x)$$

$$= \sqrt{1 + (\mu^2 - 1)\sin^2(k\Delta x)}$$

$\Rightarrow$ $|\lambda_{FDA}(k)| \leq 1$ WHEN $\mu \leq 1$

$\Rightarrow$ $\boxed{\Delta t \leq \dfrac{\Delta x}{a}}$ STABILITY CONDITION

COURANT-FRIEDRICHS-LEWY (CFL) CONDITION

TIMESTEP MUST RESOLVE CROSSING TIME OF A CELL FOR STABILITY

WHY DID THE MODIFICATION $u_j^n \rightarrow \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right)$

STABILIZE THE SCHEME?

REARRANGE DIFFERENCE EQUATION TO LOOK LIKE FTCS SCHEME PLUS EXTRA TERMS

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -a\left(\frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}\right) + \frac{1}{2}\left[\frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{\Delta t}\right]$$

NAIVE DISCRETIZATION
FTCS SCHEME

NUMERICAL DISSIPATION

$$\frac{\Delta x^2}{2\Delta t}\frac{\partial^2 u}{\partial x^2}$$

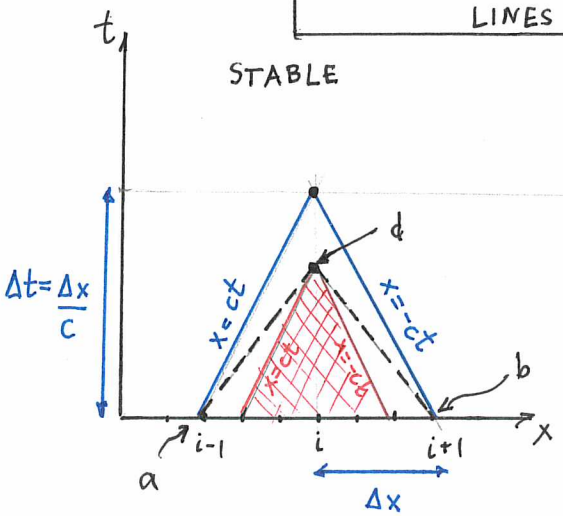
NUMERICAL DISSIPATION DAMPS GROWING (SMALL SCALE) MODES.

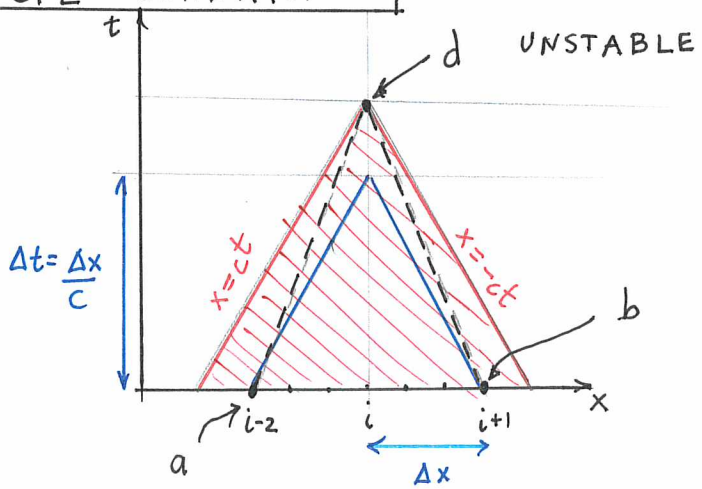
THE SCALES WE CAN RESOLVE, i.e. THOSE WITH $k\Delta x \ll 1$

HAVE $|\lambda_{FDA}(k)| \sim 1$

APPROXIMATING A PDE IS AN ART!

CONNECTION BETWEEN CHARACTERISTIC LINES & CFL CONDITION





Δ_{abd} ≡ NUMERICAL DOMAIN FOR POINT d (SCHEME USES INFO FROM i-1 & i+1)

RED SHADED TRIANGLE = ANALYTICAL DOMAIN

FOR STABILITY NUMERICAL DOMAIN MUST INCLUDE ANALYTICAL DOMAIN

THEORETICALLY POINTS OUTSIDE ANALYTICAL DOMAIN SHOULDN'T INFLUENCE SOLUTION.

PARTICLE SIMULATIONS

CLASSICAL N-BODY PROBLEM

HAVE N $(i = 1, \ldots, N)$ POINT MASSES

EACH WITH MASS m_i AND

INITIAL POSITIONS & VELOCITIES

$x_i(t=0)$ AND $v_i(t=0)$

THE POINT MASSES MOVE IN RESPONSE TO FORCES EXERTED BY THE OTHER PARTICLES.

TAKE EXAMPLE OF STARS IN GALAXIES, THE ACCELERATION OF "STAR PARTICLE" i DUE TO ALL THE OTHER "STAR PARTICLES" IN THE GALAXY IS GIVEN BY

$$\frac{d^2 x_i}{dt^2} = -\sum_{\substack{j=1 \\ j \neq i}}^{N} \frac{G m_j (\vec{x}_i - \vec{x}_j)}{|\vec{x}_i - \vec{x}_j|^3}$$

FOR TWO-BODY PROBLEM, CAN GET SOLUTION IN CLOSED FORM.

FOR $\geq$ THREE-BODY PROBLEM, GENERAL SOLUTION CAN ONLY BE OBTAINED NUMERICALLY.

$\Longrightarrow$ PROBLEM IS HIGHLY NON-LINEAR. SMALL CHANGES IN INITIAL CONDITIONS CAN LEAD TO VERY DIFFERENT RESULTS.

TWO CASES

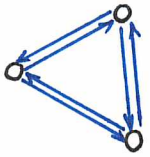
FEW BODY SYSTEMS : CARE ABOUT SUBTLE INTERPLAY OF PERTURBATIONS UNFOLDING OVER MANY, MANY ORBITS.

MANY BODY SYSTEMS: CARE ABOUT COLLECTIVE BEHAVIOUR OF AN ENORMOUS NUMBER OF PARTICLES

CHALLENGING BECAUSE

(i) FORCE CALCULATION SCALES AS N^2

3 BODIES

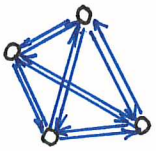


$3(2) = 6$ FORCES

↑ # OF OBJECTS N

↖ EACH OBJECT EXERTS FORCE ON N-1 OBJECTS

4 BODIES



$\frac{1}{2}(4)(3) = 6$ CALCULATION

ONLY HAVE TO DO $\frac{1}{2}$ OF THE CALCULATIONS BC OF SYMMETRY → $\frac{6}{2}$ CALCULATIONS

N BODIES REQUIRE $\frac{1}{2}N(N-1)$ CALCULATIONS

(ii) POSSIBILITY OF MULTIPLE TIME SCALES

E.G. IN A SELF-GRAVITATING SYSTEM SUCH AS A STAR CLUSTER, STARS THAT ENTER INTO A TIGHTLY BOUND ORBIT EXPERIENCE LARGE GRAVITATIONAL FORCES. TO ACCURATELY FOLLOW THESE, NEED TO USE A SMALL TIME STEP, BUT SUCH A SMALL TIMESTEP WOULD BE AN UNNECESSARY EXPENSE FOR THE VAST MAJORITY OF PARTICLES.

N-BODY PROBLEM DIVIDES INTO 2 BASIC PARTS:

1. CALCULATING THE NET FORCE ON A GIVEN PARTICLE AT A GIVEN TIME
2. DETERMINING THE NEW POSITION AND VELOCITY OF THE PARTICLE AT AN ADVANCED TIME

LET'S DISCUSS SECOND PART FIRST.

REWRITE 2ND ORDER ODE

$$\ddot{\vec{r}}_i = -G \sum_{j \neq i} m_j \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3} \longrightarrow$$

$$\dot{V}_i = \dot{x}_i$$

$$\dot{V}_i = -\sum \frac{G m_j}{r_{ij}^3} \vec{x}_{ij}$$

AS TWO 1st ORDER ODES

LET'S REWRITE TWO 1st ORDER ODEs EVEN MORE SIMPLY

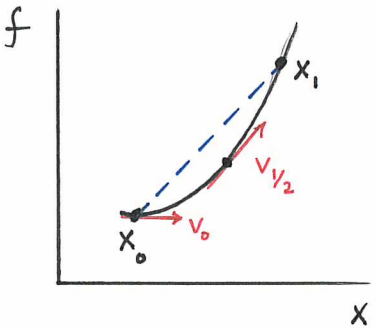
$$\frac{dx}{dt} = v$$

$$\frac{dv}{dt} = F(x) \qquad \text{WHERE} \qquad F = -\frac{dU}{dx}$$

HOW DO WE SOLVE THESE COUPLED ODEs GIVEN INITIAL CONDITIONS x_0, v_0 ?

EULER METHOD ?

$$\frac{dx}{dt} = v \longrightarrow \frac{x_1 - x_0}{\Delta t} = v_0 \longrightarrow x_1 = x_0 + \Delta t\, v_0$$



BUT SLOPE AT MIDPOINT BETWEEN 2 POINTS OF A FUNCTION IS A BETTER APPROXIMATION TO SLOPE OF CHORD CONNECTING THE TWO POINTS, THAN THE SLOPE AT EITHER END OF THE CHORD.

