

Numerical Solutions of Partial Differential Equations

偏微分方程数值解

--Why PDE or NMPDE?

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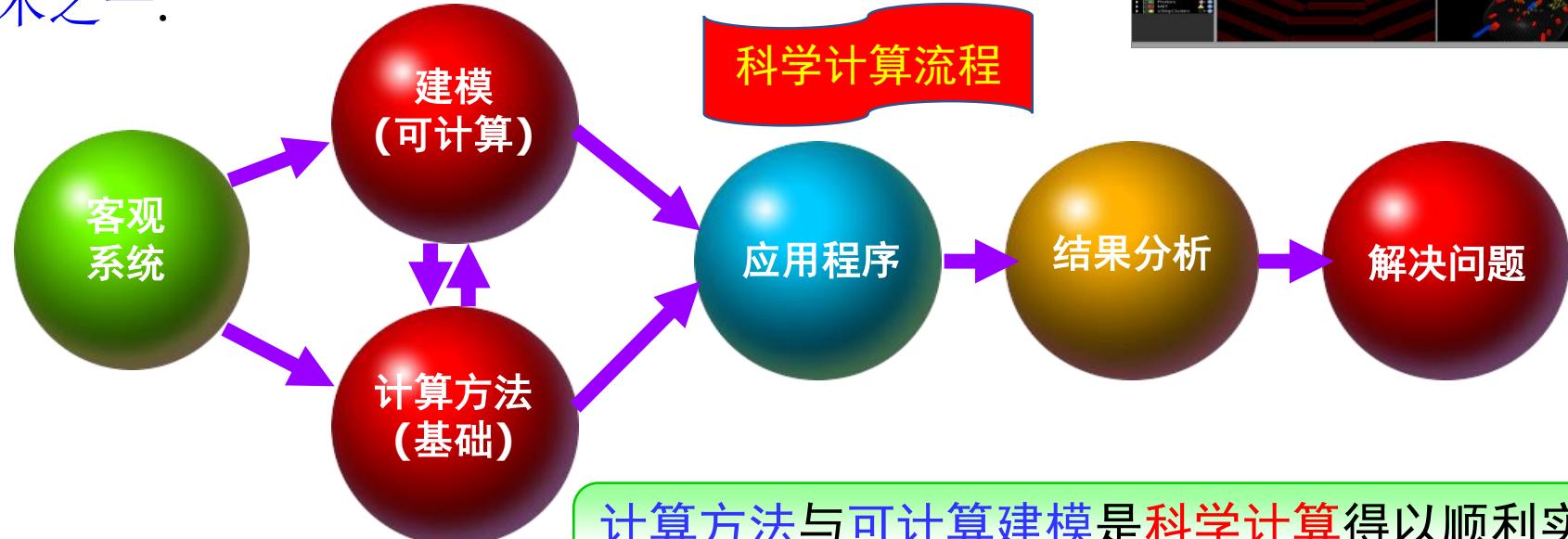
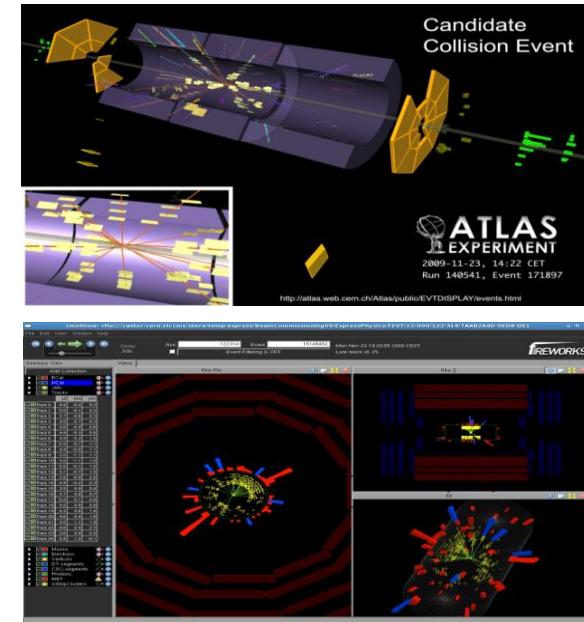
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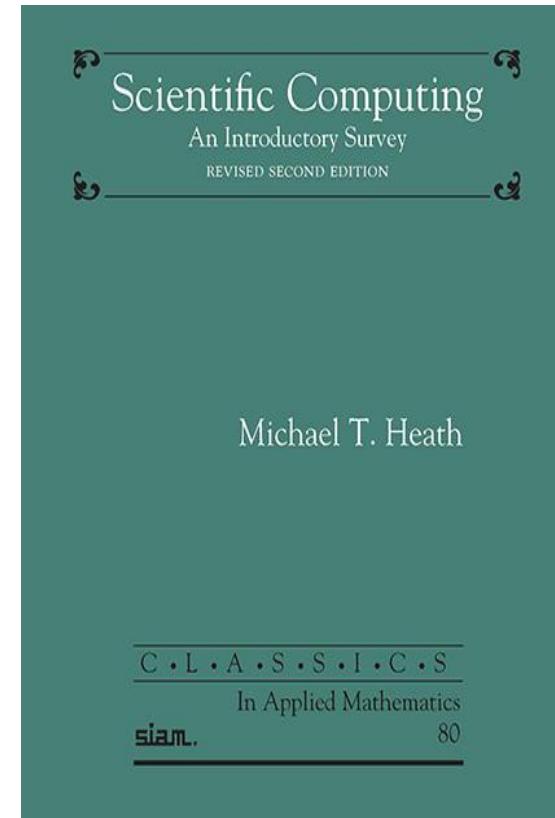
引言

- 科学计算的核心/数学基础：计算数学，有时也称为数值分析。
- 科学计算是20世纪重要科学技术进步之一，已与理论研究和实验研究相并列成为科学的研究的第三种方法。
- 在迅猛发展的高性能计算技术推动下，**计算科学**将是21世纪确保国家核心竞争能力的战略技术之一。



SCIENTIFIC COMPUTING: AN INTRODUCTORY SURVEY

1. [Scientific Computing](#)
2. [Systems of Linear Equations](#)
3. [Linear Least Squares](#)
4. [Eigenvalue Problems](#)
5. [Nonlinear Equations](#)
6. [Optimization](#)
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9. [Initial Value Problems for ODEs](#)
10. [Boundary Value Problems for ODEs](#)
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微分方程

- ✓ ODE/PDE是用于对自然界问题进行建模的最广泛工具之一，它出现在许多物理、化学和生物现象的数学模型（例如污染物在湖泊和河流中的扩散、疾病的传播、天气预报、武器研制等）中，如Euler及Navier-Stokes方程、Maxwell方程、Boltzmann方程、Einstein方程等，这也体现科学与工程技术及诸多领域与偏微分方程的“难分难舍”。
- ✓ PDE和计算数学是数学研究中的两大领域。二者亟待解决的问题很多，是大有可为的领域。PDE研究人员要了解计算科学，从事计算的人员也应时刻关注PDE的现状和进展。
- ✓ 实际的PDE往往非常复杂，对高维PDE存在众所周知的被称为“维数灾难”的困难（量子多体物理中“指数墙”困难）：求解这些高维PDE的计算成本随着维数呈指数增长。

微分方程数值方法

- **有限差分法**: FDM中的未知量为微分方程定解问题的解的离散点值/网格点值。差商近似微商、待定系数(Taylor展开确定)、插值法(插值出多项式后再求导)、积分法(后来的有限体积做法)等。
- **有限元方法**: 包括连续有限元方法、不连续有限元方法(间断 Galerkin方法); 协调FE, 非协调FE, 混合(mixed, hybrid) FE....。在 FEM函数空间(有限维的具有局部紧致性的函数空间)中近似微分方程定解问题的解, FE方程中未知量是自由度或基函数展开系数。
- **有限体积方法**: 包括格点FVM和格心FVM。FV方程中的未知量为微分方程定解问题的解的单元(控制体)平均值。
- **谱(spectral)方法**: 包括配置法, tau方法, 拟谱方法/配置(谱)方法(1970), Galerkin型方法。与FEM类似, 利用正交函数逼近微分方程定解问题的解, 但不同于FEM的是, 是在整个区域中逼近。
- **边界积分方法**: 问题化为区域边界上积分方程, 离散区域边界和积分方程
- **无网格方法**: 区域内散乱地撒点, 点之间不连线, 离散问题
- **随机模拟方法、快速方法、.....**

计算：无限化有限，连续化离散

- 处理连续量，考虑近似或离散的影响（例如近似解和精确解的差多大，是否可控制等）

例1: $y = \sin(x), x \in [0, 2\pi]$

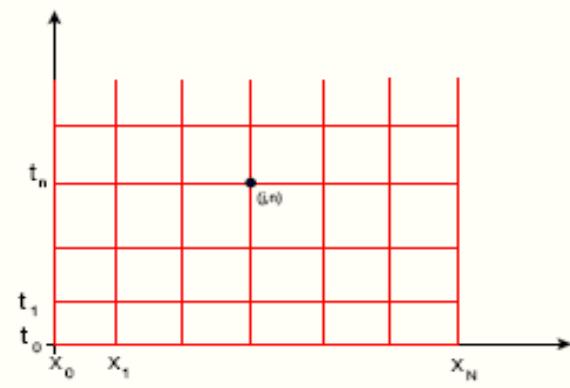
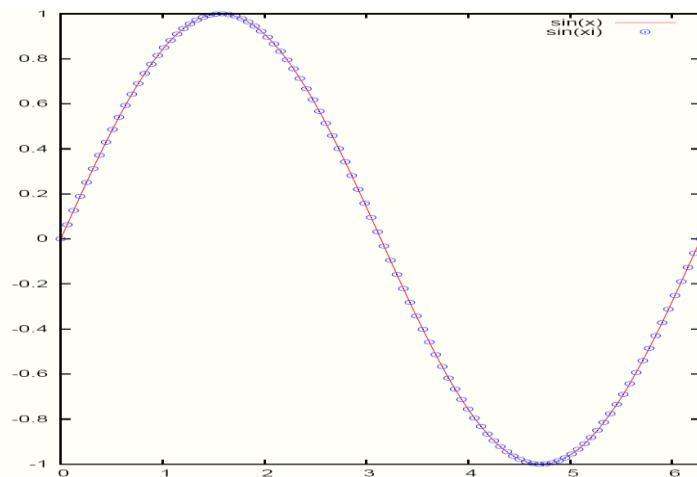


$$y_i = \sin(x_i), x_i = ih, h = \frac{2\pi}{N}$$

例2: $(x, t) \in [0, 2\pi) \times [0, T]$



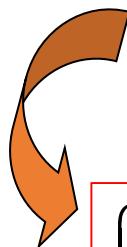
$$x_i = ih, t_n = n\tau; i = 0, 1, \dots, N; n = 0, 1, \dots$$



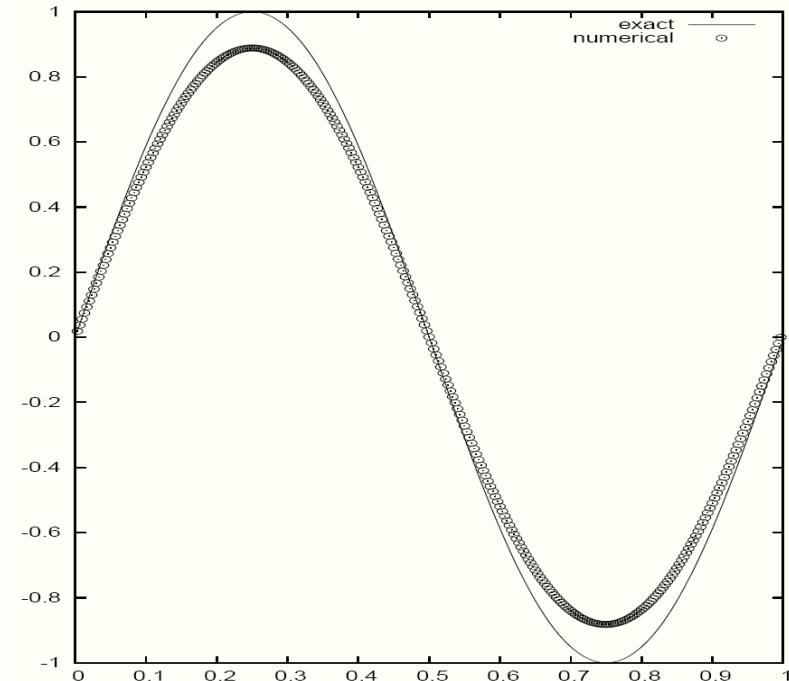
- 优点：简单、便宜；
- 缺点：只得到近似解、对计算机的硬件和软件有一定依赖。

