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Content

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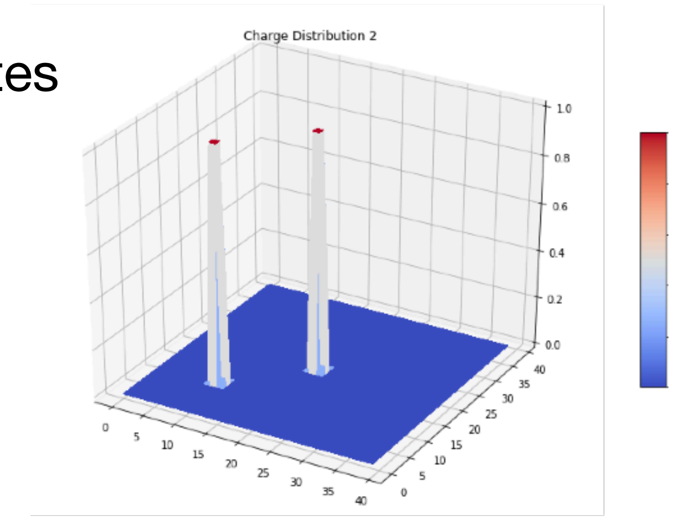
Partial differential equations

1st, 2nd derivatives of spatial and time coordinates



- Poisson equation

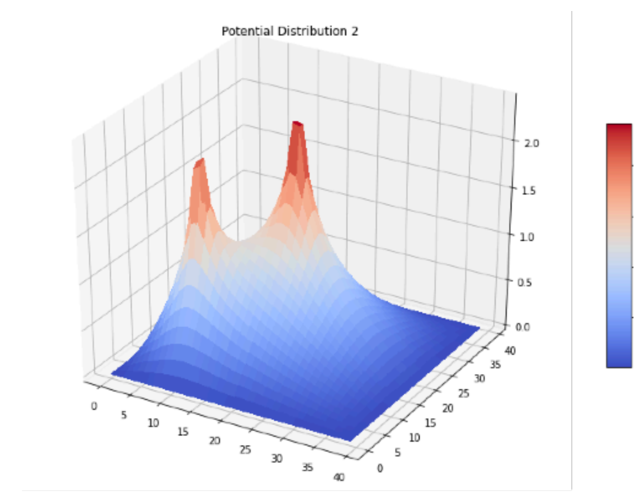
$$\Delta\phi(\vec{r}) = -\frac{1}{\epsilon_0}\rho(\vec{r})$$

Laplacian $\Delta = \sum_{i=1}^{d} \frac{\partial^2}{\partial x_i^2}$

$\rho(\vec{r})$ charge density inside domain V

$\phi(\vec{r})$ electrostatic potential

elliptic PDE



Dirichlet boundary condition $\phi(\vec{r}), \vec{r} \in \partial V$

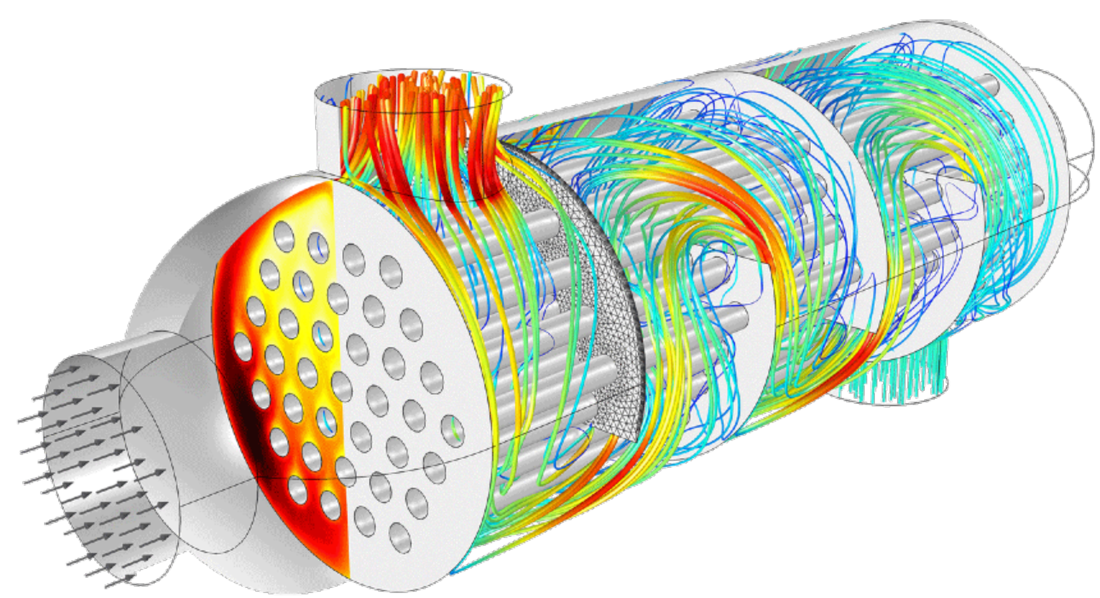
Neumann boundary condition $(\vec{n} \cdot \vec{\nabla})\phi(\vec{r}), \vec{r} \in \partial V$

- Diffusion equation

$$\frac{\partial u(\vec{r},t)}{\partial t} - D\Delta u(\vec{r},t) = S(\vec{r},t)$$

$u(\vec{r},t)$ concentration of a substance at position $\vec{r}$ and time t

$S(\vec{r},t)$ source/drain D diffusion coefficient



parabolic PDE asymmetrical under time-reversal $t \to -t$

Cauchy initial value problem $u(\vec{r}, t=0)$ on domain V

Neumann boundary condition $(\vec{n} \cdot \vec{\nabla})u(\vec{r}) = 0\,, \vec{r} \in \partial V$

Initial configuration must be consistent with the boundary condition

- Wave equation $$\frac{1}{c^2}\frac{\partial^2 u(\vec{r},t)}{\partial t^2} - \Delta u(\vec{r},t) = S(\vec{r},t)$$

c wave velocity

Hyperbolic PDE symmetrical under time-reversal $t \to -t$

initial value problem $u(\vec{r}, t=0), \frac{\partial u(\vec{r},t)}{\partial t}|_{t=0}$

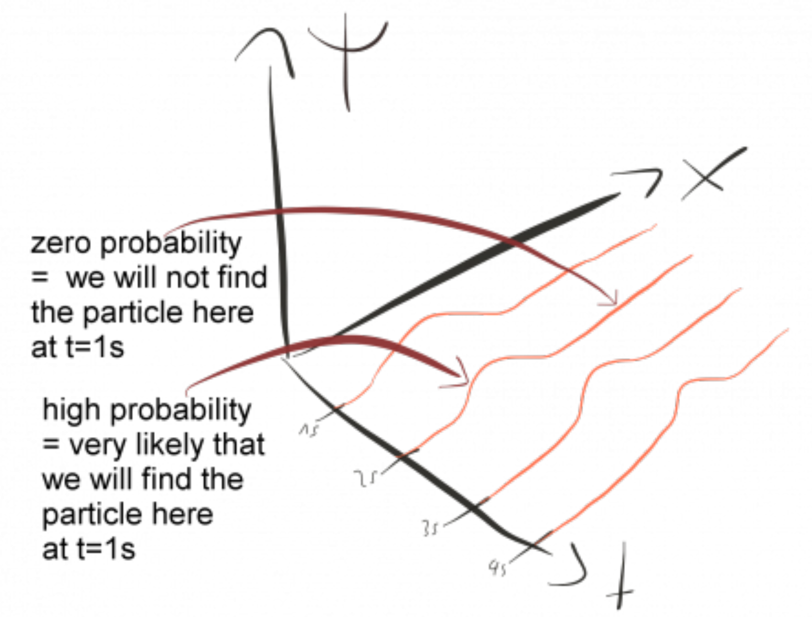
Initial configuration must be consistent with the boundary condition

浮世绘，葛饰北斋，神奈川冲浪里

- Schrödinger equation $$i\hbar\frac{\partial \Psi(\vec{r},t)}{\partial t} = H\Psi(\vec{r},t)$$