SO BETTER APPROXIMATION

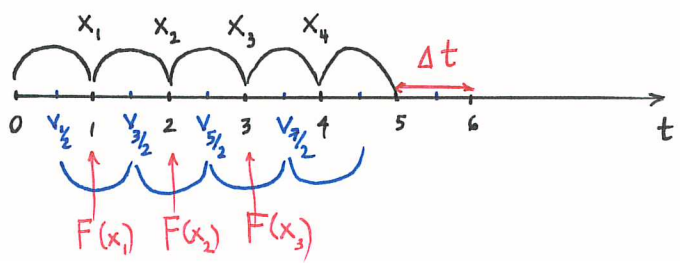
$$x_1 = x_0 + \Delta t\, v_{1/2}$$

ONCE KNOW x_1 THEN KNOW $F(x_1)$

$$v_{3/2} = v_{1/2} + \Delta t\, F(x_1)$$

ONCE KNOW $v_{3/2}$ THEN CAN USE TO GET

$$x_2 = x_1 + \Delta t\, v_{3/2}$$



LEAPFROG

x & v ARE ADVANCED SYMMETRICALLY IN TIME

$$x_{n+1} = x_n + \Delta t\, v_{n+1/2}$$

$$v_{n+3/2} = v_{n+1/2} + \Delta t\, F(x_{n+1})$$

LEAPFROG ALGORITHM

ACCURACY

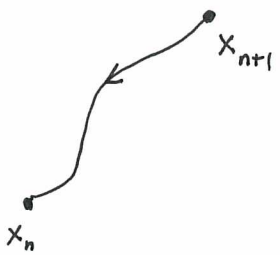
$$v_{n+1/2} = v_n + \frac{\Delta t}{2} F(x_n)$$

$$x_{n+1} = x_n + \Delta t\, v_n + \frac{1}{2}(\Delta t)^2 F(x_n)$$

SECOND ORDER ACCURATE (BETTER THAN EULER WHICH IS 1st ORDER)

WHAT ABOUT STABILITY ?

TIME REVERSIBILITY



SUPPOSE STEP BACKWARD FROM $(t_{n+1}, x_{n+1}, v_{n+3/2})$ TO $(t_n, x_n, v_{n+1/2})$

$$v_{n+1/2} = v_{n+3/2} + F(x_{n+1})(-\Delta t)$$

$$x_n = x_{n+1} + v_{n+1/2}(-\Delta t)$$

WHEN USE LEAPFROG TO STEP BACKWARDS, ARRIVE EXACTLY WHERE STARTED.

$$v_{n+3/2} = v_{n+1/2} + F(x_{n+1})\Delta t$$

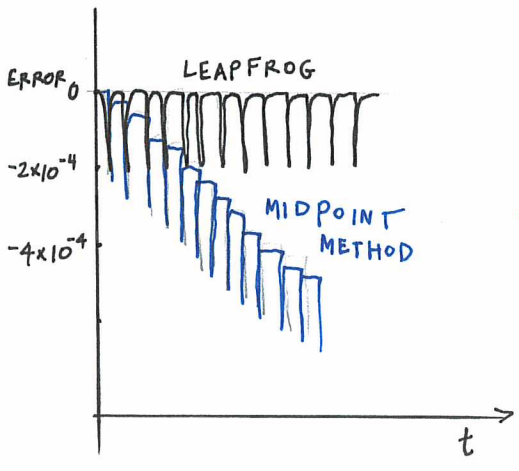
$$x_{n+1} = x_n + v_{n+1/2}\Delta t$$

WHEN REVERSE EULER, DO NOT ARRIVE AT SAME STARTING POINT WHEN COMPLETE ORBIT.

$$x_i = x_{i+1} - \Delta t\, v_{i+1} \Rightarrow x_{i+1} = x_i + \Delta t\, v_{i+1}$$

$$v_i = v_{i+1} - \Delta t\, F(x_{i+1}) \Rightarrow v_{i+1} = v_i + \Delta t\, F(x_{i+1})$$

NOT SAME x_{i+1}, v_{i+1} EULER WOULD PREDICT IF GOING FORWARD.



LEAPFROG IS ONLY SECOND ORDER ACCURATE BUT IS VERY STABLE. ERRORS INCURRED OVER OUTGOING PORTION OF ORBIT EXACTLY CANCEL THOSE PRODUCED ON INCOMING SEGMENT.

IF WANT TO KNOW X AND V AT THE SAME TIME,

TAKE $\frac{1}{2}$ A TIMESTEP WITH EULER TO GET UP TO $V_{n+1/2}$.

$h \equiv \Delta t$

$$\text{(1)}\quad V_{n+1/2} = V_n + \frac{1}{2} h F(x_n)$$

$$\text{(2)}\quad X_{n+1} = X_n + h V_{n+1/2}$$

$$\text{(3)}\quad V_{n+1} = V_{n+1/2} + \frac{1}{2} h F(x_{n+1})$$

LIOUVILLE'S THEOREM SAYS AREA IN PHASE SPACE SHOULD BE PRESERVED

CAN SHOW THAT LEAPFROG ALGORITHM CONSERVES AREA IN PHASE SPACE.

NEED TO SHOW $\iint \delta x_1 \, \delta v_1 = \iint \delta x_0 \, \delta v_0$

SUBSCRIPT FOR TIME

WHEN DO A COORDINATE TRANSFORMATION

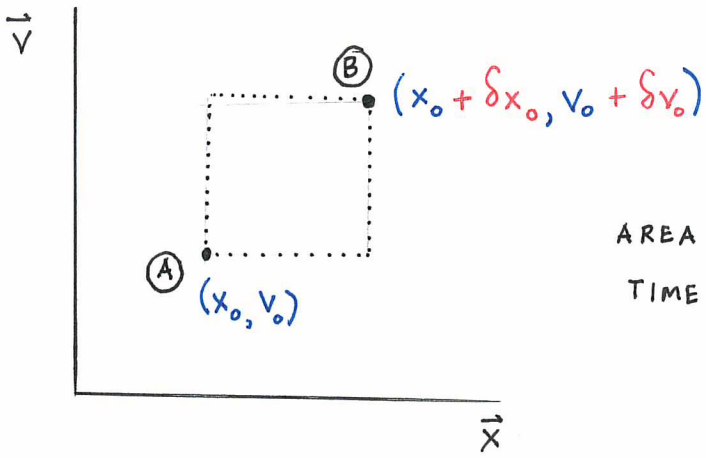
JACOBIAN

$$\iint \delta x_1 \, \delta v_1 = \iint \det J \, \delta x_0 \, \delta v_0$$

$$\begin{pmatrix} \delta x_1 \\ \delta v_1 \end{pmatrix} = \underbrace{\begin{pmatrix} \frac{\partial x_1}{\partial x_0} & \frac{\partial x_1}{\partial v_0} \\ \frac{\partial v_1}{\partial x_0} & \frac{\partial v_1}{\partial v_0} \end{pmatrix}}_{J} \begin{pmatrix} \delta x_0 \\ \delta v_0 \end{pmatrix}$$

IF AREA IN PHASE SPACE IS CONSERVED THEN $\det J = 1$

HOW DO YOU FIND J? TAKE 2 CLOSE BY COORDINATES IN PHASE SPACE



AREA AT INITIAL TIME IS $\delta x_0 \delta v_0$

EVOLVE POINT (A) (x_0, v_0) AND POINT (B) $(x_0 + \delta x_0, v_0 + \delta v_0)$ WITH LEAPFROG TO SHOW $\delta x_1 \delta v_1 = \delta x_0 \delta v_0$

FIRST STEP OF LEAPFROG $v_{n+1/2} = v_n + \frac{1}{2} h F(x_n)$

APPLY STEP 1 TO (B): $v_{1/2} + \delta v_{1/2} = v_0 + \delta v_0 + \frac{1}{2} h F(x_0 + \delta x_0)$

APPLY STEP 1 TO (A) & SUBTRACT: $-v_{1/2} = -v_0 - \frac{1}{2} h F(x_0)$

$$\delta v_{1/2} = \delta v_0 + \frac{1}{2} h \{ F(x_0 + \delta x_0) - F(x_0) \}$$

REWRITE IN MATRIX NOTATION: STEP 1

$$\begin{pmatrix} \delta x_0 \\ \delta v_{1/2} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 \\ \frac{h}{2} F'(x_0) & 1 \end{pmatrix}}_{A} \begin{pmatrix} \delta x_0 \\ \delta v_0 \end{pmatrix}$$

DON'T CHANGE δx_0 IN THIS STEP.

SECOND STEP OF LEAPFROG $x_{n+1} = x_n + h v_{n+1/2}$

APPLY STEP 2 TO (B): $x_1 + \delta x_1 = x_0 + \delta x_0 + h(v_{1/2} + \delta v_{1/2})$

APPLY STEP 2 TO (A) & SUBTRACT: $-x_1 = -x_0 - h v_{1/2}$

$$\delta x_1 = \delta x_0 + h \delta v_{1/2}$$

DON'T CHANGE $\delta v_{1/2}$ IN THIS STEP

STEP 2 $$\begin{pmatrix} \delta x_1 \\ \delta v_{1/2} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix}}_{B} \begin{pmatrix} \delta x_0 \\ \delta v_{1/2} \end{pmatrix}$$

THIRD STEP OF LEAPFROG $\quad v_{n+1} = v_{n+\frac{1}{2}} + \frac{1}{2} h F(x_{n+1})$

APPLY STEP 3 TO (B) $$v_1 + \delta v_1 = v_{1/2} + \delta v_{1/2} + \frac{1}{2} h F(x_1 + \delta x_1)$$

APPLY STEP 3 TO (A) & SUBTRACT $$-v_1 = -v_{1/2} - \frac{1}{2} h F(x_1)$$

$$\delta v_1 = \delta v_{1/2} + \frac{1}{2} h \{ F(x_1 + \delta x_1) - F(x_1) \}$$

STEP 3 $$\begin{pmatrix} \delta x_1 \\ \delta v_1 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 \\ \frac{h}{2} F'(x_1) & 1 \end{pmatrix}}_{C} \begin{pmatrix} \delta x_1 \\ \delta v_{1/2} \end{pmatrix}$$

DON'T CHANGE δx_1 IN THIS STEP

$$\therefore \quad \begin{pmatrix} \delta x_1 \\ \delta v_1 \end{pmatrix} = CBA \begin{pmatrix} \delta x_0 \\ \delta v_0 \end{pmatrix}$$

$$\det CBA = \det C \det B \det A = 1$$

HENCE LEAPFROG ALGORITHM PRESERVES AREA IN PHASE SPACE, i.e. IT IS SYMPLECTIC. SYMPLECTIC ALGORITHMS POSSESS GLOBAL STABILITY. SINCE THE AREA BOUNDED BY ADJACENT TRAJECTORIES IS PRESERVED, CANNOT HAVE THE SITUATION WHERE THE COORDINATES (AND HENCE ENERGY) INCREASE WITHOUT BOUND BC THAT WOULD EXPAND THE AREA.

