[ICP]Introduction to Computational Physics

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1. Random Number Generator

Congruential RNG

$$x_i = (cx_{i-1}) mod\ p$$

maximal period is $p-1$, maximal period reach if $c^{p-1} mod\ p = 1$

Lagged Fibonacci RNG

$$x_{b+1} = (\sum_{j \in \mathcal{J}} x_{b+1-j}) mod\ 2$$
$$j \subset \{1, \cdots, b\}$$

- initial sequence at least c bits
- usually use congruential RNG to obtain seed sequence

When $|j| = 2$

$$x_{i+1} = (x_{i-c} + x_{i-d}) mod\ 2$$
$$c, d \in \{1, \cdots, i-1\}$$

max period: $2^c - 1$

Zierler-Trinomial condition

$1 + z^c + z^d$ cannot be factorized by in subpolynomials, smallest $(c, d) = (250, 103)$

Square/Cubic Test

- square test:(s_i, s_{i+1})
- cubic test: (s_i, s_{i+1}, s_{i+2})

χ^2 test

fluctuation of mean value, mean value should be gaussian

$$\chi^2 = \sum_{i=1}^{k} \frac{N_i - \frac{n}{k}}{\frac{n}{k}}$$

n : number of samples

N_i : count number for each bin

k : number of bins

Monte Carlo

expected error for MC sampling is $\mathcal{O}(\frac{1}{\sqrt{N}})$

error bound in quasi-MC is $\mathcal{O}(\frac{(log\ N)^d}{N})$

D-star Discrepency

$$D_N^* = \underset{0\le v_j\le 1}{max}\left|\frac{1}{N}\sum_{i=1}^{N}\prod_{j=1}^{d}1_{0\le x_j^i\le v_j} - \prod_{j=1}^{d}v_j\right|$$

it measure how dense the points distributed inside a given volume

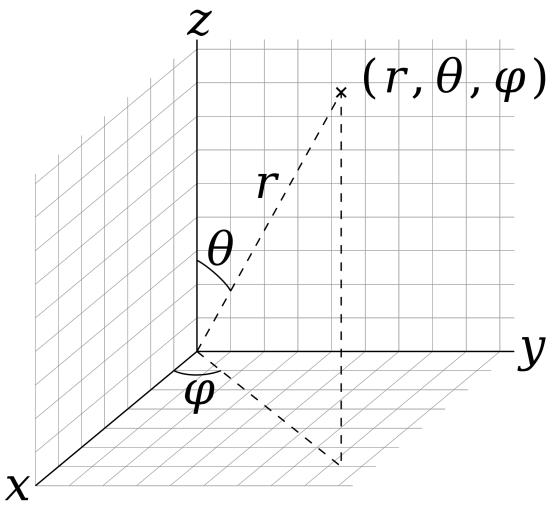
N : number of dataset points $\{x^1, \cdots, x^n\}$

d : dimension of the points

low-discrepancy : $D_N^* \le c(d)\frac{log(N)^d}{N}$

Uniform Sphere Shell

given uniform distribution $X, Y \sim Unif(0,1)$, get 3d sphere uniform distribution



$$\int_0^X\int_0^Y dxdy = \int_0^\Phi\int_0^\Theta \frac{1}{4\pi}sin\theta d\phi d\theta$$

$$\Rightarrow XY = \frac{1}{4\pi}(1-cos\Theta)\Phi$$

let $\Phi = 2\pi X$ then $\Theta = acos(1-2Y)$

$\therefore S \sim [Rsin\Theta cos\Phi, Rsin\Theta sin\Phi, Rcos\Theta]$

Uniform Ellipse

1. rejection sampling, sample $X \sim Unif(-a, a), Y \sim Unif(-b, b)$, accept the points inside ellipse
2. draw $X, Y \sim Unif(0,1)$, $\psi = atan(\frac{b}{a}tan(2\pi X))$, $r = \sqrt{Y}\frac{ab}{\sqrt{(bcos\psi)^2+(a\sin\psi)^2}}$, $E \sim [rcos\psi, rsin\psi]$

Uniform to Gaussian

$$y_1 = \sqrt{-\sigma\, ln(1-z_2)}sin(2\pi z_1)$$
$$y_2 = \sqrt{-\sigma\, ln(1-z_2)}cos(2\pi z_1)$$

using uniform z_1 and z_2 could get two gaussian y_1 and y_2

2. Percolation

- *cirtical point* p_c: occupation probabilty p, a phase transition from non-percolated system to percolated system containing an infinitely-sized cluster
- *percolation strength* β: $P(p \gtrsim p_c) \sim |p - p_c|^{\beta}$, how fast the transition
- *wrapping probability* : $W(p) = \begin{cases} 0 & 0 \leq p < p_c \\ 1 & p_c < p \leq 1 \end{cases}$
- *cluster-size distribution*: $n_s(p) = \lim_{L\to\infty} \frac{N_s(p,L)}{L}$, $N_s(p, L)$ is the number of cluster of size s given occupation probability p and system's side length L

