1. PDE方程的分类

2. PDE求解　　　　　　　　　　引言讲完

3. 网格.

4. verification, validation

1. PDE 分类

Pantankar

- one way
- two way

阅读 2. 5 段

单向坐标 t，时间

自变 t，因变量

抛物

双向坐标 x, y, z 空间

椭圆

双曲 单向

特征线方程

$T(x, y, t)$

物理本质

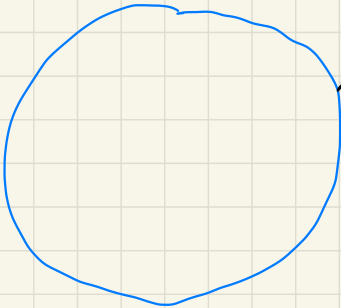
$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}$$

抛物 时间 椭圆型

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}$$

初始条件 I. V. P $\leftarrow$ t

边界条件 B. V. P $\leftarrow$ x, y



边界对整个有影响

双曲 $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$ (1D)

不可压 可压

空间 椭圆

时间 抛物

数学形：

$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial x\partial y} + C\frac{\partial^2\phi}{\partial y^2} + \cdots = 0.$$

x, y. 自变量　ϕ 因变量　$f(x, y)$　t 时间.

$B^2 - 4AC < 0$　椭圆

$B^2 - 4AC = 0$　抛物

$B^2 - 4AC > 0$　双曲

例1.　二维扩散(稳态)

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = S\phi \qquad S\phi\begin{cases} = 0 & \text{laplacian} \\ = C & \text{poisson} \\ = a\phi + b & \end{cases}$$

$A = 1,\quad B = 0,\quad C = 1$

$B^3 - 4AC = 0 - 4 = -4 < 0$　椭圆型

例 2. $$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}=S_\phi$$

仍然是椭圆型方程

例 3. 二维非稳态 常数

$$\underbrace{\frac{\partial\phi}{\partial t}}=\Gamma\underbrace{\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)}+S_\phi$$

自变量 (x, y) $A=\Gamma$, $B=0$, $C=\Gamma$

$B^2-4AC=-4\Gamma^2<0$ 椭圆

自变量 (t, x) $A=0$, $B=0$, $C=-\Gamma$

$$\frac{\partial\phi}{\partial t}-\Gamma\frac{\partial^2\phi}{\partial x^2}=\Gamma\frac{\partial^2\phi}{\partial y^2}+S_\phi$$

$A=0$, $B=0$, $C=-\Gamma$

$B^2-4AC=0$ 抛物

时间 抛物， 空间，椭圆

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2} \qquad \nabla^2\phi \qquad \nabla\cdot(\nabla\phi)$$

ν 运动粘度

例 4.

$$\underbrace{u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}}_{\text{对流项}}=\frac{\mu}{\rho}\frac{\partial^2 u}{\partial x^2}$$

$$\vec{U}\cdot\nabla\vec{U}$$

$A=\frac{\mu}{\rho}$，$B=0$，$C=0$ $\qquad B^2-4AC=0 \Rightarrow$ 抛物型

例5 $\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0 \Rightarrow$ (欧拉方程)

自变量 (t, x), 因变量 u

$$\frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t}\frac{\partial u}{\partial x} + u\frac{\partial^2 u}{\partial t\partial x} = 0$$

$A=1$, $B=u$. $C=0$ $\quad B^2-4AC = u^2 > 0$ 双曲型

例6. 波动方程

$$\frac{\partial^2 u}{\partial t^2} = \Delta u = \nabla\cdot(\nabla u) = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

自变量 t, x, $\quad \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$

$A=1$, $B=0$, $C=-1$

$B^2-4AC = 4 > 0$ 双曲型.

2. PDE 求解,

有网格. 有差分 有限体积、有限元.

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$$

强形式 FDM $\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$

$$\frac{d^2\phi}{dx^2}=0 \quad (\text{Laplace})$$

$$\frac{d\phi}{dx}=c$$

$$\phi=cx+b$$ 解析解

弱

FVM $\int_V \left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)dV=\underbrace{\int_V 0\,dV}$

守恒性

FEM $\int_V v\left(\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}\right)dV=\int_V 0\cdot v\,dV$

试函数 trival function

二阶 FDM.

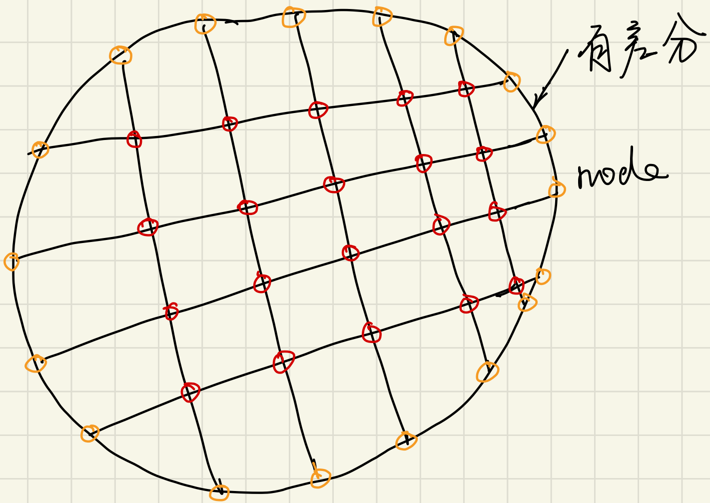
二阶 FVM.

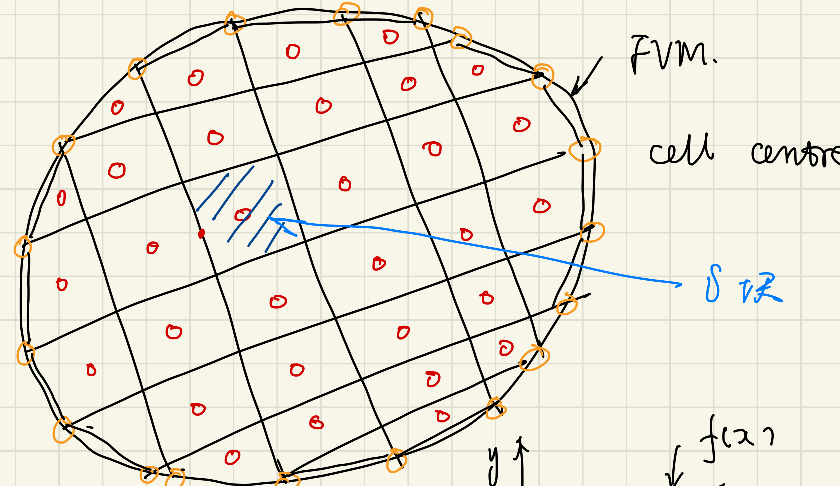
taylor. 保性

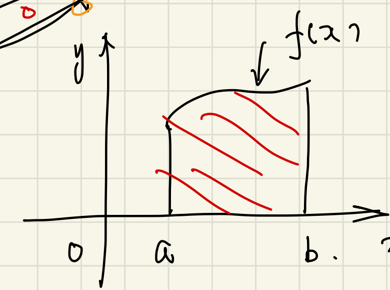
$$\frac{\partial\rho\vec{U}}{\partial t}+\nabla\cdot(\rho\underbrace{\vec{U}\vec{U}}_{\text{速度张量}})$$

$\vec{U}\cdot\nabla\vec{U}$

非守恒型







例 7. $\nabla^2\phi = S$ $\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = S_\phi$

$$\int_{V_i} \nabla\cdot(\nabla\phi)\,dV = \underline{\int_{V_i} S\,dV} \doteq S_i V_i$$

$$\int_a^b f(x)\,dx$$

1 $\Downarrow$

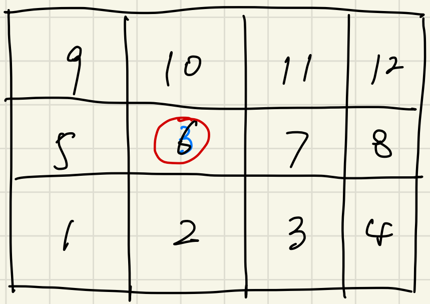
$$\int_{\partial V_i} \nabla\phi\cdot\hat{n}\,dA \xrightarrow{2} = \sum_f^n (\nabla\phi)_f \cdot \vec{S}_f$$

W即 1个离散积分点 $= \underbrace{f(\xi)}_{S_i}\underbrace{(b-a)}_{V_i}$

$\#$ $\nabla\phi_f$

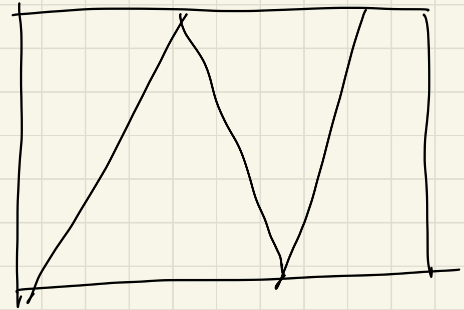
$\phi = \vec{U}$ $\nabla\phi$

3. mesh 网格



1

不是结构化

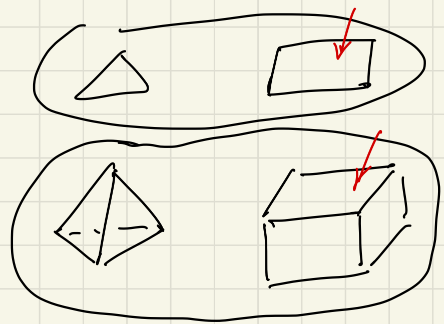


2

结构化

非结构化

owner neighbour



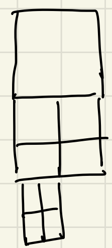
2D

3D

网格 → 学科 计算几何 邓俊辉

OpenFOAM → shm.

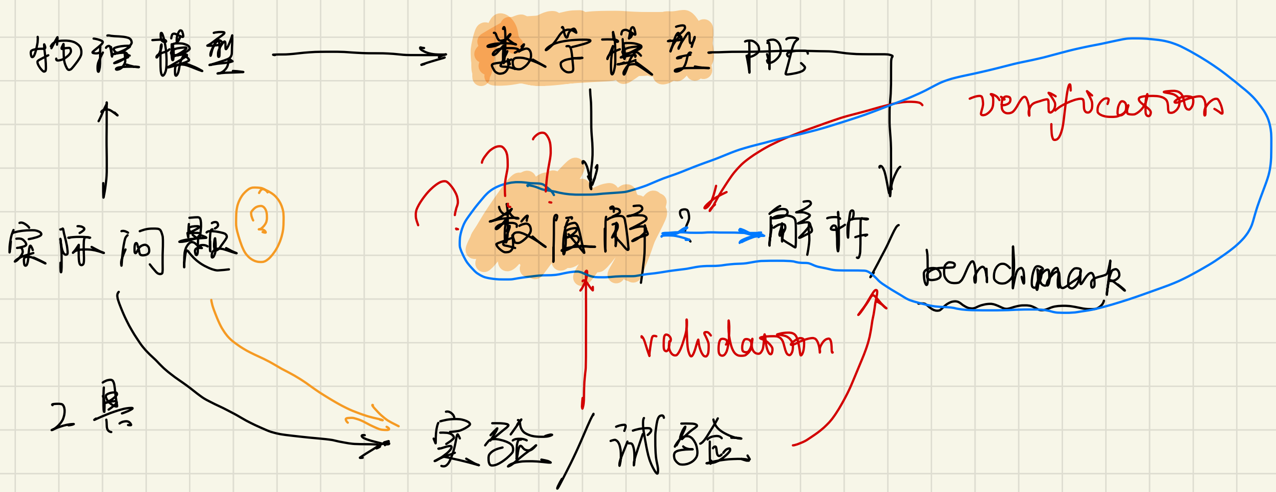
Cartesian mesh



非结构化网格

C, O, H,

4. verification and validation



1. PDE分类

帕理卡. 单双

$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial x\partial y} + C\frac{\partial^2\phi}{\partial y^2} + \cdots = 0$$

$\Delta < 0$ 椭
$\Delta = 0$ 抛
$\Delta > 0$ 双

2. PDE求解. FDM, FVM, FEM. / FDM 和 FEM
node cell

3. 网格. 结构，非结构化

4. verification, validation

下一次课. FDM. $\nabla^2\phi = S$. (二维离散)，三类边界条件.

第二次课 有限差分 一.

差分机　CFL./ Courant 数　1928 文章　德文版

FDM $\begin{cases} \text{FVM} & \text{（有限体积）} \\ \text{FEM} & \text{（有限元）} \end{cases}$

FDTD
前左. FDM

1. 差分近似和截断误差.

2. 广义差分近似推导

3. 三类边界条件的应用（下一次课）

1. 差分近似和截断误差

(1D) $\frac{\partial^2\phi}{\partial x^2}$ $\frac{d^2\phi}{dx^2} = S\phi$, $\frac{d^2\phi}{dx^2} = \underbrace{e^{-x}}$ ($\overset{P}{O}\overset{P}{P}\overset{E}{E}$)

ϕ, x. $S = a + bx$. 源项. e^{-x} 线性函数

$S = 0$. 拉普拉斯,

$S = a$. 泊松方程

$S = e^{-x}$ non-linear $\sin x$, $\cos x$

N-S $\frac{\partial\rho\vec{U}}{\partial t} + \nabla\cdot(\rho\vec{U}\vec{U}) = -\nabla p + \nabla\cdot(\mu\nabla\vec{U}) + \vec{g}$

1 2 3 4 5

$$\frac{d^2\phi}{dx^2} = S\phi \qquad \phi(x_L) = \phi_L, \quad \phi(x_R) = \phi_R$$

N.

uniform Δx

non-uniform Δx

equal spacing.

$$\Delta x = \frac{L}{N-1} \qquad x_i = x_L + (i-1)\Delta x$$

$$\begin{cases} i = 1, \cdots, N. \\ i = 0 \\ i = 0, \cdots N-1, \end{cases}$$

i. $=0$, 1 开始.

matlab. 1. 开始

python 0 开始.

C / C++ 0 开始.

编程.

$$\left.\frac{d\phi}{dx}\right|_{x=i} \approx \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}$$

泰勒公式 （只用这一个数学工具）.

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(x_0)}{n!}(x-x_0)^{n}$$

W ϕ_{i-1} O ϕ_i E ϕ_{i+1}

$i-1$ i $i+1$

$$\frac{d^2\phi}{dx^2} \longrightarrow \text{代数形式}$$

$$\phi_{i+1} = \phi_i + (x_{i+1} - x_i)\left.\frac{d\phi}{dx}\right|_i + \frac{(x_{i+1}-x_i)^2}{2!}\left.\frac{d^2\phi}{dx^2}\right|_i + \frac{(x_{i+1}-x_i)^3}{3!}\left.\frac{d^3\phi}{dx^3}\right|_i + \cdots$$

$$\boxed{\phi_{i+1} = \phi_i + \Delta x\frac{d\phi}{dx} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots}$$

$$\phi_{i-1} = \phi_i + (x_{i-1} - x_i)\left.\frac{d\phi}{dx}\right|_i + \frac{(x_{i-1}-x_i)^2}{2!}\left.\frac{d^2\phi}{dx^2}\right|_i + \frac{(x_{i-1}-x_i)^3}{3!}\left.\frac{d^3\phi}{dx^3}\right|_i + \cdots$$

$$\boxed{\phi_{i-1} = \phi_i - \Delta x\frac{d\phi}{dx} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} - \frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots}$$

$$\phi_{i+1} = \phi_i + \cancel{\Delta x \frac{d\phi}{dx}} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \cancel{\frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3}} + \frac{\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots \quad 1$$

a

$$\frac{d\phi}{dx} = \frac{\phi_{i+1}-\phi_i}{\Delta x} - \frac{\Delta x}{2}\frac{d^2\phi}{dx^2} + \cdots \qquad O(\Delta x)$$

$$\phi_{i-1} = \phi_i - \cancel{\Delta x \frac{d\phi}{dx}} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} - \cancel{\frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3}} + \frac{\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots \quad 2.$$

b

$$\frac{d\phi}{dx} = \frac{\phi_i-\phi_{i-1}}{\Delta x} + \frac{\Delta x}{2}\frac{d^2\phi}{dx^2} + \cdots \qquad O(\Delta x)$$

round off error

truncation error

截断误差

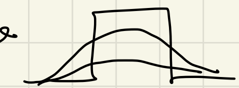
$$\phi_{i+1} + \phi_{i-1} = 2\phi_i + \Delta x^2 \frac{d^2\phi}{dx^2} + \frac{\Delta x^4}{12}\frac{d^4\phi}{dx^4} + \cdots$$

C.

$$\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{\Delta x^2} - \frac{\Delta x^2}{12}\frac{d^4\phi}{dx^4}\Big|_i + \cdots$$

人 2 精准.

stable



中央差分

central differential scheme

$$\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{\Delta x^2} + O(\Delta x^2) \quad 二阶$$

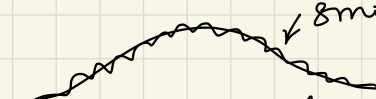
C

$O(\Delta x^2)$

c

$$\frac{d\phi}{dx} = \frac{\phi_{i+1}-\phi_{i-1}}{2\Delta x} + \frac{\Delta x^2}{6}\frac{d^3\phi}{dx^3}\Big|_i + \cdots$$

smooth

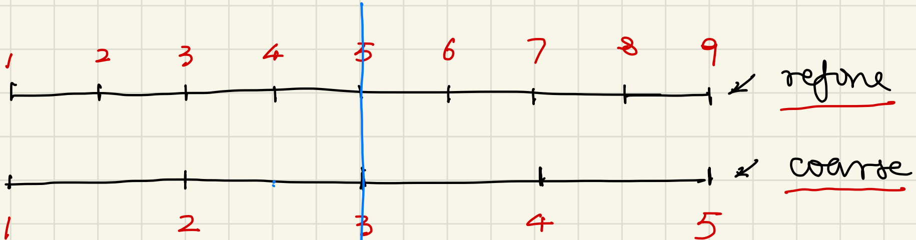


wiggle

$$\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{\Delta x^2} - \underbrace{\frac{\Delta x^2}{12}\frac{d^4\phi}{dx^4}\Big|_{x=i}} + \cdots$$

$$\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1}+\phi_{i-1}-2\phi_i}{\Delta x^2} + O(\Delta x^2)$$

中央差分格 二阶精度



$$\varepsilon = -\frac{\Delta x^2}{12}\left(\frac{d^4\phi}{dx^4}\right)_{x=i}$$

$$\frac{d^2\phi}{dx^2} = \frac{\phi_6+\phi_4-2\phi_5}{\Delta x^2} - \boxed{\frac{\Delta x^2}{12}\frac{d^4\phi}{dx^4}\Big|_{x=5}}$$ ε_1

$$\frac{d^2\phi}{dx^2} = \frac{\phi_4+\phi_2-2\phi_3}{(2\Delta x)^2} - \boxed{\frac{(2\Delta x)^2}{12}\frac{d^4\phi}{dx^4}\Big|_{x=3}}$$ ε_2

相等. 不等

truncation error 截断

round off error 舍入

1. 8. 23.