例3：

$$\begin{cases} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, x \in (0, 2\pi), \\ u(x, 0) = \sin(x), u(0, t) = u(2\pi, t) \end{cases}$$



$$\begin{cases} \frac{u_i^{n+1} - u_i^n}{\tau} + \frac{u_i^n - u_{i-1}^n}{h} = 0, i = 1, 2, \dots, N \\ u_i^0 = \sin(x_i), u_0^{n+1} = u_N^{n+1} \end{cases}$$



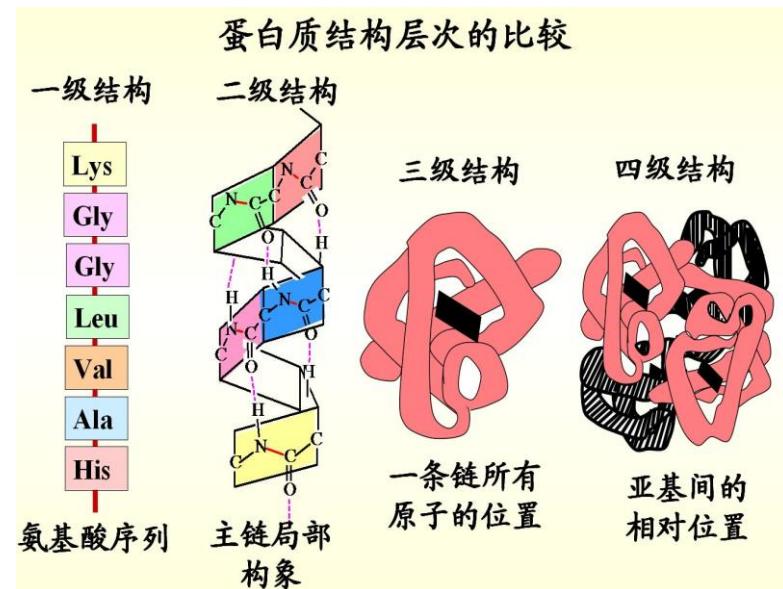
FDM思想

$$\frac{df(x)}{dx} = \lim_{\Delta x \rightarrow 0} \frac{\Delta f}{\Delta x} \approx \frac{\Delta f}{\Delta x}$$

The “**differential**” $\frac{df(x)}{dx} \approx \frac{\Delta f}{\Delta x}$ The “**difference**”

问题1：如何理解蛋白质折叠？

- 蛋白质折叠是21世纪生物学的重要课题.



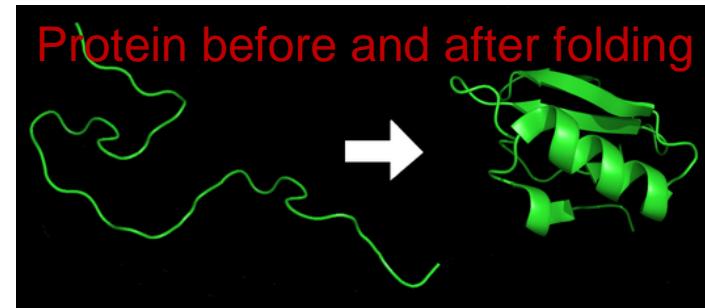
蛋白质折叠定义

- 蛋白质折叠：从一条结构松散的多肽链折叠成具有天然空间结构（三级和四级）的蛋白质分子的过程称为蛋白质折叠（protein folding）。
- 狭义是蛋白质特定三维空间结构形成的规律、稳定性和与其生物活性的关系。
- 蛋白质折叠是物理过程。多肽折叠成特定功能的三维结构，
- “分子伴侣”的发现和鉴定改变了蛋白质折叠研究的经典概念

意义：蛋白质折叠机制的阐明将揭示生命体内的第二套遗传密码, 对包涵体的复性会由重要帮助. 蛋白质高级结构的预测. 按照自己意愿设计所需要的、具有特定功能的蛋白质.....

Molecular Dynamics is an important tool for studying protein folding and dynamics in silico[生物信息学].

H.A. Scheraga, M. Khalili, and A. Liwo, Protein-Folding Dynamics: Overview of Molecular Simulation Techniques, Annu. Rev. Phys. Chem. 2007. 58:57–83.



ODE数值求解

- 考虑一阶ODE初值问题

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0.$$

- Euler 方法

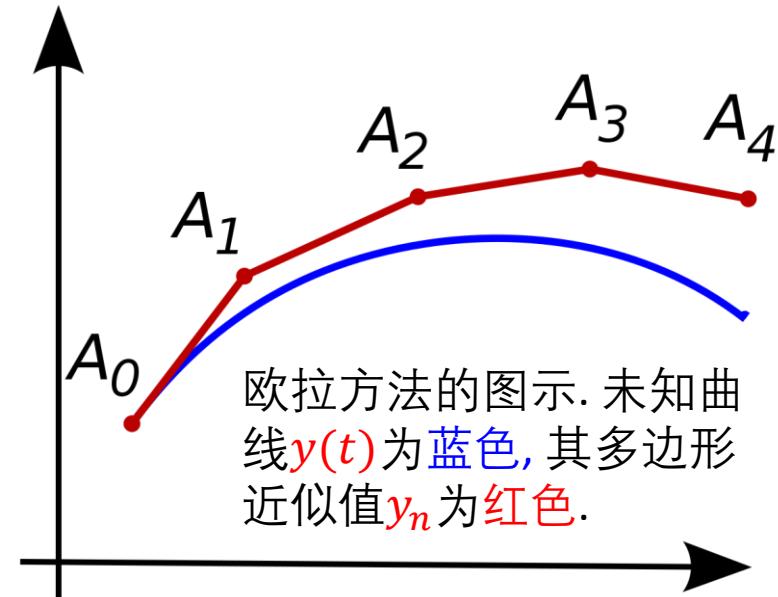
$$y_{n+1} = y_n + h f(t_n, y_n).$$

- 如何应用到N阶ODE

$$y^{(N)}(t) = f(t, y(t), y'(t), \dots, y^{(N-1)}(t)).$$

- 引入辅助变量

$$z_1(t) = y(t), z_2(t) = y'(t), \dots, z_N(t) = y^{(N-1)}(t)$$



$$\mathbf{z}'(t) = \begin{pmatrix} z'_1(t) \\ \vdots \\ z'_{N-1}(t) \\ z'_N(t) \end{pmatrix} = \begin{pmatrix} y'(t) \\ \vdots \\ y^{(N-1)}(t) \\ y^{(N)}(t) \end{pmatrix} = \begin{pmatrix} z_2(t) \\ \vdots \\ z_N(t) \\ f(t, z_1(t), \dots, z_N(t)) \end{pmatrix}$$

ODE数值求解

- 考虑一阶ODE初值问题

$$y'(t) = f(t, y(t)), \quad y(t_0) = y_0.$$

- 其它方法

$$y_{n+1} = y_n + h f(t_{n+1}, y_{n+1}). \quad \text{backward Euler方法}$$

$$y_{n+1} = y_n + h f\left(t_n + \frac{1}{2}h, y_n + \frac{1}{2}h f(t_n, y_n)\right). \quad \text{midpoint方法}$$

$$y_{n+1} = y_n + \frac{3}{2}h f(t_n, y_n) - \frac{1}{2}h f(t_{n-1}, y_{n-1}). \quad \text{2-step Adams–Bashforth方法}$$

$$y_{n+1} = y_n + h \sum_{i=1}^s b_i k_i, \quad \text{family of explicit Runge–Kutta方法}$$

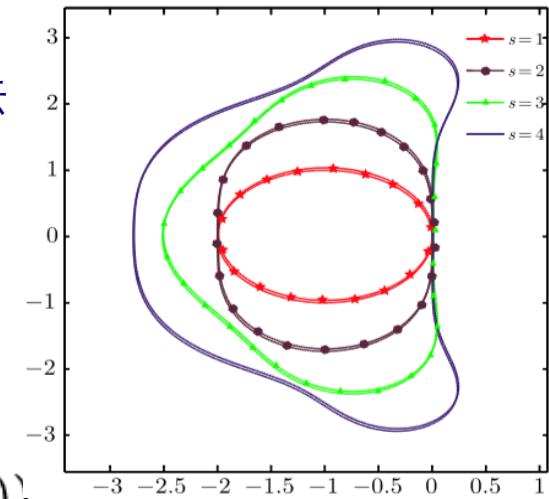
$$k_1 = f(t_n, y_n),$$

$$k_2 = f(t_n + c_2 h, y_n + h(a_{21} k_1)),$$

$$k_3 = f(t_n + c_3 h, y_n + h(a_{31} k_1 + a_{32} k_2)),$$

⋮

$$k_s = f(t_n + c_s h, y_n + h(a_{s1} k_1 + a_{s2} k_2 + \cdots + a_{s,s-1} k_{s-1})).$$



ODE数值求解

例4: 求解Lorenz方程组的初值问题

含时间参数的形式: Lorenz方程

$$\begin{aligned}\frac{dx}{dt} &= -10x + 10y, & \frac{dy}{dt} &= 28x - y - x \\ x(0) &= 10, & y(0) &= -10, & z(0) &= 20,\end{aligned}$$

$$\begin{cases} \frac{dx(t)}{dt} = \sigma(y(t) - x(t)) \\ \frac{dy(t)}{dt} = \rho x(t) - y(t) - x(t)z(t) \\ \frac{dz(t)}{dt} = x(t)y(t) - \beta z(t) \end{cases}$$

by using the 4th order accurate, explicit F

$$x^{(1)} = x^n + \frac{1}{2}\tau f(x^n),$$

$$x^{(2)} = x^n + \frac{1}{2}\tau f(x^{(1)}),$$

$$x^{(3)} = x^n + \tau f(x^{(2)}),$$

$$x^{n+1} = \frac{1}{3} \left(x^{(1)} + 2x^{(2)} + x^{(3)} \right)$$

σ 称为普兰特尔数, ρ 称为瑞利数。所有的 $\sigma, \rho, \beta > 0$ 但通常 $\sigma = 10, \beta = 8/3, \rho$ 不定。若 $\rho < 1$, 则吸引子为原点, 没有任何其他稳定点。 $1 \leq \rho < 13.927$ 时, 螺线轨迹接近两点 (这相当于存在阻尼振子), 两点的位置由下列式子决定: $x = \pm \sqrt{b(\rho - 1)}$ 、 $y = \pm \sqrt{b(\rho - 1)}$ 、 $z = \rho - 1$ 。系统在 $\rho = 28$ 时表现出混沌特性, 但 ρ 为其他值时会显示出具扭结的周期轨道。例如, 当 $\rho = 99.96$ 时,