Burning Method

```python
def burning_method(lattice):
    """
        lattice:    np.ndarray[L, L]
                    0 means empty, 1 means occupied
    """
    t = 2
    lattice[0, lattice[0, :] == 1] == t
    while True:
        t += 1
        has_changed = False
        for node in np.where(lattice == t):
            for neighbor in get_neighbors(node):
                if lattice[neighbor] == 1:
                    lattice[neighbor] = t
                    has_changed       = True
        at_bottom = (node[0] == lattice.shape[0] - 1).any()
        if not has_changed or at_bottom:
            break

```

Hoshen-Kopelman Algorithm

compute how many clusters

```python
def hoshen_kopelman_algorithm(lattice):
    """
        lattice:    np.ndarray[L, L]
                    0 means empty, 1 means occupied
    """
    cluster_sizes = [None, None] # starts with 2
```

```
    k = 2
    for i in range(lattice.shape[0]):
        for  j in range(lattice.shape[1]):
            if is_top_and_left_empty(lattice[i, j]): # new cluster
                lattice[i, j] = k
                cluster_sizes.append(1)
                k += 1
            else is_top_left_same_cluster(lattice[i, j]): # one neighbor in
cluster or neighbors in same cluster
                lattice[i, j] = get_top_left_cluster(lattice[i,j])
                cluster_sizes[lattice[i, j]] += 1
            else: # neighbors in different cluster
                k1, k2 = get_top_left_cluster(lattice[i, j])
                lattice[i, j] = k1
                cluster_sizes[k1] += cluster_sizes[k2]
                mark_cluster_size_as_transferred(cluster_sizes, k2)

```

3. Fractals

- *fractal dimension* d_f: stretch the object by a, the volume grows a^{d_f}

$$\frac{V_\varepsilon^*}{\varepsilon^d} = \left(\frac{L}{\varepsilon}\right)^{d_f}$$

- *correlation function* $c(r)$: number of filled sites with in sphere r shell Δr normalized by surface

$$c(r) \propto \begin{cases} C + exp(-\frac{r}{\xi}) & p < p_c \\ r^{-(d-2+\eta)} & p \approx p_c \end{cases}$$

  ξ is the correlation length

$$\xi \propto |p - p_c|^\nu \; where \; \nu = \begin{cases} \frac{4}{3} & 2d \\ 0.88 & 3d \end{cases}$$

$$\eta = \begin{cases} \frac{5}{24} & 2d \\ -0.05 & 3d \end{cases}$$

$$d_f = d - \frac{\beta}{\nu}$$

  β : percolation strength

  d : dimension

Sandbox Method

```
def sandbox_method(lattice):
    """
        lattice:    np.ndarray[L, L]
                    0 means empty, 1 means occupied
    """
    R  = []
    N_R = []
    c = lattice.shape[0]/2 - 1 # as python starts from 0
    for r in range(1, int(L//2)): # increase the sanbox size over iteration
        R.append(r)
        N_R.append(sum(lattice[c-r:c+r, c-r:c+r]==1))
    plot_log(R, N_R) # the fractal dimension d_f is the slope
```

Box Counting Method

```
def box_counting_method(lattice):
    """
        lattice:    np.ndarray[L, L]
                    0 means empty, 1 means occupied
    """
    epsilon_inv = []
    N_epsilon   = []
    for epsilon in range(1, lattice.shape[0]):
        boxes = maxpool2d(lattice, kernel=np.ones([epsilon, epsilon]),
padding=0) # use the pooling to compute box
        N_epsilon.append(sum(boxes > 0))
        epsilon_inv.append(1 / epsilon)
    plot_log(epsilon_inv, N_epsilon) # the fractal dimension d_f is the slope

```

4. Cellular Automata

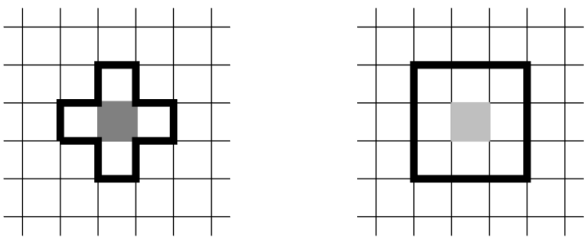
cellular automata:$(\mathcal{L}, \psi, R, \mathcal{N})$

$\mathcal{L}$: d dimension lattice of cells

ψ : m dimension boolean state for each site at time t

R : m rules to update the ψ

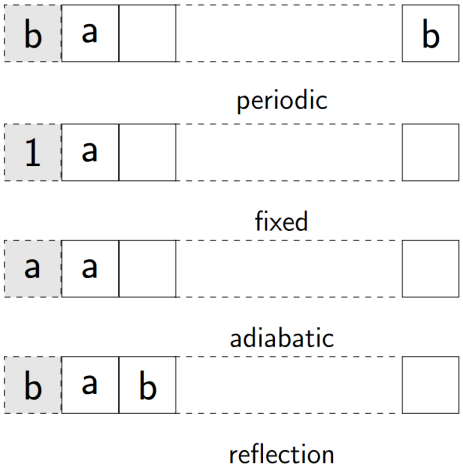
neighborhoods



- left:*Von Neumann neighborhood* : 4 (north-east-south-west)