For free particle $H = -\frac{\hbar^2}{2m}\Delta$

diffusion equation in imaginary time

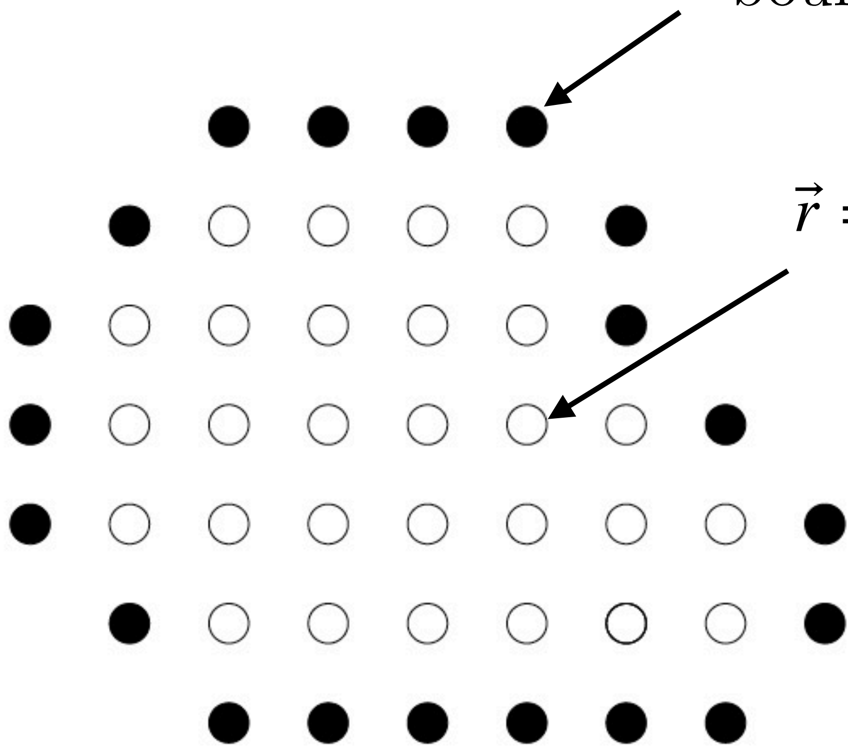


Animating Schrödinger's Equation

- Fluid Dynamics, Navier-Stokes equation

https://www.youtube.com/watch?v=Xj9PdeY64rA

Discretization



$\overrightarrow{e}_i, i = 1, \cdots, d$ unit vectors of a d-dimensional hyper cubic lattice

$$\vec{r} = \sum_{i=1}^{d=2} h_i r_i \overrightarrow{e}_i = \sum_{i=1}^{d=2} r_i \overrightarrow{e}_i$$

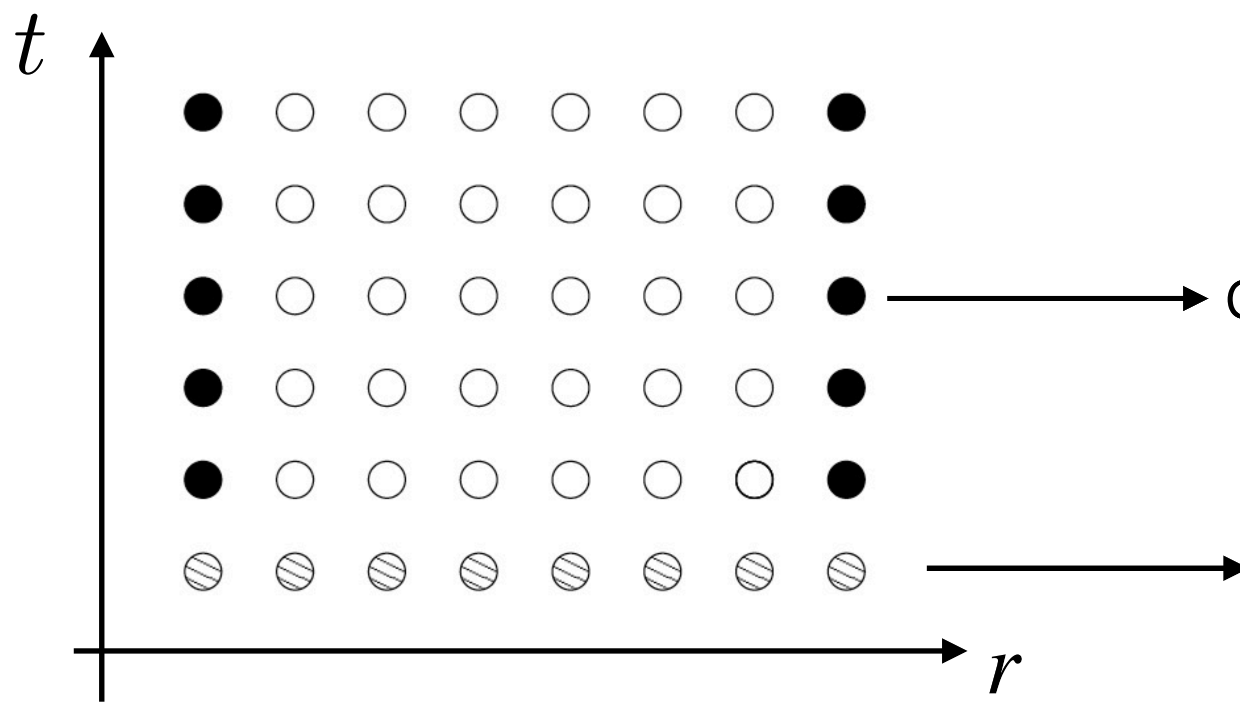
$h_i = h = 1$ lattice spacing

r_i defines the domain V

$$t_n = n\tau, n = 0, 1, 2, \cdots$$

$$u(\vec{r}, t) \rightarrow u(\vec{r}_i, t_n)$$

Discretisation of space-time domain



$$u(\vec{r}, t = 0), \frac{\partial u(\vec{r}, t)}{\partial t}\Big|_{t=0}$$

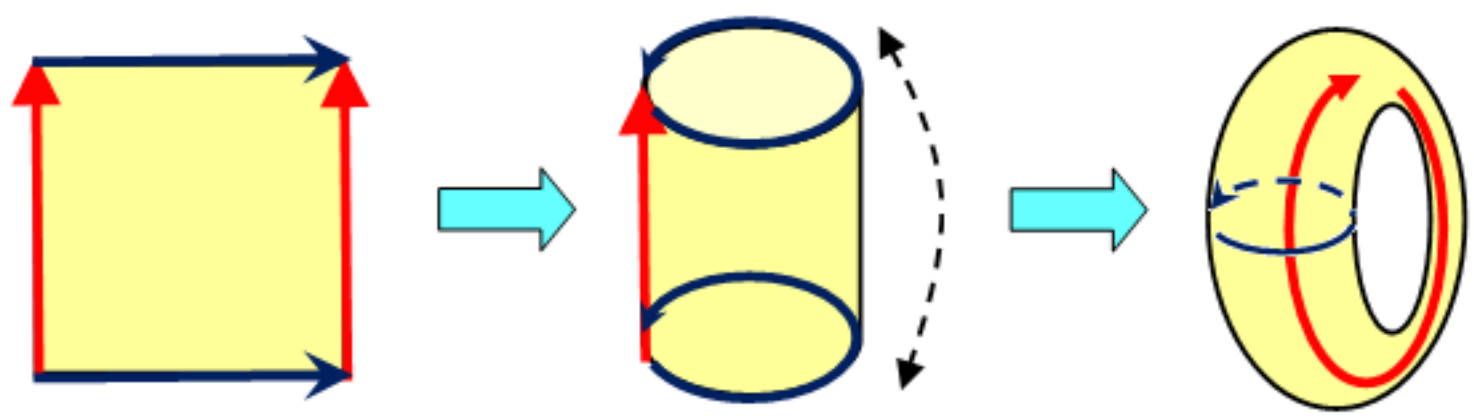
Forward time (FT) discretisation
$$\frac{\partial u(\vec{r}, t_n)}{\partial t} \rightarrow \frac{u(\vec{r}, t_{n+1}) - u(\vec{r}, t_n)}{\tau} + O(\tau)$$

Centered space (CS) discretisation
$$\frac{\partial u(\vec{r}, t_n)}{\partial x_i} \rightarrow \frac{u(\vec{r} + h_i \vec{e}_i, t_n) - u(\vec{r} - h_i \vec{e}_i, t_n)}{2h_i} + O(h)$$

$$\frac{\partial^2 u(\vec{r}, t_n)}{\partial x_i^2} \rightarrow \frac{u(\vec{r} + h_i \vec{e}_i, t_n) + u(\vec{r} - h_i \vec{e}_i, t_n) - 2u(\vec{r}, t_n)}{h_i^2} + O(h^2)$$