for $n = 0, 1, \dots, 1000$, where $\tau = 10/100$ 图像变为一个 $\pi(3,2)$ 环面扭结。

ODE数值求解

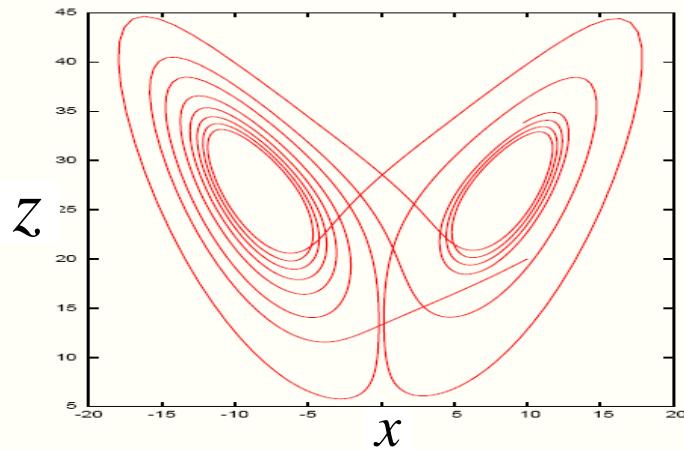
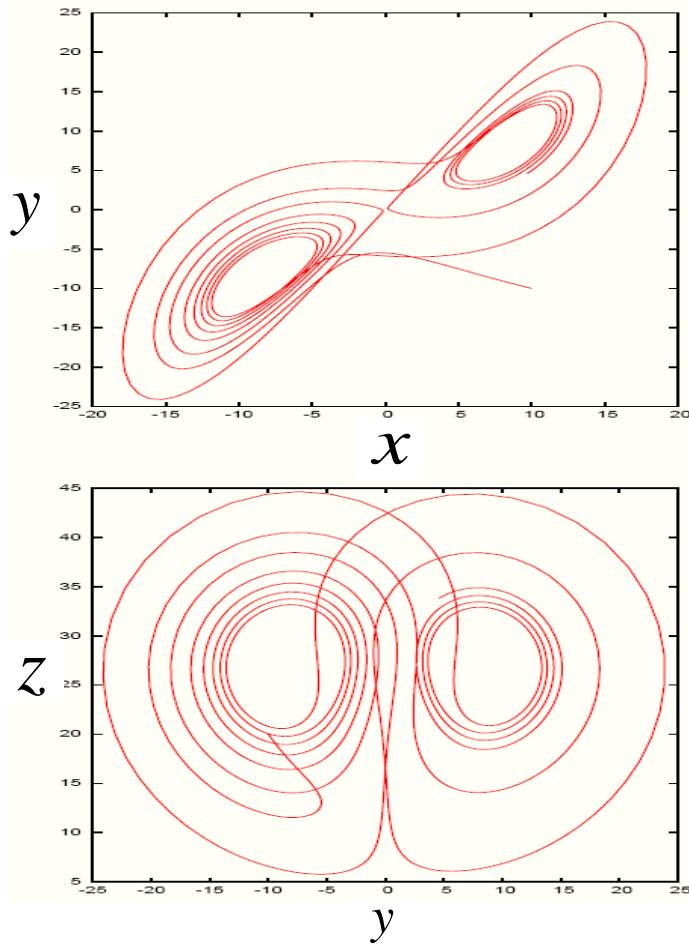
FORTRAN程序

```
x(1,1)=10.0  
x(2,1)=-10.0  
x(3,1)=20.0  
  
do n=2,np  
xx=x(1,n-1)  
yy=x(2,n-1)  
zz=x(3,n-1)  
rhs1=fx(xx,yy,zz)  
rhs2=fy(xx,yy,zz)  
rhs3=fz(xx,yy,zz)  
xx01=xx+0.5*dt*rhs1  
yy01=yy+0.5*dt*rhs2  
zz01=zz+0.5*dt*rhs3  
  
rhs1=fx(xx01,yy01,zz01)  
rhs2=fy(xx01,yy01,zz01)  
rhs3=fz(xx01,yy01,zz01)
```

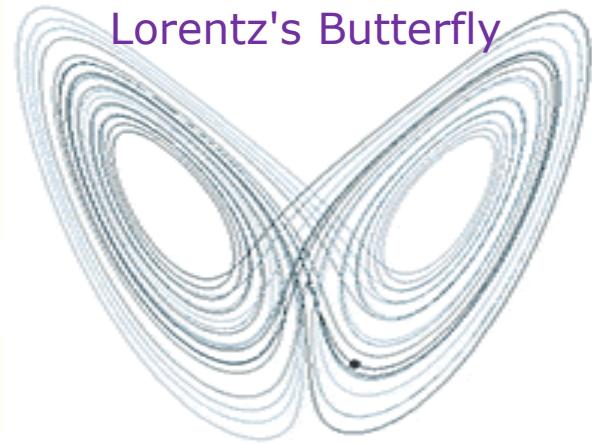
```
xx02=xx+0.5*dt*rhs1  
yy02=yy+0.5*dt*rhs2  
zz02=zz+0.5*dt*rhs3  
  
rhs1=fx(xx02,yy02,zz02)  
rhs2=fy(xx02,yy02,zz02)  
rhs3=fz(xx02,yy02,zz02)  
xx03=xx+dt*rhs1  
yy03=yy+dt*rhs2  
zz03=zz+dt*rhs3  
  
rhs1=fx(xx03,yy03,zz03)  
rhs2=fy(xx03,yy03,zz03)  
rhs3=fz(xx03,yy03,zz03)  
x(1,n)=(xx01+2.*xx02+xx03-xx+0.5*dt*rhs1)/3.  
x(2,n)=(yy01+2.*yy02+yy03-yy+0.5*dt*rhs2)/3.  
x(3,n)=(zz01+2.*zz02+zz03-zz+0.5*dt*rhs3)/3.  
enddo
```

/test/lorenz-attractor.f

ODE数值求解



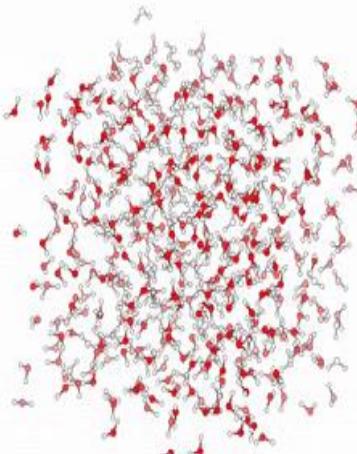
Lorentz's Butterfly



Lorenz系统是一个ODE/动力系统, 对于某些参数值和初始条件具有混沌解是值得注意的. 尤其是Lorenz吸引子(Lorenz振子的长期行为对应的分形结构)是Lorenz系统的一组混沌解. “蝴蝶效应”源于Lorenz吸引子的真实含义, 即在任何物理系统中, 在缺乏对初始条件的完全了解(甚至是蝴蝶拍打翅膀而造成的微小空气扰动的情况下, 能够预测它的未来路线总是失败的.

ODE数值求解

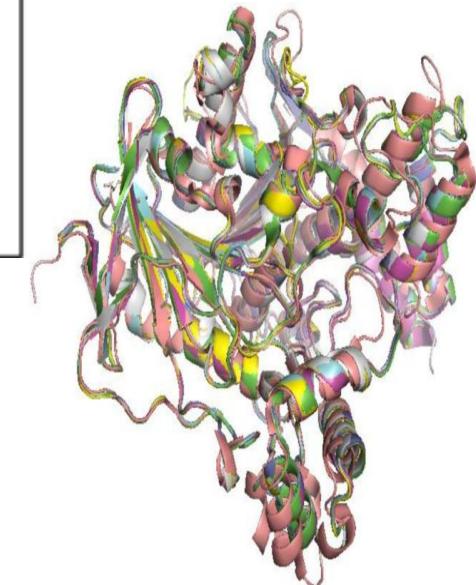
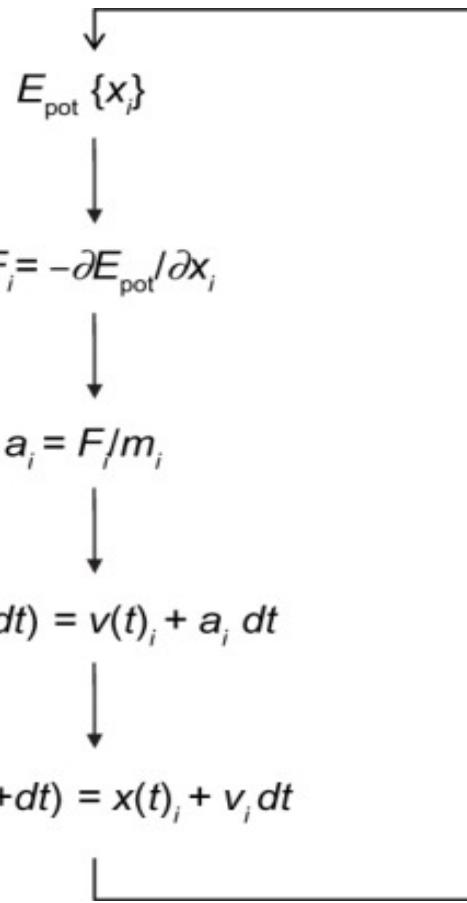
Molecular dynamics (MD) 基本算法



Energy calculation
(force-field)

Forces

Numerical
integration



MD模拟常用于研究生物物理系统。
上图描述的是水的100皮秒模拟。

<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC4655909/>

蛋白质家族的结构变异

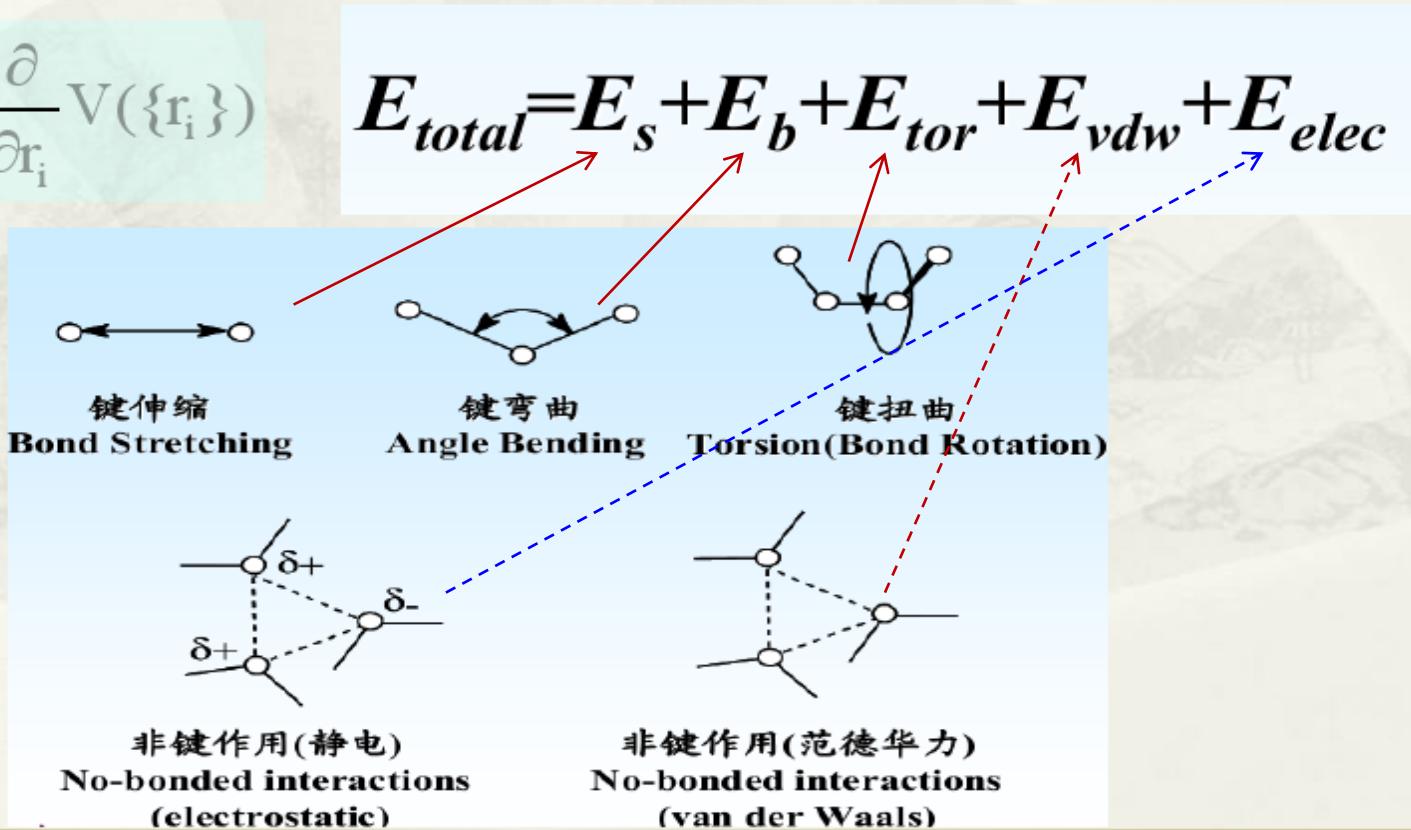
ODE数值求解

势能函数形式

- * 分子力学中势能面是用解析经验势函数来描述的，体系的势函数可以分解成多种势函数的共同作用。通常分为键伸缩能 E_s 、键弯曲能 E_b 、二面角扭曲能 E_{tor} 、范德华作用能 E_{vdw} 和静电作用能 E_{elec}

$$m_i \frac{d^2}{dt^2} r_i = -\frac{\partial}{\partial r_i} V(\{r_i\})$$

$$E_{total} = E_s + E_b + E_{tor} + E_{vdw} + E_{elec}$$



ODE数值求解

简单力场的函数形式

$$V(r^N) = \sum_{bond} \frac{k_i}{2} (l_i - l_{i,0})^2 + \sum_{angles} \frac{k_i}{2} (\theta_i - \theta_{i,0})^2 + \sum_{torsion} \frac{V_n}{2} (1 + \cos(n\omega - \gamma)) \\ + \sum_{i=1}^N \sum_{j=i+1}^N \left(4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r_{ij}} \right)$$

