① 含时问题 ⇒ Runge-kutta ⇒ $y' = f(t, y)$

Crank-Nialson $\partial_t u = a^2 \frac{\partial^2}{\partial x^2} u$.

② 本征值 $H\psi_n = \varepsilon_n \psi_n$.

基态 $E = \langle\psi|H|\psi\rangle / \langle\psi|\psi\rangle$

③ 统计力学.

$$H = p^2 + x^2 + \alpha x^4$$

$$Z = \int dp\, dx\, e^{-\beta H}$$

MC方法 (Monte-Carlo方法)

计算 $\int dx_1 dx_2 dx_3 dx_4 dx_5\, f(x_1 \cdots x_5)$

Runge-kutta.

1) $O(h^3)$

2) 稳定性. ⇒ 简单.

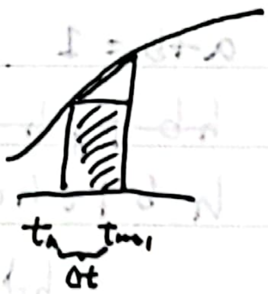
构造:

$$y' = f(t, y)$$

$$y_{n+1} = y_n + \int_{t_n}^{t_n+\Delta t} f(t, y)\, dt.$$

$$y_{n+1} = y_n + f(t_n, y_n)\Delta t.$$

$$y_{n+1} = y_n + \frac{1}{2}[f(t_n, y_n) + f(t_{n+1}, y_{n+1})] \times \Delta t$$



$$y_{n+1} = y_n + \frac{1}{2}[f(t_n, y_n) + f(t_n+\Delta t, y_n + \Delta t f(t_n, y_n))] + O(\Delta t^3)$$

迭代

没有导数

只要算2次f

Runge-kutta 23 (rk23). 2阶算法. 精度3阶.

令 $h=\Delta t$

$$y(t_{n+1}) = y_i(t_n) + \int_{t_n}^{t_{n+1}} f(t, y(t))\,dt.$$

$$\begin{aligned} y(t_{n+1}) &= y(t_n+h) \\ &= y(t_n) + y'h + \tfrac{1}{2}y''h^2 + O(h^3). \\ &= y(t_n) + f(t_n, y_n)h + \tfrac{1}{2}y''h^2 + O(h^3) \\ &= y + fh + \tfrac{1}{2}(f_t + f_y f)h^2 + O(h^3) \end{aligned}$$

$\Rightarrow$ 算3次.

$y' = f(t, y)$.

$y'' = f_t + f_y y' = f_t + f_y f$

导数.

RK算法核心

出发点: 不算导数.

rk23 = 梯形.

$$y(t_{n+1}) = y(t_n) \cancel{+f(t_n)} fh + \tfrac{1}{2}(f_t + f_y f)h^2 +$$

$$= y(t_n) + h[af(t_n, y_n) + bf(t_n + h\,dx, y_n + h\,dy)] + O(h^3)$$

$$= y(t_n) + h(af(t_n, y_n) + bf(t_n, y_n) + bf_t h\,dx + bf_y h\,dy] + O(h^3)$$

$a+b=1$.

$\cancel{hbf_y h\,dy}$

$h\,b f_t h\,dx = \tfrac{1}{2} f_t h^2$

$b\,dx = \tfrac{1}{2} \Rightarrow dx = 1$.

$\tfrac{1}{2} f_y f h^2 = b f_y h^2 dy$

$dy = f$.

~~$\Rightarrow y_{n+1} = y$~~

$\Rightarrow y(t_{n+1}) = y(t_n) + h[a f(t_n, y_n) + b f(t_n+h, y_n+hf)] + O(h^3)$

与之前结果相同.

Rk45.

$y(t_n+h) = y(t_n) + y'h + \frac{1}{2} y''h^2 + \frac{1}{3!} y'''h^3 + \frac{1}{4} y^{(4)}h^4 + O(h^5)$

$y_{n+1} = y_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)$.

