含时演化问题

$$\begin{cases} y' = f(t, y). & \Rightarrow RK\ 45 \quad O(h^5). \\ \frac{\partial u}{\partial t} = a_i \frac{\partial^2 u}{\partial x^2} & \text{Crank-Nicolson 方法 } O(\Delta t^2) \text{ or } O(\Delta x^3) \end{cases}$$

迭代问题

$$\frac{u^{n+1} - u^n}{\Delta t} = f(u^n) \quad \text{or} \quad u^{n+1} = u^n + f(u^n)\Delta t.$$

"梯形" $u_{n+1} = u_n + \frac{\Delta t}{2}[f(u^{n+1}) + f(u^n)]$

核心 code. Do: i=1:N

$a_1^i = a_0^i + f_i(\vec{a}_0)\Delta t.$

$a_0 = a_1^i$

End Do.

应用：ⓃN体.

$$\ddot{\vec{r}}_i = \frac{1}{m_i}\sum_j \vec{F}_{ij}.$$

$$\vec{r}_i^{\,n+1} + \vec{r}_i^{\,n-1} - 2\vec{r}_i^{\,n} = \frac{\Delta t^2}{m_i}\sum_j \vec{F}(\vec{r}_i^{\,n} - \vec{r}_j^{\,n})$$

八个因素.

1) m_i 大, $|\vec{r}_i - \vec{r}_j|$ 大

2) 时间长.

3) 归一化

② Kuramoto model.

$$\dot{\theta}_i = \omega_i - \frac{K}{N}\sum_j \sin(\theta_i - \theta_j)$$

1) 相变(非同步—同步)

2) 可解.

$(t^n + t^{n+1}) \times \frac{1}{2}$

$$\theta_i^{n+1} = \theta_i^n + \Delta t\left[\omega_i - \frac{K}{N}\sum_j \sin(\theta_i^n - \theta_j^n)\right]$$

③ 病毒 SIR

$$\begin{cases} \dot{S} = -cSI \\ \dot{I} = cSI - gI \\ \dot{R} = gI \end{cases} \Rightarrow \quad \begin{aligned} S^{n+1} &= S^n - \Delta t\, c S^n I^n \\ I^{n+1} &= I^n + \Delta t(cS^n I^n - gI^n) \\ R^{n+1} &= R^n + gI^n \Delta t \end{aligned}$$

④ Lorenz eq:

chaos

定义: 混沌.

Fixed point. $\begin{cases} \dot{x} = 0 \\ \dot{y} = 0 \\ \dot{z} = 0 \end{cases}$

$\begin{cases} x^{n+1} \to x^* ; \\ \lim\limits_{n \to \infty} x^n \text{ 不存在}. \end{cases}$

⑤ Logistic map.

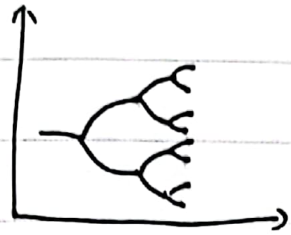
$$\frac{dx}{dt} = 4\gamma x(1-x)$$ 韦吕勒 verhulst 1845

分岔

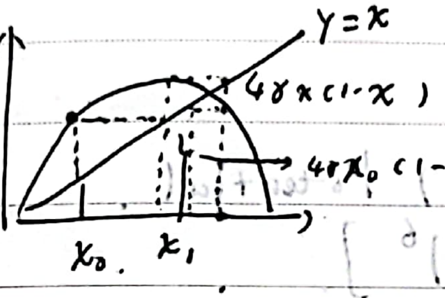
Feigenbaum $\delta = 4.6692$.

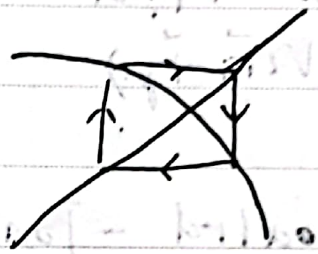
$x_{n+1} = 4\gamma x_n(1-x_n)$.

$\Rightarrow$



分叉 Bification.





⑥ Bak-Tong-Wiesenfeld (BTW) model.

沙堆模型. sand pile model

相变 沙堆可以堆多高?

$h_{\vec r}$ $\vec r \in$ D-dimensional space

随机 $\vec r \Rightarrow$ ~~$h_{\vec r} \to h_{\vec r}+1$~~ $h_{\vec r} \to h_{\vec r}+1$

$h_{\vec r} > h_c$ $h_{\vec r} \to h_{\vec r} - h_c$.

周围点 $h_{\vec r+\vec n} \to h_{\vec r+\vec n} + 1$.

⑦ Flocking behavior:

Vicsek model

生物物理

$\vec r_i^{\,n+1} = \vec r_i^{\,n} + \vec v_i^{\,n+1}\Delta t$. $\vec M_i^{\,n+1} = \Big(\sum_{|\vec r_j - \vec r_i|<R} \vec v_j^{\,n}\Big)/N + \xi_i$ → 随机修正 可以修改

$\vec r = \vec r_0 + \vec v t$.