NOW THAT WE'VE OUTLINED A METHOD TO UPDATE POSITIONS AND VELOCITIES, WE NEED TO DISCUSS HOW TO COMPUTE FORCES.

TWO APPROACHES:

PARTICLE APPROACH: SOLVE FOR FORCE

$$\vec{F}(\vec{r}) = -\sum_{i \neq j} \frac{G m_i m_j}{(r_i - r_j)^3} (\vec{r}_i - \vec{r}_j)$$

- DIRECT PARTICLE-PARTICLE SUMMATION SCALES $\sim N^2$ (N is # OF PARTICLES)
- TREE CODE: SCALES AS $N \log N$

GRID APPROACH: SOLVE FOR POTENTIAL

$$\vec{\nabla}^2 \phi(\vec{r}_{i,j,k}) = 4\pi G \rho(\vec{r}_{i,j,k})$$

$$\vec{F}(\vec{r}_{i,j,k}) = -m \vec{\nabla} \phi(\vec{r}_{i,j,k})$$

SCALES AS N_{grid} (NUMBER OF GRID POINTS)

LET'S LOOK AT GRID METHOD FIRST

PARTICLE MESH METHOD

4 STEPS

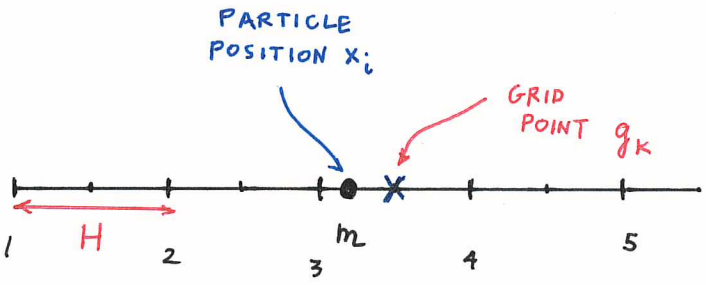
(PARTICLE MASSES, PARTICLE POSITIONS, GRID POSITIONS)

1. CALCULATE MASS DENSITY ON GRID $m_i, x_i \longrightarrow \rho(g_{k,l,m})$
2. SOLVE POISSON'S EQU. ON GRID $\Phi(g_{k,l,m})$
3. DIFFERENTIATE POTENTIAL TO GET FORCES ON GRID $\vec{F}(g_{k,l,m})$
4. INTERPOLATE FORCES BACK TO PARTICLES $\vec{F}(g_{k,l,m}) \longrightarrow \vec{F}(x_i)$

STEP 1 CALCULATING MASS DENSITY ON GRID

THERE'S A HIERARCHY OF MASS ASSIGNMENT SCHEMES

CONSIDER 1 PARTICLE ON 1D GRID



$$m(g_k) = m\,W(d)$$

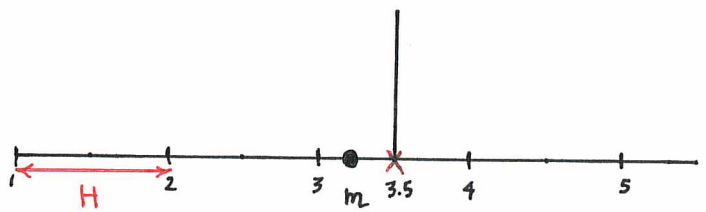
MASS ASSIGNMENT FUNCTION

WHERE $d = |x_i - g_k|$

$$\rho(g_k) = \frac{m(g_k)}{H}$$

(i) NEAREST GRID POINT

$$W(d) = \begin{cases} 1 & d \le H/2 \\ 0 & \text{OTHERWISE} \end{cases}$$



ASSIGN ALL MASS TO NEAREST GRID POINT

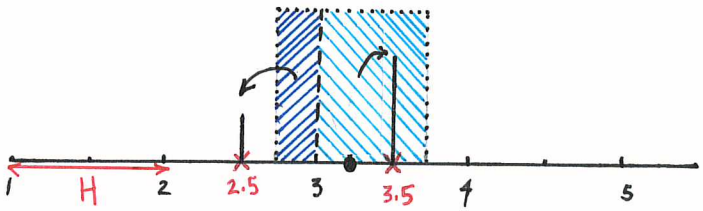
LET $x_i = 3.2$, $H = 1$

$$d = |3.2 - 3.5| = .3$$

(x_i, g_k)

(ii) CLOUD IN CELL

$$W(d) = \begin{cases} 1 - d/H & d \le H \\ 0 & \text{OTHERWISE} \end{cases}$$

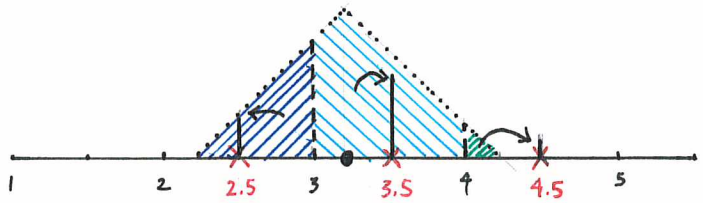


$$d = |3.2 - 3.5| = .3 \Rightarrow 1 - \frac{d}{H} = 0.7 \Rightarrow \rho(g_{3.5}) = 0.7$$

$$d = |3.2 - 2.5| = .7 \Rightarrow 1 - \frac{d}{H} = 0.3 \Rightarrow \rho(g_{2.5}) = 0.3$$

(iii) TRIANGULAR SHAPED CLOUD

$$W(d) = \begin{cases} \frac{3}{4} - \left(\frac{d}{H}\right)^2 & d \le H/2 \\ \frac{1}{2}\left(\frac{3}{2} - \frac{d}{H}\right)^2 & H/2 \le d \le 3H/2 \\ 0 & \text{OTHERWISE} \end{cases}$$



FOR N PARTICLES ON 3D GRID

$$\rho(g_{k,l,m}) = \frac{1}{H^3} \sum_{i=1}^{N} m_i \, W(|d_x|) \, W(|d_y|) \, W(|d_z|)$$

STEP 2 SOLVE POISSON'S EQU ON GRID

[I] METHOD 1 : BY FOURIER TRANSFORM

KEY TO SOLUTION OF

$$\Phi(x,y,z) = -\int \frac{G\rho(x',y',z')}{|\vec{x}-\vec{x}'|}\,dx'dy'dz'$$

IS THE CONVOLUTION THEOREM
IF $g(x)$ AND $h(x)$ ARE FUNCTIONS, THEIR CONVOLUTION IS:

$$g * h = \int_{-\infty}^{+\infty} g(x')\,h(x-x')\,dx'$$

AND THE FOURIER TRANSFORM OF THE CONVOLUTION IS $G(k)H(k)$ WHERE G & H ARE THE FOURIER TRANSFORMS OF g AND h RESPECTIVELY.

LET $g(x') = \rho(x',y',z')$

$$h(x-x') = \frac{-G}{|\vec{x}-\vec{x}'|}$$

GREEN'S FUNCTION

$$\hat{\Phi}(k) = \hat{\rho}(k)\,\hat{h}(k)$$

INSTEAD OF DOING INTEGRAL IN REAL SPACE, DO SIMPLE MULTIPLICATION IN FOURIER SPACE.

FFT OF GREEN'S FUNCTION NEEDS TO BE COMPUTED ONLY ONCE.

IN EACH TIMESTEP: FFT FORWARD DENSITY FIELD

↓

MULTIPLY WITH GREEN'S FUNCTION

↓

FFT BACKWARD TO OBTAIN POTENTIAL

FFT REQUIRES A UNIFORM GRID

STEP 3 DIFFERENTIATE POTENTIAL TO GET FORCES

APPROXIMATE FORCE FIELD ON GRID BY

FINITE DIFFERENCING

X-COMPONENT OF FORCE

$$F^{(x)}_{k,l,m} = -\frac{\left(\Phi_{k+1,l,m} - \Phi_{k-1,l,m}\right)}{2\Delta x}$$

CENTERED DIFFERENCE SCHEME (2ND ORDER ACCURATE)

$$F^{(x)}_{k,l,m} = -\frac{4}{3}\frac{\left(\Phi_{k+1,l,m} - \Phi_{k-1,l,m}\right)}{2\Delta x} + \frac{1}{3}\frac{\left(\Phi_{k+2,l,m} - \Phi_{k-2,l,m}\right)}{4\Delta x}$$

4th ORDER ACCURATE SCHEME

STEP 4 INTERPOLATE FORCES BACK TO PARTICLES

$$F(x_i) = \sum W(x_i - g_{k,l,m})\, F_{k,l,m}$$

NOTE: INTERPOLATION KERNEL W MUST BE THE SAME ONE USED FOR MASS ASSIGNMENT TO ENSURE THAT THERE'S NO SELF-FORCE (I.E. TWO INTERACTING PARTICLES FEEL EQUAL BUT OPPOSITE FORCES, NO SELF-FORCE)

II METHOD 2 TO SOLVE FOR POTENTIAL : RELAXATION SOLVERS

- NOT LIMITED TO UNIFORM GRID
- METHOD APPLICABLE FOR ANY ELLIPTIC PDE

CHANGE TIME-INDEPENDENT PROBLEM (ELLIPTIC PDE) INTO A PSEUDO-TIME DEPENDENT PROBLEM (PARABOLIC PDE)

$$\frac{\partial \Phi}{\partial \tau} = \nabla^2 \Phi - 4\pi G\rho$$

PSEUDO-TIME

SOLVE PDE FOR SEQUENCE OF VALUES OF PSEUDO-TIME STEPS $\Delta\tau$ UNTIL Φ COMES TO A STEADY-STATE.

i.e. ρ IS CONSIDERED TO BE A CONSTANT AS A FUNCTION OF PSEUDO-TIME (ALTHOUGH IT MAY BE A FUNCTION OF PHYSICAL TIME).