单精度 float 32 4 byte

双精度 double 64 8 byte

16th.

1. $\varepsilon_2 = 4\varepsilon_1 \Rightarrow \varepsilon \propto (\Delta x)^2$

$\varepsilon \propto (\Delta x)^n$

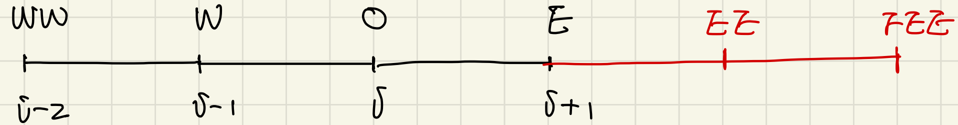
99% round off

$\frac{d^2\phi}{dx^2}$ 10^{-6}

$$\left(\frac{d^2\phi}{dx^2}\right)_{coarse} - \left(\frac{d^2\phi}{dx^2}\right)_{fine} = \varepsilon_{相} < 0.1\%$$

2. 广义差分格式推导

$$\left.\frac{d^3\phi}{dx^3}\right|_0$$



$$A\times\left[\phi_E = \phi_0 + \Delta x\left.\frac{d\phi}{dx}\right|_0 + \frac{\Delta x^2}{2}\left.\frac{d^2\phi}{dx^2}\right|_0 + \frac{\Delta x^3}{6}\left.\frac{d^3\phi}{dx^3}\right|_0 + \frac{\Delta x^4}{24}\left.\frac{d^4\phi}{dx^4}\right|_0 + \cdots\right]$$

$$B\times\left[\phi_W = \phi_0 - \Delta x\left.\frac{d\phi}{dx}\right|_0 + \frac{\Delta x^2}{2}\left.\frac{d^2\phi}{dx^2}\right|_0 - \frac{\Delta x^3}{6}\left.\frac{d^3\phi}{dx^3}\right|_0 + \frac{\Delta x^4}{24}\left.\frac{d^4\phi}{dx^4}\right|_0 + \cdots\right]$$

$$C\times\left[\phi_{WW} = \phi_0 - (2\Delta x)\left.\frac{d\phi}{dx}\right|_0 + \frac{(-2\Delta x)^2}{2}\left.\frac{d^2\phi}{dx^2}\right|_0 + \frac{(-2\Delta x)^3}{6}\left.\frac{d^3\phi}{dx^3}\right|_0 + \frac{(-2\Delta x)^4}{24}\left.\frac{d^4\phi}{dx^4}\right|_0 + \cdots\right]$$

$$\begin{cases} A\Delta x + B(-\Delta x) + C(-2\Delta x) = 0 & 1 \\ A\dfrac{\Delta x^2}{2} + B\dfrac{\Delta x^2}{2} + C\,2\Delta x^2 = 0 & 2. \\ A\dfrac{\Delta x^3}{6} + B\dfrac{-\Delta x^3}{6} + C\dfrac{(-2\Delta x^3)}{6} = 1 \end{cases}$$

$$\downarrow$$

$$A - B - 2C = 0$$

$$A + B + 4C = 0$$

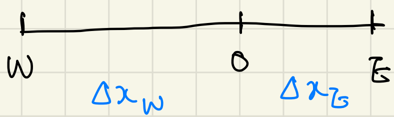
$$A - B - 8C = \frac{6}{\Delta x^3}$$

$$\begin{array}{ccc} A & x & b \\ \begin{bmatrix} 1 & -1 & -2 \\ 1 & 1 & 4 \\ 1 & -1 & 8 \end{bmatrix} & \begin{bmatrix} A \\ B \\ C \end{bmatrix} = & \begin{bmatrix} 0 \\ 0 \\ \frac{6}{\Delta x^3} \end{bmatrix} \end{array}$$

$$A = \frac{1}{(\Delta x)^3} \qquad B = \frac{1}{(\Delta x)^3} \qquad C = -\frac{1}{(\Delta x)^3}$$

$$\frac{d^3\phi}{dx^3} = \frac{1}{(\Delta x)^3}\phi_E + \frac{3}{(\Delta x)^3}\phi_W - \frac{1}{(\Delta x)^3}\phi_{WW} - \frac{3}{(\Delta x)^3}\phi_0 + \frac{1}{2}\Delta x \left.\frac{d^4\phi}{dx^4}\right|_0$$

$$\varepsilon = \frac{\Delta x}{2}\left.\frac{d^4\phi}{dx^4}\right|_0 + \cdots$$



不等间距 $\frac{d^2\phi}{dx^2}$

$$\Delta x_W \left[\phi_E = \phi_0 + (\Delta x_E)\frac{d\phi}{dx} + \frac{(\Delta x_E)}{2}\frac{d^2\phi}{dx^2} + \cdots \right]$$

$$\Delta x_E \left[\phi_W = \phi_0 - (\Delta x_W)\frac{d\phi}{dx} + \frac{(\Delta x_W)^2}{2}\frac{d^2\phi}{dx^2} - \cdots \right.$$

$$\varepsilon_i = -\frac{1}{3}(\Delta x_E - \Delta x_W)\left.\frac{d^3\phi}{dx^3}\right|_0 \qquad 0$$

$$\frac{\Delta x^2}{12}\frac{d^4\phi}{dx^4}$$

$\Delta x_E - \Delta x_W$ 很小

总结.

1. 有限差分.

2. $\frac{d\phi}{dx}$, $\frac{d^2\phi}{dx^2}$ 中央差分(2阶). 前.向(1阶)

3. 方法. A. B, C, ~~/~~ A, B, C, D, E, $Ax=b$ => matlab / python.

4. 不等间距网格 精度退化 -> (2阶 - 1阶)

上午. 周三. 三类边界

第三次课 有限差分二.

1. 三类边界条件

   a. Dirichlet 德国人

   b. Neumann 德国人

   c. Robin 法国人

2. 系数矩阵组装

$Ax = b.$

直接法

间接法 高斯-塞德尔. 雅克比

cg , mg.

数学的较难, 软件实现 ✓

数学的较易 —— 很难

并行. 指令集优化.

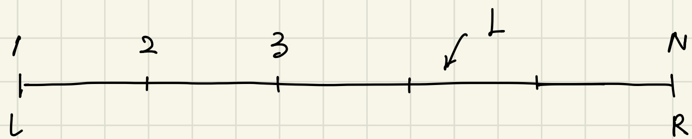
cache 友好

a. Dirichlet 边界条件

$\phi_1 = \phi_L$, $\phi_N = \phi_R$ $\phi_L = 200$, $\phi_R = 400$

b. Neumann 边界条件

通量边界条件 $\frac{d\phi}{dx}$ $\frac{\partial \phi}{\partial n}$

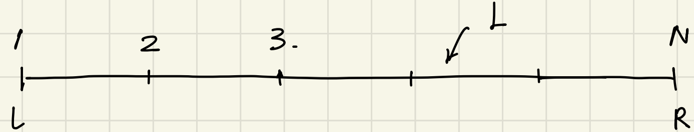


$$\frac{\phi_2 - \phi_1}{\Delta x} = C$$

$\frac{d\phi}{dx}$ 是一个定值 $\left.\frac{d\phi}{dx}\right|_{x=1} = C$.

$$\phi_2 = \phi_1 + \Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{(\Delta x)^2}{2} \left.\frac{d^2\phi}{dx^2}\right|_{x=1} + \cdots$$

$$C = \left.\frac{d\phi}{dx}\right|_{x=1} = \frac{\phi_2 - \phi_1}{\Delta x} - \frac{\Delta x}{2} \left.\frac{d^2\phi}{dx^2}\right|_{x=1} + \cdots$$



$$\frac{d\phi}{dx}\Big|_{x=1} = C. \qquad \frac{\phi_2 - \phi_1}{\Delta x} = C \qquad (1阶)$$

a b c

$$A\ \phi_2 = A\phi_1 + A\Delta x \frac{d\phi}{dx}\Big|_{x=1} + \cancel{A\frac{(\Delta x)^2}{2}\frac{d^2\phi}{dx^2}\Big|_{x=1}} + A\frac{(\Delta x)^3}{6}\frac{d^3\phi}{dx^3} + \cdots \quad 1$$

$$B\ \phi_3 = B\phi_1 + B\,2\Delta x \frac{d\phi}{dx}\Big|_{x=1} + \cancel{B\frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2}\Big|_{x=1}} + B\frac{(2\Delta x)^3}{6}\frac{d^3\phi}{dx^3} + \cdots \quad 2$$

$$\begin{cases} A\Delta x + 2B\Delta x = 1 & 1 \\ A\frac{\Delta x^2}{2} + B\frac{(2\Delta x)^2}{2} = 0\ ? & 2 \end{cases}$$

$$A\phi_2 + B\phi_3 = (A+B)\phi_1 + \Delta x\frac{d\phi}{dx}\Big|_{x=1} + 0\ \frac{d^2\phi}{dx^2}\Big|_{x=1} + (A + 4B)\frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3}.$$

$$\frac{A\phi_2 + B\phi_3 - (A+B)\phi_1}{\Delta x} - (A+4B)\frac{\Delta x^2}{6}\frac{d^3\phi}{dx^3} = \frac{d\phi}{dx}\Big|_{x=1}$$

$$\frac{d\phi}{dx} = \frac{\phi_2 - \phi_1}{\Delta x} \quad 1阶.$$

$$\frac{d\phi}{dx} = \frac{\phi_{i+1} - \phi_i}{\Delta x} \qquad \frac{d\phi}{dx} = \frac{\phi_i - \phi_{i-1}}{\Delta x} \qquad \frac{d\phi}{dx} = \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

$e^x = 1$

$$\boxed{\left.\frac{d\phi}{dx}\right|_{x=1} = \frac{4\phi_2 - \phi_3 - 3\phi_1}{2\Delta x} + \frac{1}{3}\frac{(\Delta x)^2}{1}\left.\frac{d^3\phi}{dx^3}\right|_{x=1} + \cdots}$$

$\frac{1}{3}$

一阶导函数的二阶精度

边节点，内节点 离散，精度不一致，就会导致一些问题

$$\left.\frac{d\phi}{dx}\right|_{x=1} = J. \quad A \quad \phi_2 = \phi_1 + \Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{(\Delta x)^2}{2}\frac{d^2\phi}{dx^2}\bigg|_{x=1} + \frac{(\Delta x)^3}{6}\frac{d^3\phi}{dx^3}\bigg|_{x=1} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4}$$

$$B \quad \phi_3 = \phi_1 + 2\Delta x J + \frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2}\bigg|_{x=1} + \frac{(2\Delta x)^3}{6}\frac{d^3\phi}{dx^3}\bigg|_{x=1} + \frac{(2\Delta x)^4}{4}\frac{d^4\phi}{dx^4}$$

$$A\phi_2 = A\phi_1 + A\Delta x J + A\frac{(\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + A\frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3} + \frac{A\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots$$

$$B\phi_3 = B\phi_1 + 2B\Delta x J + B\,2\Delta x^2\frac{d^2\phi}{dx^2} + B\frac{8\Delta x^3}{6}\frac{d^3\phi}{dx^3} + B\frac{16\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots$$

2 dx

$$A\phi_2 = A\phi_1 + A\Delta x J + A\frac{(\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + A\frac{\Delta x^3}{6}\frac{d^3\phi}{dx^3} + A\frac{\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots$$

$$B\phi_3 = B\phi_1 + 2B\Delta x J + B\,2\Delta x^2\frac{d^2\phi}{dx^2} + B\frac{8\Delta x^3}{6}\frac{d^3\phi}{dx^3} + B\frac{16\Delta x^4}{24}\frac{d^4\phi}{dx^4} + \cdots$$

$$A\frac{\Delta x^2}{2} + 2B\Delta x^2 = 1$$

$$A\frac{\Delta x^3}{6} + \frac{4}{3}B\Delta x^3 = 0$$

$$A + 4B = \frac{1}{\Delta x^2}$$

$$A + 8B = 0$$

$\cancel{e^{x}}$

$$J \not\propto \left.\frac{d\phi}{dx}\right|_{x=1}$$

$$\left.\frac{d^2\phi}{dx^2}\right|_{x=1} = \frac{8\phi_2 - \phi_3 - 7\phi_1 - (6\Delta x)J}{2(\Delta x)^2} + \frac{\cancel{(\Delta x)^2}}{6}\left.\frac{d^4\phi}{dx^4}\right|_{x=1} + \cdots$$

$$\frac{1}{6}$$

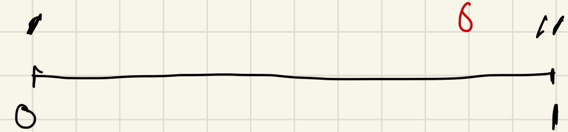
$$cJ = \frac{d\phi}{dx}$$

$$J = \frac{1}{c}\frac{d\phi}{dx}$$

$$\neq$$

$$J = -k\frac{d\phi}{dx}$$

$$\frac{d^2\phi}{dx^2} = \exp(-x)$$



0 1

$$\left.\frac{d\phi}{dx}\right|_{x=1} = 2.$$

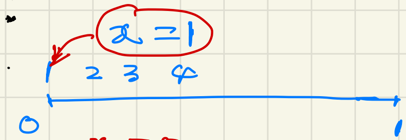
边界处理非常重要

例题. $\frac{d^2\phi}{dx^2} = e^x$ $[0, 1]$ 右, Neumann $\frac{d\phi}{dx} = 1$

2

~~2x~~ $\cancel{+1}$

左 Dirichlet $\phi = 1$.



1. 左结点, $\left.\frac{d\phi}{dx}\right|_{x=1} = \frac{4\phi_2 - 3\phi_1 - \phi_3}{\Delta x} = 1$ 2阶 A

2. 左结点 $\left.\frac{d^2\phi}{dx^2}\right|_{x=1} = \frac{8\phi_2 - 7\phi_1 - \phi_3 - (6\Delta x)J}{2(\Delta x)^2} = 1 = e^x = e^0$ B

2阶.

$x = 0$

中间结点 $\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{(\Delta x)^2}$

$\phi = ax^2 + bx + C \Rightarrow \frac{d^3\phi}{dx^3} = 0$ A = B.

第三类 robin 就是第一类 + 第二类

2. 系数矩阵的组装 PDE $\xRightarrow{FDM}$ Algebra Equations

discretization

$$Ax = b.$$

未知结点

系数矩阵

右边列向量

$$a_{1,1}\phi_1 + a_{1,2}\phi_2 + \cdots + a_{1,n}\phi_n = b_1$$

$$a_{2,1}\phi_1 + a_{2,2}\phi_2 + \cdots + a_{2n}\phi_n = b_2$$

$$\vdots$$

$$a_{n1}\phi_1 + a_{n2}\phi_2 + \cdots + a_{nn}\phi_n = b_n.$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

$$e^{x=0}$$

$$\frac{8\phi_2 - 7\phi_1 - \phi_3 - (6\Delta x) J}{2(\Delta x)^2} = 1$$

$$\frac{8\phi_2 - 7\phi_1 - \phi_3}{2\Delta x^2} = 1 + \frac{3}{\Delta x}$$

$$a_{11} = -\frac{7}{2\Delta x^2} \qquad b_1 = 1 + \frac{3}{\Delta x}$$

$$a_{12} = \frac{8}{2\Delta x^2}$$

$$a_{13} = -\frac{1}{2\Delta x^2}$$

$$\left.\frac{d^2\phi}{dx^2}\right|_{x=2} = \frac{\phi_3 - 2\phi_2 + \phi_1}{\Delta x^2} = \cancel{e^{x}} = e^{\frac{L}{n-1}}$$

$$= S_2$$

$L = 1$

$1 \quad 2 \quad n$

$$\frac{L}{n-1} = \Delta x.$$

$$a_{21} = \frac{1}{\Delta x^2} \qquad a_{22} = -\frac{2}{\Delta x^2} \qquad a_{23} = \frac{1}{\Delta x}$$

$$\phi_n = 1 \quad \Rightarrow \quad a_{nn} = 1 \qquad a_{n1} \;--\; a_{n\,n-1}$$

$$a_{11} = -\frac{7}{2\Delta x^2} \qquad b_1 = 1 + \frac{3}{\Delta x}$$

$$a_{12} = \frac{8}{2\Delta x^2}$$

$$a_{13} = -\frac{1}{2\Delta x^2}$$

$$\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & 1 & -2 & & 1 \\ & & & 1 & -2 \end{bmatrix}$$

$$A = \begin{bmatrix} -\frac{7}{2\Delta x^2} & \frac{4}{\Delta x^2} & -\frac{1}{2\Delta x^2} & & \\ \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x} & & \\ & \ddots & \ddots & \ddots & \\ & & & & 1 \end{bmatrix}$$

1. toeplitz([-2 1 zeros(1, 6)])   n = 100

$$\text{zeros}(1,\ \underset{\uparrow\ n}{6})$$

2. $-2 \times \underbrace{\text{eye}(10)} + \text{diag}(\text{ones}(9, 1), 1) + \text{diag}(\text{ones}(9, 1), -1)$

$$\begin{bmatrix} -2 & +1 & 1 & & & \\ +1 & -2 & 1 & 1 & & \\ & +1 & \ddots & 1 & 1 & \\ & & +1 & -2 & 1 & 1 \\ & & & +1 & -2 & \\ & & & & +1 & \end{bmatrix}$$

```
for i = 2 : N-1
    A(i, i) = -2
    A(i, i+1) = 1
    A(i, i-1) = 1
end
```

O(N)

1. Dirichlet 定值 $\phi_L = \phi$

2. Neumann $\left.\frac{d\phi}{dx}\right|_{x=1} =$ 2阶

$\left.\frac{d^2\phi}{dx^2}\right|_{x=1}$

3. $Ax = b$ A，怎么实现

高维 $\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = S_\phi$

1. 30% 上课听得有意思

2. 看书. 5% - 10%.