兰纳-琼斯势 范德华作用

第一项表示成键原子间的相互作用

第二项表示分子中所有键角的贡献，用的均为谐振子模型

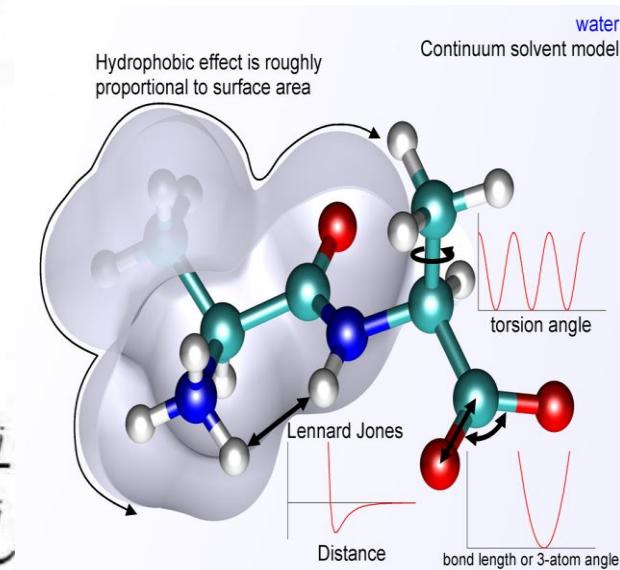
第三项为扭曲势，表示键旋转时的能量变化

第四项是非键项，在简单力场中，用Lennard-Jones势描述van der Waals作用,库仑势描述静电相互作用。

ODE数值求解

通过(化学)键连接的原子间的相互作用
+ 描述静电与范德华力的非键作用部分

$$U(\vec{R}) = \underbrace{\sum_{bonds} k_i^{bond} (r_i - r_0)^2}_{U_{bond}} + \underbrace{\sum_{angles} k_i^{angle} (\theta_i - \theta_0)^2}_{U_{angle}} + \underbrace{\sum_{dihedrals} k_i^{dih} [1 + \cos(n_i \phi_i + \delta_i)]}_{U_{dihedral}} + \underbrace{\sum_i \sum_{j \neq i} 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \sum_i \sum_{j \neq i} \frac{q_i q_j}{\epsilon r_{ij}}}_{U_{nonbond}}$$



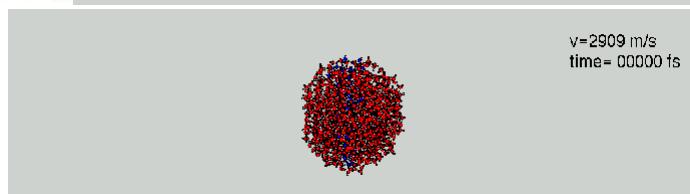
U_{bond} = oscillations about the equilibrium bond length

U_{angle} = oscillations of 3 atoms about an equilibrium bond angle

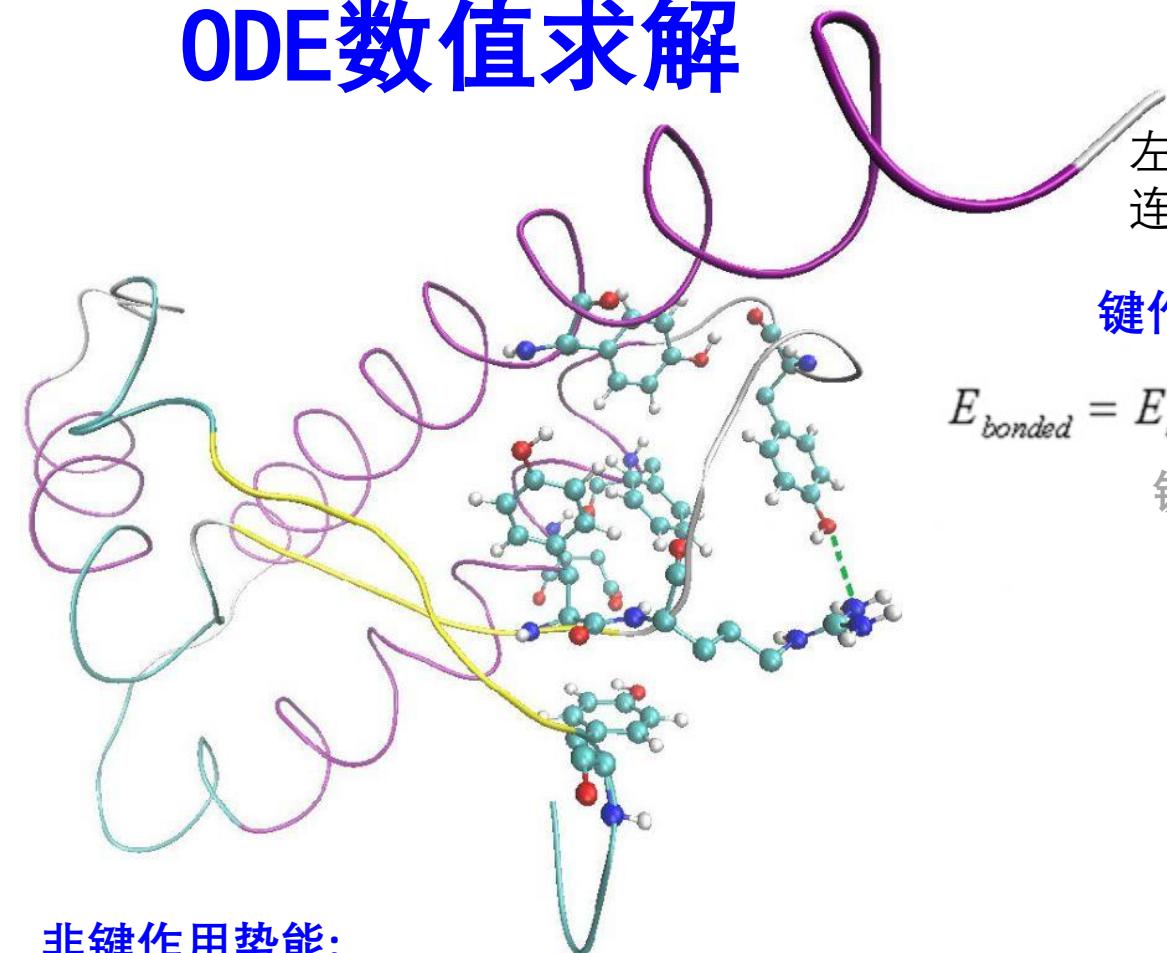
$U_{dihedral}$ = torsional rotation of 4 atoms about a central bond

$U_{nonbond}$ = non-bonded energy terms (electrostatics and Lenard-Jones)

MD模拟：由1032个分子组成的冷结晶水团，
它们以2909 m/s的撞击速度与排斥壁相撞。
<http://www2.mpq.mpg.de/~ant/MD.html>



ODE数值求解

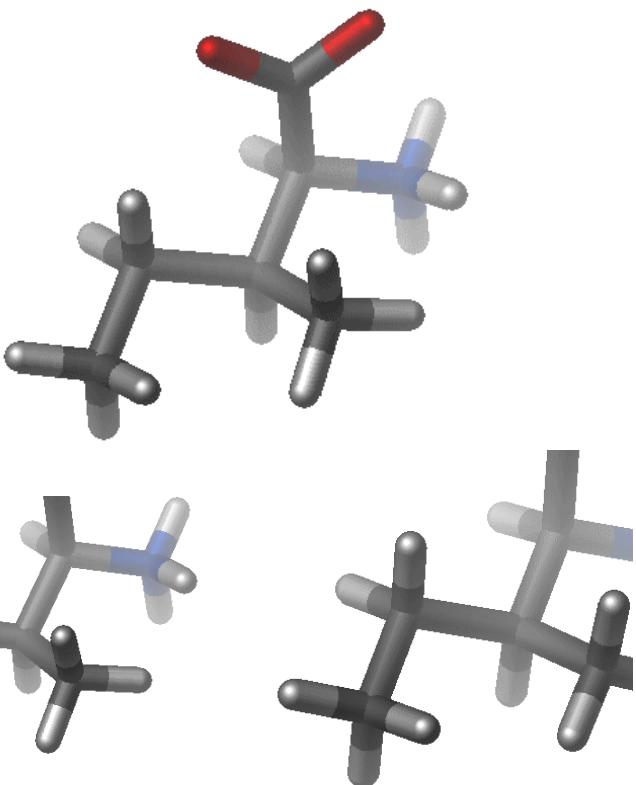


左图中的小球(原子)间的棒就是键;
连接两小球的那个虚线, 就不是键.

键作用势能:

$$E_{bonded} = E_{bond-stretch} + E_{angle-bend} + E_{rotate-along-bond}$$

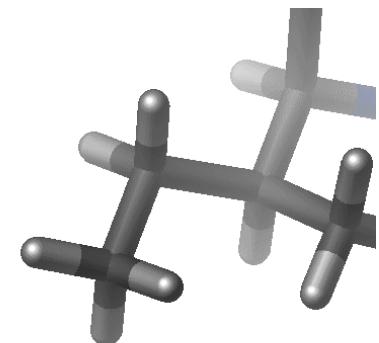
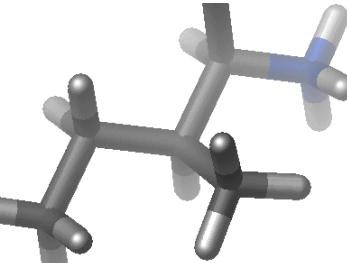
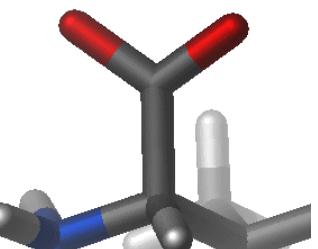
键伸展, 键弯曲, 绕键旋转/扭曲



非键作用势能:

$$E_{non-bonded} = E_{van-der-Waals} + E_{electrostatic}$$

$$= \sum_{i,j} \left\{ 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{\epsilon D r_{ij}} \right\}$$



ODE数值求解

- Hamilton 系统

$$\dot{p} = -\frac{\partial H}{\partial q} \quad \text{and} \quad \dot{q} = \frac{\partial H}{\partial p},$$

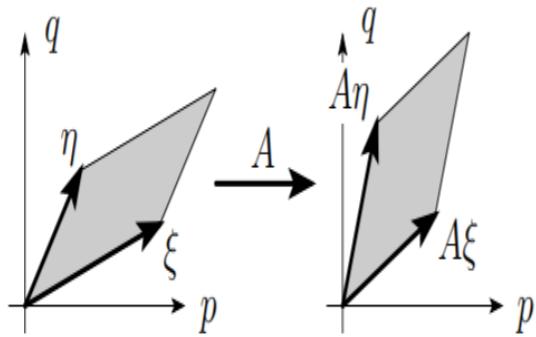
其中 q 表示位置坐标, p 表示动量坐标,
 H 表示哈密顿量.

辛同构或辛映射是辛流形范畴中的同构. 在经典力学中, 辛同构表示相空间的一种变换, 它是保持体积的, 并保留了相空间的辛结构, 称为正则变换.

- 辛Euler 方法

$$\begin{aligned} p_{n+1} &= p_n - h \nabla_q H(p_{n+1}, q_n) & p_{n+1} &= p_n - h \nabla_q H(p_n, q_{n+1}) \\ q_{n+1} &= q_n + h \nabla_p H(p_{n+1}, q_n) & \text{or} & \\ & & q_{n+1} &= q_n + h \nabla_p H(p_n, q_{n+1}) \end{aligned}$$

- 韦尔雷(Verlet)方法



Symplecticity (area preservation) of a linear mapping.