Boundary conditions

Periodic boundary conditions (PBC) $u(\vec{r} + N_i h_i \vec{e}_i) = u(\vec{r})$



1d ring
2d torus (donut)
higher-d tori

Hyperbolic PDEs

Wave equation

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

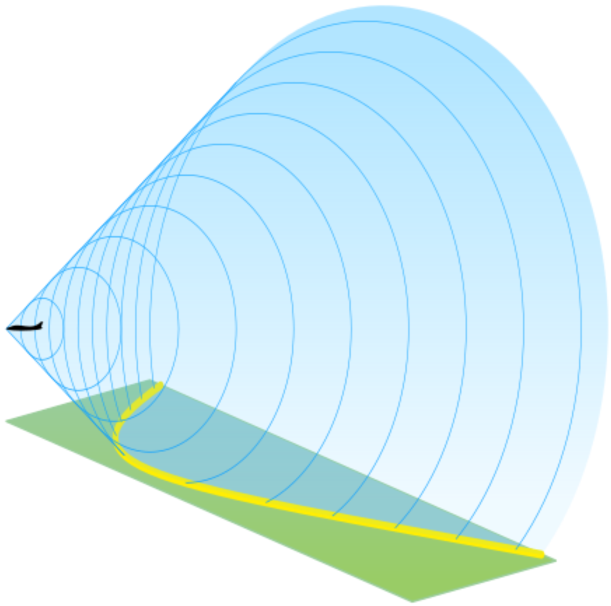
Advection equation

$$\frac{\partial u}{\partial t} = - c \frac{\partial u}{\partial x}$$

Evolution of passive field $u(t, x)$

https://en.wikipedia.org/wiki/Advection

Mach wave (shock wave)



Traffic jam

Watch these

https://www.youtube.com/watch?v=6ZC9h8jgSj4

https://www.youtube.com/watch?v=goVjVVaLe10

FTCS schemes wouldn't work

$$\frac{u(n+1,r)-u(n,r)}{\tau} = -c\frac{u(n,r+1)-u(n,r-1)}{2h}$$

$$u(n+1,r) = u(n,r) - \frac{c\tau}{2h}(u(n,r+1)-u(n,r-1))$$

von Neumann stability analysis $\quad u(n,r) = A^n e^{ikrh}$

$$A = 1 - \frac{c\tau}{2h}(e^{ikh}-e^{-ikh}) = 1 - i\frac{c\tau}{h}\sin(kh)$$

FTCS is unstable for hyperbolic equations

$$|A| = \sqrt{1+(\frac{c\tau}{h})^2\sin^2(kh)} > 1$$

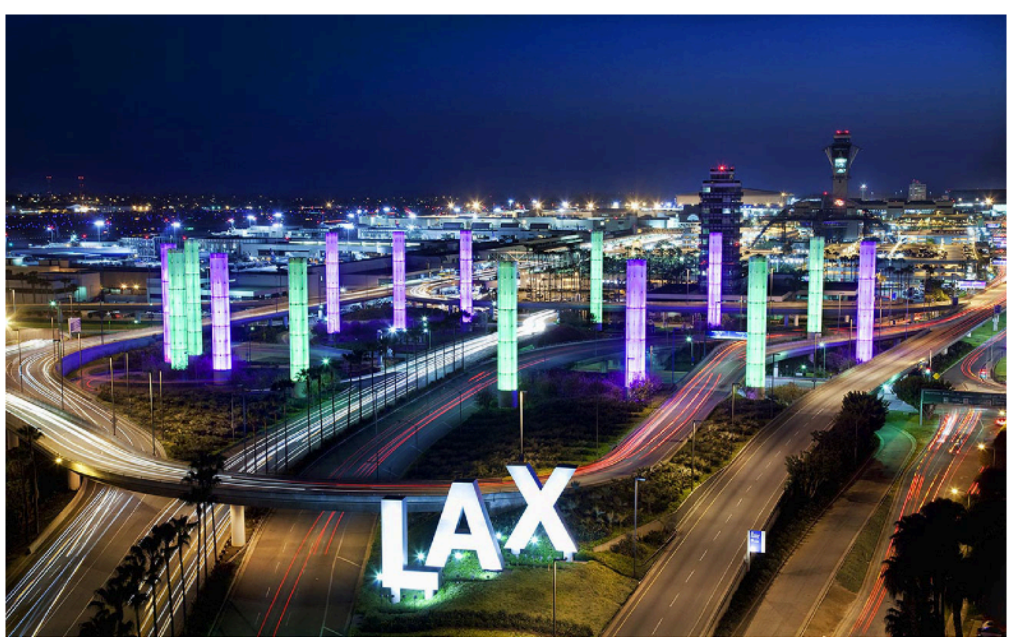
Is FTFS Stable ? $\quad \frac{u(n+1,r)-u(n,r)}{\tau} = -c\frac{u(n,r+1)-u(n,r)}{h}$

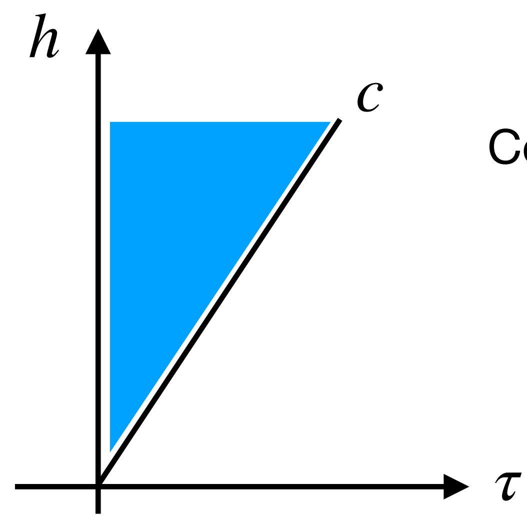
Lax method

$$u(n+1,r) = \frac{1}{2}(u(n,r+1)+u(n,r-1)) - \frac{c\tau}{2h}(u(n,r+1)-u(n,r-1))$$

$$A = \cos(kh) - i\frac{c\tau}{h}\sin(kh)$$

$$|A| = \sqrt{\cos^2(kh)+(\frac{c\tau}{h})^2\sin^2(kh)}$$





Courant-Friedrichs-Lewy (CFL) stability criterion

$$\frac{c\tau}{h} \leq 1 \qquad \frac{h}{\tau} \geq c$$

Numerical information flow is within the physical information flow

Differencing PDE
an art as much as a science

$$u(n+1,r) = \frac{1}{2}(u(n,r+1)+u(n,r-1)) - \frac{c\tau}{2h}(u(n,r+1)-u(n,r-1))$$

Equals to
$$\frac{u(n+1,r)-u(n,r)}{\tau} = -c\frac{u(n,r+1)-u(n,r-1)}{2h} + \frac{u(n,r+1)-2u(n,r)+u(n,r-1)}{2\tau}$$

Equals to FTCS of
$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \underline{\frac{h^2}{2\tau}\Delta u}$$
artificial dissipation term, suppress the unstable modes

$$|A|^2 = \cos^2(kh) + (\frac{c\tau}{h})^2\sin^2(kh)$$

$kh \ll 1, |A|^2 \approx 1$ longwavelength mode conserved

$kh \sim 1, |A|^2 < 1$ shortwavelength mode damped

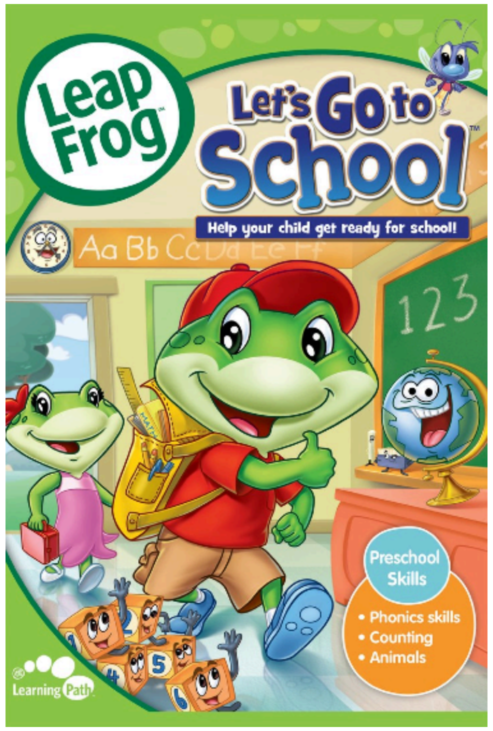
Exactly at the Courant-Friedrichs-Lewy (CFL) stability criterion $c\tau = h$ Lax becomes $u(n+1,r) = u(n,r-1)$