$\vec v^{\,n+1} = \dfrac{\vec r^{\,n+1} - \vec r^{\,n}}{\Delta t}$.

⑧ 分子动力学模拟.

$$m_i \ddot{\vec{r}}_i = \sum_j \vec{F}_{ij}$$

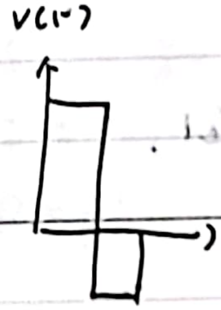
$$\vec{F}_{ij} = -\nabla_i U = -\nabla_{\vec{r}_i} U$$

$$U(\vec{r}) = \sum_{i,j} V(\vec{r}_i - \vec{r}_j)$$

常见 (a) Legenadlrd - Jones (LJ) Potential.

$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right].$$

(b)



(c) Morse potential

$$V_0\left[1 - e^{-a(r-r_e)}\right]^2 - V_0$$

Verles 算法.

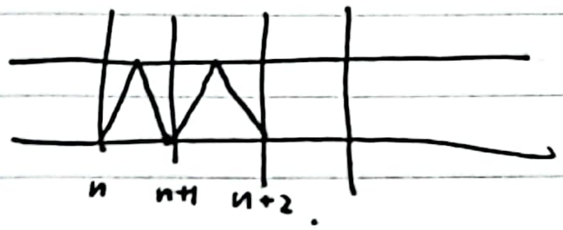
$$\vec{x}(t+dt) + \vec{x}(t-dt) = 2\vec{x}(t) + \ddot{\vec{x}}\,\Delta t^2 + O(\Delta t^4)$$

$$\ddot{\vec{x}} \to f/m$$

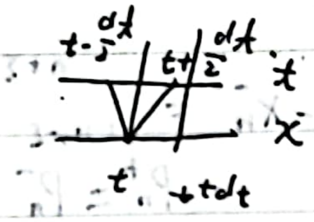
多粒子:

$$\vec{x}_i(t+dt) + \vec{x}_i(t-dt) = 2\vec{x}_i(t) + \frac{\vec{f}_i}{m_i}\Delta t^2 + O(\Delta t)^4$$

leap frog 算法.



$$\vec{v}\left(t+\frac{dt}{2}\right) = \vec{v}\left(t-\frac{dt}{2}\right) + \frac{\vec{f}}{m}\,dt$$



$$\vec{f} = \vec{f}(\vec{x}(t))$$

$$\vec{x}(t+dt) = \vec{x}(t) + \vec{v}\left(t+\frac{dt}{2}\right)dt$$ $U(\vec{x}) \to -\nabla U = \vec{f}$.

$$i\frac{\partial}{\partial t}\psi = H(t)\psi$$

$$\psi = \sum_n c_n|\varphi_n\rangle$$

↳ 不含时.

$$\sum_n i\dot{c}_n|\varphi_n\rangle = \sum_m H|\varphi_m\rangle c_m$$

$$\Downarrow$$

$$i\dot{c}_n = \langle\varphi_n|H|\varphi_m\rangle c_m = \sum_m h_{nm}(t)\,c_m$$

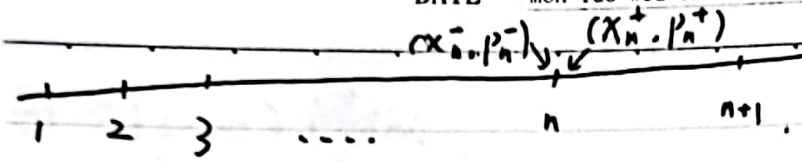
$$c_n^{k+1} = c_n^k - i\sum_m h_{nm}(t^k)\,c_m^k\,dt$$

kicked rotor model.

$$H = \frac{p^2}{2} + K\cos(x)\sum_n \delta(t-n)$$

Equation of motion.

$$\begin{cases} \dot{x} = \frac{\partial H}{\partial p} = p \\ \dot{p} = -\frac{\partial H}{\partial x} = K\sin x\sum_n\delta(t-n) = F \end{cases}$$



$$\begin{cases} p_{n+1}^- = p_n^+ \\ x_{n+1}^- = x_n^+ + p_n^+ \end{cases}$$

$\dot{x} = p$

$$x_n^+ - x_n^- = \int_{n-\varepsilon}^{n+\varepsilon} p\,dt = 0 \quad \therefore X_n^- = X_n^+$$

$$p_n^+ = p_n^- + k\sin(x_n^-)$$

$$\Rightarrow \begin{cases} p_{n+1} = p_n + k\sin(x_n) \\ x_{n+1} = x_n + p_{n+1} \end{cases}$$

唯一参数 k.

讨论.

作业：
1)
2) Logistic map. 分叉现象.