Φ IS CONSIDERED TO BE A FUNCTION OF PSEUDO-TIME.

ITERATE UNTIL $\frac{\partial \Phi}{\partial \tau} = 0$

AT WHICH POINT POISSON EQUATION IS SATISFIED.

IT'S FORMALLY LIKE A DIFFUSION EQUATION.

IN 2D

$$\frac{\Phi_{j,k}^{n+1} - \Phi_{j,k}^{n}}{\Delta\tau} = \frac{\Phi_{j+1,k}^{n} - 2\Phi_{j,k}^{n} + \Phi_{j-1,k}^{n}}{(\Delta x)^2} + \frac{\Phi_{j,k+1}^{n} - 2\Phi_{j,k}^{n} + \Phi_{j,k-1}^{n}}{(\Delta y)^2} - 4\pi G \rho_{j,k}$$

LET $\Delta x = \Delta y$

$$\Phi_{j,k}^{n+1} = \Phi_{j,k}^{n}\left\{1 - \frac{4\Delta\tau}{(\Delta x)^2}\right\} + \frac{\Delta\tau}{(\Delta x)^2}\left[\Phi_{j+1,k}^{n} + \Phi_{j-1,k}^{n} + \Phi_{j,k+1}^{n} + \Phi_{j,k-1}^{n} - 4\pi G \rho_{j,k} (\Delta x)^2\right]$$

RECALL THE EXPLICIT SOLUTION OF A DIFFUSION EQUATION INVOLVES A LIMITATION ON THE TIMESTEP

IN 1D (TAKE DIFFUSION COEFFICIENT TO BE 1) $\frac{\Delta\tau}{(\Delta x)^2} \leq \frac{1}{2}$. IN 2D $\frac{\Delta\tau}{(\Delta x)^2} + \frac{\Delta\tau}{(\Delta y)^2} \leq \frac{1}{2}$ IF $\Delta x = \Delta y$ $\Rightarrow \frac{\Delta\tau}{(\Delta x)^2} \leq \frac{1}{4}$

TAKE MAXIMUM PSEUDO-TIMESTEP $\Delta\tau = \frac{1}{4}(\Delta x)^2$ TO GET

JACOBI METHOD

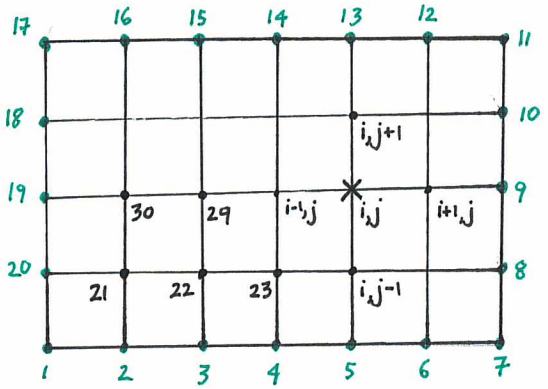
$$\Phi_{i,j}^{n+1} = \frac{1}{4}\left[\Phi_{j+1,k}^{n} + \Phi_{j-1,k}^{n} + \Phi_{j,k+1}^{n} + \Phi_{j,k-1}^{n} - 4\pi G \rho_{i,j} (\Delta x)^2\right]$$

ITERATION NUMBER

SUM OF POTENTIALS AT 4 POINTS SURROUNDING i,j

DENSITY FROM MASS ASSIGNMENT SCHEME

BOUNDARY CONDITIONS MUST BE SPECIFIED OVER ENTIRE BOUNDARY ENCLOSING THE DOMAIN FOR ELLIPTIC PDE.



BOUNDARY CONDITIONS SPECIFIED FOR Φ_1 THROUGH Φ_{20}

$\Phi_{i,j}$ AT ALL OTHER GRID POINTS IS UNKNOWN

USE JACOBI METHOD TO COMPUTE $\Phi_{i,j}$ AT INTERIOR GRID POINTS

FOR EXAMPLE

ITERATION NUMBER

KNOWN FROM BOUNDARY CONDITIONS

$$\Phi_{21}^{n+1} = \frac{1}{4}\left[\Phi_{22}^{n} + \Phi_{20} + \Phi_{30}^{n} + \Phi_{2} - 4\pi G \rho_{21} (\Delta x)^2\right]$$

$$\Phi_{22}^{n+1} = \frac{1}{4}\left[\Phi_{23}^{n} + \Phi_{21}^{n} + \Phi_{29}^{n} + \Phi_{3} - 4\pi G \rho_{22} (\Delta x)^2\right]$$

AND REPEAT FOR NEXT GRID POINT UNTIL COMPLETE ITERATION.

IF $\text{MAX}\left|\Phi_{i,j}^{n+1} - \Phi_{i,j}^{n}\right| \leq \varepsilon$

A PRESCRIBED THRESHOLD

THEN HAVE CONVERGENCE

GAUSS-SEIDEL

$$\Phi_{22}^{n+1} = \frac{1}{4}\left[\Phi_{23}^{n} + \Phi_{21}^{n+1} + \Phi_{29}^{n} + \Phi_{3} - 4\pi G \rho_{22} (\Delta x)^2\right]$$

USE ALREADY UPDATED VALUE!

NOTHING MAGIC ABOUT SWEEPING DIRECTION.

JACOBI METHOD CONVERGES VERY SLOWLY FOR LARGE GRIDS AND IS VERY SENSITIVE TO INITIAL GUESS.

GAUSS-SEIDEL IMPROVES CONVERGENCE RATE BY FACTOR 2.

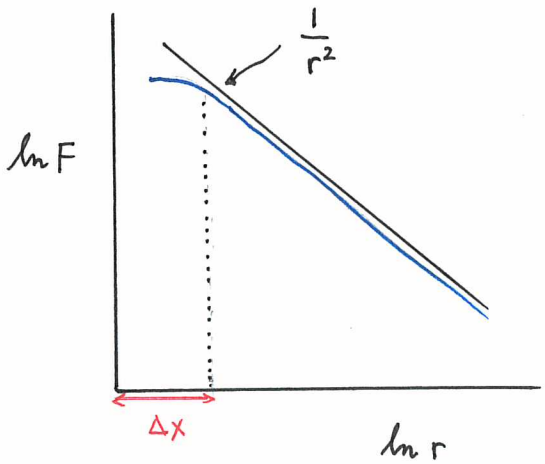
BOTH METHODS QUICKLY ELIMINATE SHORT WAVELENGTH ERRORS (THOSE ON SCALE OF GRID SPACING) BUT ARE INEFFICIENT AT ELIMINATING ERRORS WITH LONG WAVELENGTHS BECAUSE ONE CELL INTERACTS ONLY WITH ITS NEIGHBORS DURING ONE ITERATION.

MULTIGRID TECHNIQUES USE COARSER GRIDS TO SPEED UP CONVERGENCE.

OVERLAY SERIES OF COARSER AND COARSER GRIDS ON TOP OF ORIGINAL GRID.
SWITCH BETWEEN THESE GRIDS ACCORDING TO SOME ORDERED PROCEDURE & OBTAIN APPROXIMATE SOLUTION ON EACH GRID.

SHORT WAVELENGTH ERRORS ELIMINATED ON FINE GRIDS, AND LONG WAVELENGTH ERRORS ARE ELIMINATED ON COARSE GRIDS.

FORCE RESOLUTION FOR GRID METHODS



FOR GRID METHODS FORCE IS SOFTENED ON SCALE OF LOCAL GRID SIZE

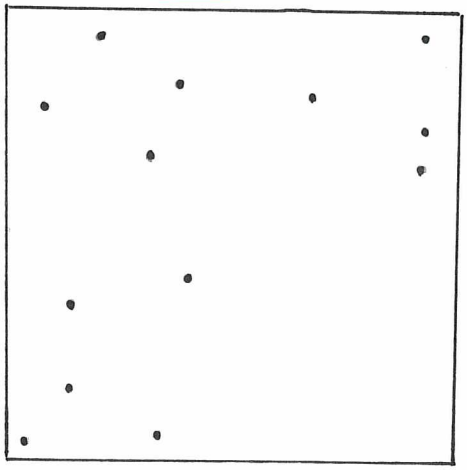
TREE ALGORITHM FOR FORCE CALCULATION

TO OVERCOME THE "N^2" ISSUE OF (GRAVITATIONAL) FORCE CALCULATION BY DIRECT SUMMATION, e.g.

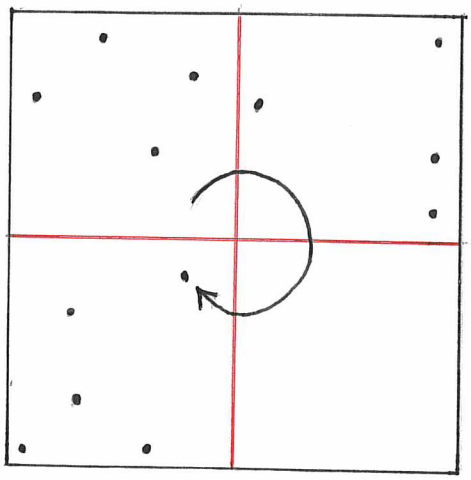
$$\vec{F}_i(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{(r_i - r_j)^3} (\vec{r}_i - \vec{r}_j)$$

ONE CAN ORGANIZE PARTICLES INTO A TREE STRUCTURE.