$k_1 = f(t_n, y_n)$.

$k_2 = f(t_n + \frac{1}{3}h, y_n + \frac{1}{3}hk_1)$.

$k_3 = f(t_n + \frac{2}{3}h, y_n - \frac{1}{3}hk_1 + hk_2)$.

$k_4 = f(t_n+h, y_n + hk_1 - hk_2 + hk_3)$

①最广泛应用. ②形式不唯一. $\rightarrow a+b=1$.

代码 code.

ode(f, eqn, y, t, tout, relerr, abserr, iflag, work, iwork).

变步长 rk45.

Runge-Kutta可以用来算积分. $f(t, y) = f(t)$

$\int_0^t f(t)\,dt$.

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

$$\frac{\partial^2}{\partial x^2}\psi = E\psi$$

$\Downarrow$

对角阵

$$\frac{\partial^2}{\partial x^2}\psi = \frac{\psi_{n+1}+\psi_{n-1}-2\psi_n}{\Delta x^2}.$$

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

符号：u_i^n $n \to$ 时间，$i \leftarrow$ 空间.

$$\frac{u_i^{n+1}-u_i^n}{\Delta t} = a^2 \frac{u_{i+1}^n+u_{i-1}^n-u_i^n}{\Delta x^2}$$

$$y_{n+1} = y_n + h f(t_n, y_n)$$
$$= y_n + \frac{h}{2}[f(t_n, y_n) + f(t_{n+1}, y_{n+1})].$$

$$\gamma = \frac{\Delta t}{\Delta x^2} a^2$$

$$u_i^{n+1} = u_i^n + \gamma(u_{i+1}^n + u_{i-1}^n - 2u_i^n)$$
$$= \gamma(u_{i+1}^n + u_{i-1}^n) + (1-2\gamma)u_i^n.$$
$$u^{n+1} = Tu^n = T^2u^{n-1} = \cdots = T^n u^1$$

T: 三对角阵

$$T = U^+ \lambda U \qquad T^n = U^+ \lambda^n U.$$

Crank-Nicolson method.

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

同样 $r = \frac{\Delta t\, a^2}{\Delta x^2}$

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

$T_L U^{n+1} = T_R U^n$. T_L, T_R 三对角

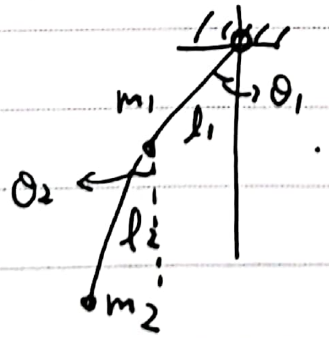
$U^{n+1} = T_L^{-1} T_R U^n = T U^n$.

应用:

mma, NSolve
NDSolve.

Integrate. 解析
NIntegrate. 数值
Solve. 解析 NSolve 数值. DSolve 微分方程.

作业: 1)



2d. 3d.

$\mathcal{L} = T - V$

$x_1 = l_1 \sin\theta_1 \quad y_1 = -l_1 \cos\theta_1$

$x_2 = l_1 \sin\theta_1 + l_2 \sin\theta_2$.

$y_2 = -l_1 \cos\theta_1 - l_2 \cos\theta_2$.

$T = \frac{1}{2} m_1(\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2} m(\dot{y}_2^2 + \dot{x}_2^2)$

$U = -m_1 g y_1 - m_2 g y_2$. ⇒ 运动方程.

2). 求 $\frac{\partial}{\partial t}u = a^2\frac{\partial^2}{\partial x^2}u$ 扩散方程.

$u \sim e^{-x^2/4at} \Rightarrow \langle x^2\rangle \propto t$.

数值结果与手推结果作比对.
h 对精度的影响.
空间, 时间的间隔对精度的影响.

计算物理从简单到复杂:

时) 分子动力学
一样(: flocking behavior
复杂系统. Lorentz model.
⇓
chaos.