FTCS and Lax are all 1st order accuracy in τ

Leap-Frog method

is of 2nd order accuracy in τ

$$\frac{\partial u}{\partial t} = -\frac{\partial F(u)}{\partial x}$$
$F(u) = cu$ for advection equation



CTCS
$$\frac{u(n+1,r)-u(n-1,r)}{\tau} = -\frac{F(n,r+1)-F(n,r-1)}{h}$$

$$u(n+1,r) = u(n-1,r) - \frac{\tau}{h}(F(n,r+1)-F(n,r-1))$$

Not self-starting, use Lax to start

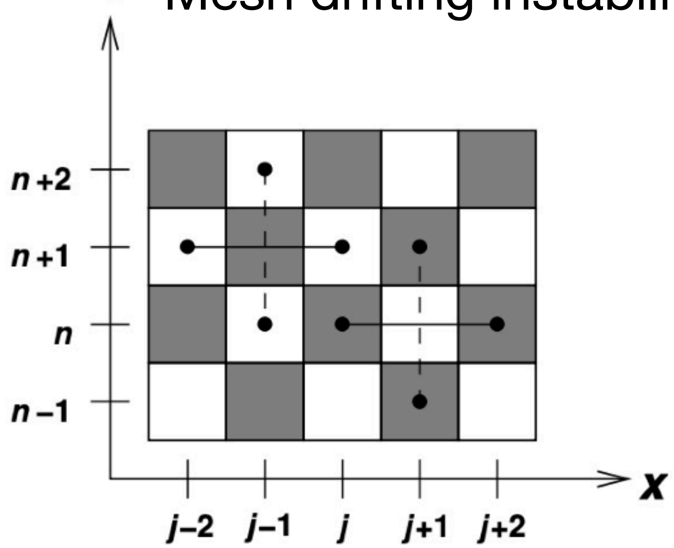
Leap-Frog method

$$A^2 = 1 - 2iA\frac{c\tau}{h}\sin(kh) \qquad A = -i\frac{c\tau}{h}\sin(kh) \pm \sqrt{1 - (\frac{c\tau}{h}\sin(hk))^2}$$

Performing von Neumann stability analysis on Leap-Frog, stable when $c\tau/h \leq 1$

$|A|^2 = 1 \qquad c\tau/h \leq 1$ No amplitude dissipation (can you see this ?)

t Mesh drifting instability



introduce artificial dissipation to couples the sublattices

Chap.20.1.

http://numerical.recipes/book/book.html

Lax-Wendroff method

$$\frac{\partial u}{\partial t} = -\frac{\partial F(u)}{\partial x}$$

Taylor expansion of $u(x, t)$ in t

$$u(t+\tau, x) = u(t, x) + \tau\frac{\partial u(x,t)}{\partial t} + \frac{\tau^2}{2}\frac{\partial^2 u(t,x)}{\partial t^2} + O(\tau^3)$$

$$= u(t,x) - \tau\frac{\partial}{\partial x}F(t,x) + \frac{\tau^2}{2}(\frac{\partial}{\partial x}[F'\frac{\partial F}{\partial x}](t,x))$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\frac{\partial u}{\partial t} = -\frac{\partial}{\partial t}\frac{\partial}{\partial x}F = -\frac{\partial}{\partial x}\frac{\partial}{\partial t}F \qquad \frac{\partial F}{\partial t} = \frac{dF}{du}\frac{\partial u}{\partial t} = F'\frac{\partial u}{\partial t} = -F'\frac{\partial F}{\partial x}$$

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}[F'\frac{\partial F}{\partial x}]$$

$F(u)$ only depends on u

Lax-Wendroff method

$$u(n+1,r) = u(n,r) - \tau \frac{F(n,r+1) - F(n,r-1)}{2h} + \frac{\tau^2}{2}\left(\frac{[F' \frac{\partial F}{\partial x}](n,r+1/2) - [F' \frac{\partial F}{\partial x}](n,r-1/2)}{h}\right)$$

$$= u(n,r) - \tau \frac{F(n,r+1) - F(n,r-1)}{2h} + \frac{\tau^2}{2h}\left(F'(n,r+1/2)\frac{F(n,r+1) - F(n,r)}{h} - F'(n,r-1/2)\frac{F(n,r) - F(n,r-1)}{h}\right)$$

where $F'(n,r \pm 1/2) = F'\left(\frac{u(n,r\pm 1) + u(n,r)}{2}\right)$

For advection equation $F(u) = cu \qquad F'(u) = c$

$$u(n+1,r) = u(n,r) - \frac{c\tau}{2h}(u(n,r+1) - u(n,r-1)) + \frac{c^2\tau^2}{2h^2}(u(n,r+1) + u(n,r-1) - 2u(n,r))$$

Performing von Neumann stability analysis on Lax-Wendroff, obtain CFL $c\tau/h \le 1$

$$A = 1 - i\frac{c\tau}{h}\sin(kh) - \left(\frac{c\tau}{h}\right)^2(1-\cos(kh))$$

$$|A|^2 = 1 - \left(\frac{c\tau}{h}\right)^2\left(1 - \left(\frac{c\tau}{h}\right)^2\right)(1-\cos(kh))^2$$

$kh \ll 1 \qquad |A|^2 = 1 - \left(\frac{c\tau}{h}\right)^2\left(1 - \left(\frac{c\tau}{h}\right)^2\right)\frac{(kh)^4}{4} + \cdots$

(can you see these ?)

Damping is smaller than in the Lax method $|A|^2 = 1 - \left(1 - \left(\frac{c\tau}{h}\right)^2\right)(kh)^2 + \cdots$

At the CFL stability threshold $c\tau/h = 1$ Lax-Wendroff becomes $u(n+1,r) = u(n,r-1)$

Physics of Traffic flow

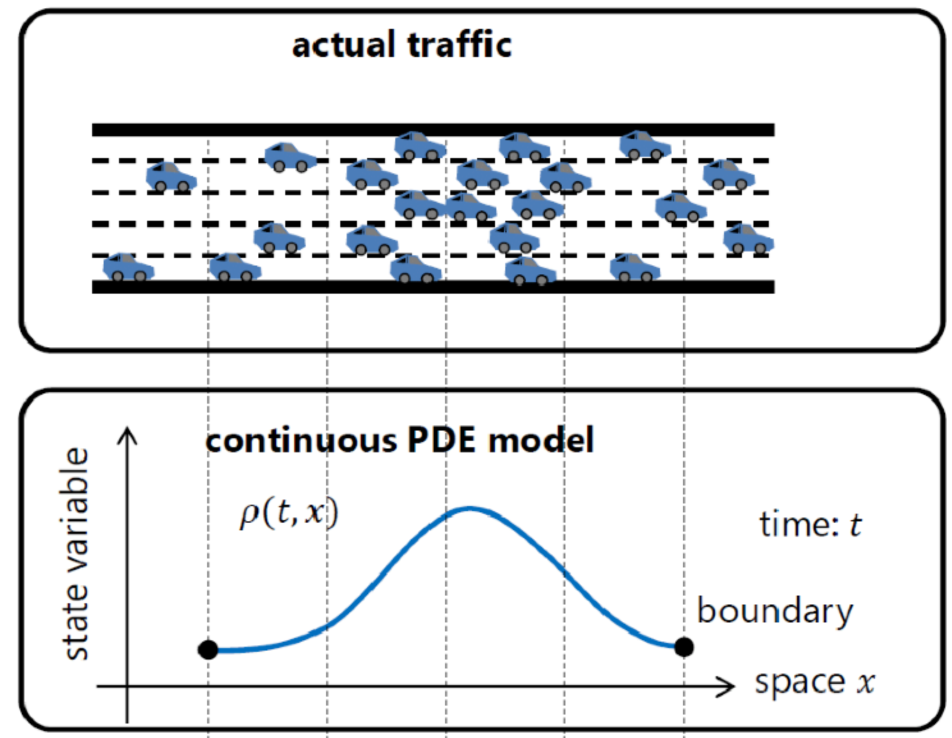
Number of vehicles

$$N(t,x_1,x_2) = \int_{x_1}^{x_2} \rho(t,x)dx$$

$$\frac{d}{dt}N(t,x_1,x_2) = \frac{d}{dt}\int_{x_1}^{x_2} \rho(t,x)dx = \int_{x_1}^{x_2} \frac{\partial \rho(t,x)}{\partial t}dx = -F(t,x_2) + F(t,x_1)$$