ROOT GRID

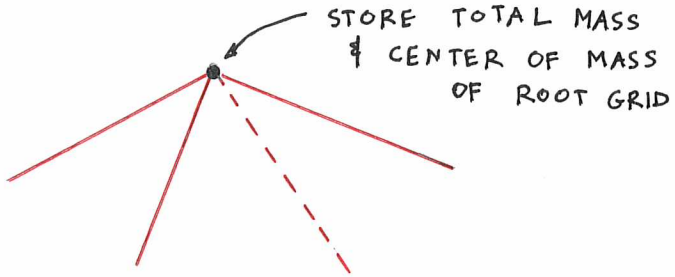


"BUILDING" THE TREE

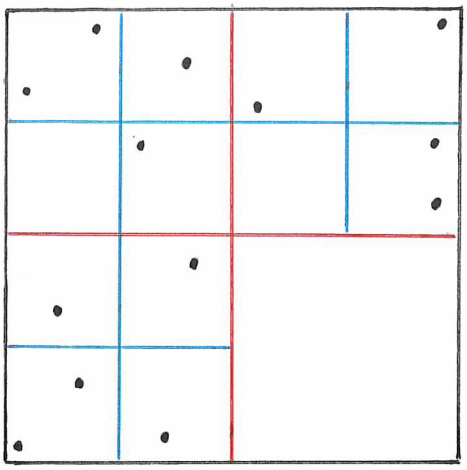


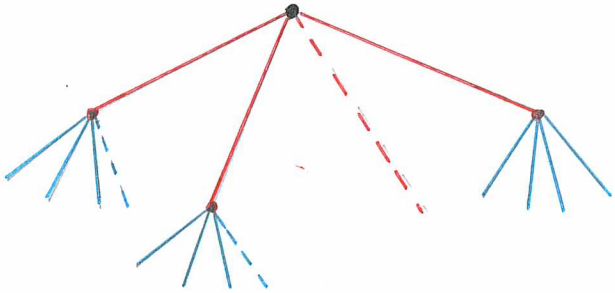
IDEA DON'T NEED TO ESTIMATE FORCE EXERTED BY EACH SINGLE PARTICLE. WE CAN ESTIMATE THE FORCE EXERTED BY GROUPS OF PARTICLES IF THEY ARE SUFFICIENTLY FAR.

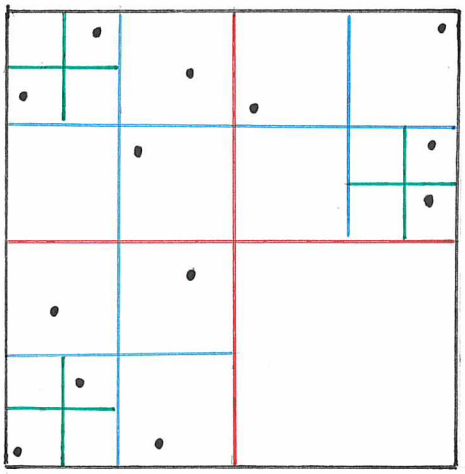
A GROUP OF PARTICLES AT A DISTANCE EXERTS ALMOST THE SAME FORCE AS A LARGE SINGLE PARTICLE AT THE GROUP'S CENTER OF MASS.

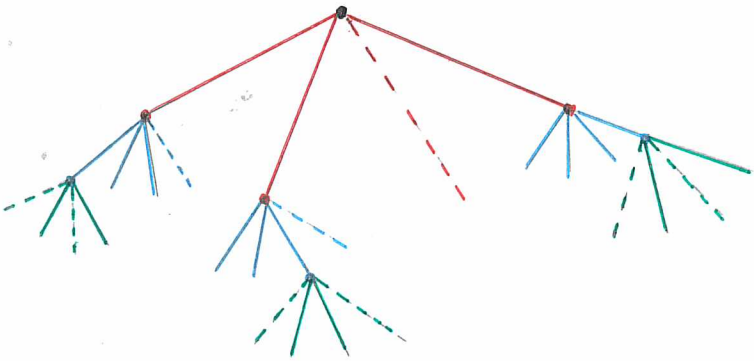


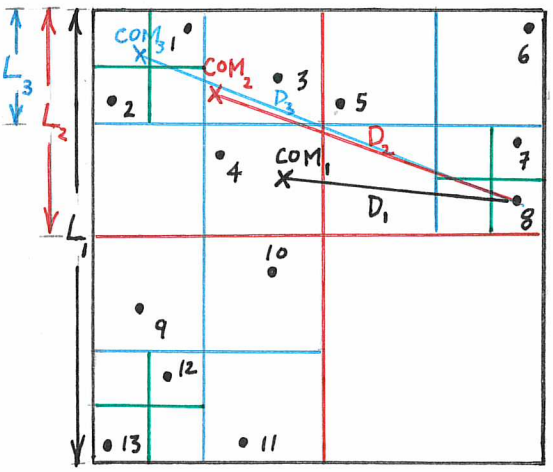
DIVIDE SPACE INTO 4 CELLS (IN 2D) MOVING IN CLOCKWISE DIRECTION FROM TOP LEFT. EACH BRANCH STORES MASS & CENTER OF MASS OF CELL ON THAT LEVEL. EMPTY CELLS ARE INDICATED BY A DASHED LINE.

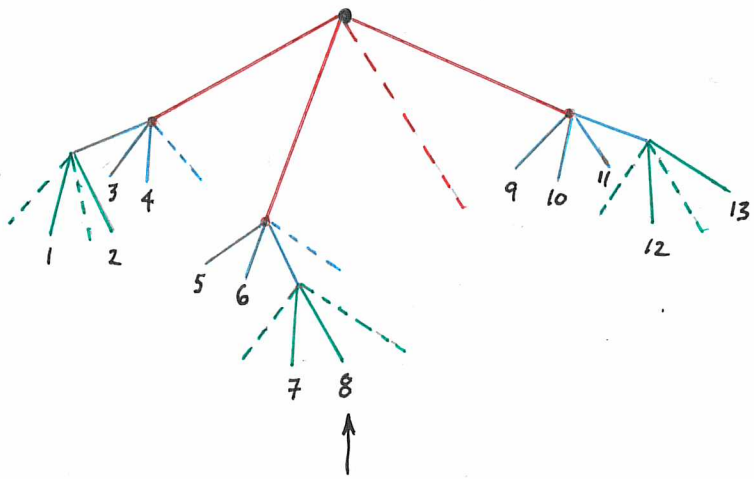









COM3
COM2
COM1
L3
L2
L1
D3
D2
D1
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2
3
4
5
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7
8
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13

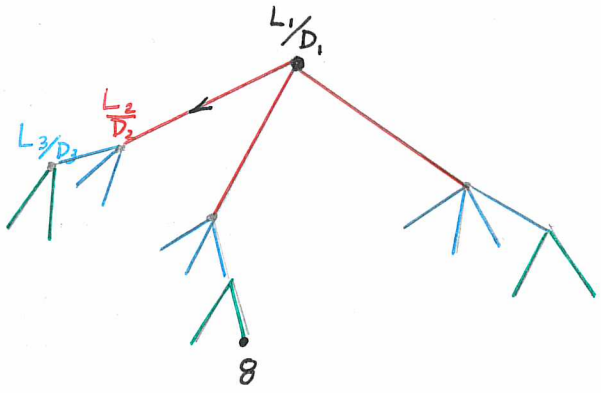

1
2
3
4
5
6
7
8
9
10
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12
13

"WALKING THE TREE"

FOCUS ON PARTICLE 8

START WITH TOP NODE (i.e. ROOT NODE)

IF $\frac{L_1}{D_1} > \theta$ ← OPENING ANGLE



THEN GO TO NEXT NODE IN TREE.

IF $\frac{L_2}{D_2} > \theta$

THEN DESCEND TO NEXT NODE IN TREE.

IF $\frac{L_3}{D_3} < \theta$

THEN STOP OPENING THAT BRANCH AND ADD FORCE CONTRIBUTION FROM "SUPER-PARTICLE"

BUT THEN STILL NEED TO ADD REMAINING CONTRIBUTIONS FROM THAT BRANCH

IF PARTICLE IS ALONE IN A CELL THEN DO DIRECT CALCULATION. THEN WALK THE OTHER BRANCHES.

HOW MANY STEPS, x, TO ORGANIZE N PARTICLES IN A TREE?

$$N\left(\frac{1}{2}\right)^x = 1 \quad \Rightarrow \quad x = \log_2 N$$

WHAT DETERMINES RESOLUTION OF FORCE CALCULATION?

FORCE IS SOFTENED WITH SOFTENING PARAMETER ε TO AVOID THE SINGULARITY FOR $r_i = r_j$.

$$\vec{F}(\vec{r}_i) = -\sum_{i \neq j} \frac{G m_i m_j}{\left\{ (r_i - r_j)^2 + \varepsilon^2 \right\}^{3/2}} (\vec{r}_i - \vec{r}_j)$$

AND TO PREVENT THE TIMESTEP FROM BECOMING TOO SHORT $\Delta t \simeq \sqrt{\frac{\varepsilon}{a}}$ (WHERE $a \equiv$ ACCELERATION)

RULE OF THUMB FOR CHOOSING SOFTENING LENGTH

$\varepsilon \sim$ AVERAGE DISTANCE BETWEEN PARTICLES

$$N \varepsilon^3 \sim \frac{4\pi}{3} R_{vir}^3$$

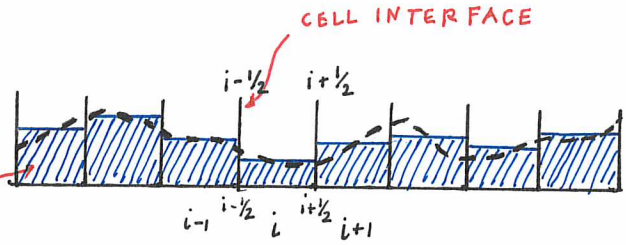
R_{vir} ← VIRIAL RADIUS

$$\varepsilon \sim \left(\frac{4\pi}{3} R_{vir}^3 \right)^{1/3} N^{-1/3}$$

N ← NUMBER OF PARTICLES IN SIMULATION

ε DETERMINES FORCE RESOLUTION OF SIMULATION

FINITE VOLUME METHODS



STORE THE AVERAGE IN EACH CELL

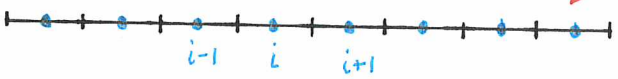
TIME

$$\langle U \rangle_i^n = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t^n)\, dx$$

SPACE

VERSUS

FINITE DIFFERENCE METHOD



$$U_i^n = U(x_i, t^n)$$

REPLACE DERIVATIVES IN PARTIAL DIFFERENTIAL EQUATION BY DIFFERENCES BETWEEN NEIGHBOURING GRID POINTS.