- right:*Moore neighborhood* : 8 (3x3 region)

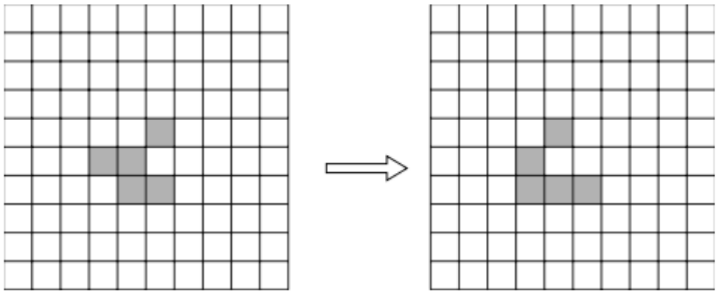
boundary conditions



assume `x[1:]` is the actual space

- *periodic* : `x[0] = x[-1]`
- *fixed* : `x[0] = c`
- *adiabtic* : `x[0] = x[1]`
- reflection: `x[0] = x[2]`

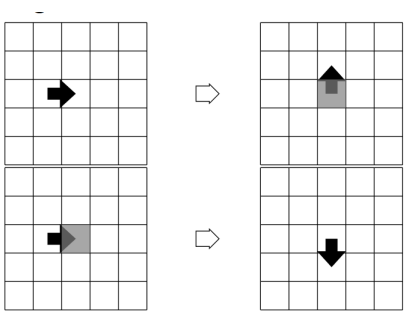
Game of Life



moore neighborhood

- $n < 2$: 0 dead because of isolation
- $n = 2$: stay as before
- $n = 3$: 1 birth
- $n > 3$: 0 dead because of over population

Langton Ant

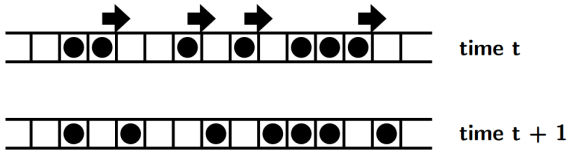


- enter white cell, turn left and paint cell gray
- enter gray cell, turn right and paint cell white

observation

- chaotic phase of about 10000 steps
- formation highway
- walking on highway

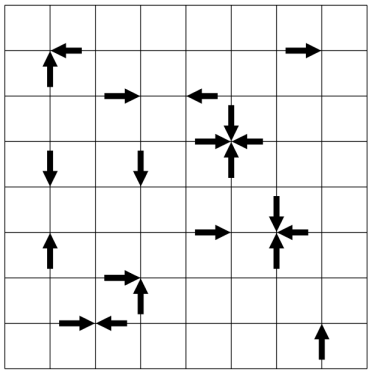
Traffic Models

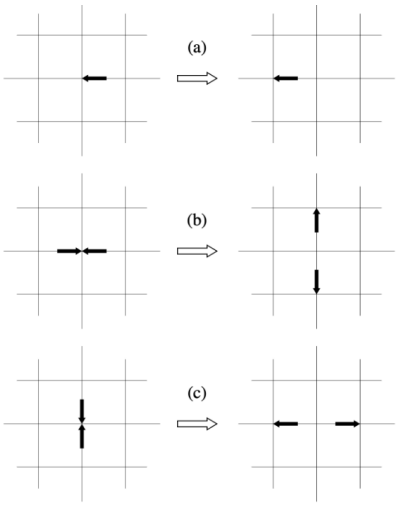


$$(\psi_{i-1}, \psi_i, \psi_{i+1})_t \rightarrow (\psi_i)_{t+1}$$

rule \$(\psi_{i-1}\psi_i\psi_{i+1})_t$	111	110	101	100	011	010	001	000
184 $(\psi_i)_t$	1	0	1	1	1	0	0	0

Gas of Particles (HPP model)