Traffic density $\rho(t,x)$

Traffic Flux $F(t,x)$



Equation of continuity $$\frac{\partial \rho}{\partial t} + \frac{\partial F}{\partial x} = 0$$

Local velocity of the vehicles $$v(t,x) = \frac{F(t,x)}{\rho(t,x)}$$

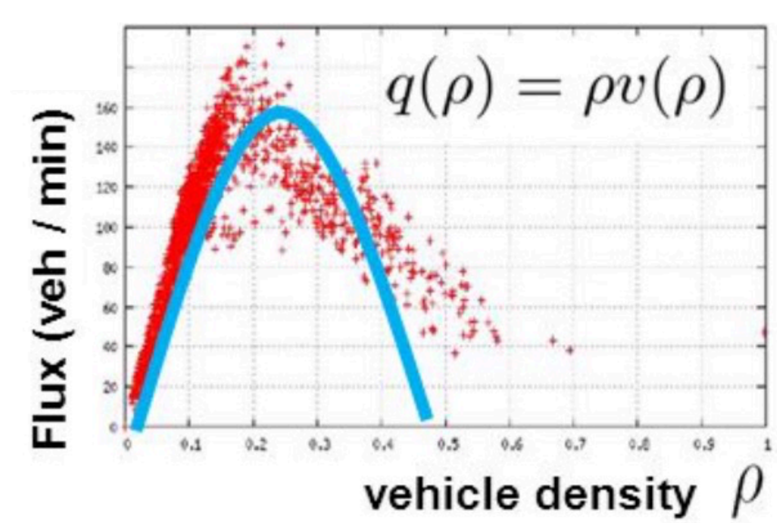
Lighthill and Whitham (1955)

Local flux depends on local density $F(t,x) = F(\rho(t,x))$

$$F(\rho) = 4F_{\max}[\frac{\rho}{\rho_{\max}} - (\frac{\rho}{\rho_{\max}})^2]$$

$\rho_{\max} = 100$ **vehicles/km**

$F_{\max} = 3000$ **vehicles/h**



$$v(\rho) = \frac{F(\rho)}{\rho} = \underbrace{\frac{4F_{\max}}{\rho_{\max}}}_{v_{\max}=120} (1 - \frac{\rho}{\rho_{\max}})$$

$v_{\max}=120$ **km/h**

Increasing the density, the velocity decreases linearly
Until vanishes at $\rho = \rho_{\max}$ (bumper-to-bumper)

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F(\rho)}{\partial x}$$

density wave in the vehicle density: kinematic waves

$$F(\rho) = 4F_{\max}\left[\frac{\rho}{\rho_{\max}} - \left(\frac{\rho}{\rho_{\max}}\right)^2\right]$$

$$\frac{\partial \rho}{\partial t} = -\frac{dF(\rho)}{d\rho}\frac{\partial \rho}{\partial x}$$

$$c(\rho) = v_{\max}\left(1 - \frac{2\rho}{\rho_{\max}}\right)$$

$$v(\rho) = \frac{F(\rho)}{\rho} = \underbrace{\frac{4F_{\max}}{\rho_{\max}}}_{v_{\max}=120\ \text{km/h}}\left(1 - \frac{\rho}{\rho_{\max}}\right)$$

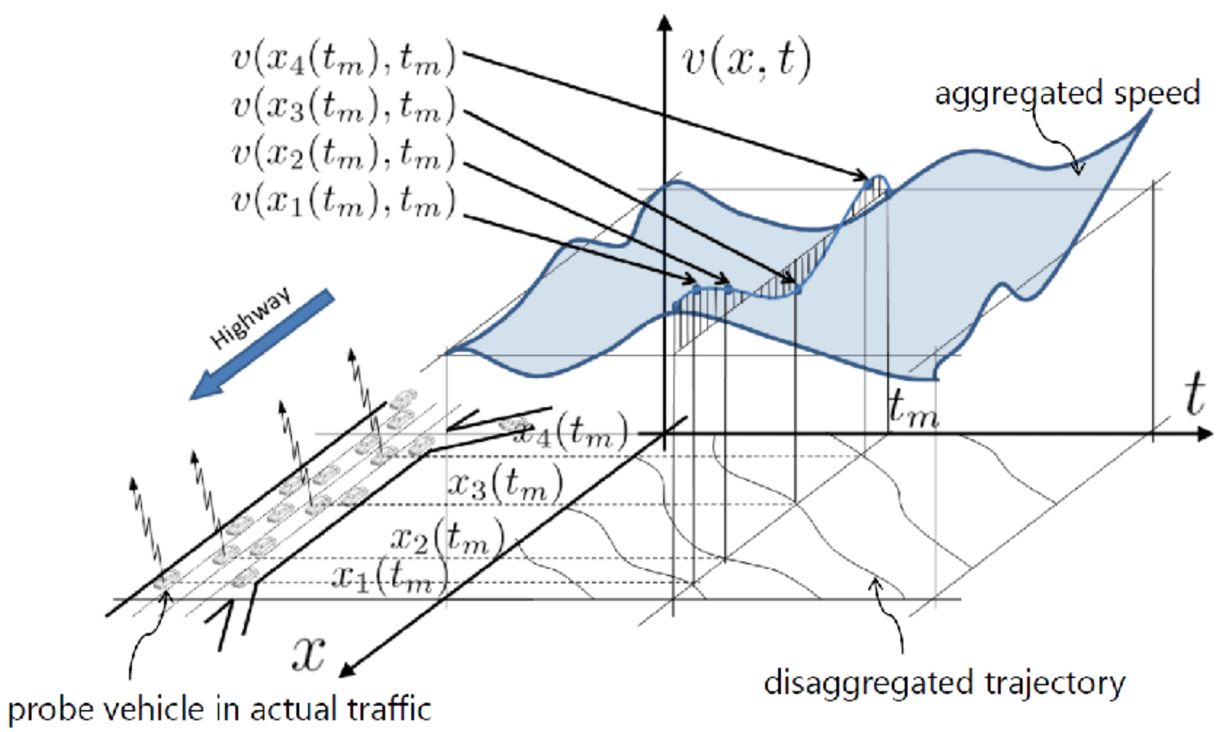
$$= -\frac{d(\rho v(\rho))}{d\rho}\frac{\partial \rho}{\partial x}$$

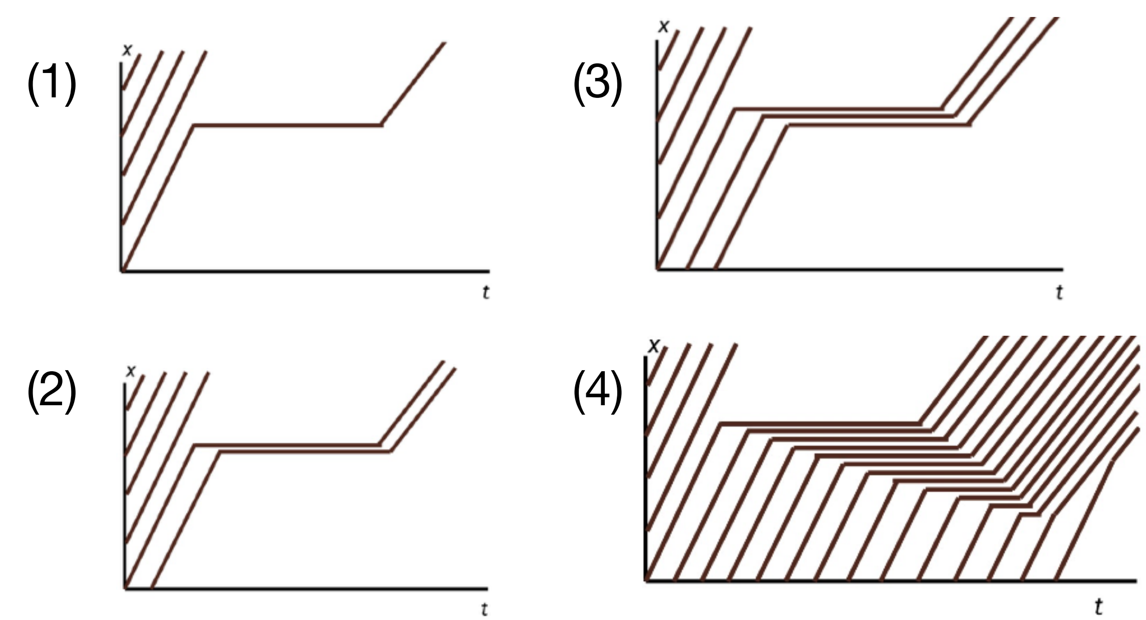
$$= -\left(v(\rho) + \rho\underbrace{\frac{dv(\rho)}{d\rho}}_{-\frac{v_{\max}}{\rho_{\max}} < 0}\right)\frac{\partial \rho}{\partial x}$$