3. 推导 10% - 20%

4. 做作业. (精进) 30% 手动, 70% (编程)

两周交.人 2 → 没有上限

markdown / Latex (有一点模板)

代码. 测试. 功能,

→ 并行. 100 × 100 matlab parallel par for

图. → SCI. / Journal of numerical analysis

计数 ~~JCI~~ 第一档

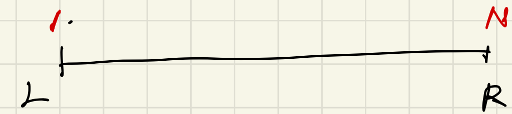
思考结果

第四次课

1. 第三类边界条件 $\alpha\phi(x_L) + \beta\frac{d\phi}{dx}\Big|_{x=L} = \gamma$

N−1 块. $\Delta x = \frac{L}{N-1}$

2. 二维问题. $\nabla^2\phi = S\phi$



$$\alpha\phi(x_L) + \beta\frac{d\phi}{dx}\Big|_{x=L} = \gamma \Rightarrow \frac{d\phi}{dx}\Big|_{\substack{x=L\\x=1}} = \boxed{\frac{\gamma - \alpha\phi_1}{\beta}}$$

robin

法国科学家

$$\frac{d\phi}{dx} = \frac{4\phi_2 - \phi_3 - 3\phi_1}{\Delta x} + O(\Delta x^2)$$

$$\frac{d^2\phi}{dx^2} = \frac{8\phi_2 - \phi_3 - 7\phi_1 - 6\Delta x\, J}{2(\Delta x)^2} + O(\Delta x^2)$$

$$\phi_3 = \phi_1 + (2\Delta x)\frac{d\phi}{dx}\Big|_{x=1} + \frac{(2\Delta x)^2}{2!}\frac{d^2\phi}{dx^2}$$

$$\phi_2 = \phi_1 + \Delta x\frac{d\phi}{dx}\Big|_{x=1} + \cdots$$

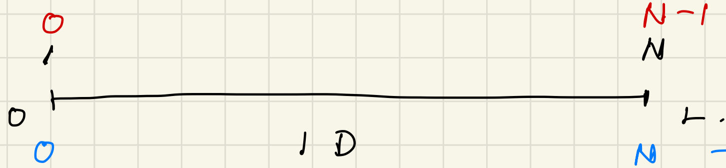
$$\frac{d^2\phi}{dx^2}\Big|_{x=1} = \frac{8\phi_2 - \phi_3 - (7 - 6\Delta x\frac{\alpha}{\beta})\phi_1 - 6\Delta x(\frac{\gamma}{\beta})}{2(\Delta x)^2} = S_1$$

第二类 多维问题 (2D)

$$\nabla^2\phi = S_\phi$$

1D $\Rightarrow$ $\dfrac{d^2\phi}{dx^2} = S_\phi$ (ODE)

2D $\Rightarrow$ $\dfrac{\partial^2\phi}{\partial x^2} + \dfrac{\partial^2\phi}{\partial y^2} = S_\phi$ (PDE)

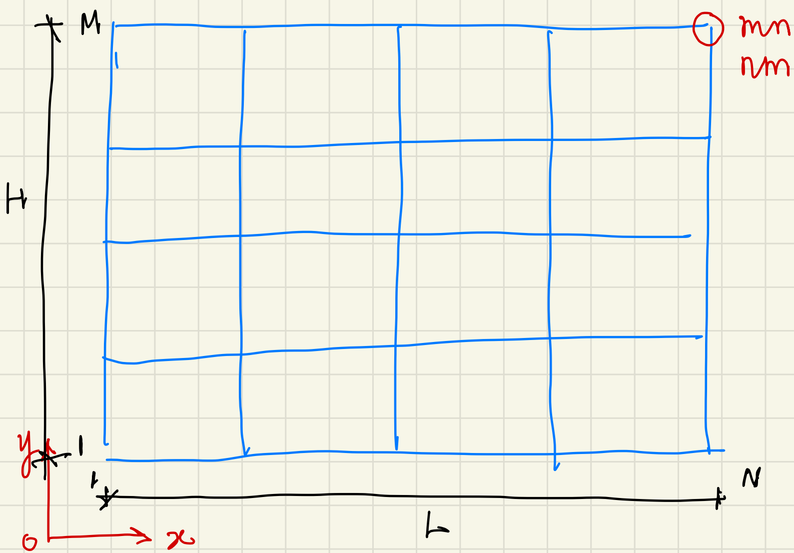


$\Delta x = \dfrac{L}{N-1}$ (matlab) N−1

N $\to$ N+1 个节点 网格 N

matlab (用得人多)

0 $\to$ 1, 1 $\to$ 100



column-wise

row-wise

$$\begin{array}{cccccc} 1 & 2 & 3 & 4 & 5 & 6 \end{array}$$

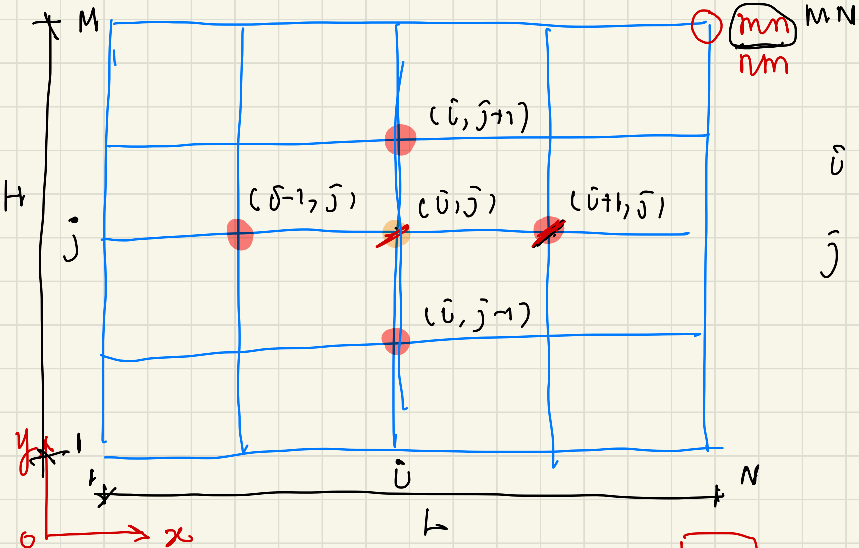
$A = [1\ 2\ 3\ 4\ 5\ 6]$

$A = \mathrm{reshape}(A, [2, 3])$

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix} \qquad \begin{array}{c} \begin{array}{ccc} 1 & 3 & 5 \end{array} \\ \begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix} \end{array}$$

A B

列优



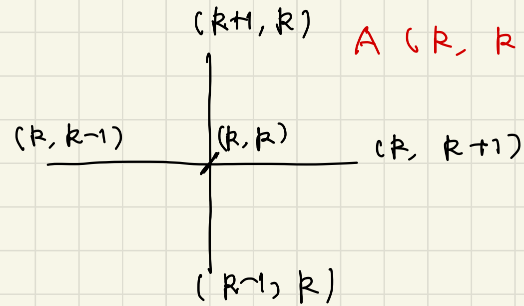
$$\Delta x = \frac{L}{N-1} \qquad \Delta y = \frac{L}{m-1}$$

$i \in 1,\ N.$

$\quad\quad\quad\ \ \|$

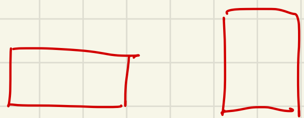
$j \in 1,\ M.$

$A(k, k)$ 列 行



$A(k, k+1)$

$N = M \Rightarrow$



泰勒展开. 下册

$$\phi_{i+1,j} = \phi_{i,j} + (x_{i+1,j} - x_{i,j})\frac{\partial\phi}{\partial x}\Big|_{i,j} + \cancel{(y_{i+1,j} - y_{i,j})}\frac{\partial\phi}{\partial y}\Big|_{i,j} \quad 0$$

$$+ \frac{1}{2}(x_{i+1,j} - x_{i,j})^2\frac{\partial^2\phi}{\partial x^2}\Big|_{i,j} + \frac{1}{2}\cancel{(y_{i+1,j} - y_{i,j})^2}\frac{\partial^2\phi}{\partial y^2}\Big|_{i,j} + \frac{1}{2}(x_{i+1,j} - x_{i,j})\cancel{(y_{i+1,j} - y_{i,j})}\frac{\partial^2\phi}{\partial x\partial y} \quad 0 \quad 0$$

$$+ \frac{1}{3!}(x_{i+1,j} - x_{i,j})^3\frac{\partial^3\phi}{\partial x^3}\Big|_{i,j} + \frac{1}{3!}\cancel{(y_{i+1,j} - y_{i,j})^3}\frac{\partial^3\phi}{\partial y^3}\Big|_{i,j} + \frac{1}{3!}(x_{i+1,j} - x_{i,j})^2\cancel{(y_{i+1,j} - y_{i,j})}\frac{\partial^3\phi}{\partial x^2\partial y} + \quad 0 \quad 0$$

$$\frac{1}{3!}(x_{i+1,j} - x_{i,j})\cancel{(y_{i+1,j} - y_{i,j})^2}\frac{\partial^3\phi}{\partial x\partial y^2} \quad 0$$

$$\phi_{i+1,j} = \phi_{i,j} + (\overset{\Delta x}{x_{i+1,j} - x_{i,j}}) \frac{\partial \phi}{\partial x}\Big|_{i,j} + \frac{1}{2}(\overset{\Delta x}{x_{i+1,j} - x_{i,j}})^2 \frac{\partial^2 \phi}{\partial x^2}\Big|_{i,j}$$

$$+ \frac{1}{3!}(\overset{\Delta x}{x_{i+1,j} - x_{i,j}})^3 \frac{\partial^3 \phi}{\partial x^3}\Big|_{i,j} + \cdots$$

$$\phi_{i+1,j} = \phi_{i,j} + \Delta x \frac{\partial \phi}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 \phi}{\partial x^2} + \frac{1}{3!} \Delta x^3 \frac{\partial^3 \phi}{\partial x^3} + \frac{1}{4} \Delta x^4 \frac{\partial^4 \phi}{\partial x^4} \quad 1$$

$$\phi_{i-1,j} = \phi_{i,j} - \Delta x \frac{\partial \phi}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 \phi}{\partial x^2} - \frac{1}{3!} \Delta x^3 \frac{\partial^3 \phi}{\partial x^3} + \frac{1}{4!} \Delta x^4 \frac{\partial^4 \phi}{\partial x^4} \quad 2.$$

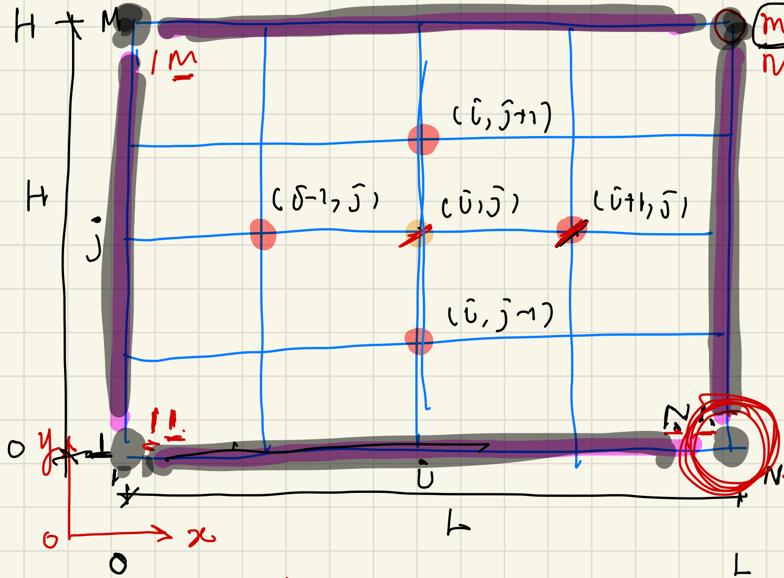
$$1+2 \Rightarrow \boxed{\frac{\partial^2 \phi}{\partial x^2} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} - \frac{1}{12} \Delta x^2 \frac{\partial^4 \phi}{\partial x^4}} \quad x \rightarrow$$

$$\boxed{\frac{\partial^2 \phi}{\partial y^2} = \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} - \frac{1}{12} \Delta y^2 \frac{\partial^4 \phi}{\partial y^4}} \quad y \rightarrow$$

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = S_\phi \Rightarrow \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta x^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta y^2} = S_{i,j}$$

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} = S_\phi$$

内结点. 边结点



四个角点.

四条边. { left, right, top, bottom, front, back

左: $\phi(0, y) = \phi_L$ Dirichlet

右: $\left.\frac{\partial \phi}{\partial x}\right|_{L,y} = J_R$ Neumann

上: $\phi(x, H) = \phi_T$ Dirichlet

下: $\alpha \phi(x, 0) + \beta \left.\frac{\partial \phi}{\partial y}\right|_{x,0} = \gamma$ Robin

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = S_{N,1}$$

1M $\frac{\phi_L + \phi_T}{2}$.

11 ϕ_L

NM ϕ_T

N1

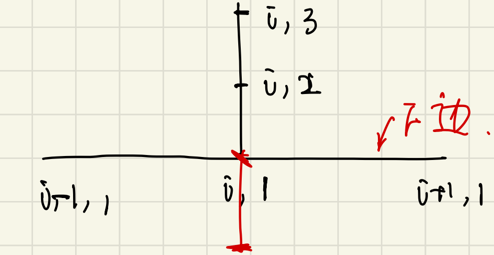
[i = 1, j = 2, --- M-1.] 左.

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = S\phi$$

[i = N, j = 2, --- M-1] 右

[j = 1, i = 2 --- N-1] 下

[j = M, i = 2 --- N-1] 上

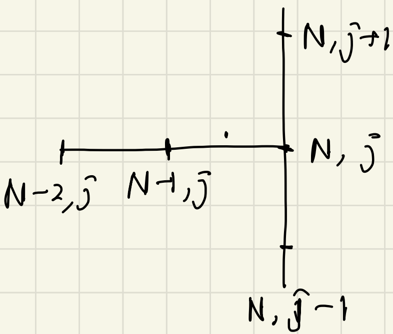


下 $a\phi(x,0) + \beta \frac{\partial\phi}{\partial y}\Big|_{x,0} = \gamma$ Robin

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = S_\phi \Rightarrow \frac{\partial^2\phi}{\partial x^2} = \frac{\phi_{i+1,1} - 2\phi_{i,1} + \phi_{i-1,1}}{\Delta x^2}$$

$+$

$$\frac{\partial^2\phi}{\partial y^2} = \frac{8\phi_{i,2} - \phi_{i,3} - (7 - 6\Delta y\frac{a}{\beta})\phi_{i,1} - 6\Delta y(\frac{\gamma}{\beta})}{2\Delta y^2} = S_{i,1}$$



右 : $\frac{\partial\phi}{\partial x}\Big|_{L,y} = J_R$ Neumann

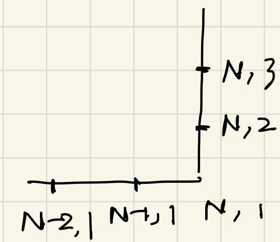
$$\left.\begin{aligned} &\frac{\partial^2\phi}{\partial y^2} = \frac{\phi_{N,j+1} - 2\phi_{N,j} + 2\phi_{N,j-1}}{\Delta y^2} \\ &+ \\ &\frac{\partial^2\phi}{\partial x^2} = \frac{8\phi_{N-1,j} - \phi_{N-2,j} + 7\phi_{N,j} + 6\Delta x J_R}{2\Delta x^2} \end{aligned}\right\} = S_{N,j}$$

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = S_\phi$$

$$\frac{d^2\phi}{dx^2}\Big|_{x=1} = \frac{8\phi_2 - \phi_3 - (7 - 6\Delta x\frac{a}{\beta})\phi_1 - 6\Delta x(\frac{\gamma}{\beta})}{2(\Delta x)^2} = S_1$$

$$\frac{8\phi_{N-1,1}-\phi_{N-2,1}-7\phi_{N,1}+6\Delta x J_R}{2\Delta x^2}+\frac{8\phi_{N,2}-\phi_{N,3}-\left(7-6\Delta y\frac{\alpha}{\beta}\right)\phi_{N,1}-6\Delta y\left(\frac{\gamma}{\beta}\right)}{2\Delta y^2}=S_{N,1}$$

$\left(\frac{\partial^2\phi}{\partial x^2}\right)$ 右 $\left(\frac{\partial^2\phi}{\partial y}\right)$ 下



1. 补 第三类边界

2. 二维有限差分.

