分子动力学，次量64
Flocking
随机数

含时问题

① $y' = f(t,y)$ → Runge-Kutta Method RK45 $O(h^5)$

② $\frac{\partial y}{\partial t} = \alpha^2 \frac{\partial^2}{\partial x^2} u$ → Crank-Nicolson 方法

迭代问题，

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

"梯形"

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

核心代码（迭代）

```
Do i = 1:N
a_1^i = a_0^i + f(a_0^i)Δt ;
a_0^i = a_1^i
End Do.
```

应用 ① 天体 $\ddot{r}_i = \frac{1}{m_i} \sum_j \vec{f}_{ij}$

① $\begin{cases} \dot{v}_i = \frac{1}{m_i} \sum_j \vec{f}_{ij} \\ \dot{x} = v_i \end{cases}$

② $r_i^{n+1} + r_i^{n-1} - 2 r_i^n = \frac{\Delta t^2}{m_i} \sum_j \vec{f}_{ij}$

耗时的几个因素

1> m_i 大 $|\vec{r}_i - \vec{r}_j|$ 大

2> 时间长

3>

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.

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

③ 病毒模型. SIR

$$\begin{cases} \dot{S} = -cSI \\ \dot{I} = cSI - gI \\ \dot{R} = gI \end{cases} \quad \text{OR} \quad \begin{cases} S^{n+1} = S^n - c^n S^n I^n \Delta t \\ I^{n+1} = I^n + c^n S^n I^n \Delta t - gI^n \Delta t \\ R^{n+1} = R^n + gI^n \Delta t \end{cases}$$

④ Lorenz 模型. Chaos.

fixed point $\begin{cases} \dot{x} = 0 \\ \dot{y} = 0 \\ \dot{z} = 0 \end{cases}$ $\lim_{n\to\infty} x^n \to x^*$

⇒ Infinite.

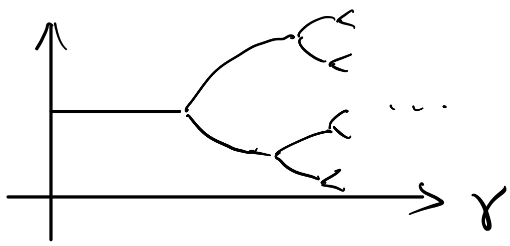
⑤. Logistic map.

$$\frac{dx}{dt} = 4rx(1-x)$$

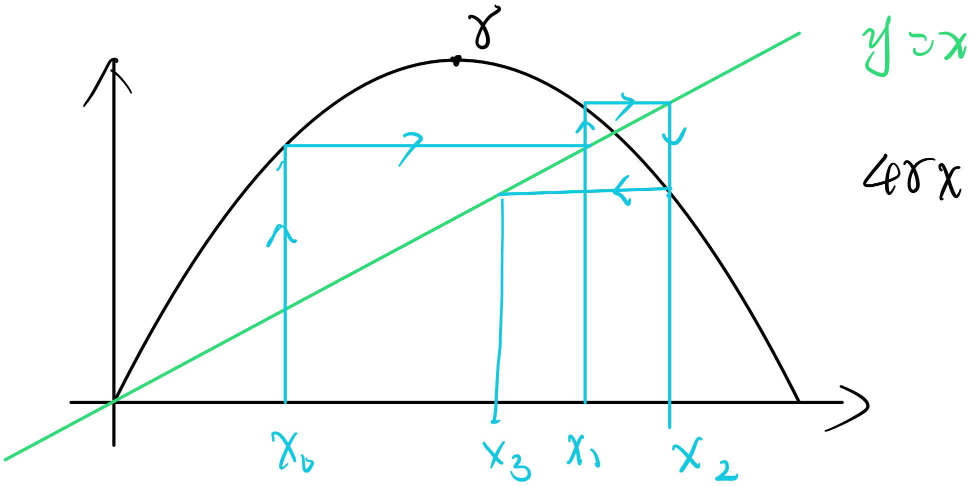
Verhulst.

Feigenbaum

$$X_{n+1} = 4rX_n(1-X_n)$$



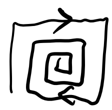
分叉 Bification.



$4rx(1-x) < r$

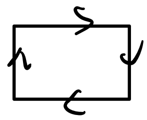
迭代过程.

①



迭代结果收敛

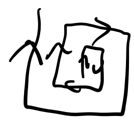
②.



振荡解.

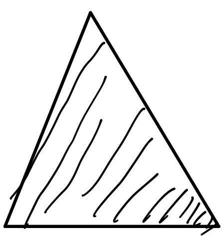
$\lim_{n\to\infty} x_n$ 不存在

③.



⑥. Bak - Tong - Wiesenfield Model

(BTW) [沙堆模型]



沙堆可以堆多高?

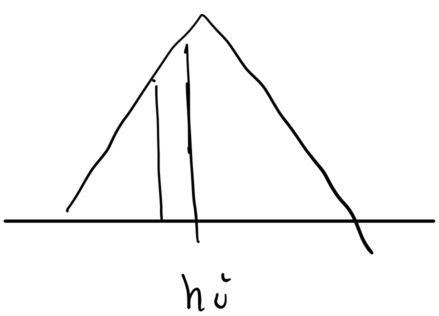
$h_{\vec{r}}$, $\vec{r} \in$ D-dimensional space.

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

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

周围点

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



⑦ Flocking Behavior.

Vissek model

$\nearrow \vec{r}_i^{\,n+1}$.（抽象对象的坐标）

$$\vec{r}_i^{\,n+1} = \vec{r}_i^{\,n} + \vec{u}^{\,n+1}\Delta t$$

$$\vec{u}_i^{\,n+1} = \left(\sum_{|\vec{r}_i-\vec{r}_j|<R} \vec{v}_j^{\,n}\right)\Big/N + \vec{\xi}_i \qquad (\vec{r} = \vec{r}_0 + \vec{v}t)$$

随机修正.