$\rho < \rho_{\max}/2$ low traffic densities, $c(\rho) > 0$ vehicle density move to right

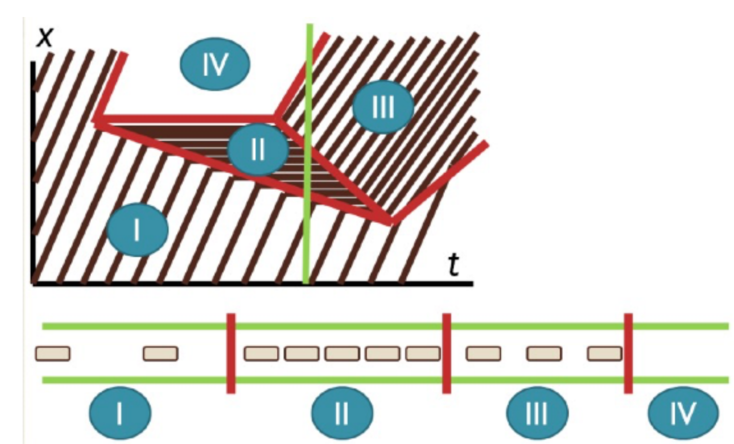
$\rho > \rho_{\max}/2$ high traffic densities, $c(\rho) < 0$ vehicle density move to left

$\rho = \rho_{\max}/2$ medium traffic density, $c(\rho) = 0$ vehicle density stationary



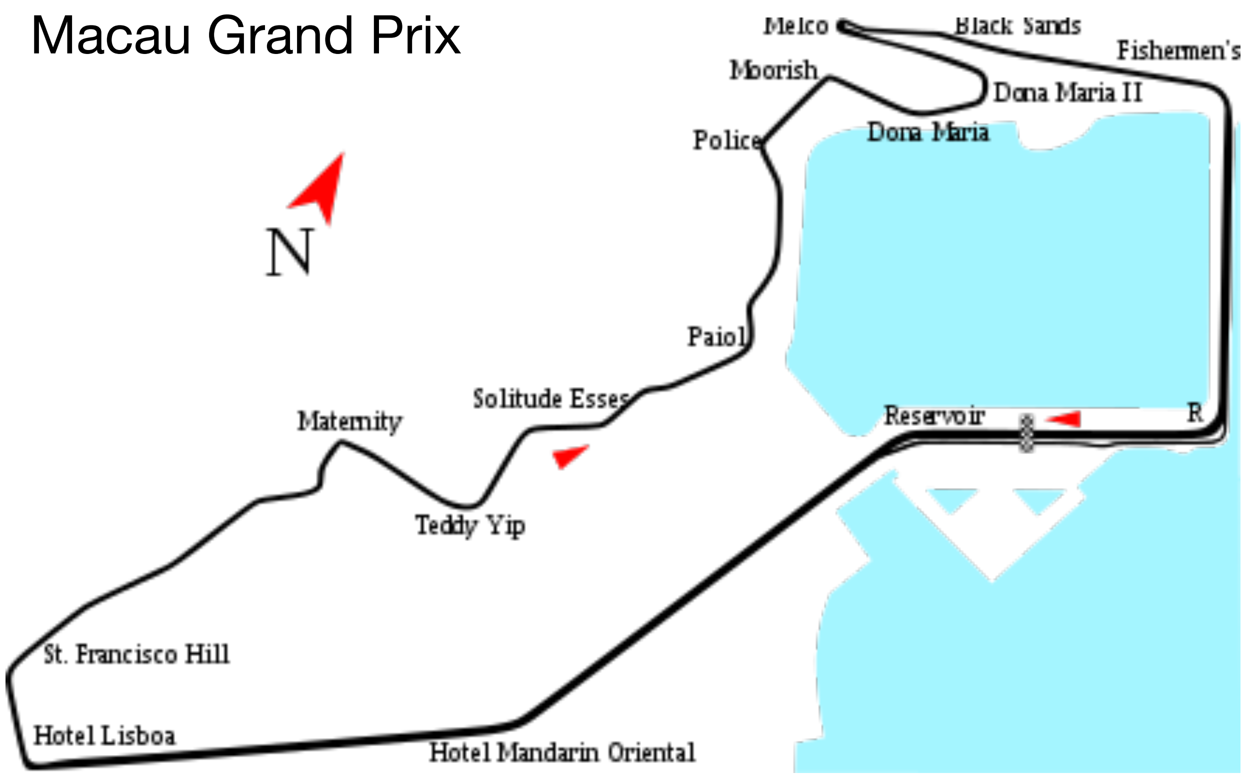


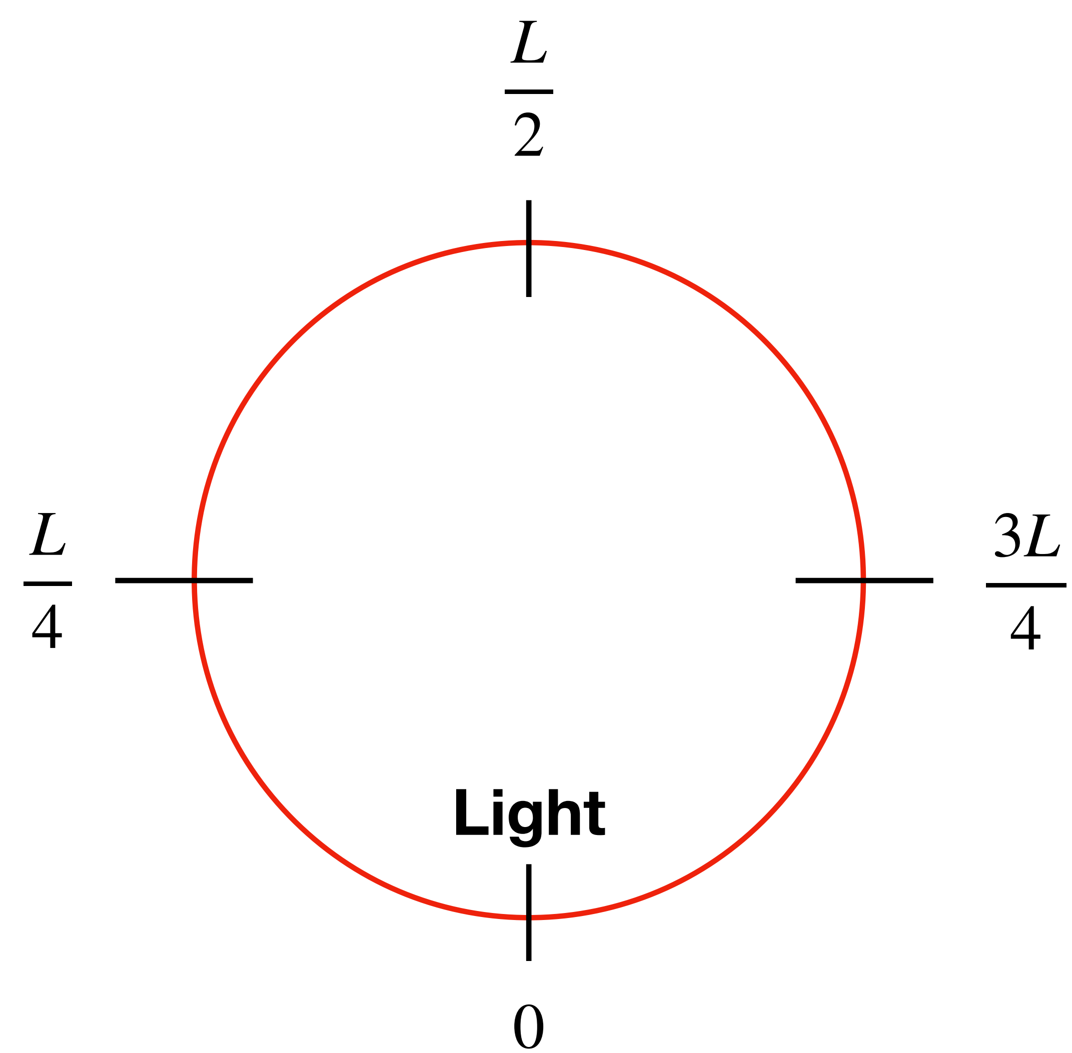
Traffic jam = shock wave



Traffic light simulation Ring-road with circumference L

Macau Grand Prix





$$F(\rho) = v(\rho)\rho = v_{\max}(1 - \frac{\rho}{\rho_{\max}})\rho$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial F(\rho)}{\partial x}$$