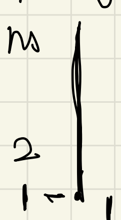
for $i = 2$ — $N-1$

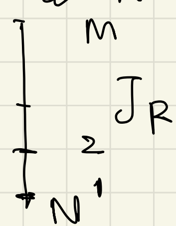
for $j = 2$ — $M-1$

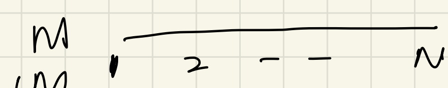
22, 23, -- 2-M-1

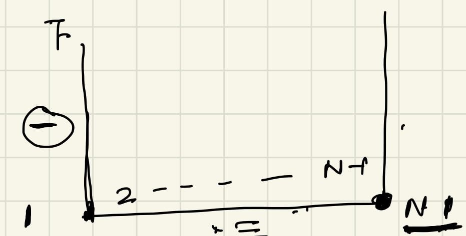
$i = 2$ -- $N-1$
$j = 2$ — $M-1$ } 内结点 中央差分. 5点格式

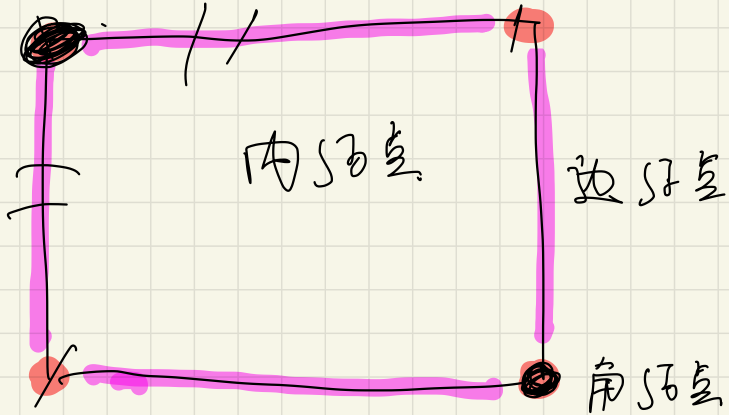
$i=1$. $j = 1$ --- M $i=N$ $j=M$ $i=1$ -- N $j=1$ $i=1$ -- N










内结点
边结点
角结点

第五次课 线性矩阵求解

真实生活中 ⟶ 物理模型 ⟶ 数学模型（PDE）$\xrightarrow[\text{离散}]{\text{FDM, FVM}}$ 代数方程组.

$Ax=b$.

$$Ax = b. \quad (\text{求解})$$

$Ax=b$ 不用自己写. eigen3.（C++） $A \backslash b$ PETSc.

OpenFOAM（界） CFD

1. grid（mesh）
2. fields（u, v, p, T etc）
3. matrix fvMatrix
4. boundary
5. solution
6. output

1. preprocessor.
2. solver
3. postprocessing

$Ax = b.$

$$\begin{cases} 1.\ \text{直接法} \quad \text{高斯消元} \quad \text{TDMA} \\ 2.\ \text{间接法}\ (\text{迭代法}).\ \text{Jacobi.} \quad \text{Gauss-Seidel} \end{cases}$$

CGS

CG. MG $\begin{cases} \text{GMG} \\ \text{AMG} \end{cases}$

GMRS.

Jacobi. GS, ADI. stone's, CG. CGS multi grid

1. 直接法 求逆. $\begin{cases} \text{sparse} \\ \text{dense.} \end{cases}$ 线代 18.06 (Gilbert Strang)

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \quad (1) \Rightarrow x_1 = \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}}x_2 - \frac{a_{13}}{a_{11}}x_3 - \cdots - \frac{a_{1n}}{a_{11}}x_n$$

$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \quad 2 \Rightarrow \left(a_{22} - a_{12}\frac{a_{21}}{a_{11}}\right)x_2 + \left(a_{23} - a_{13}\frac{a_{21}}{a_{11}}\right)x_3$$

$$a_{31}x_1 + a_{32}x_2 + \cdots + a_{3n}x_n = b_3 \qquad + \cdots + \left(a_{2n} - a_{1n}\frac{a_{21}}{a_{11}}\right)x_n \qquad i,\ j$$

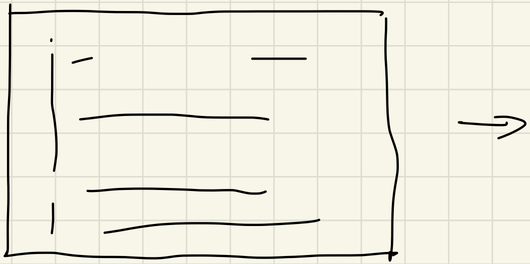
$$a_{n1}x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n \quad n \qquad = b_2 - b_1\frac{a_{21}}{a_{11}} \qquad b_j - b_i\frac{a_{ji}}{a_{ii}}$$

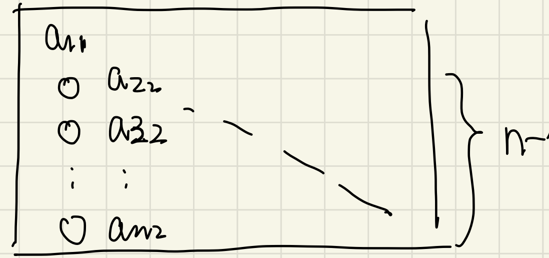
$$\left(a_{32} - a_{12}\frac{a_{31}}{a_{11}}\right)x_2 + \left(a_{23} - a_{13}\frac{a_{31}}{a_{11}}\right)x_3$$

$$+ \cdots + \left(a_{3n} - a_{1n}\frac{a_{31}}{a_{11}}\right)x_n$$

$$= b_3 - b_1\frac{a_{31}}{a_{11}}$$

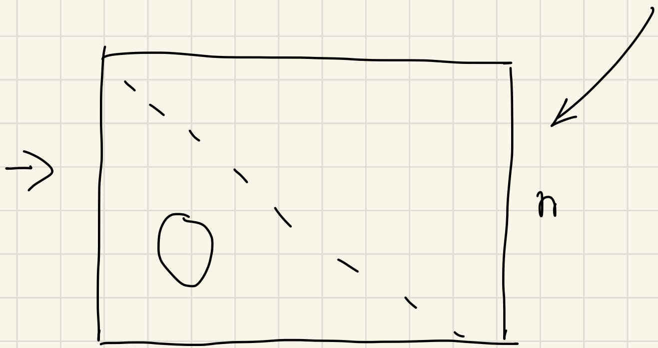
$$a_{n-1\,n-1}x_{n-1} + a_{n-1\,n}x_{nn} = b_{n-1} \qquad x_{nn} = \frac{b_n}{a_{nn}}$$





$a_{21} - a_{n1} = 0$

x_1



$$a_{ij}^{*} = a_{ij} - a_{1j}\frac{a_{j1}}{a_{11}}$$

$$(a_{22} - a_{12}\frac{a_{21}}{a_{11}})x_2 + \boxed{(a_{23} - a_{13}\frac{a_{21}}{a_{11}})}x_3$$

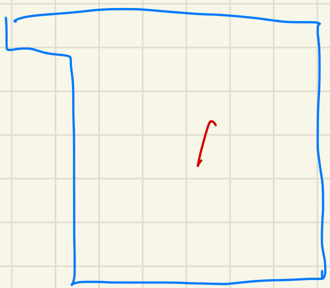
$$+\cdots+(a_{2n} - a_{1n}\frac{a_{21}}{a_{11}})x_n \qquad i, \quad j$$

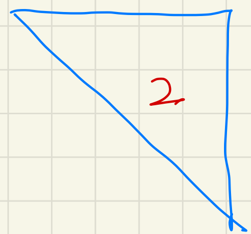
$$= b_2 - b_1\frac{a_{21}}{a_{11}} \qquad b_j - b_i\frac{a_{ji}}{a_{ii}}$$

$$(a_{32} - a_{12}\frac{a_{31}}{a_{11}})x_2 + (a_{23} - a_{13}\frac{a_{31}}{a_{11}})x_3$$

$$+\cdots+(a_{3n} - a_{1n}\frac{a_{31}}{a_{11}})x_n$$

$$= b_3 - b_1\frac{a_{31}}{a_{11}}$$





$$a^*_{i,j} = a_{i,j} - \frac{a_{ip}}{a_{pp}}a_{p,j}$$

$$a^*_{23} = a_{23} - \frac{a_{2,p}}{a_{pp}}a_{p,3}$$

$$0x_1 + a^*_{22}x_2 + a^*_{23}x_3 + \cdots + a^*_{2n}x_n = b^*_2$$

a''_{ii}

$$a^*_{22} = (a_{22} - a_{12}\frac{a_{21}}{a_{11}})$$

$$a^*_{23} = (a_{23} - a_{13}\frac{a_{21}}{a_{11}})$$

$$a^*_{ij} = a_{ij} - a_{1j}\frac{a_{i1}}{a_{11}}$$

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$$a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n = b_2$$
$n-1$
$$a_{n1}x_1 + a_{n2}x_2 \cdots + a_{nn}x_n = b_n$$

$\Rightarrow$

$$a_{11}x_1 + a_{12}x_2 \cdots + a_{1n}x_n = b_1$$
$$0x_1 + a_{22}^{*}x_2 \cdots + a_{2n}x_n = b_2$$
$n-2$
$$\vdots$$
$$0x_1 + a_{n2}x_2 + \cdots + a_{nn}x_n = b_n$$

$$a_{22}^{*} = a_{22} - a_{12}\frac{a_{21}}{a_{11}}$$

$$x_2 = \frac{b_2}{a_{22}} - \frac{a_{23}}{a_{22}}x_3 - \frac{a_{24}}{a_{22}}x_4 - \frac{a_{2n}}{a_{22}}x_n$$

$A(i,j) = A(i,j) + C$

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$\Rightarrow$
$$a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \quad n-1$$
$$\vdots$$
$$0 x_n + a_{n3}x_n + \cdots + a_{nn}x_n = b_n$$

0

n^3

$\Rightarrow$
$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \vdots \\ a_{n,n-1} \quad a_{nn}x_n = b_n \end{cases}$$
1

$n-1$ 循环

$(n-1) + (n-2) \;—\; 1 \quad \frac{n^2}{2}$

$$(n-1) + (n-2) + \cdots + 1 = \frac{1}{2}(n-1)n = \frac{n^2}{2}$$

$n-1$

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1 \\ \quad a_{22}x_2 + \cdots + a_{2n}x_n = b_2 \\ \quad \vdots \\ \quad \underline{a_{nn}x_n = b_n} \end{cases}$$

$\uparrow n$

$$x_{n-1} = \frac{b_{n-1} - a_{n-1\,n}\dfrac{b_n}{a_{nn}}}{a_{n-1\,n-1}} \qquad n-1$$

$$\Rightarrow \quad x_n = \frac{b_n}{a_{nn}} \qquad 0$$

n^2

$40^2 = 1600$

$\underline{O(40^3)}$

$\underline{40^3} = 64000$

64000^2 dense sparse

TDMA

中央差分

$$\begin{bmatrix} -2 & 1 & & \\ +1 & -2 & 1 & \\ & \ddots & \ddots & \\ & & -1 & -2 \end{bmatrix} \Rightarrow \begin{bmatrix} d_1 & c_1 & & 0 \\ a_1 & d_2 & c_2 & \\ & \ddots & \ddots & c_{n-1} \\ 0 & & a_{n-1} & d_n \end{bmatrix}$$

高斯消元的变种

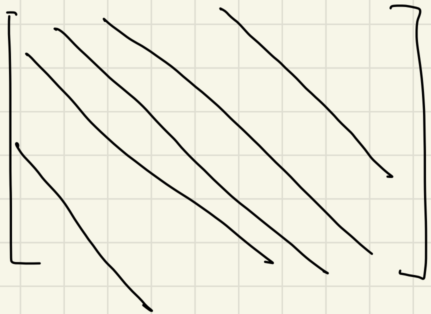
$O(n)$

$n + n-1 + n-1 = 3n-2$

1维. 内节点 $$\frac{d^2\phi}{dx^2} = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2}$$

2维 内节点 $$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = \frac{\phi_{i+1,j} - 2\phi_{i,j} + \phi_{i-1,j}}{\Delta y^2} + \frac{\phi_{i,j+1} - 2\phi_{i,j} + \phi_{i,j-1}}{\Delta x^2}$$

+1 $\quad$ 0 $\quad \underbrace{+1 \quad -2 \quad +1}$ $\quad$ 0 $\quad$ +1 $\quad$ +1 $\quad$ 0 $\quad$ +1 $\quad$ -2 $\quad$ 1 $\quad$ 0 $\quad$ +1



一维 $\frac{d^2\phi}{dx^2}$ → 四阶

$\phi_{i+2} + \phi_{i+1} + \phi_i + \phi_{i-1} + \phi_i$

间接法. 迭代算法.

Jacobi Gauss - Seidel ADI. Stone's MSD. CG. CGS.

求解问答问题.

$5x + 2y = 3$.
$2x + 3y = 1$

消元法.

$$\begin{cases} 5x + 2y + 2z = 9 \\ 2x - 6y + 3z = -1 \\ x + 2y + 7z = 10 \end{cases}$$

guess ( ).

$$\begin{bmatrix} 5 & 2 & 2 \\ 2 & -6 & 3 \\ 1 & 2 & 7 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 9 \\ -1 \\ 10 \end{bmatrix}$$

$$\begin{cases} x = \dfrac{9 - 2y - 2z}{5} \\ y = \dfrac{-1 - 2x - 3z}{-6} \\ z = \dfrac{10 - x - 2y}{7} \end{cases}$$

$$\begin{cases} x = \dfrac{9-2y+2z}{5} \\ y = \dfrac{-1-2x-3z}{-6} \\ z = \dfrac{10-x-2y}{7} \end{cases}$$

1. 假设 $(0,0,0)^T$

2. 第一次迭代 $y = \dfrac{-1-2\cdot 0-3\cdot 0}{-6}$

① $x = 1.8$, $y = 0.16667$, $z = 1.4285$

3. 第二次迭代

4. 迭代停止

Jacobi

$$\begin{cases} x = \dfrac{9-2y+2z}{5} \\ y = \dfrac{-1-2x-3z}{-6} \\ z = \dfrac{10-x-2y}{7} \end{cases}$$

第二次迭代

$x = 1.8$, $y = \dfrac{-1-2\cdot 1.8-3\cdot 0}{-6} = \dfrac{4.6}{6}$

Gauss-seidel

$$\begin{cases} 5x + 2y + 2z = 9 \\ 2x - 6y + 3z = -1 \\ 0x + 2y + \boxed{7}z = 10 \end{cases}
\qquad
\begin{bmatrix} 5 & 2 & 2 \\ 2 & -6 & 3 \\ \cancel{1} & 2 & 7 \end{bmatrix}$$

$\rightarrow$ divergence, convergence

diagonal dominance 对角占优 Scarborough criterion

$$|a_{i,i}| \geq \sum_{\substack{j=1 \\ i \neq j}}^{j=n} |a_{i,j}| \quad \forall\ i = 1, 2, \dots n.$$

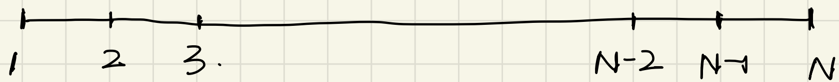
$$|a_{i,i}| > \sum |a_{i,j}| \quad \text{at least one}$$

$$\begin{bmatrix} & +1 & -2 & 1 & \end{bmatrix}$$

1. 直接法. 高斯消元
2. 间接法. Jacobi. Gauss-Seidel

residual

$$\frac{d\phi}{dx} = J_L = 1 \qquad \frac{d^2\phi}{d^2x} = S \qquad \frac{d\phi}{dx} = J_R$$



$$\phi_2 = \phi_1 + \Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \frac{\Delta x^3}{3!}\frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_3 = \phi_1 + 2\Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \frac{(2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3} + \frac{(2\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_2 = \phi_1 + \Delta x \overset{J}{\cancel{\left.\frac{d\phi}{dx}\right|_{x=1}}} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \frac{\Delta x^3}{3!}\frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_3 = \phi_1 + 2\Delta x \overset{J}{\cancel{\left.\frac{d\phi}{dx}\right|_{x=1}}} + \frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \frac{(2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3} + \frac{(2\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$A\left[\phi_2 = \phi_1 + \Delta x\right] + A\frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \cancel{A\frac{\Delta x^3}{3!}\frac{d^3\phi}{dx^3}} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4} + \cdots\Big]$$

$$B\left[\phi_3 = \phi_1 + 2\Delta x\right] + B\frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \cancel{B\frac{(2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3}} + \frac{(2\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots\Big]$$

$$\frac{d^2\phi}{dx^2} = \frac{8\phi_2 - \phi_3 - 7\phi_1 - (6\Delta x)J_L}{2\Delta x^2} + O(\Delta x^2)$$

$$\frac{d^2\phi}{dx^2} = \frac{8\phi_{n-1} - \phi_{n-2} - 7\phi_n + (6\Delta x)J_R}{2\Delta x^2}$$

$\to N$

$$\phi_{n-1} = \phi_n - \Delta x \left.\frac{d\phi}{dx}\right|_x + \frac{(-\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \frac{(-\Delta x)^3}{3!}\frac{d^3\phi}{dx^3} + \frac{(-\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_{n-2} = \phi - 2\Delta x \left.\frac{d\phi}{dx}\right|_x + \frac{(-2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \frac{(-2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3} + \frac{(-2\Delta x)^4}{4}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_2 = \phi_1 + \Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \frac{\Delta x^3}{3!}\frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$\phi_3 = \phi_1 + 2\Delta x \left.\frac{d\phi}{dx}\right|_{x=1} + \frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \frac{(2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3} + \frac{(2\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots$$

$$A\left[\phi_2 = \phi_1 + \Delta x \quad + A\frac{\Delta x^2}{2}\frac{d^2\phi}{dx^2} + \cancel{A\frac{\Delta x^3}{3!}\frac{d^3\phi}{dx^3}} + \frac{\Delta x^4}{4!}\frac{d^4\phi}{dx^4} + \cdots\right]$$

$$B\left[\phi_3 = \phi_1 + 2\Delta x \quad + B\frac{(2\Delta x)^2}{2}\frac{d^2\phi}{dx^2} + \cancel{B\frac{(2\Delta x)^3}{3!}\frac{d^3\phi}{dx^3}} + \frac{(2\Delta x)^4}{4!}\frac{d^4\phi}{dx^4} + \cdots\right]$$

第六次课 迭代解法

精典解法
1. Jacobi
2. Gauss-Seidel
3. ADI

二维泊松方程　$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} = S\phi$
二阶格式　$\Delta\phi = S$.
三类边界条件

Stone's 不讲.

常用
1. conjugate gradient　CG
2. multi grid (MG)
   - GMG　几何多重网格
   - AMG　代数 - - (?)

学会. 作业　poisson + FDM. (二维)　$\Delta u = f$.