CONSIDER THE CONSERVATIVE FORM OF THE PDE

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0$$

CONSERVATIVE VARIABLES $U = \begin{pmatrix} \rho \\ \rho v_i \\ \varepsilon \end{pmatrix}$

MASS, MOMENTUM & ENERGY DENSITY UPDATED BY DERIVATIVES OF MASS, MOMENTUM AND ENERGY FLUXES.

EXAMPLE: EULER EQUATIONS

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0$$

$$\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\rho v_i v_j + P\delta_{ij}) = 0$$

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial}{\partial x_i}((\varepsilon + P) v_i) = 0$$

WHERE $\varepsilon = e + \frac{1}{2}\rho v^2$

INTERNAL ENERGY

$P = (\gamma - 1) e$ EQUATION OF STATE

RATHER THAN SOLVING THE DIFFERENTIAL FORM OF A PDE, FINITE VOLUME SCHEMES SOLVE THE INTEGRAL FORM OF THE PDE.

INTEGRATE $\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$ OVER A

TIME INTERVAL $\Delta t = t^{n+1} - t^n$

AND A CELL SIZE $\Delta x = x_{i+1/2} - x_{i-1/2}$

$$\int_{t^n}^{t^{n+1}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left(\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} \right) dt\, dx = 0$$

SPATIAL INTEGRATION

$$\int_{t^n}^{t^{n+1}} \left[\frac{\partial}{\partial t} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x,t)\, dx + \int_{x_{i-1/2}}^{x_{i+1/2}} \frac{\partial F}{\partial x}\, dx \right] dt = 0$$

DEFINE SPATIAL AVERAGE

$$\langle U \rangle_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x,t)\, dx$$

$$\int_{t^n}^{t^{n+1}} \left[\Delta x \frac{\partial}{\partial t} \langle U \rangle_i + \left(F_{i+1/2} - F_{i-1/2} \right) \right] dt = 0$$

TIME INTEGRATION

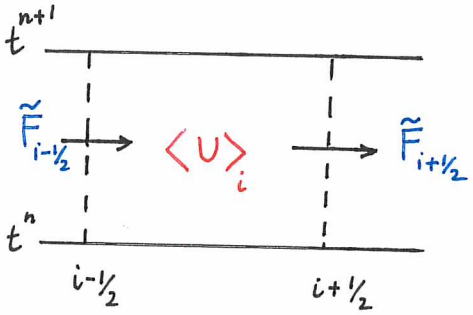
$$\Delta x \left(\langle U \rangle_i^{n+1} - \langle U \rangle_i^{n} \right) + \Delta t \left(\tilde{F}_{i+1/2}^{n+1/2} - \tilde{F}_{i-1/2}^{n+1/2} \right) = 0$$

WHERE $\tilde{F}_{i\pm 1/2}^{n+1/2} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} F\left(U(x_{i\pm 1/2}) \right) dt$

REARRANGING TERMS

$$\langle U \rangle_i^{n+1} = \langle U \rangle_i^n - \frac{\Delta t}{\Delta x}\left(\tilde{F}_{i+1/2}^{\,n+1/2} - \tilde{F}_{i-1/2}^{\,n+1/2} \right)$$

INTEGRAL REPRESENTATION OF ORIGINAL PDE DOES NOT MAKE USE OF PARTIAL DERIVATIVES.



EXPRESSING PDE IN INTEGRAL OR CONSERVATION FORM ENSURES (1) GLOBAL CONSERVATION (E.G. FOR EULER EQUATIONS NO MASS, MOMENTUM OR ENERGY IS CREATED OR DESTROYED UNLESS THERE IS A NET FLUX) (2) CORRECT DESCRIPTION OF DISCONTINUOUS FLOWS (SPEEDS & JUMPS)

TO UPDATE $\langle U \rangle_i^n$ IN A CELL, THE CHALLENGE IS TO CONSTRUCT APPROXIMATIONS TO THE FLUXES $\tilde{F}_{i\pm1/2}$ THROUGH THE CELL WALLS.

CHARACTERISTIC ANALYSIS OF THE EULER EQUATIONS

RECAST EULER EQUATIONS IN PRIMITIVE VARIABLES (DENSITY ρ, VELOCITY $\vec{v}$, & PRESSURE P)

$$\frac{D\rho}{Dt} = -\rho \vec{\nabla}\cdot\vec{v}$$

$$\rho \frac{Dv_i}{Dt} + \frac{\partial P}{\partial x_i} = 0$$

$$\frac{De}{Dt} = -(e+P)\vec{\nabla}\cdot\vec{v}$$

WHERE

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + \vec{v}\cdot\vec{\nabla}$$

LAGRANGIAN DERIVATIVE

IN 1D

$$\frac{\partial \rho}{\partial t} + v_x \frac{\partial \rho}{\partial x} + \rho \frac{\partial v_x}{\partial x} = 0$$

$$\rho \frac{\partial v_x}{\partial t} + \rho v_x \frac{\partial v_x}{\partial x} + \frac{\partial P}{\partial x} = 0$$

$$\frac{\partial e}{\partial t} + v_x \frac{\partial e}{\partial x} + (e + P) \frac{\partial v_x}{\partial x} = 0$$

BUT $P = (\gamma - 1) e$ ← INTERNAL ENERGY DENSITY

$$\Longrightarrow \quad \frac{\partial P}{\partial t} + v_x \frac{\partial P}{\partial x} + (\gamma P) \frac{\partial v_x}{\partial x} = 0$$

REWRITE IN MATRIX NOTATION

VECTOR OF PRIMITIVE VARIABLES

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ v_x \\ P \end{pmatrix} + \begin{pmatrix} v_x & \rho & 0 \\ 0 & v_x & 1/\rho \\ 0 & \gamma P & v_x \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} \rho \\ v_x \\ P \end{pmatrix} = 0$$

3×3 CHARACTERISTIC MATRIX

LINEARIZE EULER EQUATIONS

ASSUME SOLUTION

$$\begin{pmatrix} \rho(x,t) \\ v_x(x,t) \\ P(x,t) \end{pmatrix} = \begin{pmatrix} \rho_0 \\ v_{x0} \\ P_0 \end{pmatrix} + \begin{pmatrix} \rho_1 \\ v_{x1} \\ P_1 \end{pmatrix} e^{i(kx - \omega t)}$$

SMALL FLUCTUATION ABOUT A CONSTANT STATE

$$-i\omega \begin{pmatrix} \rho_1 \\ v_{x1} \\ p_1 \end{pmatrix} + ik \underbrace{\begin{pmatrix} v_{x0} & \rho_0 & 0 \\ 0 & v_{x0} & 1/\rho_0 \\ 0 & \gamma p_0 & v_{x0} \end{pmatrix}}_{A} \begin{pmatrix} \rho_1 \\ v_{x1} \\ p_1 \end{pmatrix} = 0$$

let $\lambda = \omega/k$

$$\begin{pmatrix} v_{x0}-\lambda & \rho_0 & 0 \\ 0 & v_{x0}-\lambda & 1/\rho_0 \\ 0 & \gamma p_0 & v_{x0}-\lambda \end{pmatrix} \begin{pmatrix} \rho_1 \\ v_{x1} \\ p_1 \end{pmatrix} = 0 \qquad \star$$

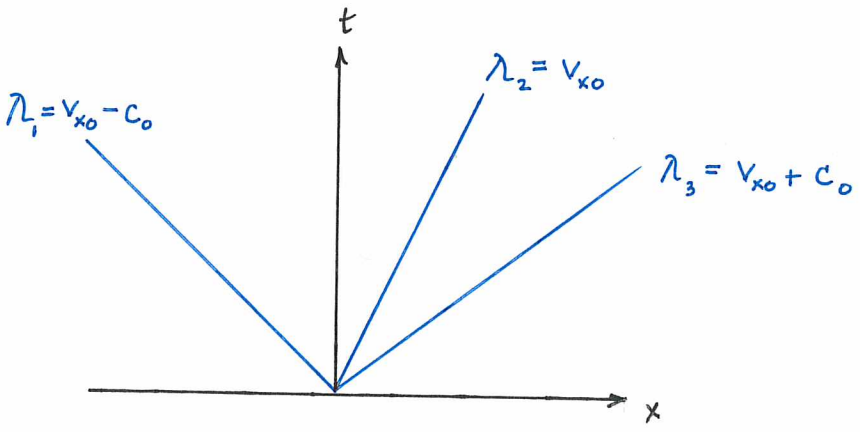
DETERMINANT YIELDS CHARACTERISTIC EQUATION FOR EIGENVALUES

$\lambda_1 = v_{x0} - c_0$ LEFT GOING SOUND WAVE

$\lambda_2 = v_{x0}$ ENTROPY WAVE (CONTACT DISCONTINUITY)

$\lambda_3 = v_{x0} + c_0$ RIGHT GOING SOUND WAVE

WHERE $c_0 = \sqrt{\dfrac{\gamma p_0}{\rho_0}}$



EIGENVALUES GIVE CHARACTERISTIC SPEEDS OF SYSTEM, I.E. SPEEDS AT WHICH INFORMATION PROPAGATES.