$$\rho(t=0,x) = \begin{cases} \rho_{max}, 0 < x < \frac{2L}{3} \\ 0, else \end{cases}$$

$L = 400\, m$

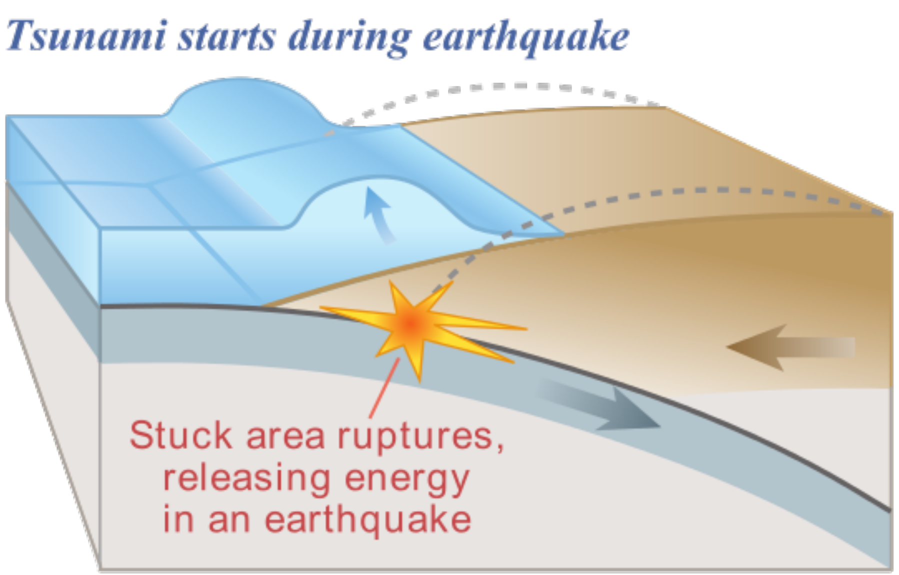
$h = 1\, m$

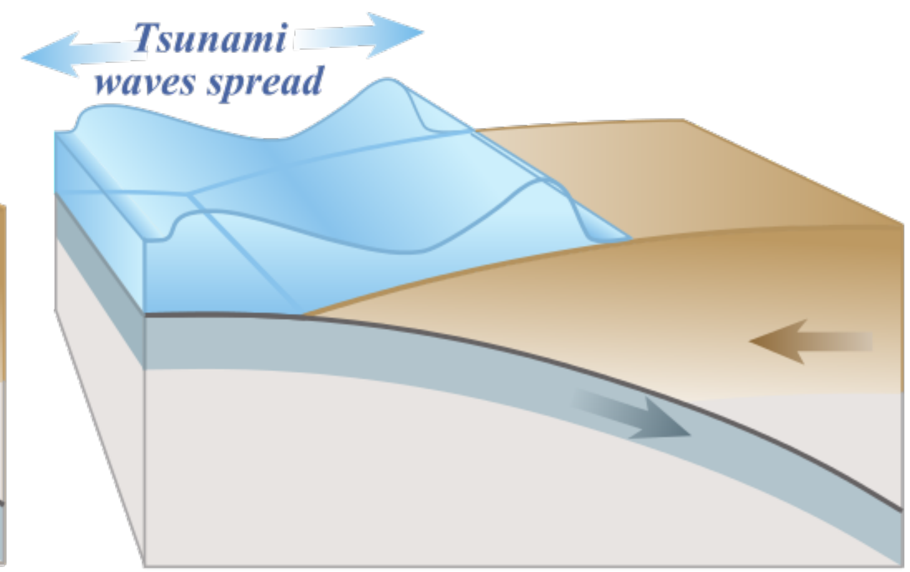
$\rho_{\max} = 1$

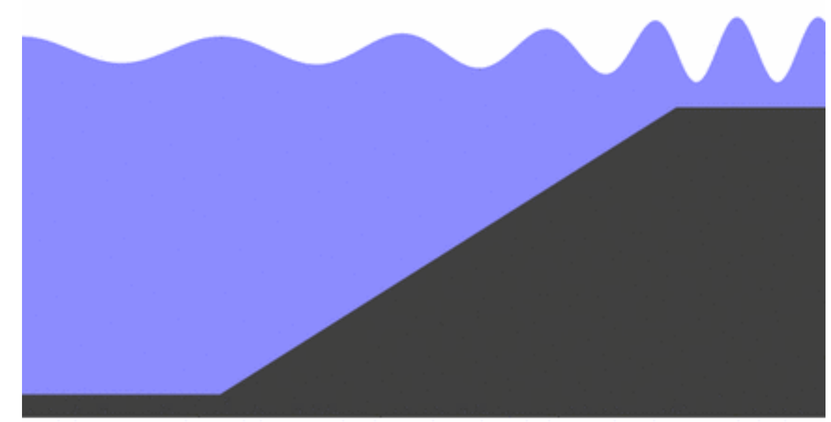
$\tau = h/v_{\max} = 1/33\, s$

$v_{\max} = 33\, m/s$

Physics of Tsunami waves







Watch the 3D animation https://en.wikipedia.org/wiki/Tsunami

- caused by submarine earthquake, vertical shift of a whole water column (~ 1 m)
- Reaching the shall shore of the ocean, the wave slows down, but the amplitude increases (~ 10 m)

https://en.wikipedia.org/wiki/Viscosity

equ. continuity $$\frac{\partial \rho}{\partial t} + \nabla \cdot \underbrace{(\rho \vec{v})}_{flux} = 0$$

volume viscosity

shear viscosity

Navier-Stokes equ. $$\frac{d}{dt}\vec{v} = \frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} = \frac{\vec{f}}{\rho} - \frac{1}{\rho}\nabla P + \frac{\zeta + \frac{1}{3}\eta}{\rho}\nabla(\nabla \cdot \vec{v}) + \eta \Delta \vec{v}$$