$\psi(r,t) = (1011)$

- collision
- propagation

5. Monte Carlo Method

Error

$$\Delta \propto \frac{1}{\sqrt{N}}$$

π Buffon's Needle Experiment

$$\pi(N) = 4\frac{N_c(N)}{N}$$

N_c : points in the quarter circle

Monte Carlo Integral

$$\int_a^b g(x)dx \approx \frac{b-a}{N}\sum_{i=1}^{N} g(x_i) \equiv Q$$

x_i is uniform sampled in $[a,b]$

N is the number of samples

error $\propto (\Delta x)^2 \propto N^{-\frac{2}{d}}$

Center Limit Theorem

$$\delta Q = (b-a)\frac{\sigma}{\sqrt{N}} = V\frac{\sigma}{\sqrt{N}}$$

$$\sigma^2 = \frac{1}{N-1}\sum_{i=1}^{N}\left(g(x_i) - \frac{Q}{N}\right)$$

V : is the volume of hypercube for integration in high dimension

the error independent of dimension d

cirtical point

$$N^{-\frac{2}{d}} \overset{crit}{=} \frac{1}{\sqrt{N}}$$

for $d > 4$, MC more efficient

high dimension integration

hard-sphere, overlap $\rightarrow$ rejective

Importance Sampling

$$\int_a^b f(x)dx \approx \frac{1}{N}\sum_{i=1}^{N}\frac{f(x_i^G)}{g(x_i^G)}$$

x_i^G is sampled according to distribution $g(x)$

$G(x)$ is the cdf of $g(x)$, $G(x) = \int_a^x g(x)dx$

f and g need to be positively correlated

Control Variates

$$\int_a^b f(x)dx = \int_a^b (f(x) - g(x))dx + \int_a^b g(x)dx$$

f and g need to be positively coorelated

- $Var(f-g) < Var(f)$
- $\int_a^b g(x)dx$ is known

Quasi Monte Carlo

$$D_N^* = \mathcal{O}\left(\frac{(logN)^d}{N}\right)$$

$$\mathcal{O}(\frac{(logN)^d}{N}) < \mathcal{O}(\frac{1}{\sqrt{N}}) \Rightarrow N > 2^d$$

Markov Chain

$$\frac{dp(X,\tau)}{d\tau} = \sum_{Y\neq X} p(Y)W(Y\rightarrow X) - \sum_{Y\neq X} p(X)W(X\rightarrow Y)$$

$$W(X\rightarrow Y) = T(X\rightarrow Y)A(X\rightarrow Y)$$

$A(X\rightarrow Y)$ means the accpet probability from X to Y

$T(X\rightarrow Y)$ means the transition probablity from X to Y

- ergodicity: $\forall X, Y : W(X\rightarrow Y) > 0$
- normalization: $\sum_Y W(X\rightarrow Y) = 1$
- homogeneity: $\sum_Y p(Y)W(Y\rightarrow X) = p(X)$

Detailed Balance : $\frac{d\,p(X,\tau)}{d\tau} = 0$

M(RT)^2 Algorithm

1. random choose a configuration X
2. compute $\Delta E = E(Y) - E(X)$
3. spinflip if $\Delta E < 0$ else accept iwth probability $exp(-\frac{\Delta E}{k_B T})$

Ising Model

simulate the magnetic properties of a material

$$\mathcal{H} = -J \sum_{i,j} S_i S_j - H \sum_i S_i$$

S_i means the spin at position i

j : is the neighbor off i

```
def ising_model(lattice, M, E, J, beta, steps):
    """
        lattice:    np.ndarray[L, L]
                    1 means spin up, -1 means spin down
        M:          float
                    magnetic field
        E:          float
                    energy
        J:          float
                    coupling constant
        beta:       float
                    inverse of temperature `beta = 1 / T / kB`
        steps:      int
    """
    L = lattice.shape[0]
    for i in range(steps):
        x, y = np.random.randint(0, L, [2])
        sigma_j = lattice[get_neighbors(lattice, x, y)].sum()
        sigma_i = lattice[x, y]
        delta_E = 2 * J * sigma_i * sigma_j
        accept = min(1., exp(-beta * delta_E)) > rand()
        if accpet:
            M -= 2*lattice[x, y]
            E += delta_E
            lattice[x, y] *= -1
   return M, E
```

1. random choose a configuration X
2. compute $\Delta E = E(Y) - E(X) = 2J\sigma_i\sigma_j$
3. spinflip if $\Delta E < 0$ else accept with probability $exp(-\frac{\Delta E}{k_B T})$

Multilevel Monte Carlo(MLMC)

$$\mathbb{E}[P_L] = \mathbb{E}[P_0] + \sum_{l=1}^{L} \mathbb{E}[P_l - P_{l-1}]$$

$$N_l = \mu \sqrt{\frac{V_l}{C_l}}$$

$$C = \sum_{l=1}^{L} C_l N_l$$

$$Var = \sum_{l=1}^{L} V_l N_l^{-1}$$

C_l : cost at level l

V_l : variance at level l

N_l : sample number at level l

6. Finite Difference

Error

- input data error
- rounding error
- truncation error
- simplification in mathematical model
- human & machine error

propogation

$$\varepsilon \approx \sqrt{\sum_{i}^{n} \left(\frac{\partial f}{\partial x_i} \right)^2 \varepsilon_i^2}$$

Partial Differential Equation (PDE)

- *parabolic* : $D\frac{\partial^2 \phi}{\partial^2 x} - \frac{\partial \phi}{\partial t} = 0$
- *hyperbolic* : $\frac{\partial^2 \phi}{\partial^2 x} - \frac{1}{c}\frac{\partial^2 \phi}{\partial^2 t} = 0$
  generate solution is $\phi(x,t) = \alpha f_0(x - ct) + \beta g_0(x + ct)$
- *elliptic* : $\nabla^2 \phi = 0$

Lagrange Derivative :

$$\frac{D\phi}{Dt} = \frac{\partial \phi}{\partial t} + \overrightarrow{u} \cdot \nabla \phi$$