$Ax = b$ (sparse matrix)　$x = A \setminus b$;　Eigen3. ;　numpy.　algebra <u>lone</u>

PETSc.

SPD (symmetric positive definite)
对称正定

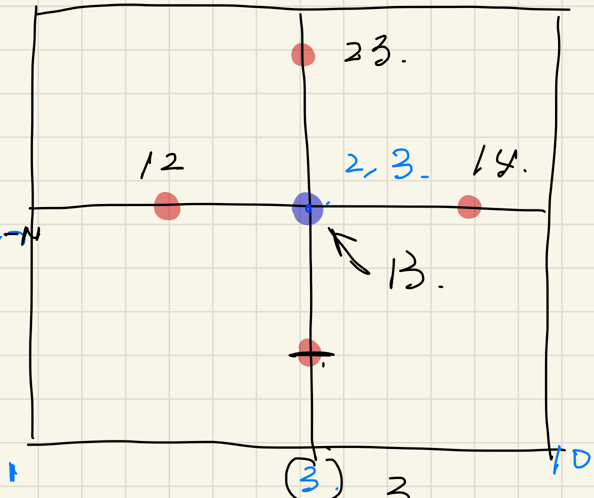
二阶. $\frac{\phi_{i+1,j}-2\phi_{i,j}+\phi_{i-1,j}}{\Delta x^2}+\frac{\phi_{i,j+1}-2\phi_{i,j}+\phi_{i,j-1}}{\Delta y^2}=S_{i,j}$

$$\boxed{\left(-\frac{2}{\Delta x^2}-\frac{2}{\Delta y^2}\right)\phi_{i,j}=S_{i,j}-\frac{1}{\Delta x^2}\phi_{i+1,j}-\frac{1}{\Delta x^2}\phi_{i-1,j}-\frac{1}{\Delta y^2}\phi_{i,j+1}-\frac{1}{\Delta y^2}\phi_{i,j-1}}$$

$$a_k\phi_k+\sum_{\substack{j=1\\ j\neq k}}^{N_{nb,k}}a_j\phi_j=S_k \qquad k=1,2,\dots,N$$

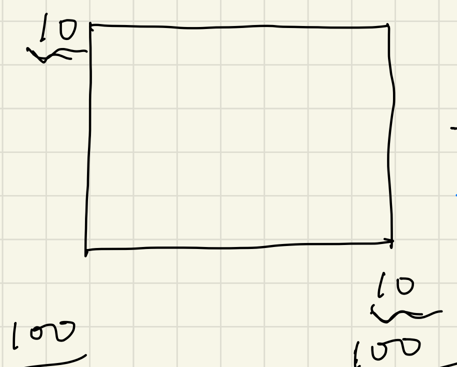
N, N

$a_k\phi_k+a_{k+1}\phi_k+a_{k-1}\phi_k+a_{k+N}\phi_{k+N}+a_{k-N}\phi_{k-N}$



3.

$\phi \sim ?$ 个



→ 矩阵

$A\overset{\phi}{x}=b$

$\begin{bmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_{100}\end{bmatrix}$

100×100

10^8

$(10^4)^2 = 10^8$

$\frac{100}{10^8}$

3N

A — 10^4 个元素

$10^4\times 8$ 个 byte

80k

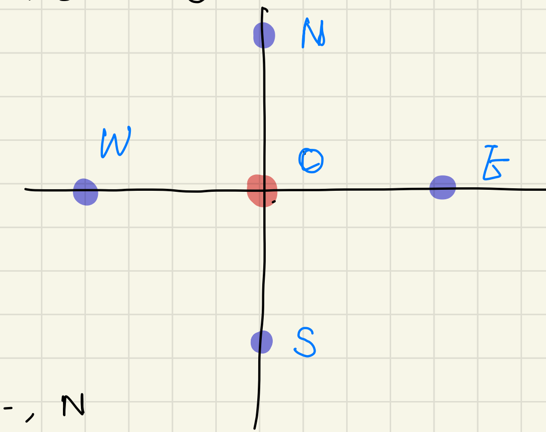
$10^3 = k$

$\frac{0.1\times G}{0.8G}$

$$a_k \phi_k + \sum_{\substack{j=1 \\ j \neq k}}^{N_{nb,k}} a_j \phi_j = S_k \qquad k = 1, 2, \cdots, N$$

$$a_k \phi_k + a_{k+1}\phi_{k+1} + a_{k-1}\phi_{k-1} + a_{k+N}\phi_{k+N} + a_{k-N}\phi_{k-N} = S_k.$$

$$\Rightarrow \quad a_O \phi_O + a_E \phi_E + a_W \phi_W + a_N \phi_N + a_S \phi_S = S_O$$



$$a_O = -\left(\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2}\right)$$

$$a_E = a_W = \frac{1}{\Delta x^2} \qquad a_N = a_S = \frac{1}{\Delta y^2}$$

$$\boxed{R_k^{(n)} = S_k - a_k \phi_k^{(n)} - \sum_{j=1}^{N} a_j \phi_j^{(n)}}$$

$k = 1 \cdots, N$

$$\begin{Bmatrix} 0.01 \\ 0.9 \\ \vdots \\ 0.333 \end{Bmatrix} = R^n \qquad R_1^{100} = 0.01$$

R^n

$R^{(n)}$ (residual vector)

$$a_k \phi_k + \sum_{\substack{j=1 \\ j \neq k}}^{N_{nb,k}} a_j \phi_j = S_k$$

$Ax = b$ $\quad A\vec{\phi} = \vec{b}$

$[\phi_1, \cdots, \phi_n]^T$ $\quad \begin{bmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_n \end{bmatrix}$

假设 $(n+1)$ 收敛 $a_k \phi_k^{n+1} + \sum a_j \phi_j^{n+1} = S_k$ $\quad \phi_k^{n+1}$

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

$$a_k \phi_k^n + a_k \phi_k' + \sum a_j \phi_j^n + \sum a_j \phi_j' = S_k$$

$$a_k \phi_k' + \sum a_j \phi_j' = \underbrace{S_k - a_k \phi_k^n - \sum a_j \phi_j^n}_{= R_k^n}$$

R^n 残差向量

$$\boxed{a_k \phi_k' + \sum a_j \phi_j' = R_k^n}$$

修正方程

correction form

L1 范数. $R1 = (r_1, r_2, \cdots r_n)^T$ abs(y - x_{new})

$$R_1 = \sum_{i=1}^{n} |r_i| \qquad R_1 = \max(|r_i|)$$

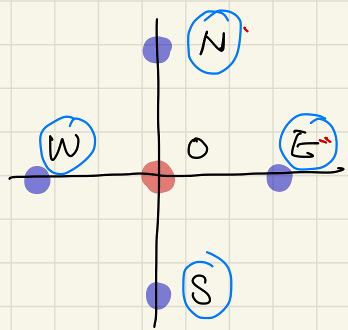
L2 范数 $$R2 = \sqrt{\sum_{i=1}^{n} r_i^2} \qquad R2 = \sqrt{R^T R}$$

$$R_2 < \varepsilon$$

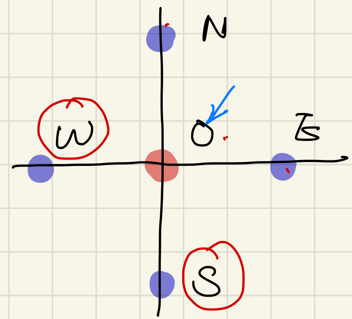
细节. C++, matlab, python

Julia. rust

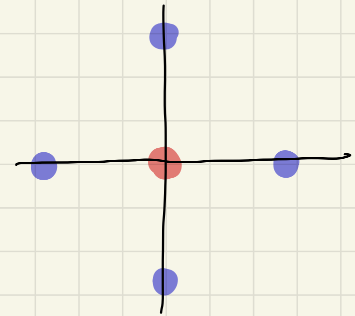
Jacobi / Gauss-Seidel / ADI (line by line)



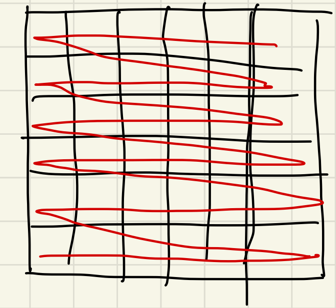
1 (初始值)



2.



3.



$$\phi_0^2 = \frac{S_0 - a_E\phi_E^1 - a_N\phi_N^1 - a_S\phi_S^1 - a_W\phi_W^1}{a_0} \quad \text{(Jacobi)}$$

point-wise

$$\phi_0^2 = \frac{S_0 - a_E\phi_E^1 - a_N\phi_N^1 - a_S\phi_S^2 - a_W\phi_W^2}{a_0} \quad \text{(Gauss-Seidel}$$

几何形状. 慢. 开销大.

算法　1. 初值（猜）$\phi_{i,j}$　$\forall\ i=1,\cdots,N,\ j=1,\cdots M.$　Gauss-Seidel

ϕ^0　第1类

2. 对内结点

$$\phi_{i,j}^{(n+1)}=\frac{S_{i,j}-a_E\phi_{i+1,j}^{n}-a_N\phi_{i,j+1}^{N}-a_S\phi_{i,j-1}^{n+1}-a_W\phi_{i-1,j}^{n+1}}{a_0}$$

$$\phi_{i,j}^{(n+1)}=\frac{S_{i,j}-a_E\phi_{i+1,j}^{n}-a_N\phi_{i,j+1}^{n}-a_S\phi_{i,j-1}^{n}-a_W\phi_{i-1,j}^{n}}{a_0}$$

对边结点. $\phi_{i,j}^{(n+1)}=\phi_{i,j}^{(n)}=\phi_{i,j}^{(0)}$

3. 计算残差向量 $\phi^{n+1}\rightarrow R2^{n+1}$

4 确定 $R2<\varepsilon$

5 结束后处理

```
for i = 1 : N - 1
    for j = 1 : M - 1
        phi(i, j) = ( S(i,j) - aE phi(i+1, j) - aW phi(i-1, j) - aN phi(i, j+1)
                    - aS phi(i, j-1) ) / aO
    end
end
```

i, j

Gauss - Seidel / jacobi

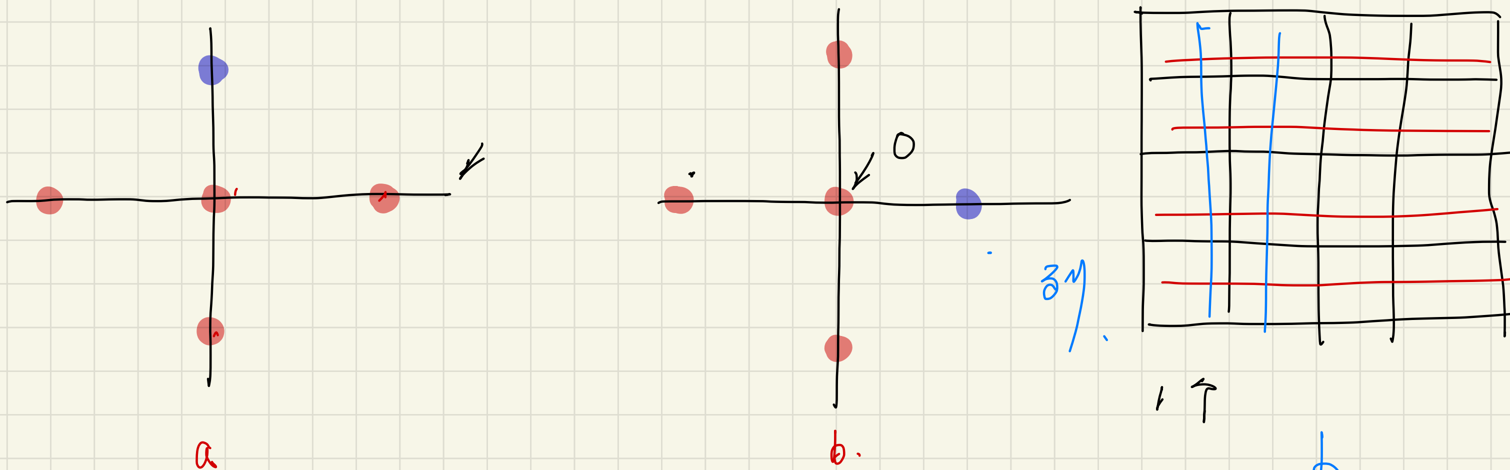
phi_new(i,j) = phi(i,j)

jacobi , Gauss - Seidel

1 2

phi(i, j) = phi_new(i, j)

线 line wise



$$\underbrace{\left(-\frac{2}{\Delta x^2}-\frac{2}{\Delta y^2}\right)}_{a_0}\phi_{i,j}^{n+1}+\underbrace{\frac{1}{\Delta x^2}}_{a_E}\phi_{i+1,j}^{n+1}+\underbrace{\frac{1}{\Delta x^2}}_{a_W}\phi_{i-1,j}^{n+1}=\boxed{S_{i,j}-\underbrace{\frac{1}{\Delta y^2}}_{a_N}\phi_{i,j+1}^{n}-\underbrace{\frac{1}{\Delta y^2}}_{a_S}\phi_{i,j-1}^{n+1}}$$

$n+1$

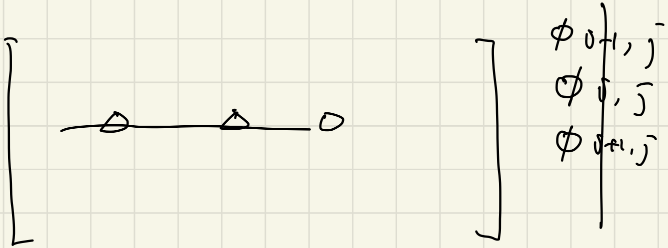
```
for i
    for j
        phi = a/b
    end
end
```

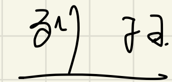
→

```
for i
    for j
        phi = a / b
    end
end
```

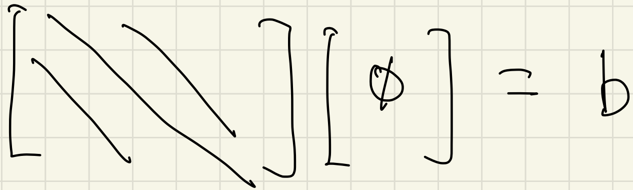
→ TDMA

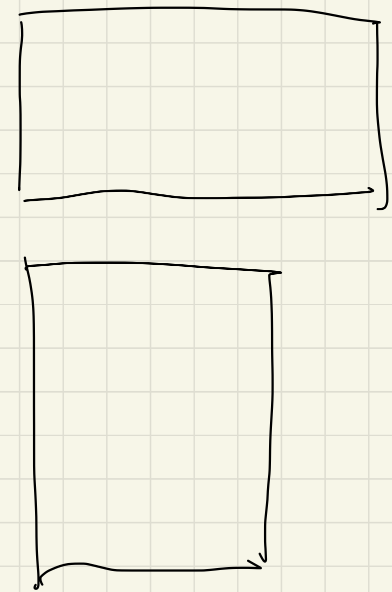
A \ b;



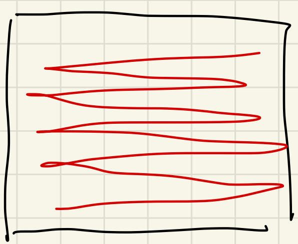


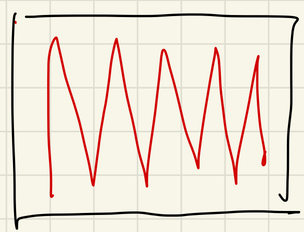
$Ax = b$





ADI (alternating direction implicit)





总结.

1. 残差向量 $R_k^n = S_k - a_k \phi_k^n - \sum a_j \phi_j^n$ R^n $R_2 = \sqrt{R^T R}$

2. 经典
$$\left\{\begin{array}{lll} \text{Jacobi} & \text{显式} & \text{并行} \\ \text{G-S} & \text{半隐式} & \text{不好并行} \\ \text{ADI} & & \end{array}\right.$$

steepest descent / conjugate method

误差. 稳定性.

第七次课. 迭代解法二

$$\left\{\begin{array}{l} \left.\begin{array}{l} \text{MSD} \\ \text{CG} \end{array}\right\} \text{一类} \\ \text{CGS} \end{array}\right.$$

$$\left\{\begin{array}{l} \cancel{\text{BCG}} \\ \text{BiCGSTAB} \ \checkmark \\ \text{GMRES} \ \checkmark \end{array}\right.$$

Lanczos 1952 MSD → CG → CGS

BiCGSTAB.