CAN SOLVE FOR 3 LINEARLY INDEPENDENT RIGHT EIGENVECTORS

$A r^m = \lambda^m r^m$

$$r_1 = \begin{pmatrix} \rho_0 \\ -c_0 \\ \rho_0 c_0^2 \end{pmatrix} \qquad r_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad r_3 = \begin{pmatrix} \rho_0 \\ c_0 \\ \rho_0 c_0^2 \end{pmatrix}$$

BY PLUGGING λ_3 INTO ★ CAN SHOW

$$\rho_1 : v_{x1} : P_1 = \rho_0 : c_0 : \rho_0 c_0^2$$

$\Rightarrow$ INCREASE IN v_{x1} CAUSES INCREASE IN ρ_1 AND P_1

"COMPRESSIVE WAVES"

BY PLUGGING λ_2 INTO ★ CAN SHOW THAT ONLY GET FLUCTUATIONS IN DENSITY AND NONE IN v_x AND P

"ENTROPY WAVE" OR "CONTACT DISCONTINUITY"

DEFINE ORTHONORMAL LEFT EIGENVECTORS $(r^j \cdot l^k = \delta_{jk})$

$$l^m A = l^m \lambda^m$$

$$l^1 = \left(0 \quad \frac{-1}{2c_0} \quad \frac{1}{2\rho_0 c_0^2}\right)$$

$$l^2 = \left(1 \quad 0 \quad \frac{-1}{c_0^2}\right)$$

$$l^3 = \left(0 \quad \frac{1}{2c_0} \quad \frac{1}{2\rho_0 c_0^2}\right)$$

$$\begin{pmatrix} l^1 \\ l^2 \\ l^3 \end{pmatrix} A \begin{pmatrix} r^1 & r^2 & r^3 \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}$$

$L \quad A \quad R \quad \Lambda$

WRITE EULER EQUATIONS IN COMPACT FORM

$\vec{V}$ is VECTOR OF PRIMITIVE VARIABLES

$$\vec{V}_t + A\vec{V}_x = 0$$

BECAUSE WE LINEARIZED THE HYPERBOLIC SYSTEM A IS A FUNCTION OF CONSTANT STATE V_0 SO CAN PULL IT OUTSIDE x DERIVATIVE.

$$\begin{pmatrix} \rho \\ v_x \\ p \end{pmatrix}$$

$$A = \begin{pmatrix} v_{x0} & \rho_0 & 0 \\ 0 & v_{x0} & 1/\rho_0 \\ 0 & \gamma p_0 & v_{x0} \end{pmatrix}$$

GIVEN INITIAL CONDITIONS

$$\vec{V}(x, t=0) = \vec{V}_0 + \vec{V}_1(x)$$

FLUCTUATION ABOUT CONSTANT STATE $\vec{V}_0$

WANT TO SOLVE FOR TIME DEPENDENT EVOLUTION OF $\vec{V}$.

$\vec{V}_0$ (THE CONSTANT STATE) SATISFIES $\vec{V}_t + A\vec{V}_x = 0$ TRIVIALLY, SO DYNAMICAL EQUATION BECOMES

$$(V_1)_t + A(V_1)_x = 0$$

$$L(V_1)_t + LA(V_1)_x = 0$$

$$L(V_1)_t + LA\underbrace{RL}_{I}(V_1)_x = 0$$

$$L(V_1)_t + \Lambda L(V_1)_x = 0$$

LET $W \equiv LV_1 = \begin{pmatrix} w^1 \\ w^2 \\ \vdots \\ w^m \end{pmatrix}$

$$W_t + \Lambda W_x = 0$$

$$w_t^m + \lambda^m w_x^m = 0$$

λ^m ↑ CONSTANT

SCALAR LINEAR ADVECTION EQUATION

SOLUTION

$$w^m(x,t) = w_o^m(x - \lambda^m t)$$

w^m ARE <u>EIGENWEIGHTS</u>

$$V_1 = w^1 r^1 + w^2 r^2 + \ldots + w^m r^m$$

$$w^1 = l^1 \cdot V_1$$
$$w^2 = l^2 \cdot V_1$$
$$\vdots$$
$$w^m = l^m \cdot V_1$$

SO SOLUTION FOR $V(x,t)$ IS

$$\boxed{V(x,t) = V_o + \sum_{m=1}^{M} w^m(x - \lambda^m t)\, r^m}$$

EXAMPLE: <u>SMOOTH INITIAL CONDITIONS</u>

$$\begin{pmatrix} \rho(x,t=0) \\ v_x(x,t=0) \\ P(x,t=0) \end{pmatrix} = \begin{pmatrix} \rho_o \\ v_{xo} \\ P_o \end{pmatrix} + \begin{pmatrix} \rho_1 \\ v_{x1} \\ P_1 \end{pmatrix} e^{-x^2} = V_o + V_1 e^{-x^2}$$

↑ AMPLITUDE OF SMALL GAUSSIAN FLUCTUATION

WRITE V_1 IN TERMS OF EIGENVECTORS

$$V_1 = w^1 r^1 + w^2 r^2 + w^3 r^3$$

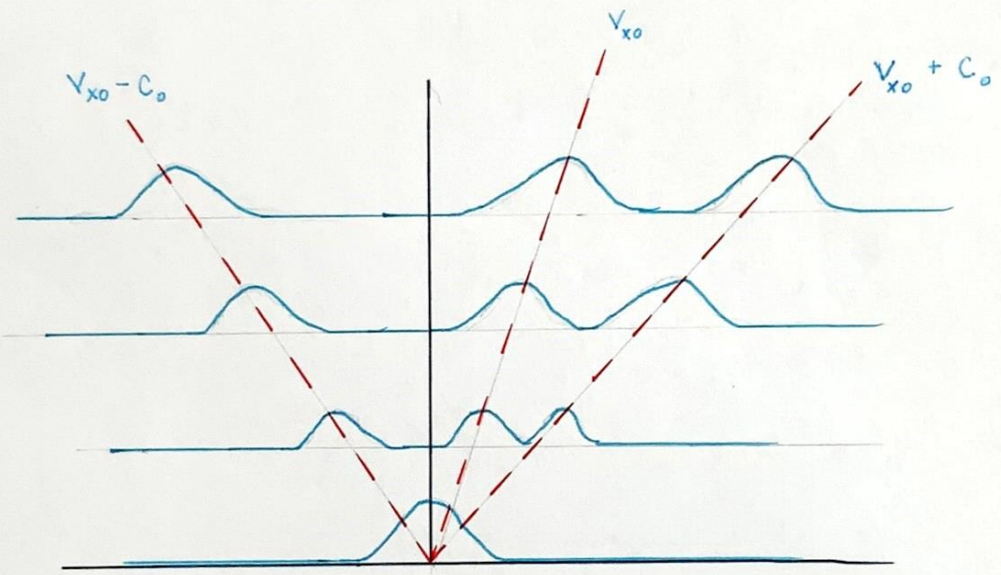
SOLVE FOR EIGENWEIGHTS w^1, w^2, w^3 BY TAKING DOT PRODUCT OF V_1 WITH LEFT EIGENVECTORS

$$w^1 = l^1 \cdot V_1$$
$$w^2 = l^2 \cdot V_1$$
$$w^3 = l^3 \cdot V_1$$

$$\begin{pmatrix} \rho(x,t) \\ v_x(x,t) \\ P(x,t) \end{pmatrix} = \begin{pmatrix} \rho_0 \\ v_{x0} \\ P_0 \end{pmatrix} + w^1 \begin{pmatrix} \rho_0 \\ -c_0 \\ \rho_0 c_0^2 \end{pmatrix} e^{-(x-\lambda_1 t)^2} + w^2 \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} e^{-(x-\lambda_2 t)^2} +$$

$$w^3 \begin{pmatrix} \rho_0 \\ c_0 \\ \rho_0 c_0^2 \end{pmatrix} e^{-(x-\lambda_3 t)^2}$$

INITIAL GAUSSIAN PULSE PROPAGATES AWAY AS 3 GAUSSIAN PULSES WITH AMPLITUDES GIVEN BY EIGENWEIGHTS AND SPEEDS GIVEN BY EIGENVALUES.

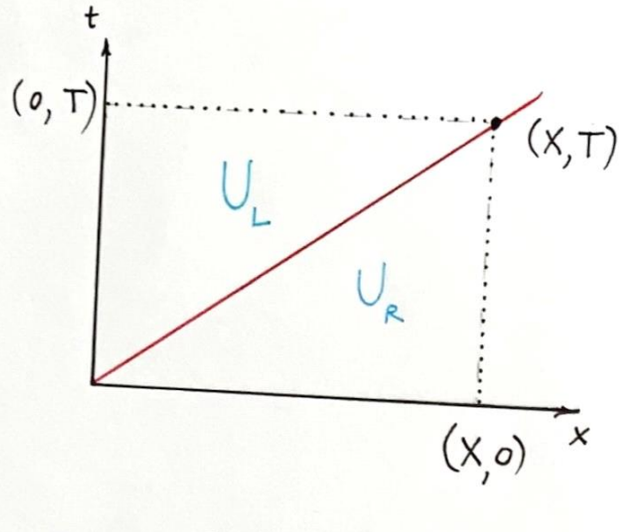


WHAT IF LINEAR HYPERBOLIC PDE HAS DISCONTINUOUS INITIAL DATA?