Forward in Time, Backward in Space (FTBS)

$$\frac{\partial \phi_j^{n+1}}{\partial t} = \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \mathcal{O}(\Delta t)$$
$$\frac{\partial \phi_j^n}{\partial x} = \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} + \mathcal{O}(\Delta x)$$

first order accurate

explicit

Centred in Time, Centred in Space (CTCS)

$$\frac{\partial \phi_j^n}{\partial t} = \frac{\phi_j^{(n+1)} - \phi_j^{(n-1)}}{2\Delta t} + \mathcal{O}(\Delta t^2)$$
$$\frac{\partial \phi_j^n}{\partial x} = \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

second order accurate

implicit

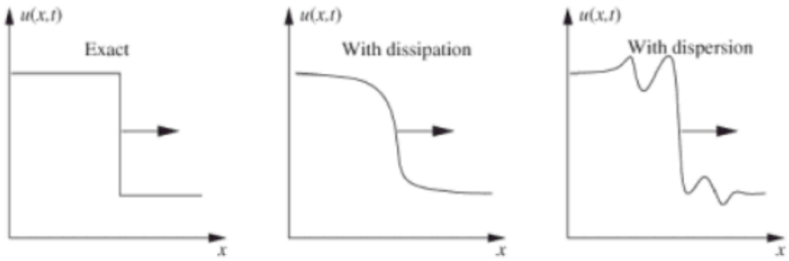
Backward in Time, Centred in Space (BTCS)

$$\frac{\partial \phi_j^n}{\partial t} = \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \mathcal{O}(\Delta t)$$
$$\frac{\partial \phi_j^n}{\partial x} = \frac{\phi_{j+1}^n - \phi_{j-1}^n}{\Delta x} + \mathcal{O}(\Delta x)$$

first order accurate

implicit

Stability



- *Dissipation* : smooth out sharp corners, gradients, discontinuities
- *Dispersion* : dependence of wave speed on wavelength

Lax-Equivalence Theorem

consistency + stability $\Leftrightarrow$ convergence

Courant-Friedrichs-Lewy(CFL) cirterion

$$C = \frac{u\Delta t}{\Delta x} \leq C_{max}$$

for explicit, $C_{max} = 1$, much larger for implicit, as it's much more stable

Domain of Dependence(DoD)

- DoD for FTBS $0 \leq c \leq 1$
- DoD for CTCS $-1 \leq c \leq 1$

Von-Neumann Stability Analysis

$$\phi^{n+1} = A\phi^n$$

- $|A|^2 < 1$ stable and damping
- $|A|^2 = 1$ neutral stable
- $|A|^2 > 1$ unstable and amplyfying

for FTBS

$$\begin{aligned} \phi_j^{n+1} &= \phi_j^n - c(\phi_j^n - \phi_{j-1}^n) \\ A^{n+1}e^{ikj\Delta x} &= A^n e^{ekj\Delta x} - cA^n\left(e^{ikj\Delta x} - e^{ik(j-1)\Delta x}\right) \\ A &= 1 - c(1 - e^{-ik\Delta x}) \\ |A|^2 &= 1 - 2c(1-c)(1 - cosk\Delta x) \end{aligned}$$

$c = \frac{u\Delta t}{\Delta x}$

if $u < 0$ or $\frac{u\Delta t}{\Delta x} > 1$ the FTBS is unstable , which is $0 \leq c \leq 1$

for FTCS

$$|A|^2 = 1 + 4c^2 sin^2(k\Delta x)$$

for CTCS

$$\begin{aligned} \phi_j^{n+1} &= \phi_j^{n-1} - c(\phi_{j+1}^n - \phi_{j-1}^n) \\ A &= -icsin(k\Delta x) \pm \sqrt{1 - c^2 sin^2 k\Delta x} \\ |A|^2 &= 2c^2 sin^2(k\Delta x) - 1 \mp sin(k\Delta x)\sqrt{c^2 sin^2(k\Delta x) - 1} \end{aligned}$$

- $|c| > 1$ unstable
- $|c| \leq 1$ stable

there are two solutions ,should ignore the spurious solution

Conservation

$$\begin{aligned} M^{n+1} &= \int_0^1 \phi_x^{n+1} dx \\ &= M^n = \int_0^1 \phi_x^n dx \end{aligned}$$

Phase Velocity

$$\phi(x,t) = \phi(x - ut, 0)$$

u: phase speed

for CTCS, small k and Δx is correct

Shallow Water Equation

$$H = H_0 + \eta$$

where H is the water height, η is the fluctuation

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u = -\frac{1}{\rho}\nabla p + g$$
$$\nabla \cdot u = 0$$
$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + g_i$$
$$\frac{\partial u_i}{\partial x_i} = 0$$

where $g = [0, 0, g_z]$ is the velocity

A-Grid(unstaggered)

$$\frac{\eta_j^n - \eta_j^{n-1}}{\Delta t} = -H_0 \frac{u_{j+1}^n - u_{j-1}^n}{\Delta x}$$
$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -g \frac{\eta_{j+1}^n - \eta_{j-1}^n}{\Delta x}$$

courant number $c = \sqrt{gH_0}\frac{\Delta t}{\Delta x}$

stable for $c \leq 2$

C-Grid(Staggered)