汉密尔顿系统的时间演化是一种辛同构, 这意味着它保持辛二形(微分形式) $dp \wedge dq$. 如果一个数值格式也能保持这个二形式, 它就是辛的.

$$\begin{aligned} p_{n+1/2} &= p_n - \frac{h}{2} \nabla_q H(p_{n+1/2}, q_n) \\ q_{n+1} &= q_n + \frac{h}{2} \left(\nabla_p H(p_{n+1/2}, q_n) + \nabla_p H(p_{n+1/2}, q_{n+1}) \right) \\ p_{n+1} &= p_{n+1/2} - \frac{h}{2} \nabla_q H(p_{n+1/2}, q_{n+1}) \\ q_{n+1/2} &= q_n + \frac{h}{2} \nabla_p H(p_n, q_{n+1/2}) \\ p_{n+1} &= p_n - \frac{h}{2} \left(\nabla_q H(p_n, q_{n+1/2}) + \nabla_q H(p_{n+1}, q_{n+1/2}) \right) \\ q_{n+1} &= q_{n+1/2} + \frac{h}{2} \nabla_p H(p_{n+1}, q_{n+1/2}) \end{aligned}$$

ODE数值求解

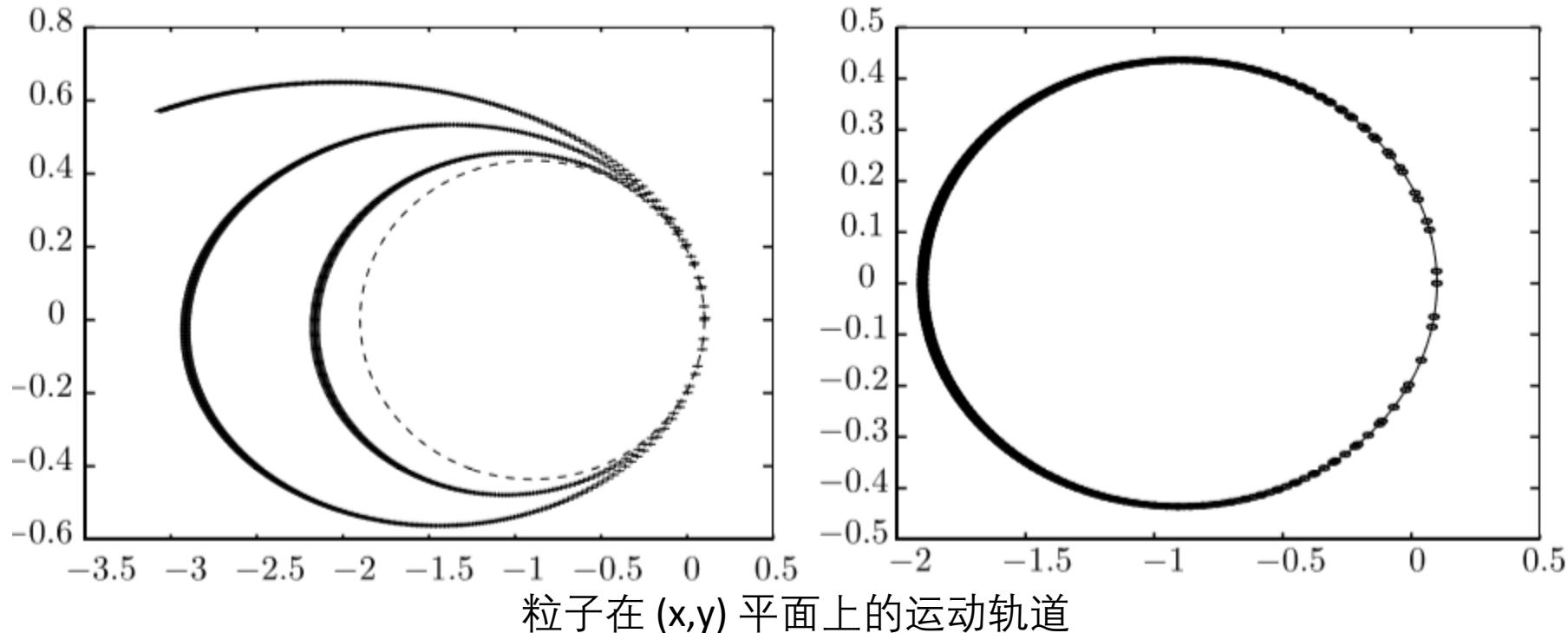
- 例5:开普勒 (Kepler) 问题 $\frac{d}{dt}\mathbf{r} = M^{-1}\mathbf{p}, \quad \frac{d}{dt}\mathbf{p} = \mathbf{f}(\mathbf{r}),$

$$\mathbf{r} = (x, y)^T, \quad \mathbf{p} = \dot{\mathbf{r}} = \frac{d}{dt}\mathbf{r}, \quad V(x, y) = -(x^2 + y^2)^{-1/2}, \quad \mathbf{f}(\mathbf{r}) = -\nabla_{\mathbf{r}}V(\mathbf{r}).$$

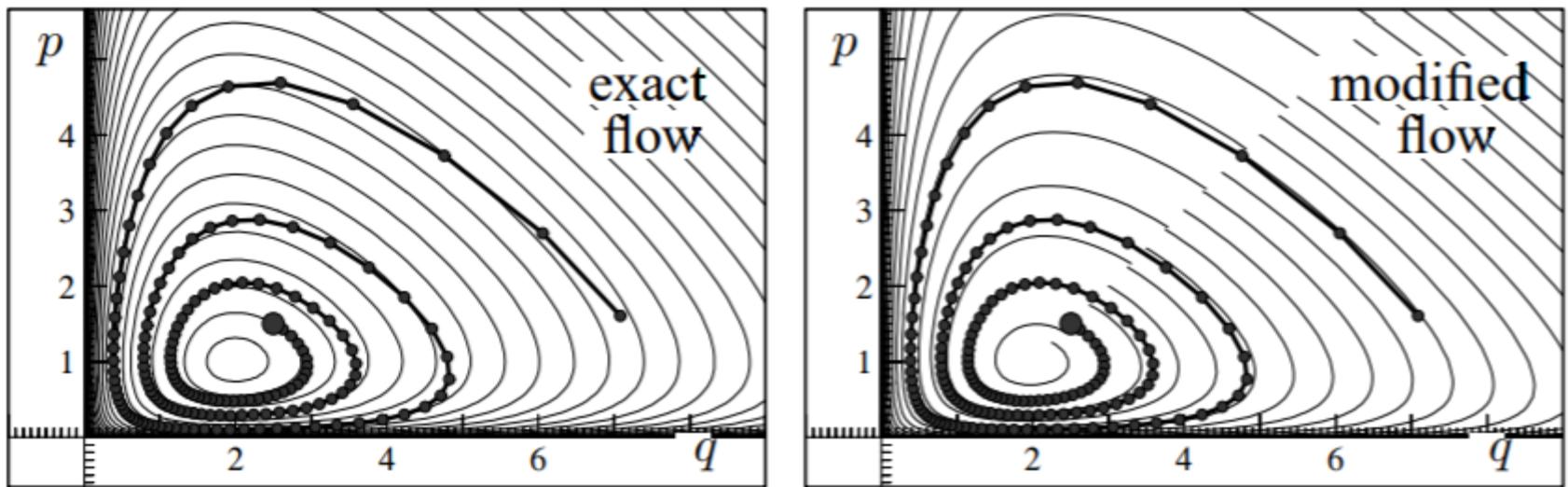
$$x(0) = 1 - a, \quad \dot{x}(0) = 0, \quad y(0) = 0, \quad \dot{y}(0) = \sqrt{(1+a)/(1-a)},$$

参数 a 表示轨道的离心率. 计算中取 $a = 0.9$, 旋转周期为 2π , M 为单位矩阵.

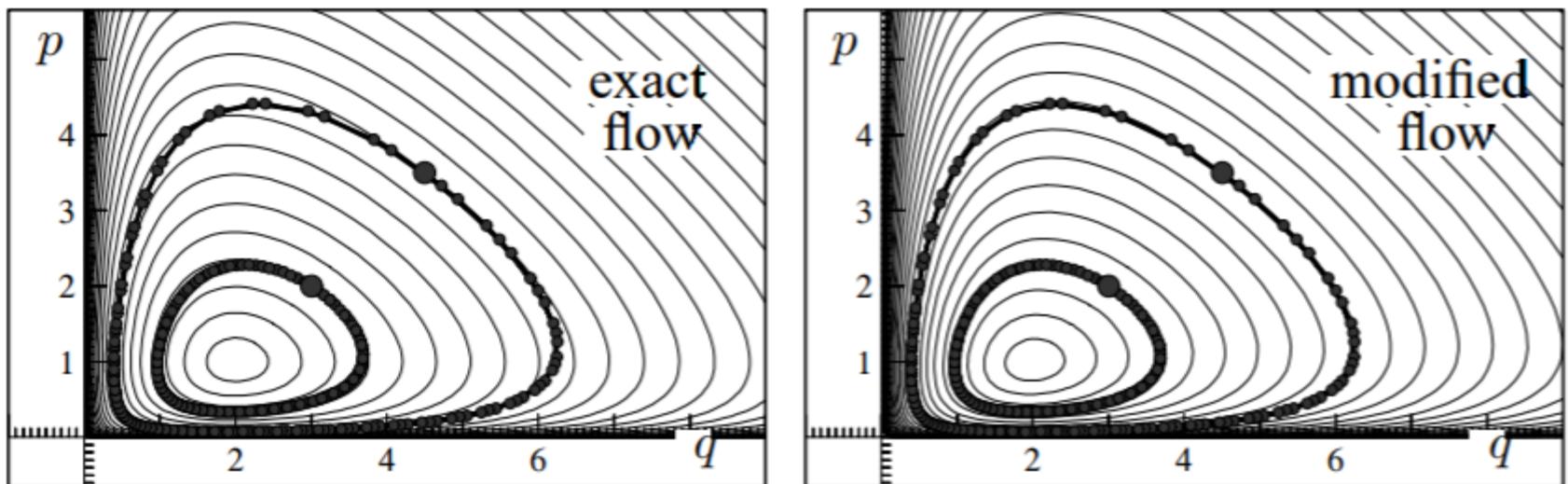
结果: 显式 Euler 方法得到了错误的轨道, 而 Verlet 方法可以获得正确轨道.



(a) explicit Euler, $h = 0.1$



(b) symplectic Euler, $h = 0.1$



图： Numerical solution compared to the exact and modified flows.

https://www.unige.ch/~hairer/poly_geoint/week3.pdf



ODE数值求解

- 2阶ODE边值问题 $y''(t) = f(t, y(t), y'(t)), \quad y(t_0) = y_0, \quad y(t_1) = y_1$
- 试射法：化为ODE初值问题求解.

为求解BVP, 先解IVP

$$y''(t) = f(t, y(t), y'(t)), \quad y(t_0) = y_0, \quad y'(t_0) = a$$

可化为1阶方程组,
再用前面初值问题
的计算方法计算.

令 $F(a) = y(t_1; a) - y_1$

如果F有根a, 则对应IVP的解 $y(t; a)$ 也是BVP的解. 反之, 如果BVP有一个解 $y(t)$, 则 $y(t)$ 也是IVP的唯一解 $y(t; a)$, 其中 $a=y'(t_0)$, 因此a是F的根.

通常的求根方法可以在这里使用, 如二分法或牛顿法.

ODE数值求解

- 二阶ODE边值问题 $y''(t) = f(t, y(t), y'(t)), \quad y(t_0) = y_0, \quad y(t_1) = y_1$
- 例6: The boundary value problem is linear if f has the form

$$f(t, y(t), y'(t)) = p(t)y'(t) + q(t)y(t) + r(t).$$

In this case, the solution to the boundary value problem is usually given by:

$$y(t) = y_{(1)}(t) + \frac{y_1 - y_{(1)}(t_1)}{y_{(2)}(t_1)}y_{(2)}(t)$$

where $y_{(1)}(t)$ is the solution to the initial value problem:

$$y''_{(1)}(t) = p(t)y'_{(1)}(t) + q(t)y_{(1)}(t) + r(t), \quad y_{(1)}(t_0) = y_0, \quad y'_{(1)}(t_0) = 0,$$

and $y_{(2)}(t)$ is the solution to the initial value problem:

$$y''_{(2)}(t) = p(t)y'_{(2)}(t) + q(t)y_{(2)}(t), \quad y_{(2)}(t_0) = 0, \quad y'_{(2)}(t_0) = 1.$$

ODE数值求解

- 二阶ODE边值问题 $y''(x) = f(x, y, y'), \quad a < x < b,$

$$y(a) = \alpha, \quad y(b) = \beta.$$

或 $\alpha_0 y(a) - \alpha_1 y'(a) = \alpha, \quad \beta_0 y(b) + \beta_1 y'(b) = \beta,$
 $\alpha_0 \alpha_1 \geq 0, \beta_0 \beta_1 \geq 0, \alpha_0 + \alpha_1 \neq 0,$ 和 $\beta_0 + \beta_1 \neq 0.$