数学 → 证明

理解 实现 multi grid

FW 优化算法,

$$f(x_1, x_2, \cdots, x_n) = \frac{1}{2}[x_1, \cdots, x_n]^T [A] \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + [b]^T \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + C$$

$$f([x]) = \frac{1}{2}[x]^T A [x] + [b]^T [x] + C$$

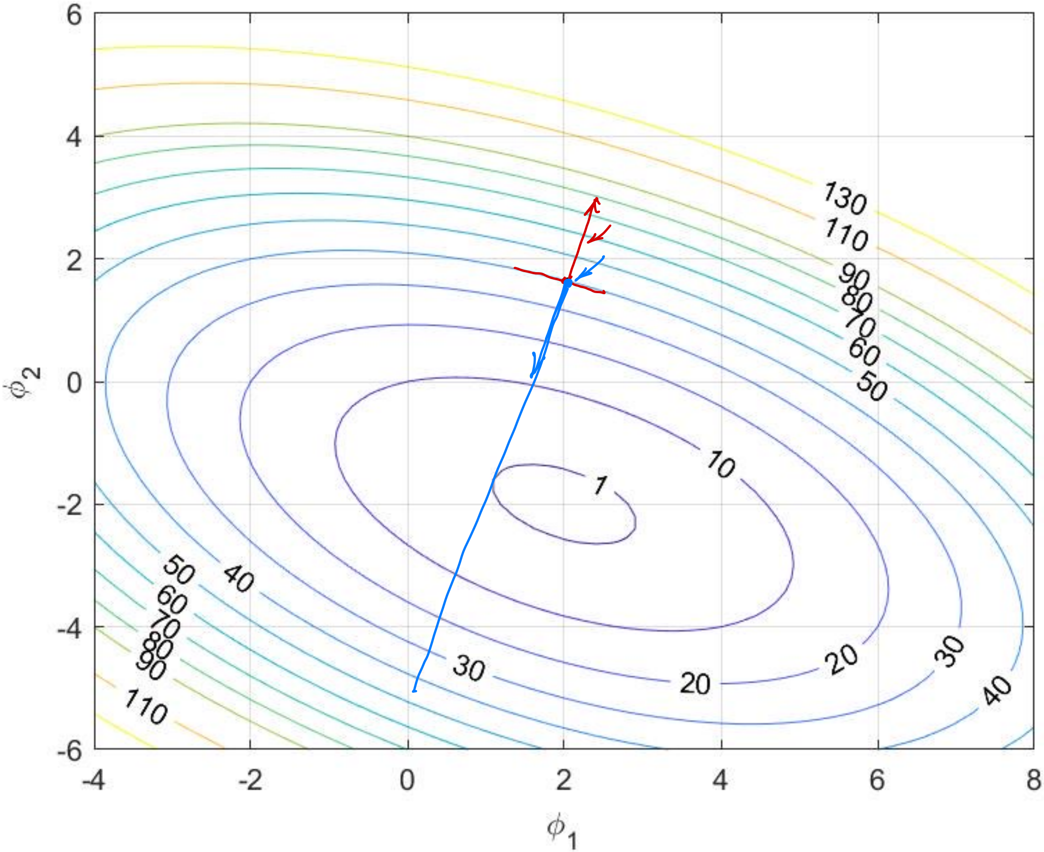
无痛入门 CG

$$[A][\phi] = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \end{Bmatrix} = b = \begin{Bmatrix} 2 \\ -8 \end{Bmatrix}$$

$$f(\phi_1, \phi_2) = [\phi_1, \phi_2] \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} + [2, -8] \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} + 10$$

$$= \frac{3}{2}\phi_1^2 + 2\phi_1\phi_2 + 3\phi_2^2 - 2\phi_1 + 8\phi_2 + C$$

$$f(x, y) = \frac{3}{2}x^2 + 2xy + 3y^2 - 2x + 8y + C$$



6
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-4
-2
0
2
4
6
8
ϕ_1
ϕ_2
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20
20
30
40

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial \phi_1} \\ \frac{\partial f}{\partial \phi_2} \\ \vdots \\ \frac{\partial f}{\partial \phi_n} \end{bmatrix} = \underbrace{\frac{1}{2} A^T \phi + \frac{1}{2} A \phi - b}\, = 0 \qquad A^T = A$$

$$\nabla f = A\phi - b$$

$$\Downarrow$$

$$A\phi = b. \quad \text{求解}$$

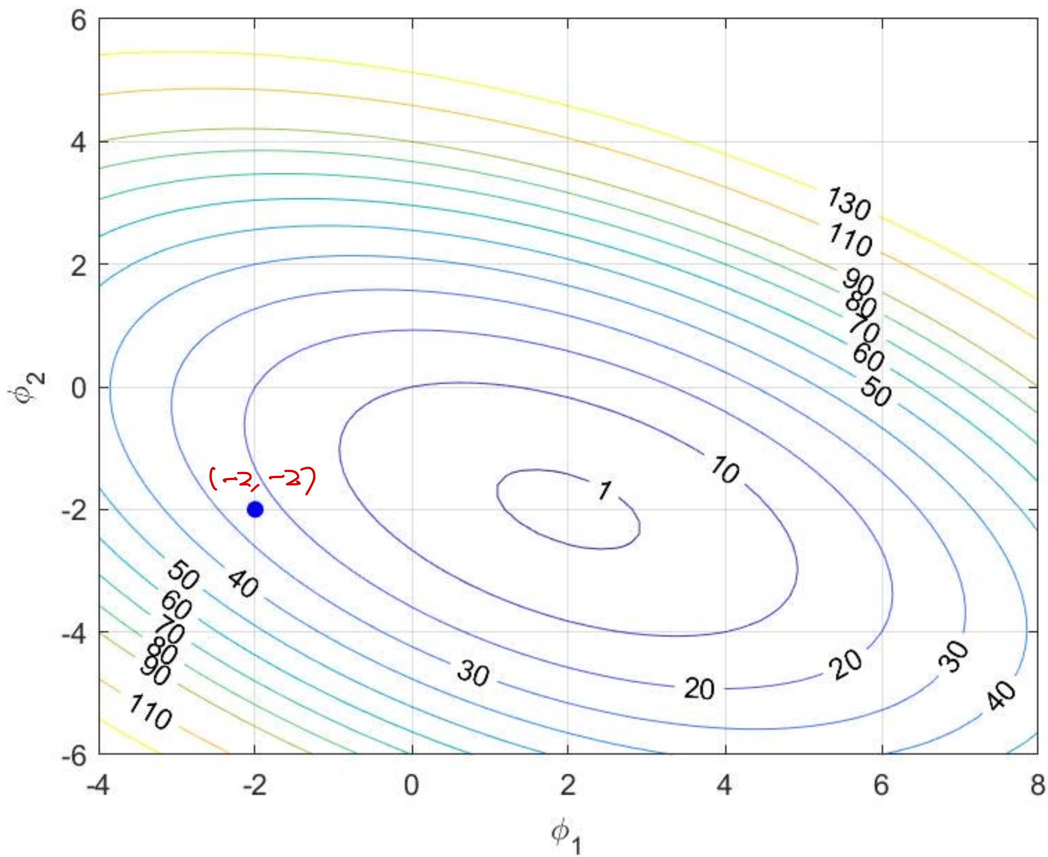
1. 给出初值 $\phi^0 \rightarrow R^0 = b - A\phi^0$

$$\nabla f^n = -R^n$$

2. $\phi^{n+1} = \phi^n - \alpha \nabla f^n = \phi^n + \alpha R^n$

$$\underbrace{f(\phi^{n+1})} \rightarrow \alpha \qquad \frac{\partial f}{\partial \alpha} = 0 \qquad \frac{df}{d\alpha} = 0$$

$$f(\phi_1, \phi_2, \cdots \phi_n) = \frac{\partial f}{\partial \phi_1}\frac{\partial \phi_1}{\partial \alpha} + \frac{\partial f}{\partial \phi_2}\frac{\partial \phi_2}{\partial \alpha} + \cdots + \frac{\partial f}{\partial \phi_n}\frac{\partial \phi_n}{\partial \alpha}$$



(-2, -2)
1
10
20
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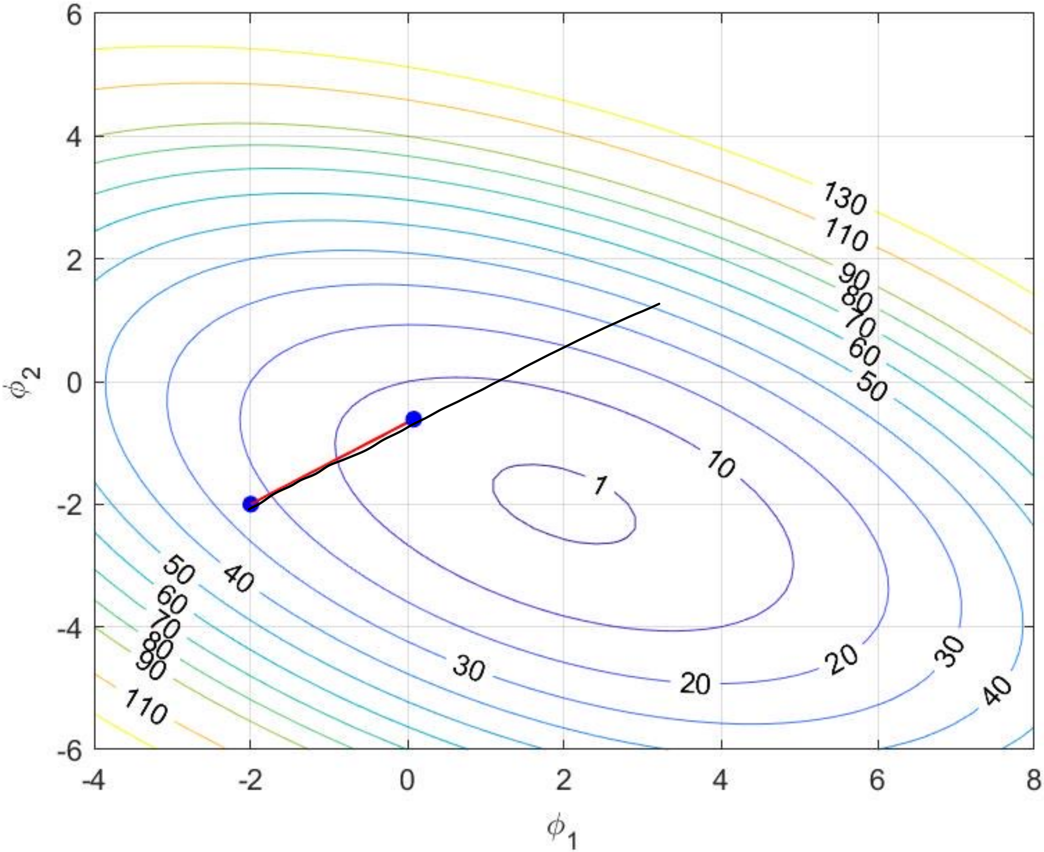
70
80
90
110
130
ϕ_1
ϕ_2



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40
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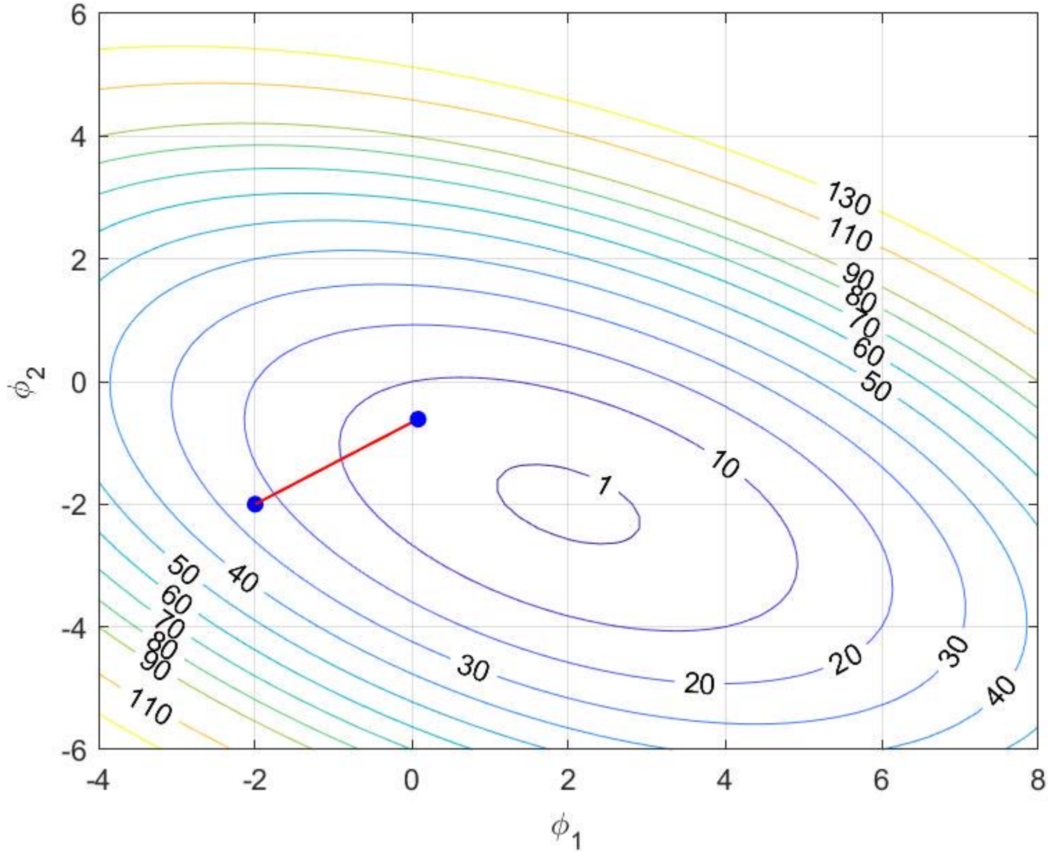
0
-2
-4
-6
-4
-2
0
2
4
6
8
ϕ_1
ϕ_2



6
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2
0
-2
-4
-6
-4
-2
0
2
4
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8
ϕ_1
ϕ_2
130
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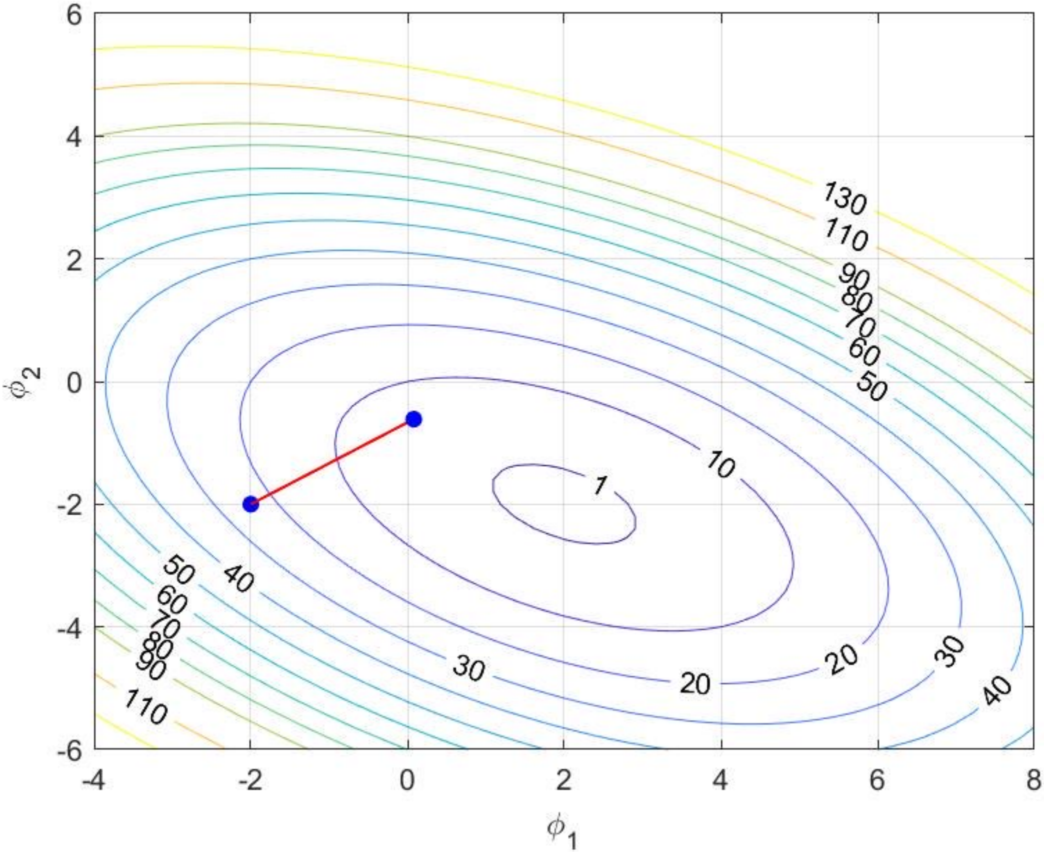
10
1



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0
2
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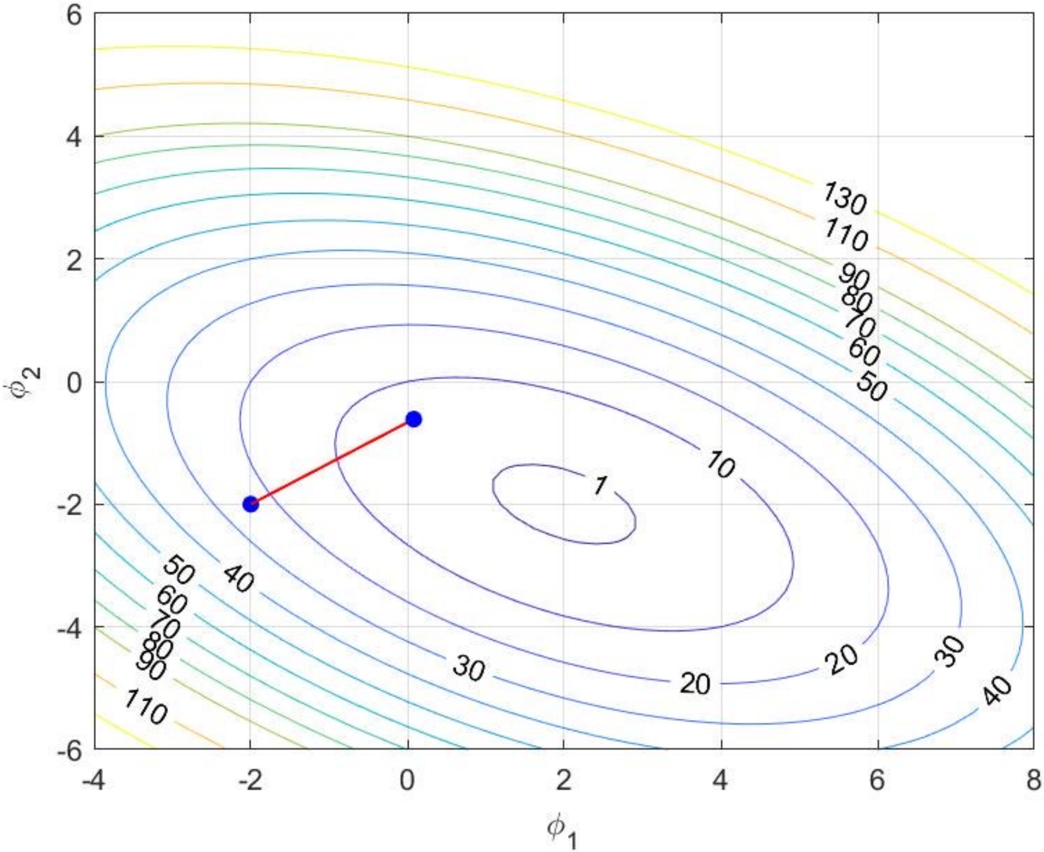
8
ϕ_1
ϕ_2