$$\frac{\eta_j^n - \eta_j^{n-1}}{\Delta t} = -H_0 \frac{u_{j+\frac{1}{2}}^n - u_{j-1}^n}{\Delta x}$$
$$\frac{u_{j+\frac{1}{2}}^{n+1} - u_{j+\frac{1}{2}}^n}{\Delta t} = -g \frac{\eta_{j+1}^n - \eta_{j-1}^n}{\Delta x}$$

stable for $c \leq 1$

7. Time Integration

error

- *truncation error* : taylor expansion in euler method, $\mathcal{O}(\Delta t^2)$ for each step, $\mathcal{O}(\Delta t)$ in total
- *round-off error* : charcteristic number η, the smallest incremental, in euler method $\mathcal{O}(\eta)$ for each step, $\mathcal{O}(\frac{\eta}{\Delta t})$ in total
- *total error* : for euler method, $\varepsilon \sim \frac{\eta}{\Delta t} + \Delta t$

one step method

for ordinary differential equatiion (ODE)

$$\frac{\partial \phi}{\partial t} = f(t, \phi(t)) \quad \phi(t_0) = \phi^0$$

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} = \gamma f(t + \Delta t, \phi^{n+1}) + (1 - \gamma) f(t, \phi^n)$$

multi step method

$$\frac{(1+\beta)\phi^{n+1}-(1+2\beta)\phi^{n}+\beta\phi^{n-1}}{\Delta t}=\gamma f(t+\Delta t,\phi^{n+1})+(1-\gamma+\alpha)f(t,\phi^{n})-\alpha f(t-\Delta t,\phi^{n-1})$$

name	α	β	γ	order
explicit euler	0	0	0	1
implicit euer	0	0	1	1
leapfrog	0	$-\frac{1}{2}$	0	2

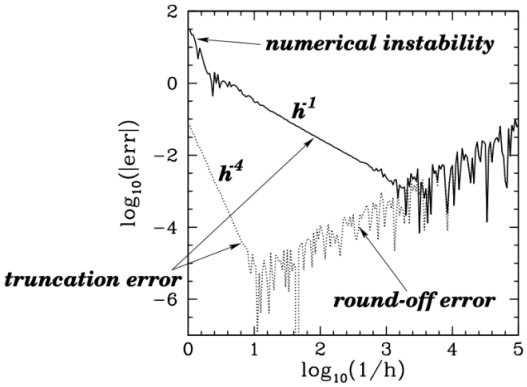
Runge-Kutta method

$$\begin{aligned}
k_1 &= \Delta t f(t_n,\phi^n)\\
k_2 &= \Delta t f(t_{n+\frac{1}{2}},\phi^n+\frac{k_1}{2})\\
k_3 &= \Delta t f(t_{n+\frac{1}{2}},\phi^n+\frac{k_2}{2})\\
k_4 &= \Delta t f(t_{n+1},\phi^n+k_3)\\
\phi^{n+1} &= \phi^n+\frac{k_1}{6}+\frac{k_2}{3}+\frac{k_3}{3}+\frac{k_4}{6}+\mathcal{O}(\Delta t^5)
\end{aligned}$$

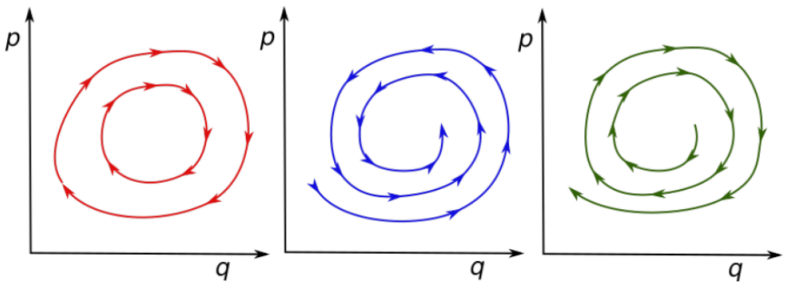
truncation error $\mathcal{O}(\Delta t^4)$

round-off error $\mathcal{O}(\frac{\eta}{\Delta t})$

minimum error is smaller with bigger Δt compared to euler



Conservation



volume ↔ energy

- left: conserve

- middle: loss energy
- right: gain energy

Symplectic

for Hamiltonian $[p, q]$ and $p = \dot{q}$

$$\begin{bmatrix} q(\tau) \\ p(\tau) \end{bmatrix} = A \begin{bmatrix} q(0) \\ p(0) \end{bmatrix}$$