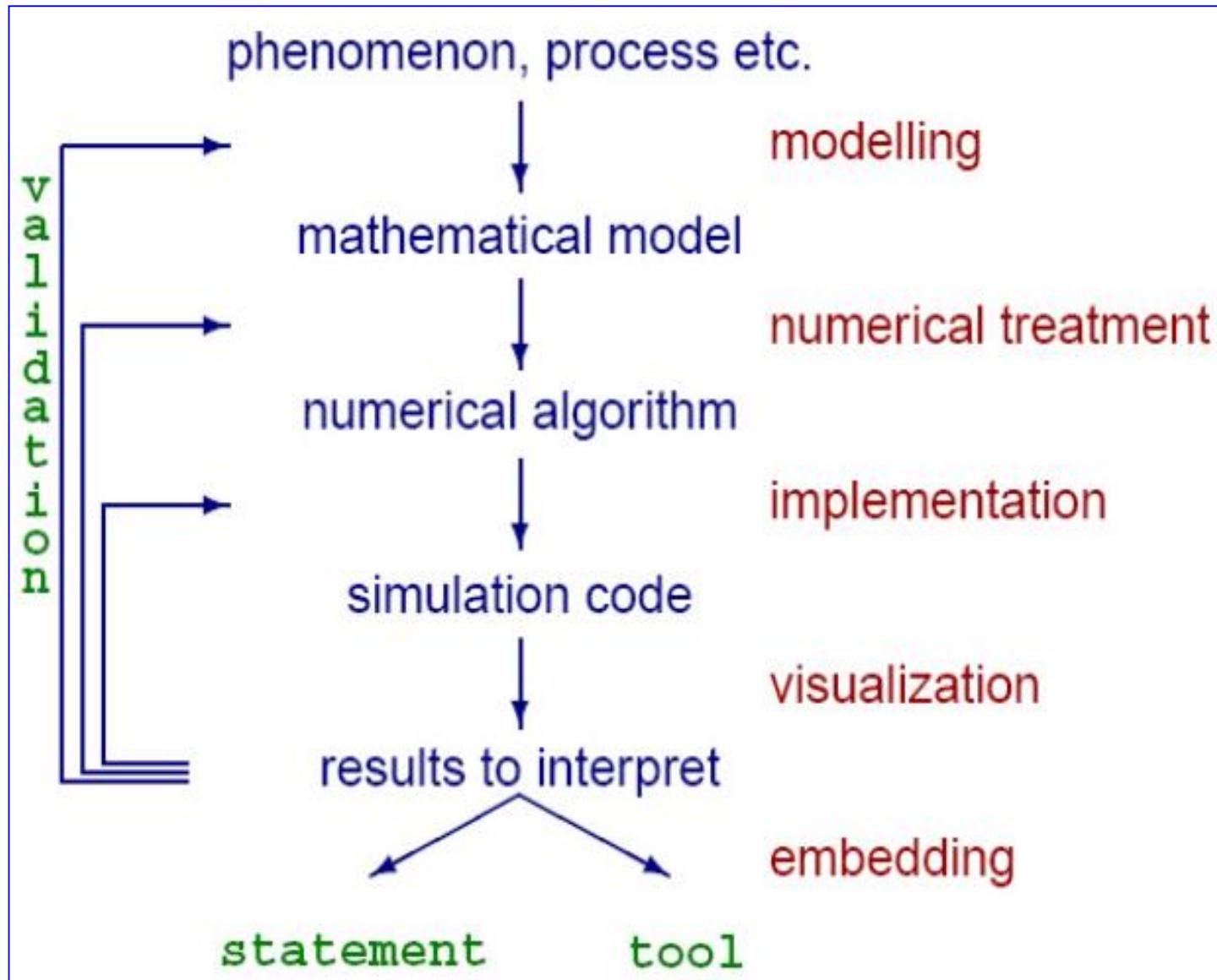
其它方法： FDS, FVM, FEM, Spectral method,

- FDS: 差商代替导数的方法

$$\begin{cases} -a_m y_{m-1} + b_m y_m - c_m y_{m+1} = g_m, & 1 \leq m \leq N-1, \\ y_0 = \alpha, \quad y_N = \beta, & a_m = \frac{2}{h} p_{m-1/2} + r_m, \quad c_m = \frac{2}{h} p_{m+1/2} - r_m, \\ & b_m = \frac{2}{h} (p_{m+1/2} + p_{m-1/2}) + 2hq_m, \quad g_m = 2hf_m. \end{cases}$$
$$\mathbf{Ay = g}, A = \begin{pmatrix} b_1 & -c_1 & & & \\ -a_2 & b_2 & -c_2 & & \\ \ddots & \ddots & \ddots & \ddots & \\ & & -a_{N-2} & b_{N-2} & -c_{N-2} \\ & & -a_{N-1} & b_{N-1} & \end{pmatrix}$$

Thomas 算法/追赶法

科学计算: 从现象到计算预报



问题2：如何解PDE?

- 基于数学模型(特别是PDE)的计算方法研究一直以来是计算数学的核心之一.
- 数学模型如牛顿运动方程、流体力学中Navier-Stokes方程、电动力学中Maxwell方程、量子力学中Schrödinger方程等.
- 三维NS方程解的正则性研究是国际数学界最具挑战性的7个重大数学问题之一.美国麻州的克雷(Clay)数学研究所各设一百万美金奖励七个重大数学问题中的每个问题的解决者： P对NP问题，霍奇猜想，庞加莱猜想，Riemann假设，杨—米尔斯理论，NS方程，BSD(Birch & Swinnerton-Dyer)猜想.

庞加莱猜想被俄罗斯数学家格里戈里·佩雷尔曼于2003年左右证明.



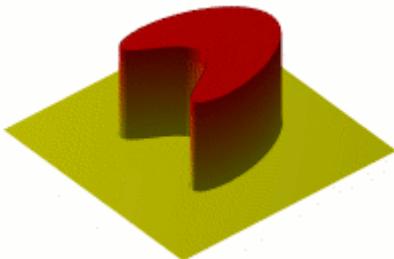
Navier–Stokes Equations 3 – dimensional – unsteady

Glenn
Research
Center

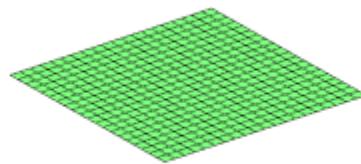
Coordinates: (x, y, z)	Time : t	Pressure: p	Heat Flux: q
	Density: ρ	Stress: τ	Reynolds Number: Re
Velocity Components: (u, v, w)	Total Energy: Et		Prandtl Number: Pr
Continuity:	$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0$		
X – Momentum:	$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2)}{\partial x} + \frac{\partial(\rho uv)}{\partial y} + \frac{\partial(\rho uw)}{\partial z} = - \frac{\partial p}{\partial x} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} \right]$		
Y – Momentum:	$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho uv)}{\partial x} + \frac{\partial(\rho v^2)}{\partial y} + \frac{\partial(\rho vw)}{\partial z} = - \frac{\partial p}{\partial y} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} \right]$		
Z – Momentum	$\frac{\partial(\rho w)}{\partial t} + \frac{\partial(\rho uw)}{\partial x} + \frac{\partial(\rho vw)}{\partial y} + \frac{\partial(\rho w^2)}{\partial z} = - \frac{\partial p}{\partial z} + \frac{1}{Re_r} \left[\frac{\partial \tau_{xz}}{\partial x} + \frac{\partial \tau_{yz}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \right]$		
Energy:	$\begin{aligned} \frac{\partial(E_T)}{\partial t} + \frac{\partial(uE_T)}{\partial x} + \frac{\partial(vE_T)}{\partial y} + \frac{\partial(wE_T)}{\partial z} = & - \frac{\partial(up)}{\partial x} - \frac{\partial(vp)}{\partial y} - \frac{\partial(wp)}{\partial z} - \frac{1}{Re_r Pr_r} \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z} \right] \\ & + \frac{1}{Re_r} \left[\frac{\partial}{\partial x} (u \tau_{xx} + v \tau_{xy} + w \tau_{xz}) + \frac{\partial}{\partial y} (u \tau_{xy} + v \tau_{yy} + w \tau_{yz}) + \frac{\partial}{\partial z} (u \tau_{xz} + v \tau_{yz} + w \tau_{zz}) \right] \end{aligned}$		

PDE

- PDE指含有未知函数及其偏导数的方程/等式：描述自变量、未知函数及其偏导数之间的关系.
- 分为线性PDE与非线性PDE.
- 线性PDE的例子(见右侧)：



2D热传导方程的解



2D波动方程的解

拉普拉斯方程

$$u_{xx} + u_{yy} + u_{zz} = 0$$

适用于重力场问题的求解

泊松方程

$$u_{xx} + u_{yy} + u_{zz} = f(x, y, z)$$

适用于所有物质或电荷的重力场或静电场。

波动方程

未知函数 $u(x, y, z, t)$:

$$u_{tt} = c^2(u_{xx} + u_{yy} + u_{zz})$$

$$\ddot{u} = c^2 \nabla^2 u$$

热传导方程

$$u_t = k(u_{xx} + u_{yy} + u_{zz})$$

其中 k 代表该材料.

PDE

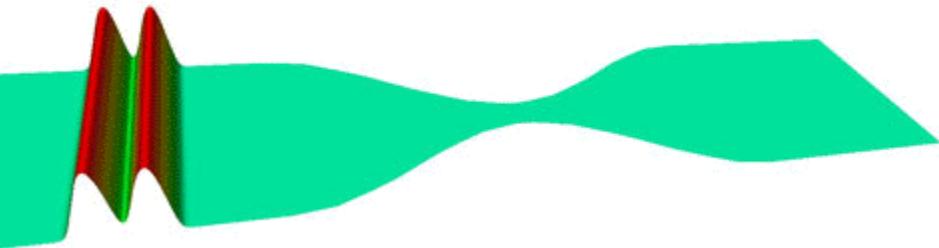
$$\frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} = 0 \text{ is linear .}$$

$$\frac{\partial u}{\partial x_1} + \left(\frac{\partial u}{\partial x_2} \right)^2 = 0 \text{ is nonlinear .}$$

$$\frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} + u^2 = 0 \text{ is nonlinear .}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} = x_1 \text{ is linear .}$$

$$\frac{\partial^2 u}{\partial x_1^2} + u \frac{\partial^2 u}{\partial x_2^2} = 0 \text{ is quasilinear .}$$

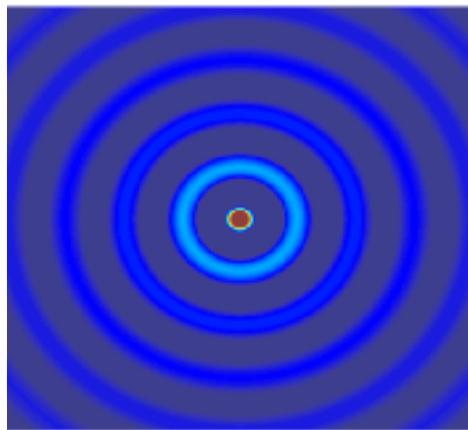


$$\frac{\partial u}{\partial x_1} - \frac{\partial u}{\partial x_2} = 0 \text{ is a first-order PDE.}$$

$$\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} + \frac{\partial^2 u}{\partial x_3^2} = 0 \text{ is a second-order PDE.}$$

$$\frac{\partial^4 u}{\partial x_1^4} + \frac{\partial^2 u}{\partial x_2^2} - u = 0 \text{ is a fourth-order PDE.}$$

$$\left(\frac{\partial u}{\partial x_1} \right)^3 + \frac{\partial u}{\partial x_2} + u^4 = 0 \text{ is a first-order PDE.}$$



Spherical waves coming from a point source.

PDE

例1. 1895年, Korteweg和de Vries研究了浅水波的运动, 建立了KdV方程

$$\frac{\partial u}{\partial t} = \frac{3}{2} \sqrt{\frac{g}{l}} \cdot \frac{\partial}{\partial x} \left(\frac{u^2}{2} + \frac{2\alpha}{3}u + \frac{\sigma}{3} \frac{\partial^2 u}{\partial x^2} \right),$$

其中 u 是波峰的高度(被称为孤立子), l 是水深.

例2. 1827年, Gauss出版了《关于曲面的一般研究》的著作, 奠定了曲面论的基础, 其中引入了预定Gauss曲率的方程—— Monge-Ampère方程

$$\frac{\partial^2 u}{\partial x^2} \cdot \frac{\partial^2 u}{\partial y^2} - \left(\frac{\partial^2 u}{\partial x \partial y} \right)^2 = K(x, y) \left(1 + \left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial u}{\partial y} \right)^2 \right)^2,$$

其中 $K(x, y)$ 是曲面 $z = u(x, y)$ 在 (x, y) 的Gauss曲率.

例3. 将偏微分方程应用于图像处理开始于上个世纪70年代末. 1993年, Alvarez, Guichard, Lions, Morel发表了论文《Axioms and fundamental equations of image processing》，建立了AMSS(仿射的形态尺度空间)模型

$$\frac{\partial u}{\partial t} = |Du| (\text{curv}(u))^{1/3},$$

被认为是基于偏微分方程的图像处理这个研究方向形成的一个标志，其中 u 表示图像的亮度值.



例4. 最优投资中的Hamilton-Jacobi-Bellman方程

$$\min \{-u_t - y^2 u_{yy} + yu_y + xu_{xx}, -au_x + u_y, bu_x - u_y\} = 0,$$

其中 u 表示回报.