$$\zeta = \eta = 0$$

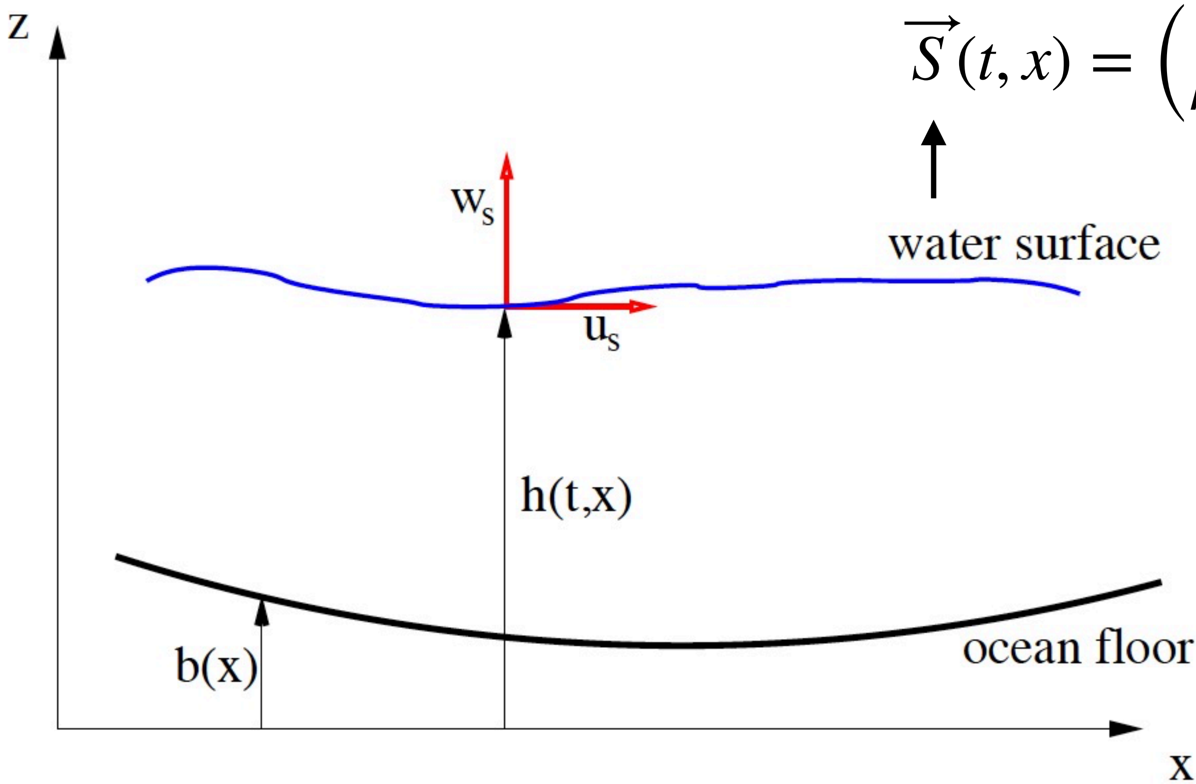
ρ const $$\frac{\partial \rho}{\partial t} = 0$$

$$\begin{pmatrix} 0 \\ 0 \\ -g \end{pmatrix}$$

local pressure

Incompressible, curl-free fluid

local external force density



$$\overrightarrow{S}(t,x) = \begin{pmatrix} x \\ h(t,x) \end{pmatrix}$$

$$\begin{pmatrix} h(t,x) \\ \bar{u}(t,x) \end{pmatrix}$$

Shallow water equations

$$\frac{\partial h(t,x)}{\partial t} + \frac{\partial}{\partial x}((h(t,x) - b(x))\bar{u}(t,x)) = 0$$

$$\frac{\partial \bar{u}(t,x)}{\partial t} + \bar{u}(t,x)\frac{\partial \bar{u}(t,x)}{\partial x} + g\frac{\partial h(x)}{\partial x} = 0$$

$$\overrightarrow{x} = \begin{pmatrix} x \\ z \end{pmatrix} \qquad \overrightarrow{v} = \begin{pmatrix} u \\ w \end{pmatrix}$$

Average horizontal velocity

$$\bar{u}(t,x) = \frac{1}{h(t,x) - b(x)} \int_{b(x)}^{h(t,x)} u(t,x,z)dz$$

C.H. Su and C.S. Gardner J. Math. Phys. 10, 536 (1969)

APPENDIX: DERIVATION OF THE CORRECTION EQUATION TO THE SHALLOW-WATER THEORY

We start with the two-dimensional incompressible inviscid hydrodynamic equations

Navier-Stokes equ. →

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -p_x, \qquad \text{(A1)}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -p_y - g, \qquad \text{(A2)}$$

equ. continuity →

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \qquad \text{(A3)}$$

$$v \rightarrow w \qquad p_x \rightarrow \frac{1}{\rho}\frac{\partial P}{\partial x}$$

In the form of advection equation

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ \bar{u} \end{pmatrix} = -\frac{\partial}{\partial x}\begin{pmatrix} (h-b)\bar{u} \\ \frac{1}{2}\bar{u}^2 + gh \end{pmatrix}$$

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ \bar{u} \\ \bar{v} \end{pmatrix} = -\frac{\partial}{\partial x}\begin{pmatrix} (h-b)\bar{u} \\ \frac{1}{2}\bar{u}^2 + gh \\ \bar{u}\bar{v} \end{pmatrix} - \frac{\partial}{\partial y}\begin{pmatrix} (h-b)\bar{v} \\ \bar{u}\bar{v} \\ \frac{1}{2}\bar{v}^2 + gh \end{pmatrix}$$

$$\frac{\partial}{\partial t}\begin{pmatrix} h \\ \bar{u} \end{pmatrix} = -\frac{\partial}{\partial x}\begin{pmatrix} (h-b)\bar{u} \\ \frac{1}{2}\bar{u}^2 + gh \end{pmatrix}$$

Boundary condition

$$h(t, x = \pm x_0) = 0$$

$$\bar{u}(t, x = \pm x_0) = 0$$

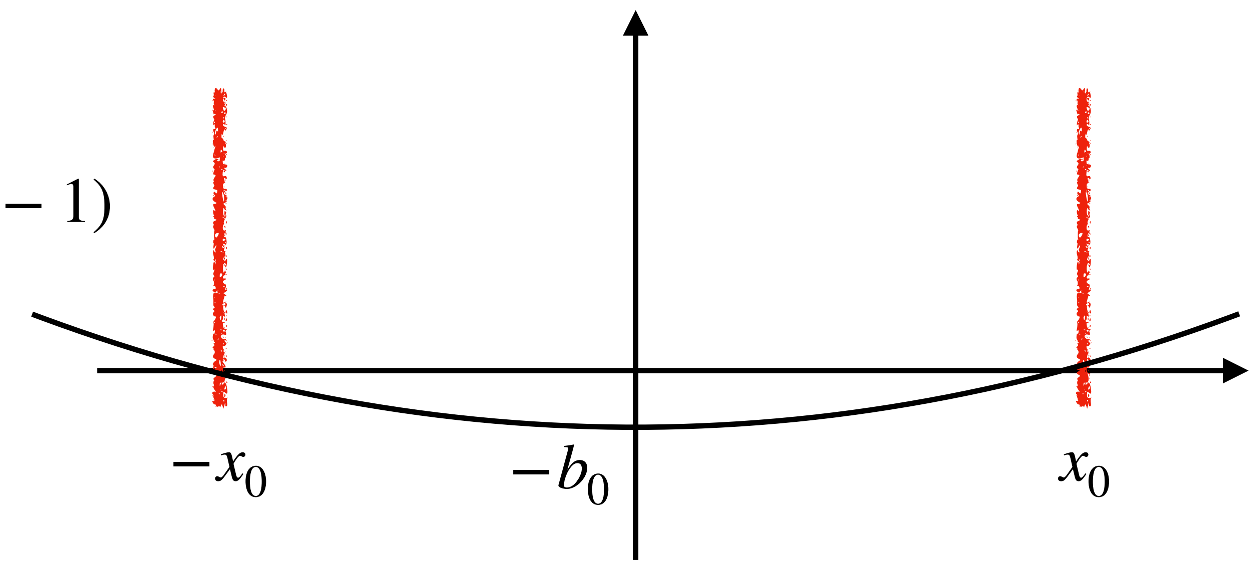
Initial condition: Gaussian

$$h(t=0,x) = h_0 e^{-x^2/D^2}$$

$$\bar{u}(t=0,x) = 0$$

Parabolic ocean floor

$$b(x) = b_0(\frac{x^2}{x_0^2} - 1)$$



$$b_0 = 1\,km \doteq 10$$

$$x_0 = 10\,km \doteq 100$$

$$h_0 = 1\,m \doteq 0.01$$

$$D = 1\,km \doteq 10$$

$$g = 10\,m/s^2 \doteq 0.1$$

$$h = 100\,m \doteq 1$$

$$\tau = 0.3\,s \doteq 0.3$$

Length unit 100 m

Time unit 1 s

$$\frac{\partial u}{\partial t} = -\frac{\partial F(u)}{\partial x}$$

Leap-Frog method is of 2nd order accuracy in τ

$$u(n+1,r) = u(n-1,r) - \frac{\tau}{h}(F(n,r+1) - F(n,r-1))$$

Shallow water equations: derivation

- C.H. Su and C.S. Gardner J. Math. Phys. 10, 536 (1969)

APPENDIX: DERIVATION OF THE CORRECTION EQUATION TO THE SHALLOW-WATER THEORY

We start with the two-dimensional incompressible inviscid hydrodynamic equations

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -p_x, \qquad (A1)$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -p_y - g, \qquad (A2)$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \qquad (A3)$$