for energy conservation $|A| = 1$

8. Maxwell Equation

Valsov-Maxwell-Bolzmann equation

computational plasma

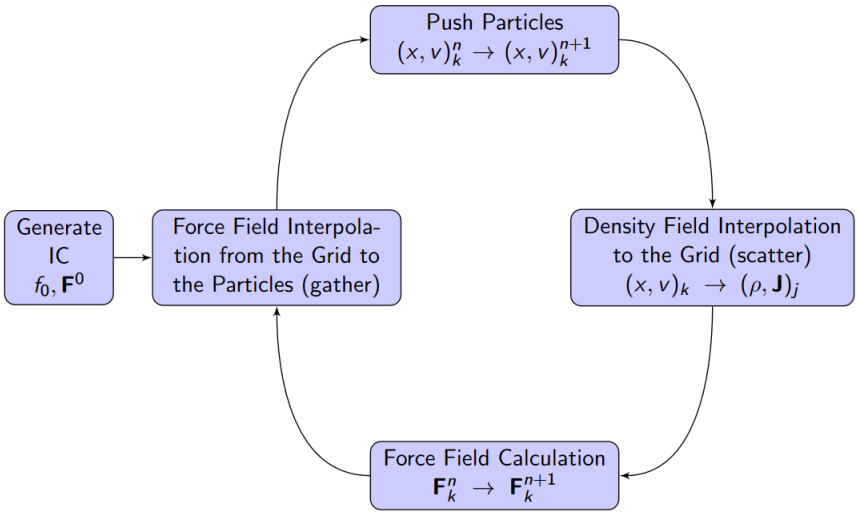
$$\begin{aligned} \frac{\partial f_s}{\partial t} + \nabla_x \cdot (\boldsymbol{v} f_s) + \nabla_{\boldsymbol{v}} \cdot ((\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) \frac{q_s f_s}{m_s}) &= (\frac{\partial f_s}{\partial t})_c \\ \nabla \cdot \boldsymbol{E} &= \frac{\rho}{\varepsilon_0} \\ \nabla \cdot \boldsymbol{H} &= 0 \\ \nabla \times \boldsymbol{E} + \frac{\partial \boldsymbol{H}}{\partial t} &= 0 \\ \nabla \times \boldsymbol{H} - \mu_0 \varepsilon_0 \frac{\partial \boldsymbol{E}}{\partial t} &= \mu_0 \sum_s q_s \int_{-\infty}^{\infty} \boldsymbol{v} f_s d\boldsymbol{v}^3 \end{aligned}$$

where $f(x, \boldsymbol{v}, t) \in \mathbb{R}^{3\times 3\times}$ is the distribution

$$\begin{aligned} \boldsymbol{D} &= \varepsilon_0 \varepsilon_r \boldsymbol{E} \\ \boldsymbol{B} &= \mu_0 \mu_r \boldsymbol{H} \end{aligned}$$

Particle In Cell Method (PIC)

$$\begin{aligned} \frac{d\boldsymbol{x}}{dt} &= \boldsymbol{v} \\ \frac{d\boldsymbol{v}}{dt} &= \frac{q}{m}(\boldsymbol{E}(\boldsymbol{x}, t), \boldsymbol{v} \times \boldsymbol{B}(\boldsymbol{x}, t)) \end{aligned}$$



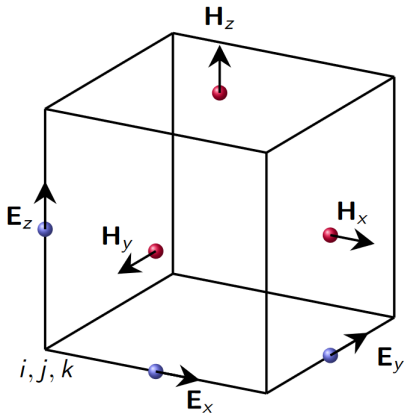
Boris algorithm

$$
\begin{aligned}
\boldsymbol{v}^{-} &= \boldsymbol{v}^{n-\frac{1}{2}} + \frac{q}{m}\boldsymbol{E}^{n}\frac{\Delta t}{2} \\
\frac{\boldsymbol{v}^{+} - \boldsymbol{v}^{-}}{\Delta t} &= \frac{q}{2m}(\boldsymbol{v}^{+} + \boldsymbol{v}^{-}) \times \boldsymbol{B}^{n} \\
\boldsymbol{v}^{n+\frac{1}{2}} &= \boldsymbol{v}^{+} + \frac{q}{m}\boldsymbol{E}^{n}\frac{\Delta t}{2}
\end{aligned}
$$

without $\boldsymbol{E}$

$$
\begin{aligned}
\boldsymbol{t} &\approx \frac{q\boldsymbol{B}\Delta t}{2m} \\
\boldsymbol{s} &= \frac{2\boldsymbol{t}}{1 + |\boldsymbol{t}|^{2}} \\
\boldsymbol{v}' &= \boldsymbol{v}^{-} + \boldsymbol{v}^{-} \times \boldsymbol{t} \\
\boldsymbol{v}^{+} &= \boldsymbol{v}^{-} + \boldsymbol{v}' \times \boldsymbol{s}
\end{aligned}
$$