PDE

例6. 极小曲面方程 在 \mathbb{R}^3 中考虑曲面 $M: z = u(x, y)$, $(x, y) \in D$, D 是 \mathbb{R}^2 中的一个区域. 1760年Lagrange利用他创立的变分法原理证明了: 若在所有定义在 D 上, 且在 ∂D 上取相同值的函数图像中, M 的面积最小, 则 u 满足极小曲面方程

$$(1 + u_y^2)u_{xx} - 2u_xu_yu_{xy} + (1 + u_x^2)u_{yy} = 0, \quad (x, y) \in D.$$

PDE

考虑二阶线性PDE

$$Au_{xx} + 2Bu_{xy} + Cu_{yy} + \dots = 0,$$

其中参数A,B,C是x,y的变量。如果在xy平面上有 $A^2 + B^2 + C^2 > 0$, 该偏微分方程在该平面上为二阶偏微分方程。二阶偏微分方程类似以下的圆锥方程:

$$Ax^2 + 2Bxy + Cy^2 + \dots = 0.$$

该二阶偏微分方程可分类为: 抛物型, 双曲型和椭圆型方程, 其分类方式是:

1. $B^2 - AC < 0$: 椭圆型方程

2. $B^2 - AC = 0$: 抛物型方程

3. $B^2 - AC > 0$: 双曲型方程

PDE

Wave eq.

$$u_{tt} - c^2 u_{xx} = 0, \quad u(x, 0) = f(x), \quad u_t(x, 0) = g(x)$$

d'Alembert公式 $u(x, t) = \frac{f(x - ct) + f(x + ct)}{2} + \frac{1}{2c} \int_{x-ct}^{x+ct} g(s) \, ds$

在点 (x_0, t_0) 处的解依赖于：

- $f(x)$ 在点 $x_0 + ct_0$ 和 $x_0 - ct_0$ 的值,
- $g(x)$ 在区间 $x_0 - ct_0 \leq x \leq x_0 + ct_0$ 内的值.

Domain of dependence and range of influence

electromagnetic wave eq.

$$\left(v_{ph}^2 \nabla^2 - \frac{\partial^2}{\partial t^2} \right) \mathbf{E} = \mathbf{0} \quad v_{ph} = \frac{1}{\sqrt{\mu\varepsilon}}$$

$$\left(v_{ph}^2 \nabla^2 - \frac{\partial^2}{\partial t^2} \right) \mathbf{B} = \mathbf{0}$$
 是具有磁导率 μ 和介电常数 ε 的介质中的光速

PDE

Heat eq.

$$\begin{cases} u_t = ku_{xx} & (x, t) \in \mathbf{R} \times (0, \infty) \\ u(x, 0) = g(x) & IC \end{cases}$$

解:

$$u(x, t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x-y)^2}{4kt}\right) g(y) dy$$

3-temperature energy equations

$$\begin{cases} C_{ve} \frac{\partial T_e}{\partial t} - \frac{1}{\rho} \nabla \cdot (K_e \nabla T_e) = \omega_{ei}(T_i - T_e) + \omega_{er}(T_r - T_e) \\ C_{vi} \frac{\partial T_i}{\partial t} - \frac{1}{\rho} \nabla \cdot (K_i \nabla T_i) = \omega_{ei}(T_e - T_i), \\ C_{vr} \frac{\partial T_r}{\partial t} - \frac{1}{\rho} \nabla \cdot (K_r \nabla T_r) = \omega_{er}(T_e - T_r) \end{cases}$$



PDE

Poisson eq.

$$\nabla^2 \varphi = f.$$

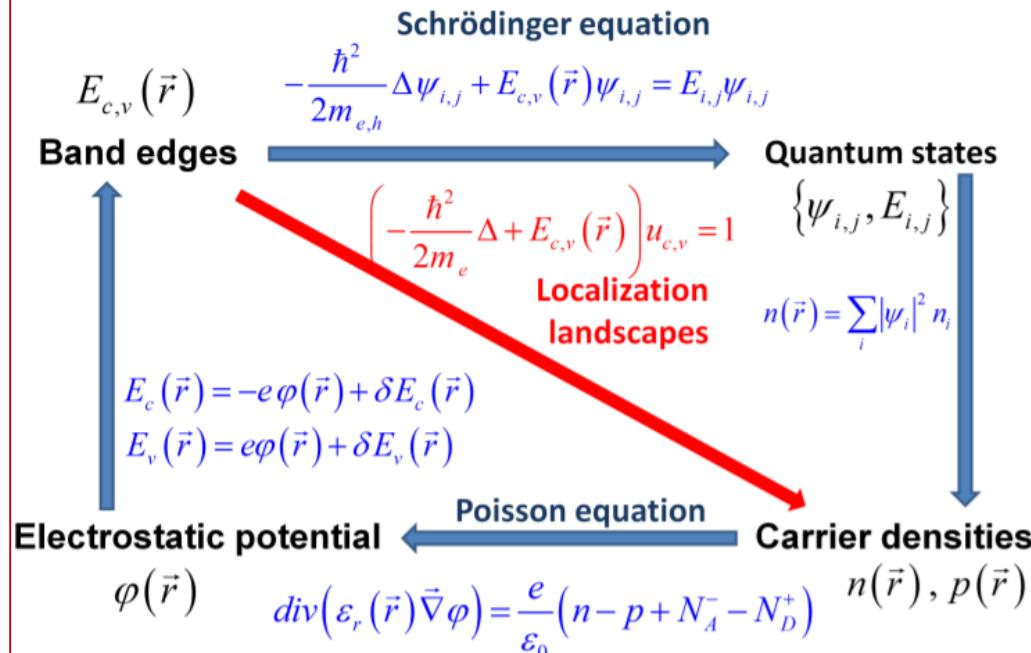
解: $\varphi(\mathbf{r}) = - \iiint_{R^3} \frac{f(\mathbf{r}')}{4\pi|\mathbf{r} - \mathbf{r}'|} d^3 r'$

$$\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \Phi(x, y) = 0$$

$$w(x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \Phi(\xi, \eta) \ln \frac{1}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} d\xi d\eta$$

半导体器件模拟

The self-consistent Poisson-Schrödinger approach



In Nitride-based semiconductors,
calculate ρ_{pol}

Solve Poisson equation

$$\nabla \cdot (\epsilon \nabla \varphi) = \frac{e}{\epsilon_0} (n - p + N_A^- - N_D^+ \pm \rho_{pol})$$

Solve landscape equations

$$\left(-\frac{\hbar^2}{2m_e^*} \Delta + E_{c,v} \right) u_{e,h} = 1 \quad W_{c,v} = \frac{1}{u_{e,h}}$$

Solve drift-diffusion equations

$$\begin{aligned} J_n &= n \mu_n \nabla E_{Fn} & \nabla \cdot J_n &= R + G_n \\ J_p &= p \mu_p \nabla E_{Fp} & \nabla \cdot J_p &= -R + G_p \end{aligned}$$

Converged?

Yes

No

PDE

Convection-diffusion eq.

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c) - \nabla \cdot (\mathbf{v} c) + R$$

对流-扩散方程是扩散和对流方程的组合，描述了粒子、能量或其他物理量由于扩散和对流两个过程在物理系统内传递的物理现象。

Fokker–Planck eq.

$$\frac{\partial}{\partial t} p(x, t) = -\frac{\partial}{\partial x} [\mu(x, t)p(x, t)] + \frac{\partial^2}{\partial x^2} [D(x, t)p(x, t)]$$

p: 概率密度

Black–Scholes eq.

$$\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0$$

V: 期权价格, 是股票价格s和时间t函数

Navier–Stokes eq.

$$\underbrace{\frac{\partial \mathbf{u}}{\partial t} + \underbrace{(\mathbf{u} \cdot \nabla) \mathbf{u}}_{\text{Convection}}}_{\text{Variation}} - \underbrace{\nu \nabla^2 \mathbf{u}}_{\text{Diffusion}} = \underbrace{-\nabla w}_{\text{Internal source}} + \underbrace{\mathbf{g}}_{\text{External source}}$$

Inertia (per volume)

Divergence of stress

PDE

consider the optimal control problem:

$$\min J(w, v) = 1/2 \|w - w_d\|_{L^2(\Omega_f)}^2 + 1/2 \|v\|_{H^3(\mathcal{D})}^2$$

subject to

$$\begin{cases} -\nu \Delta w + Dw \cdot w + \nabla p = v|_{\Omega_f} & \text{on } \Omega_f \\ \operatorname{div} w = 0 & \text{on } \Omega_f \\ w = 0 & \text{on } \Gamma := \varphi(S) \\ -\operatorname{Div} \mathcal{T} = v|_{\Omega_e} & \text{on } \Omega_e = \varphi(\mathcal{O}) \\ \mathcal{T} n = \sigma(p, w)n & \text{on } \Gamma \\ w = 0, \quad \varphi = l_{\Gamma_f} & \text{on } \Gamma_f. \end{cases}$$

- ▶ distributed control $v \in H^3(\mathcal{D})$
- ▶ $w_d \in L^2(\Omega_f)$ is a desired fluid velocity.

PDE

Optimal Shape Design in Fluid Dynamics

Consider the problem of designing one boundary S of a wind tunnel Ω with required properties (such as uniform flow) in some region of space D .

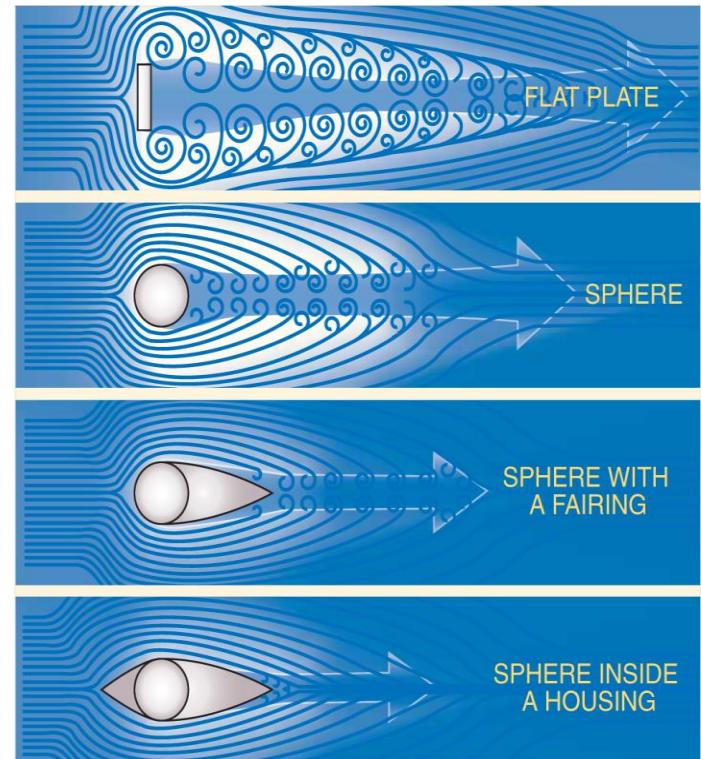
Assume that the flow is potential and 2D. With a stream function formulation this would be

$$\min_{S \in S_d} \left\{ j(S) := \int_D |\psi - \psi_d|^2 : -\Delta\psi = 0, \text{ in } \Omega \quad \psi|_S = 0 \quad \psi|_C = \psi_d \right\}$$

$C = \Gamma \setminus S$ and $\Gamma = \partial\Omega$.



Figure Inverse design for a wind tunnel with desired properties ψ_d in D .