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

⑧ 分子动力学模拟

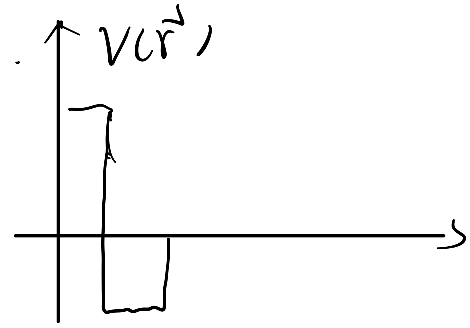
$$\begin{cases} m\ddot{\vec{r}}_i = \sum_j \vec{f}_{ij}, \\ \vec{f}_{ij} = -\nabla_i U(\vec{r}_i - \vec{r}_j) \end{cases}$$

常见的相互作用形式.

① Legenard-Janes (LJ) potential.

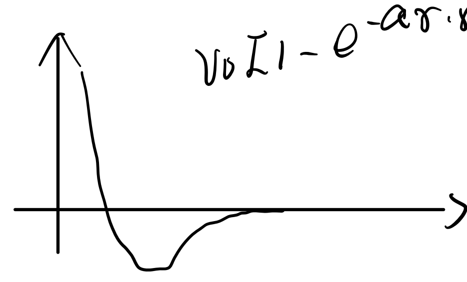
$$V(\vec{r}) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\rho}{r}\right)^{6}\right]$$

②. $V(\vec{r})$



③ Morse potential.

$$v_0\left[1 - e^{-a r \cdot r e}\right]^2 - v_0$$



Verles 算法.

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

$\uparrow$

$\frac{\vec{f}}{m}$

$\Downarrow$

$$\vec{x}(t+\Delta t)+\vec{x}(t-\Delta t)=2\vec{x}(t)+\frac{f}{m}\Delta t^2+o(\Delta t^2)$$

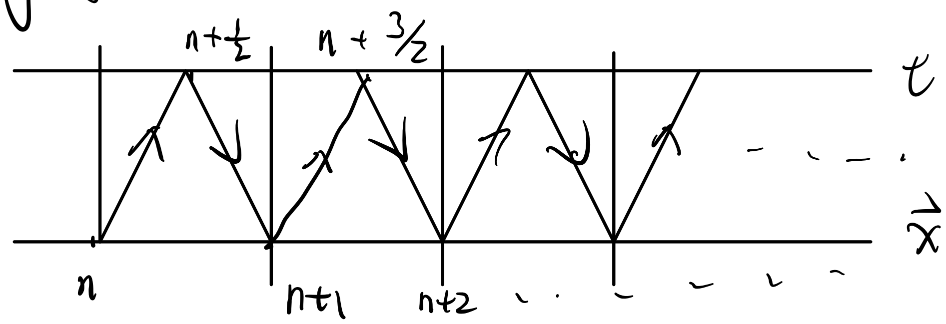
$\Downarrow$ 多粒子.

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

$\Uparrow$

和速度无关.

Leapfrog 算法.



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

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

$$\vec{x}(t+dt)=x(t)+\vec{v}(t+\tfrac{dt}{2})dt$$

Ref:

⑨ Schrödinger 方程.

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

<1> 本征基矢展开

$$|\psi\rangle = \sum_n C_n(t)|n\rangle$$

$$\Rightarrow \quad i\dot{C}_n = \sum_m \underbrace{H_{nm}(t)C_m(t)}_{\boxed{\text{矩阵形式}}}, \quad H_{nm} = \langle n|H(t)|m\rangle$$

离散化

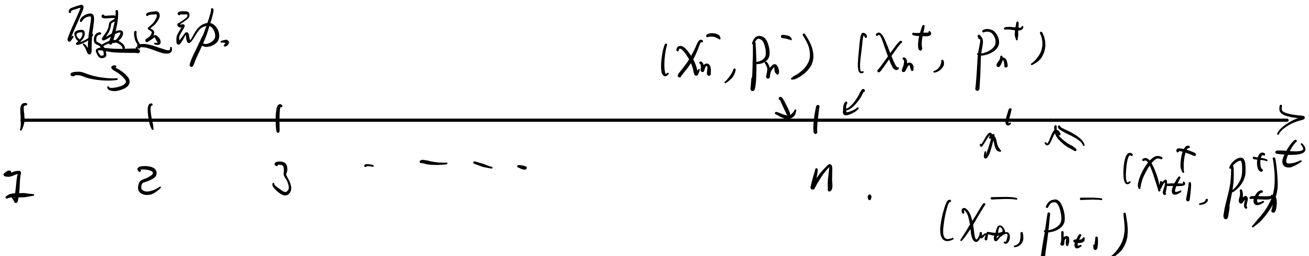
$$C_n^{k+1} = C_n^k - i\sum_m H_{nm}(t_k)C_m(t_k)\Delta t$$

⑩. Kicked - Rotor model.

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

Equation of Motion.

$$\begin{cases} \dot{x} = \dfrac{\partial H}{\partial p} \\ \dot{p} = -\dfrac{\partial H}{\partial x} \end{cases} \Rightarrow \begin{cases} \dot{x} = p \\ \dot{p} = k\sin(x)\sum_n \delta(t-n) \end{cases}$$



速度改变发生在整数时刻

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

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

一个参数k.

作业：①讨论 kick-rotor Model 中的各种情况.

②. Logistic map 的分叉现象.