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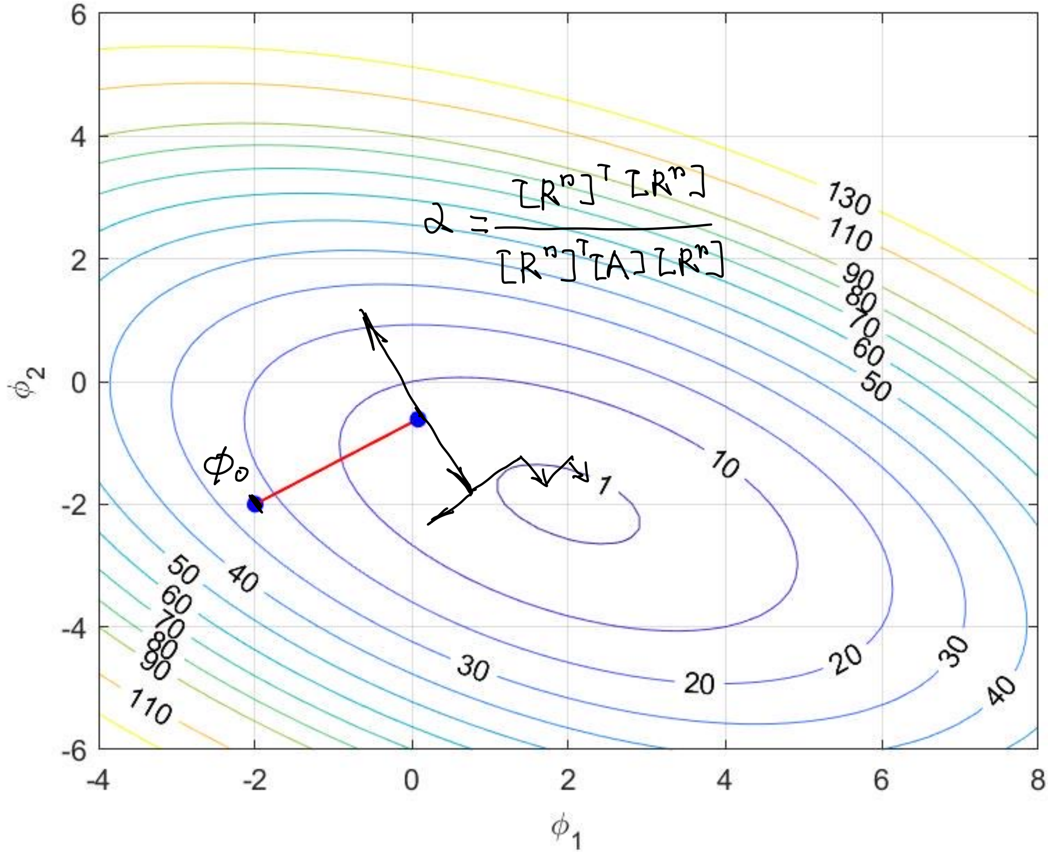
-4
-6
-4
-2
0
2
4
6
8
ϕ_2
ϕ_1



$\alpha = \dfrac{[R^n]^T [R^n]}{[R^n]^T [A] [R^n]}$
ϕ_0
ϕ_1
ϕ_2
130
110
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70
60
50
40
30
20
10
1

2. $\phi^{n+1} = \phi^{n} - \alpha \nabla f^{n} = \phi^{n} + \alpha R^{n}$

$$\begin{Bmatrix} \phi_1^{n+1} \\ \phi_2^{n+1} \\ \phi_3^{n+1} \end{Bmatrix} = \begin{Bmatrix} \phi_1^{n} \\ \phi_2^{n} \\ \phi_3^{n} \end{Bmatrix} + \alpha \begin{Bmatrix} R_1^{n} \\ R_2^{n} \\ R_3^{n} \end{Bmatrix}$$

$$\underbrace{f(\phi^{n+1})} \rightarrow \alpha \qquad \frac{\partial f}{\partial \alpha} = 0 \qquad \frac{df}{d\alpha} = 0$$

$$f(\phi_1, \phi_2, \cdots \phi_n^{n+1}) = \frac{\partial f}{\partial \phi_1}\frac{\partial \phi_1}{\partial \alpha} + \frac{\partial f}{\partial \phi_2}\frac{\partial \phi_2}{\partial \alpha} + \cdots + \frac{\partial f}{\partial \phi_n}\frac{\partial \phi_n}{\partial \alpha}$$

$$= \left[\frac{\partial f}{\partial \phi_1} R_1^{n} + \frac{\partial f}{\partial \phi_2} R_2^{n} + \cdots + \frac{\partial f}{\partial \phi_n} R_n^{n}\right]^{n+1}$$

$$= \underbrace{\left[\frac{\partial f}{\partial \phi_1}, \frac{\partial f}{\partial \phi_2}, \cdots, \frac{\partial f}{\partial \phi_n}\right]^{n+1}}_{(\nabla f)^{n+1}} \begin{bmatrix} R_1^{n} \\ R_2^{n} \\ \vdots \\ R_n^{n} \end{bmatrix} \quad R^{n}$$

$$\Rightarrow -[R^{n+1}]^{T} \cdot [R^{n}] = 0$$

$$[b - A\phi^{n+1}]^{T} [R]^{n} = 0$$

$$[b - A(\phi^{n} + \alpha R^{n})]^{T} R^{n} = 0$$

$$[b - A\phi^{n} - \alpha A R^{n}]^{T} R^{n} = 0$$

$$[b - A\phi^n - \alpha A R^n]^T R^n = 0 \qquad A^T = A$$

$$\Rightarrow (b - A\phi^n)^T R^n - \alpha (R^n)^T A^T R^n = 0$$

R^n

$$\Rightarrow (R^n)^T (R^n) = \alpha (R^n)^T A R^n \Rightarrow \alpha^n = \frac{(R^n)^T (R^n)}{(R^n)^T A R^n}$$

$$\begin{cases} R_0 = b - A\, \text{phi}0 \\ R_0 < \varepsilon \\ \text{alpha} = \dfrac{R_0' * R_0}{R_0' * A * R_0} \\ \text{phi}0 = \text{phi}0 + \alpha_0 R0 \end{cases}$$

$4 \frac{13}{3}$.

for i = 1 : iteration

alpha =

phi0 = phi0 + α0 R0

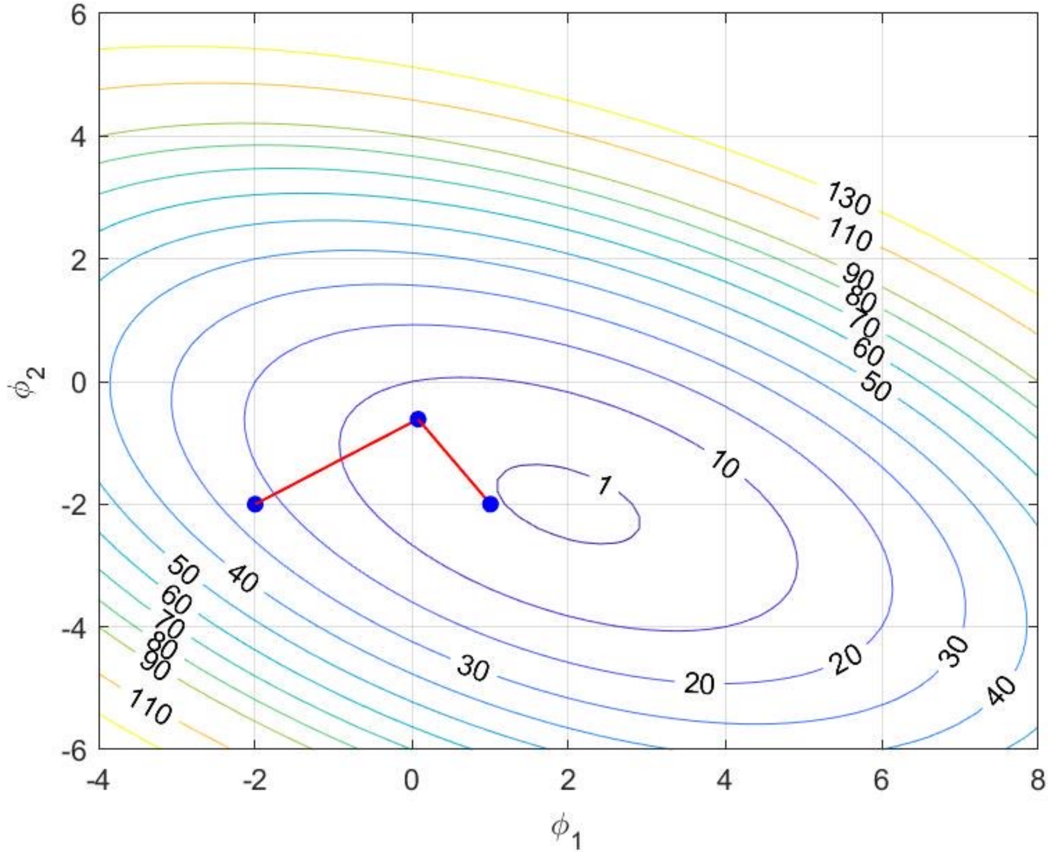
end

if residual < 1e-6

{norm(residual)

$$[A][\phi] = \begin{bmatrix} 3 & 2 \\ 2 & 6 \end{bmatrix} \begin{Bmatrix} \phi_1 \\ \phi_2 \end{Bmatrix} = b = \begin{Bmatrix} 2 \\ -8 \end{Bmatrix}$$

$$[-2, \ -2]$$



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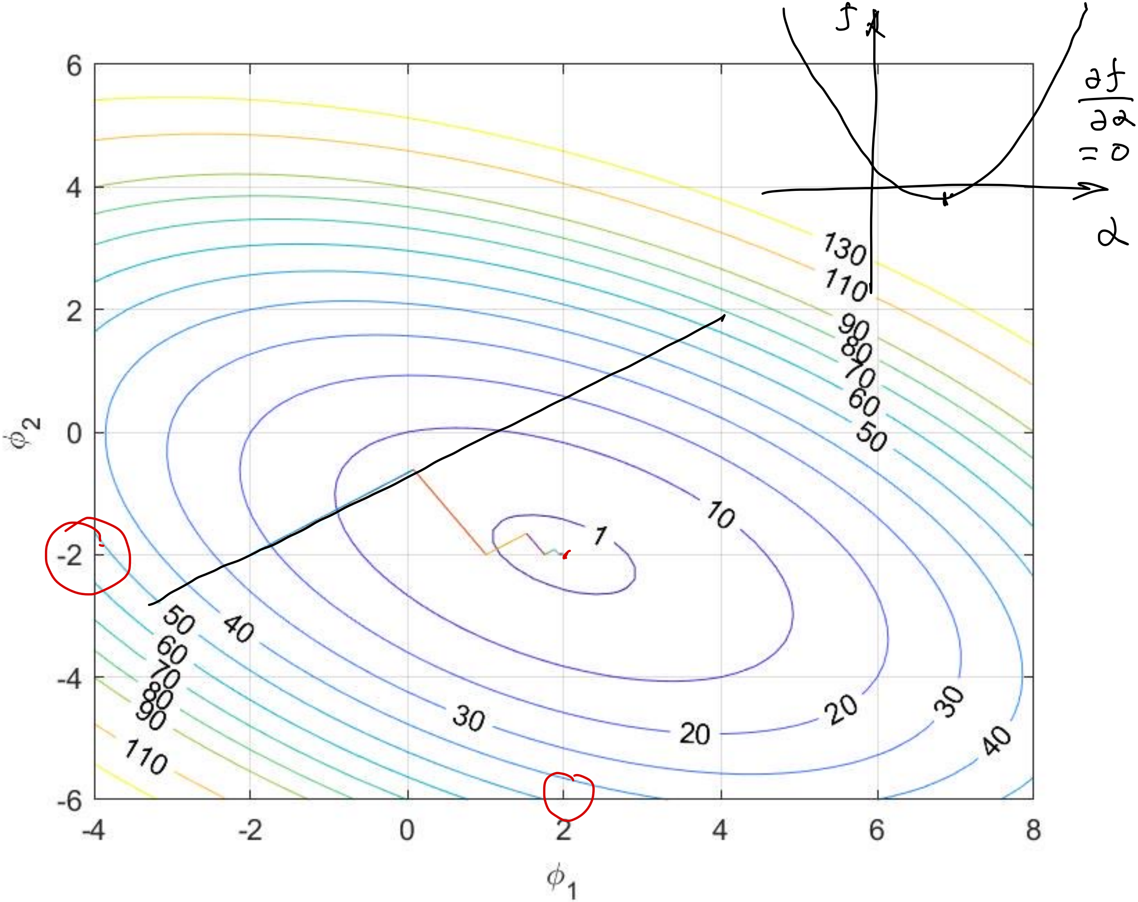
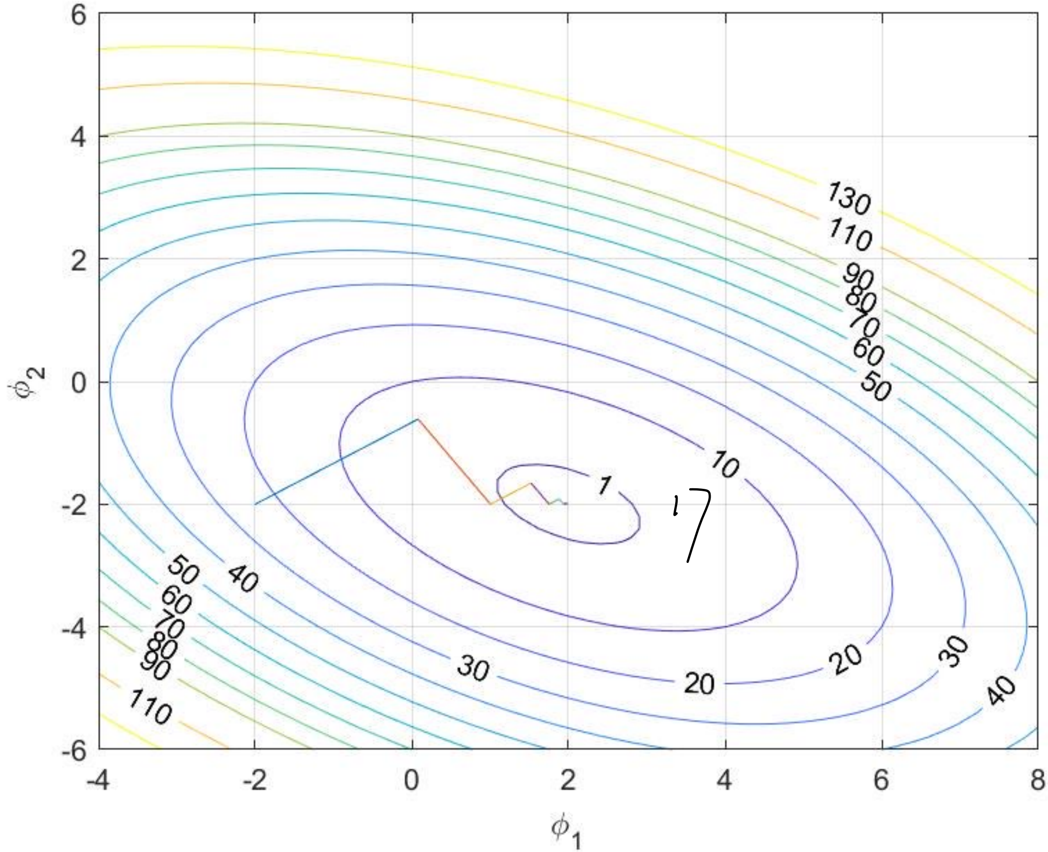
-2
-4
-6
-4
-2
0
2
4
6
8
ϕ_1
ϕ_2



ϕ_2
ϕ_1
130
110
90
80
70
60
50
40
30
20
10
1
f
$\frac{\partial f}{\partial \alpha} = 0$
α



ϕ_1
ϕ_2
-4
-2
0
2
4
6
8
-6
130
110
90
80
70
60
50
40
30
20
10
1

1. ϕ^0, $b - A\phi^0 = R^0$ MSD

2. $\alpha^0 = \dfrac{[R^0]^T [R^0]}{[R^0]^T A [R^0]}$ method of steepest_descent

no 3. $\phi^{n+1} = \phi^n + \alpha^n R^n$

4. 残差 $R^{n+1} = b - A\phi^{n+1} < \varepsilon$.

1

5 结束

三行一号.

三行一号

学生手册.

不一样. 不简单.

$$\underbrace{\underset{1\times n}{x^T}\,\underset{n\times n}{A}\,\underset{n\times 1}{x}}_{\text{scalar}} > 0 \quad (< 0)$$

positive SPD.

$A^T = A$

$Ax = b$.