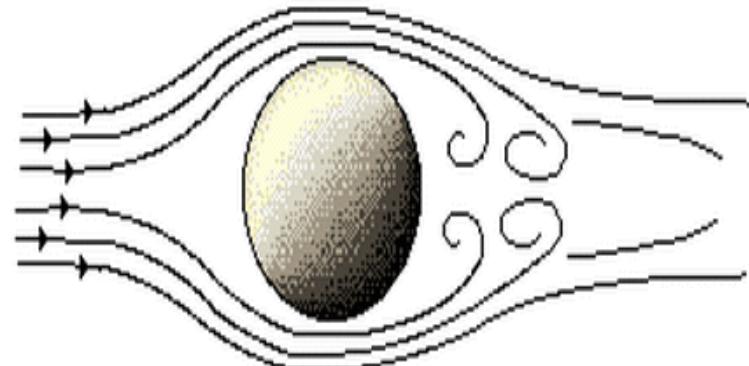


It can be discretized by

$$\min_{T_h} \left\{ j_h := \int_D |\psi - \psi_d|^2 : \int_{\Omega} \nabla \psi_h \nabla w_h + \frac{1}{\epsilon} \int_C (\psi_h - \psi_d) w_h = 0 \quad \forall w_h \in V_h \right\},$$

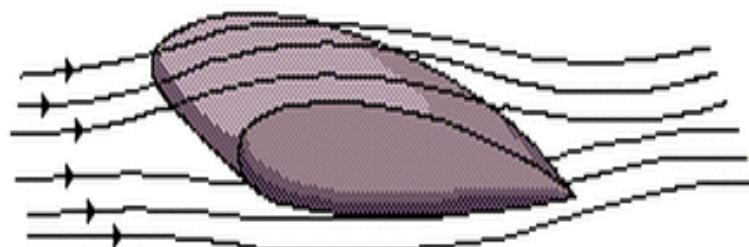
PDE

Optimal Shape Design in Fluid Dynamics



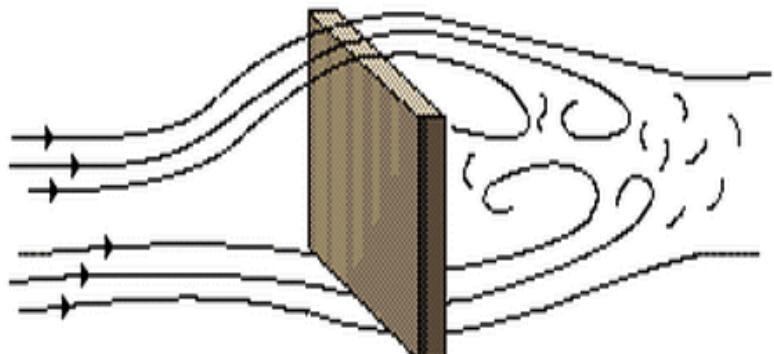
Sphere

Round objects such as baseballs experience a medium amount of drag.



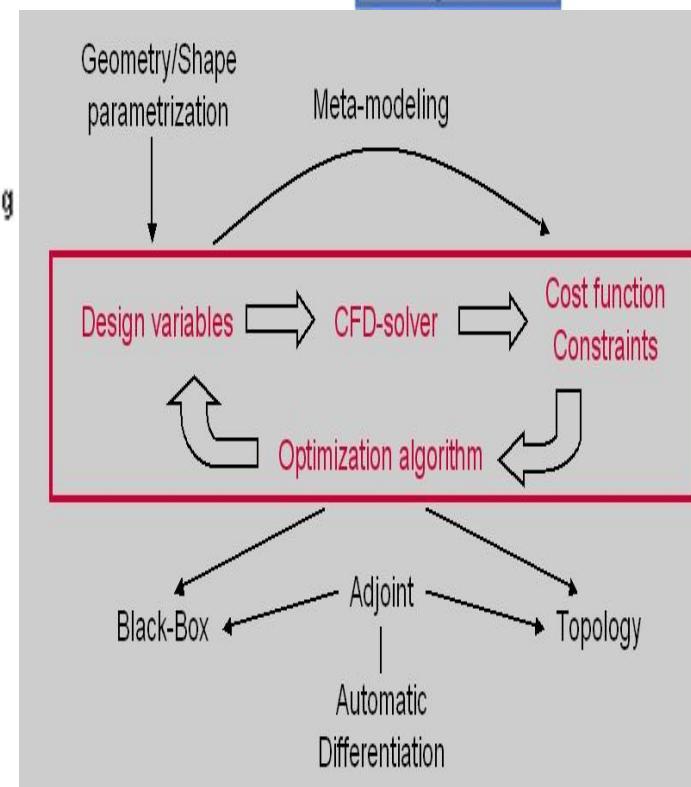
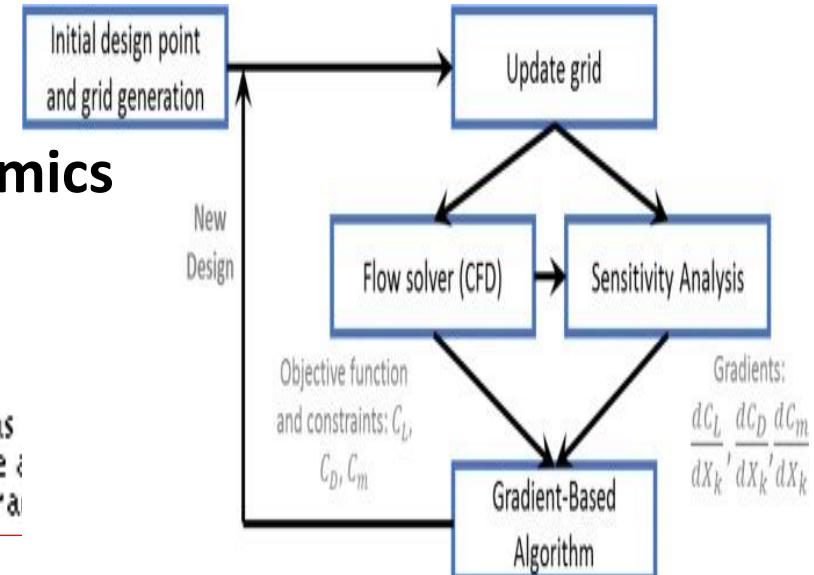
Airfoil

The shape of an airplane wing minimizes drag.



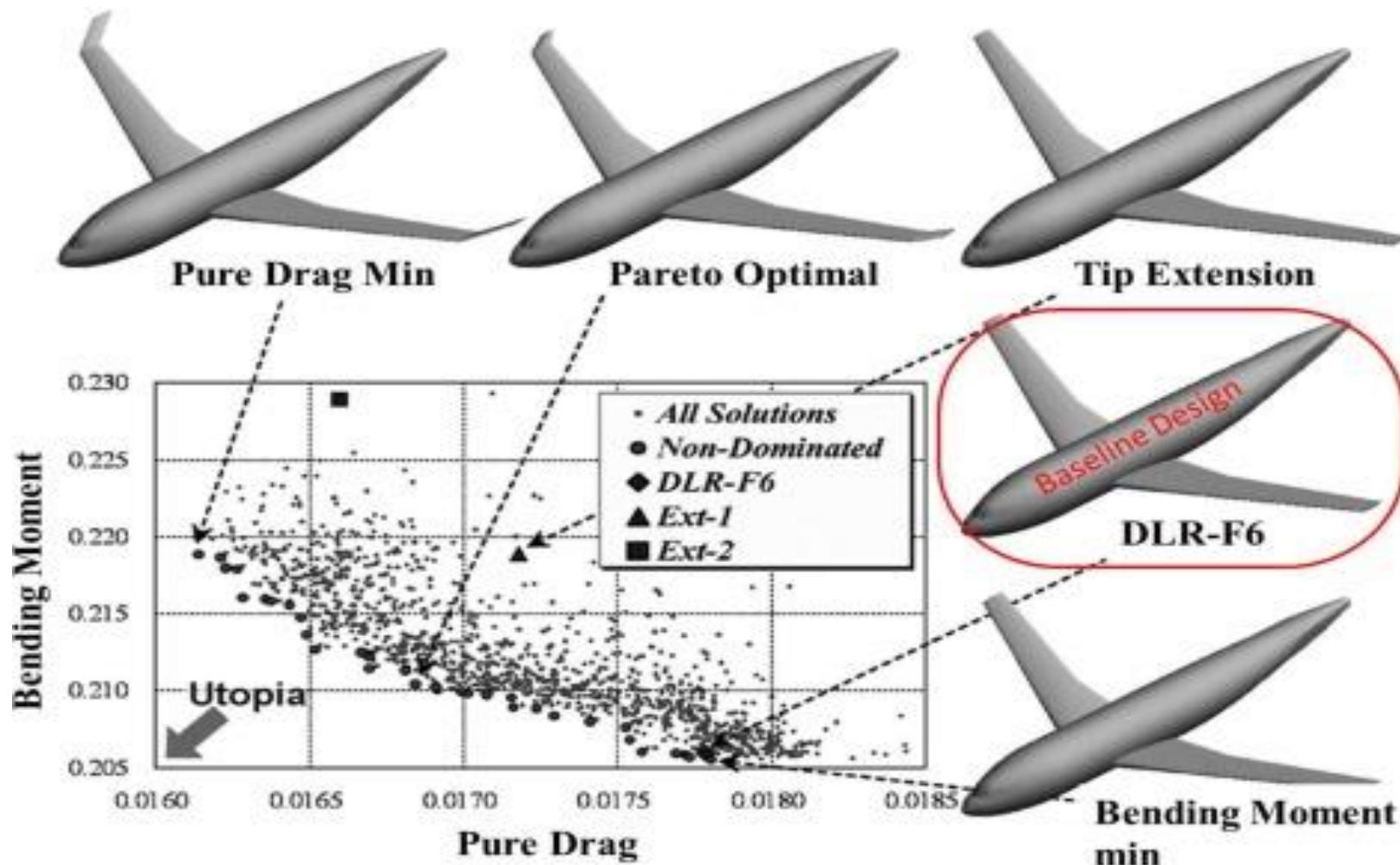
Square

Flat, edged objects such as boxes experience a high amount of drag.



PDE

Optimal Shape Design in Fluid Dynamics



PDE

Well Posed Problems (Jacques Hadamard):

If the solution exists, unique, and depends continuously on the boundary data and initial data.

Problems that are not well-posed in the sense of Hadamard are termed **ill-posed**.



反问题(**Inverse problem**)通常是不适当的. 例如从最终数据中推导出以前的温度分布的反/逆热传导方程是不适当的, 因为该解对最终数据的变化非常敏感.

direct (forward) problem of heat eq.

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} \quad 0 < x < L, t > 0$$

$$u(0, t) = 0 \quad t > 0$$

$$u(L, t) = 0 \quad t > 0$$

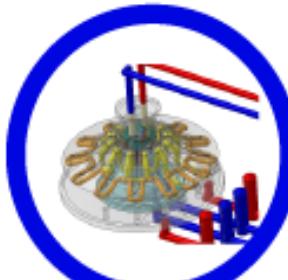
$$u(x, 0) = f(x) \quad 0 \leq x \leq L$$

Inverse (backward) problem of heat eq.

Initial condition $f(x)$ is regarded as being unknown. In addition, an overspecified condition is also considered available. To estimate the unknown coefficient $f(x)$, the additional information $u(x, T) = g(x)$.

CFD for every Industry

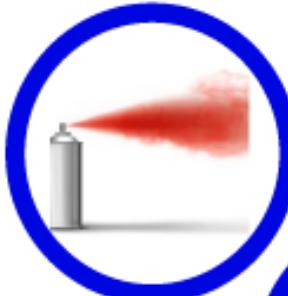
Metal chip removal
Mold cooling
Scrap chutes



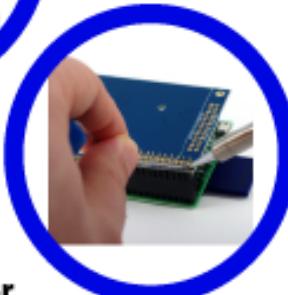
Gas liquid flow
Kneading
High-viscosity stirring



Resin injection molding
Complex material flow
Spray painting



Soldering & casting
Washing machine balancer



Transmission lubrication
Air resistance modelling
Oil Aeration



Gear oil flow
Oil tank sloshing
Car splashing



Fuel Cells
Spent fuel pool sloshing
Loss-of-coolant accident



Tsunami run-up
Debris flow
Concrete Flow



Kneading
Solvent Runoff



Blood Flow
Mouthwashing
Shape Optimization of tablets

Optimal Shape Design in Fluid Dynamics: Literature

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有限元方法在 20 世纪 50 年代诞生于结构力学, 至今它已在众多领域取得了巨大的成功. 现在, 它是求解微分方程的成熟、有效的数值方法. 在有限元方法的创立和发展过程中, 我国学者作出了重要的贡献. 冯康的有关工作是开创性的, 独立于美国和欧洲之外创立并发展了有限元方法.

有限元方法的基本思想是根据变分原理, 利用有限元空间上的离散解近似无穷维空间 V 上的连续解. 构造有限元空间的典型步骤如下:

- (1) 将连续解的定义域 Ω 剖分成若干个子区域, 称每个子区域为一个单元;
- (2) 在每个单元上, 选取一个由多项式构成的 m 维空间和 m 个节点参数, 要求空间中的每个多项式都可以由一组节点参数值唯一确定, 函数或导数在单元某些点的值可以作为节点参数;
- (3) 以某种方式连接各单元上的节点参数, 进而得到定义在 Ω 上的分片多项式空间 V_h , 称这样得到的 V_h 为有限元空间.

在有限元方法的数学理论中, 有下面著名的结果:

当 V_h 是 V 的子空间时, 有限元解对连续解的逼近性取决于有限元空间 V_h 对 V 的逼近性.