Yee Cell



$$
\begin{aligned}
\frac{\partial \boldsymbol{H}}{\partial t} &= -\frac{1}{\mu_0}\nabla \times \boldsymbol{E} \\
\frac{\partial \boldsymbol{E}}{\partial t} &= \frac{1}{\varepsilon_0}\nabla \times \boldsymbol{H}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \boldsymbol{H}_x}{\partial t} &= \frac{-1}{\mu_0}\left(\frac{\partial \boldsymbol{E}_y}{\partial z} - \frac{\partial \boldsymbol{E}_z}{\partial y}\right) \qquad \frac{\partial \boldsymbol{E}_x}{\partial t} = \frac{1}{\varepsilon_0}\left(\frac{\partial \boldsymbol{E}_y}{\partial z} - \frac{\partial \boldsymbol{E}_z}{\partial y}\right) \\
\frac{\partial \boldsymbol{H}_y}{\partial t} &= \frac{-1}{\mu_0}\left(\frac{\partial \boldsymbol{E}_z}{\partial x} - \frac{\partial \boldsymbol{E}_x}{\partial z}\right) \qquad \frac{\partial \boldsymbol{E}_y}{\partial t} = \frac{1}{\varepsilon_0}\left(\frac{\partial \boldsymbol{E}_z}{\partial x} - \frac{\partial \boldsymbol{E}_x}{\partial z}\right) \\
\frac{\partial \boldsymbol{H}_z}{\partial t} &= \frac{-1}{\mu_0}\left(\frac{\partial \boldsymbol{E}_x}{\partial y} - \frac{\partial \boldsymbol{E}_y}{\partial x}\right) \qquad \frac{\partial \boldsymbol{E}_z}{\partial t} = \frac{1}{\varepsilon_0}\left(\frac{\partial \boldsymbol{E}_x}{\partial y} - \frac{\partial \boldsymbol{E}_y}{\partial x}\right)
\end{aligned}
$$

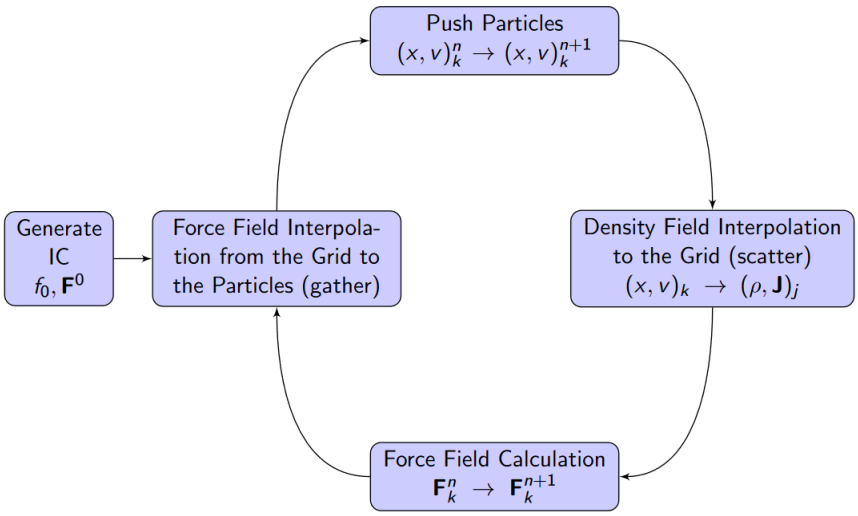
$$
\begin{aligned}
\frac{E_{x_k}^{n+\frac{1}{2}} - E_{x_k}^{n-\frac{1}{2}}}{\Delta t} &= -\frac{1}{\varepsilon_0}\frac{H_{y_{k+\frac{1}{2}}}^{n} - H_{y_{k-\frac{1}{2}}}^{n}}{\Delta z} \\
\frac{H_{y_{k+\frac{1}{2}}}^{n+1} - H_{y_{k+\frac{1}{2}}}^{n}}{\Delta t} &= -\frac{1}{\mu_0}\frac{E_{x_{k+1}}^{n+\frac{1}{2}} - E_{x_k}^{n+\frac{1}{2}}}{\Delta z}
\end{aligned}
$$

error minimized by $\tilde{E}_x = \sqrt{\frac{\varepsilon_0}{\mu_0}}E_x$

stability: $\frac{\Delta t}{\Delta x} = \frac{1}{\sqrt{d}c}$

9. N-Body Problems

Particle in Cell Method (PIC)



$$-\Delta\phi = \rho$$
$$F = -\nabla\phi$$

ρ is the mass density, ϕ is the potential field

$$\phi(x) = G(x,x') * \rho(x')$$

0. generate initial condition f_0, F^0
1. for loop
    0. force field interpolate from grid to particles
    1. push particles $(x,v)_k^n \to (x,v)_k^{n+1}$
    2. density field interpolation to grid $(x,v)_k \to (\rho, J)_j$
    3. force field calculation $F_k^n \to F_k^{n+1}$, using FFT

$$\phi(x) = \int \rho(x')G(x,x')dx' = \mathcal{F}^{-1}(\mathcal{F}(\rho)\cdot\mathcal{F}(G))$$

Particle particle Particle Mesh(P3M)

$$G(r) = \underbrace{\frac{1-erf(\alpha r)}{r}}_{G_{pp}} + \underbrace{\frac{erf(\alpha r)}{r}}_{G_{pm}}$$

G_{pp} : use the n-body solver for short-range

G_{pm} : use particle-mesh solver for long-range