TAKE AS INITIAL CONDITIONS

$$U_0(x) = \begin{cases} U_L & \text{FOR } x < 0 \\ U_R & \text{FOR } x \geq 0 \end{cases}$$

LET DISCONTINUITY PROPAGATE FROM ORIGIN IN X-DIRECTION SO THAT AT TIME T IT HAS PROPAGATED A DISTANCE X.



INTEGRATE $U_t + AU_x = 0$ OVER RECTANGLE $[0, X]$, $[0, T]$

$$\int_{t=0}^{t=T} \int_{x=0}^{x=X} (U_t + A U_x)\, dx\, dt = 0$$

$$\int_{x=0}^{x=X} \left[U(T) - U(t=0) \right] dx + A \int_{t=0}^{t=T} \left[U(X) - U(x=0) \right] dt = 0$$

$$\int_{x=0}^{x=X} (U_L - U_R)\, dx + A \int_{t=0}^{T} (U_R - U_L)\, dt = 0$$

$$(U_L - U_R) X = -A (U_R - U_L) T$$

REARRANGE $$A (U_R - U_L) = \frac{X}{T} (U_R - U_L)$$

$(U_R - U_L)$ JUMP IS PROPORTIONAL TO AN EIGENVECTOR

$\frac{X}{T}$ SPEED OF DISCONTINUITY IS AN EIGENVALUE λ

SOLUTION

$$U(x,t) = \begin{cases} U_L & x < \lambda t \\ U_R & x \geq \lambda t \end{cases}$$

WHAT OTHER DISCONTINUOUS INITIAL CONDITIONS ARE EASILY SOLVED FOR WITH $U_t + A U_x = 0$?

LET JUMP BETWEEN U_L & U_R BE EXACTLY EQUAL TO SOME SCALAR MULTIPLE OF m^{th} RIGHT EIGENVECTOR

AT $t = 0$

$$U_0(x) = \begin{cases} U_L & \text{FOR} \quad x < 0 \\ U_R = U_L + w^m r^m & \text{FOR} \quad x \geq 0 \end{cases}$$

w^m: EIGENWEIGHT, r^m: EIGENVECTOR

TO FIND TIME EVOLUTION, INTEGRATE $U_t + A U_x = 0$

$$A(U_R - U_L) = \frac{X}{T}(U_R - U_L)$$

$$A(U_L + w^m r^m - U_L) = A w^m r^m = \lambda^m w^m r^m$$

SOLUTION

$$U(x,t) = \begin{cases} U_L & \text{FOR} \quad x < \lambda^m t \\ U_R = U_L + w^m r^m & \text{FOR} \quad x \geq \lambda^m t \end{cases}$$

WHAT HAPPENS IF LEFT AND RIGHT STATES ARE CHOSEN RANDOMLY ?

RIEMANN PROBLEM

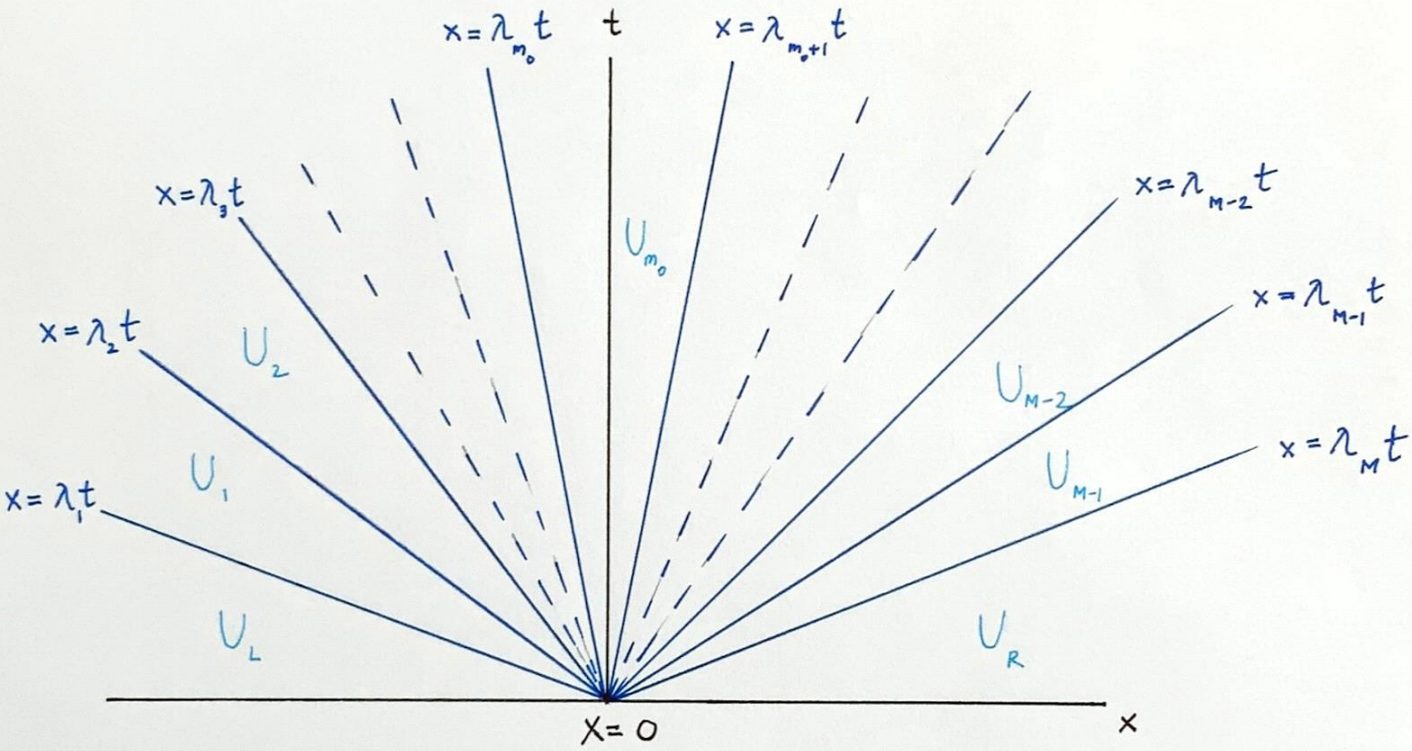
IF HAVE A COMPLETE SET OF EIGENVECTORS THEN CAN EXPRESS $U_R - U_L$ AS A LINEAR COMBINATION OF THE EIGENVECTORS

$$U_R - U_L = \sum_{m=1}^{M} w^m r^m$$

WHERE

$$w^m = l^m \cdot (U_R - U_L)$$

EACH JUMP BY $w^m r^m$ INTRODUCES ANOTHER SIMPLE WAVE MOVING AT CHARACTERISTIC SPEED λ^m.



RIEMANN FAN

THERE IS A SET OF M-1 CONSTANT STATES $\{U_1, U_2, \ldots, U_m, \ldots U_{M-1}\}$ BETWEEN U_L AND U_R

WHERE U_m LIES IN REGION BOUNDED BY $\lambda_m t < x < \lambda_{m+1} t$

SOLUTION CONSISTS OF M SIMPLE WAVES SEPARATED BY M CONSTANT STATES LYING BETWEEN U_L AND U_R.

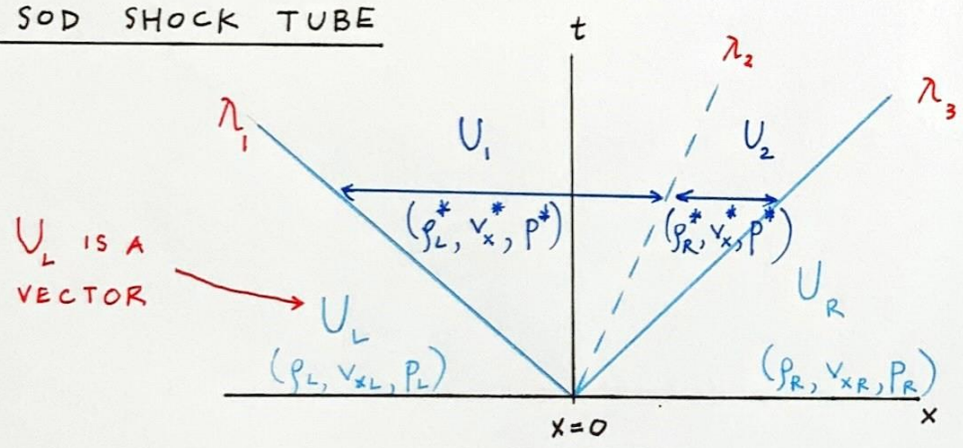
SOLUTION

$$U(x,t) = \begin{cases} U_L & \text{FOR } x/t < \lambda_1 \\ U_m = U_L + \sum_{p=1}^{m} w^p r^p & \text{FOR } \lambda_m < x/t < \lambda_{m+1},\ m = 1,\dots,M-1 \\ U_R & \text{FOR } x/t > \lambda_M \end{cases}$$

NOTE: U_m CAN BE OBTAINED BY STARTING FROM U_L AND SEQUENTIALLY ADDING CONTRIBUTIONS OF RIGHT EIGENVECTORS $w^p r^p$ WITH $p \leq m$.

CROSSING CHARACTERISTIC CURVE ASSOCIATED WITH EACH SIMPLE WAVE ADDS THE CONTRIBUTION OF THAT SIMPLE WAVE TO THE SOLUTION.

1D SOD SHOCK TUBE



$$U(x,t) = \begin{cases} U_L & \text{FOR } x/t < \lambda_1 \\ U_1 = U_L + w^1 r^1 & \text{FOR } \lambda_1 < x/t < \lambda_2 \\ U_2 = U_L + w^1 r^1 + w^2 r^2 & \text{FOR } \lambda_2 < x/t < \lambda_3 \\ U_R = U_L + w^1 r^1 + w^2 r^2 + w^3 r^3 & \text{FOR } x/t > \lambda_3 \end{cases}$$