特征值

特征向量

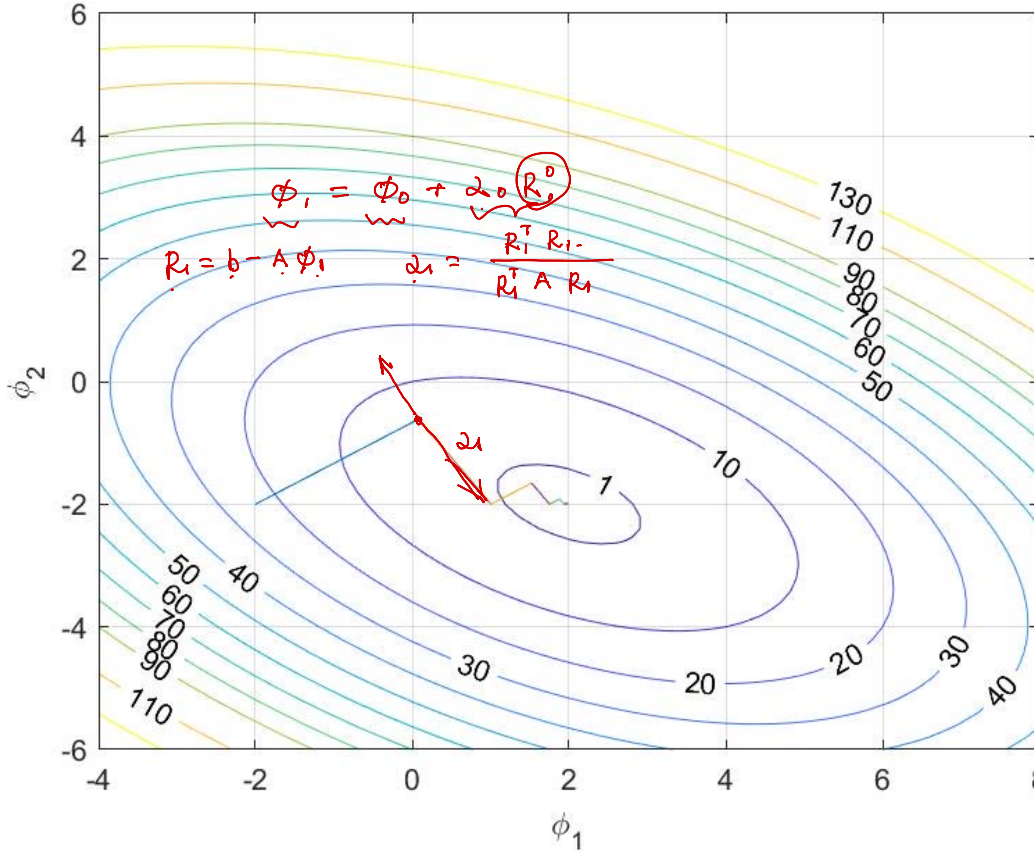
OF

$\underbrace{\text{MSD} \rightarrow \text{CG}} \rightarrow$ PBiCGSTAB.

算法

$1 \rightarrow 100\%$ 0, 1.

$20 - 30\% \rightarrow 60 \rightarrow 70\%$



$\phi_1 = \phi_0 + \alpha_0 R_0$
$R_1 = b - A\phi_1$
$\alpha_1 = \frac{R_1^T R_1}{R_1^T A R_1}$
α_1
130
110
90
80
70
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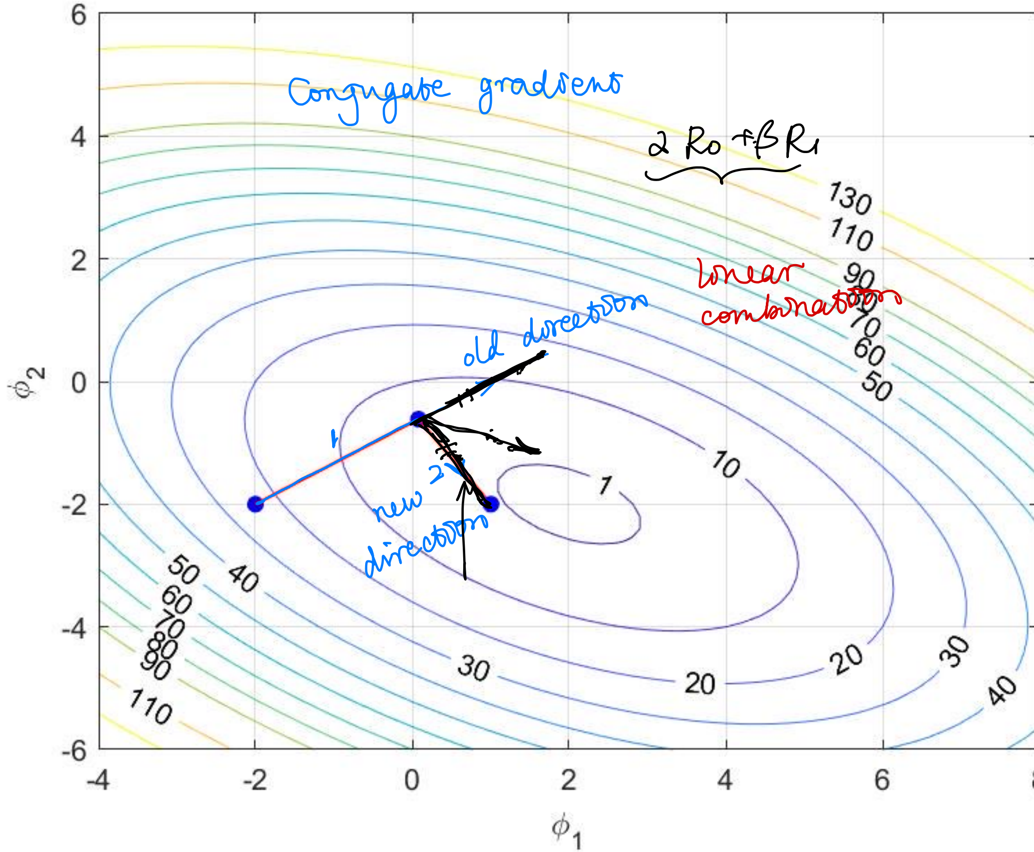
30
20
10
1
ϕ_1
ϕ_2


Conjugate gradient
$\underbrace{\alpha R_0 + \beta R_1}$
linear combination
old direction
new direction
130
110
90
70
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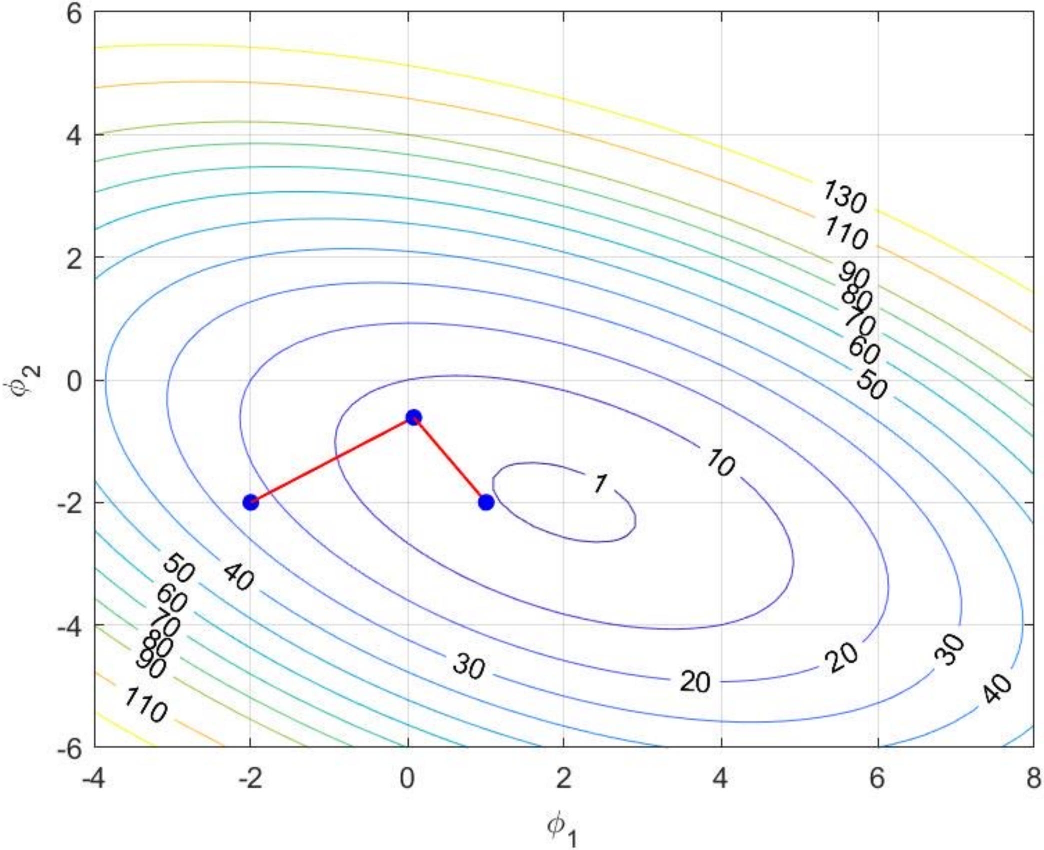
40
30
20
10
1
ϕ_1
ϕ_2



6
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-6
-4
-2
0
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6
8
ϕ_1
ϕ_2
130
110
90
80
70
60
50
10
1
40
30
20
20
30
40
50
60
70
80
90
110

matlab, python 实现. 没问题. 快

分而治之 MSD.

1 ϕ_0, b, A.

2 R_0, alpha.

3. ϕ_1

R_1 <

1 R_1, alpha1.

2. $\phi_2 = \phi_1 + \text{alpha1} \times R1$

for → MSD 函数.

循环. 分支 if

for.

MSD, CG. 的程

C++

CG 算法

$Ax = b$

$A\phi = b$

1. ϕ^0
2. $R^0 = b - A\phi^0$, $R^0 < \varepsilon$

residual r, R. a, b,

searchDirection

3. $D^0 = R^0$ direction = residual

search-direction

4. $$\alpha^{n+1} = \frac{(R^n)^T (R^n)}{(D^n)^T A D^n}$$

$$\alpha^{n+1} = \frac{(R^n)^T (R^n)}{(R^n)^T A (R^n)}$$

5. 更新 $\phi^{n+1} = \phi^n + \alpha^{n+1} D^n$
6. $R^{n+1} = b - A\phi^{n+1}$
7. $$\beta^{n+1} = \frac{(R^{n+1})^T (R^{n+1})}{(R^n)^T (R^n)}$$
8. $D^{n+1} = R^{n+1} + \beta^{n+1} D^n$
9. $R^{n+1} < \varepsilon$
10. 結束

可能CG推导 编程

CGS. 算法

1. ϕ^0
2. $R^0 = b - A\phi^0$, $R^0 < \varepsilon$

residual r, R. a, b,

searchDirection

3. $D^0 = R^0$ direction = residual

CGS.

1. ϕ^0
2. $R^0 = b - A\phi^0$, $R^0 < \varepsilon$

residual r., R. a, b,

searchDirection

3. $D^0 = R^0$ direction = residual

$D^{0*} = R^0$ 表示.

4. $\alpha^{n+1} = \dfrac{[R^0]^T[R^n]}{[R^0]^T A [D^n]}$
5. $G^{n+1} = [D^n]^* - \alpha^{n+1}[A]D^n$
6. $\phi^{n+1} = \phi^n + \alpha^{n+1}\{[D^n]^* + G^{n+1}\}$
7. $R^{n+1} = b - A\phi^{n+1}$ R2
8. $\beta^{n+1} = \dfrac{[R^0]^T[R^{n+1}]}{[R^0]^T[R^n]}$
9. $[D^{n+1}]^* = R^{n+1} + \beta^{n+1} G^{n+1}$ 表示

10. 搜索. $D^{n+1} = [D^{n+1}]^* + \beta^{n+1}\{G^{n+1} + \beta^{n+1} D^n\}$
11. $R2 < \varepsilon$.
12. 结束. full implicit solver

1个母门算完 $Ax = b$.

$A \neq A^T$

1. MSD. 收敛慢
2. CG / CGS

BCG / BiCGSTAB.

krylov subspace

span$\{q.\ Aq.\ A^2q.\ \cdots A^{n-1}q\}$

正交 orthogonal basis vector

i, j. k orthonormal

第九次课

1. 预条件：

2. 多重网格
   - 几何（GMG）
   - 代数（AMG） → pyamg. AmgX

algebraic

GMG

太极胡老师

Multigrid preconditioned conjugate gradient MGPCG.

Games 201. taichi

80分钟 300行，2020年论文.

多重网格
- preconditioner 预条件器 CGS
- solver

1. 预条件　　PCG，PBiCG　PBiCGSTAB.（OpenFOAM）fvSolution

$Ax=b$.　　A → 条件数不好，病态　ill-condition.

$A'x=b'$

$M^{-1}Ax=M^{-1}b$.　　M^{-1} preconditioner 预条件器，预条件子.

cond(A)

1.　$A \to \text{diag}(A) \Rightarrow$　　L, $U \Leftrightarrow A$

sparse 稀疏

2.　ILU(0)　　$A=LU$.　　L，U 稀疏 问题

fill-in

$A \approx LU$

3、incomplete cholesky 分解　$A \approx LL^T$　　mgpcg　icpcg

$Ax=b \Rightarrow LL^Tx=b$

M^{-1}.

CG

1. 计算残差. $R^n = M^{-1} b - M^{-1} A \phi^n$ R2.

2. $D^0 = R^0$

3. $\alpha = \dfrac{(R^n)^T R^n}{(D^n)^T M^{-1} A (D^n)}$

4. $\phi^{n+1} = \phi^n + \alpha D^n$

5. 更新残差 $R^{n+1} = M^{-1} b - M^{-1} A \phi^{n+1}$

6. $\beta^{n+1} = \dfrac{(R^{n+1})^T R^{n+1}}{(R^n)^T R^n}$

7. 更新搜索方向. $D^{n+1} = R^{n+1} + \beta^{n+1} D^n$

2. 多重网格

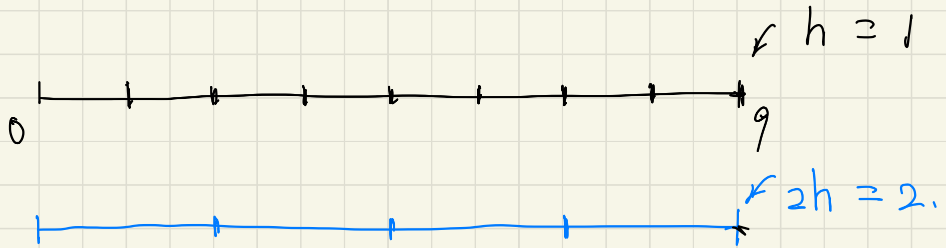
1. Jacobi. G-S. 椭圆方程. 泊松方程

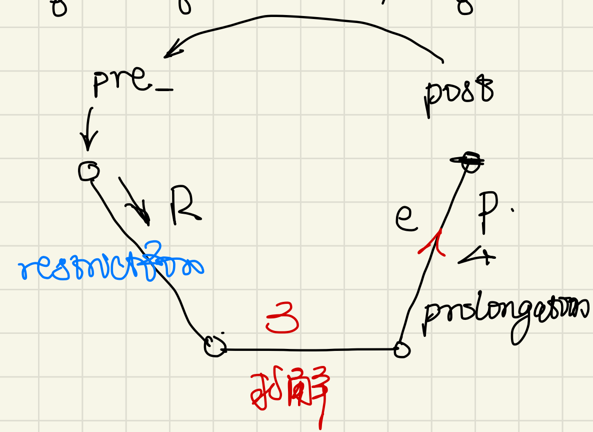
$$\Delta \phi = f \qquad 1维,\ 2维$$

高频分量 特别容易耗散掉, 低频 收敛特慢.

$$\theta_m = \frac{m\pi}{M-1} \qquad \sqrt{\frac{1}{5-4\cos\theta_m}}$$

$$\frac{\pi}{8},\ \frac{2\pi}{8},\ \cdots,\ \frac{7\pi}{8}$$





1. pre_smoothing 算一下

2. restriction 限定.

3. solve 求解.

4. prolongation 延拓.

5. post_smoothing 算一下

(V cycle, W cycle F cycle)

二层网格 V cycle, mg.

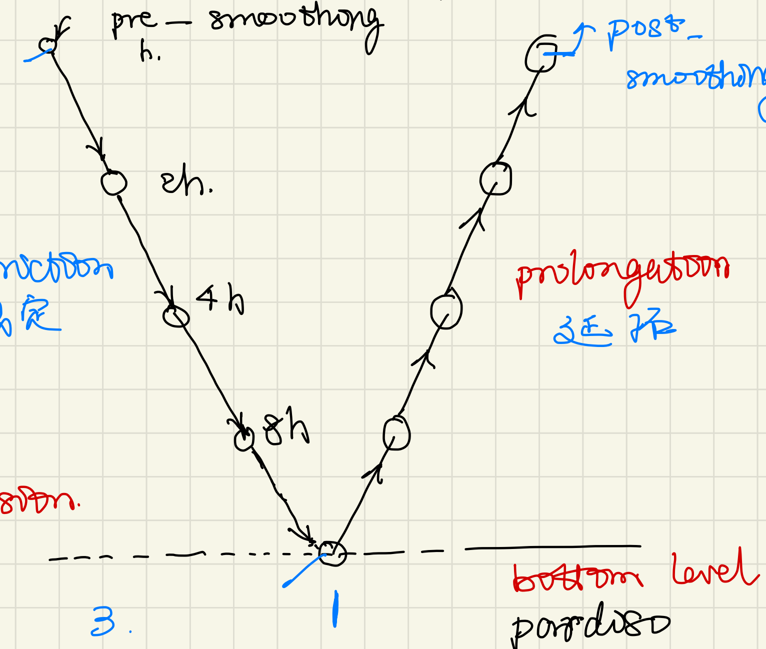
smoother 光顺器 Jacobi, G-S.

256 → 64 → 16 → 4 → 1 damped $\omega = \frac{2}{3}$.

1024

2^{10} / 2

/ 4



$2^n \longrightarrow 2^0$

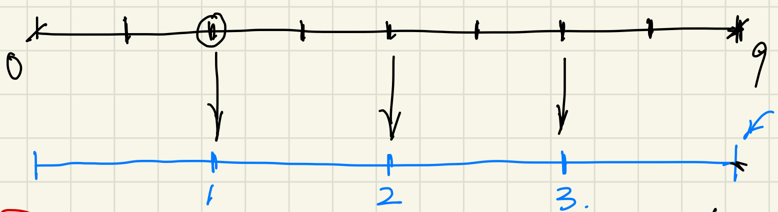
3x3.

$Ax = b$

$x = b$.

这时. 直接计算

$h = 1$ fine



$2h = 2.$ coarse

$Ae = r$

1. pre_smoothing. $Ax = b.$, 10./Jacobi, G-S.

$r = b - Ax^{10}$ 7×1. 列向量.

A 7×7.

2. restriction $r_{2h} = R\, r_h$

$$R: 3\times 7.$$

$$\begin{bmatrix} r_{2h}^1 \\ r_{2h}^2 \\ r_{2h}^3 \end{bmatrix} = \begin{bmatrix} & R & \end{bmatrix} \begin{bmatrix} r_h^1 \\ r_h^2 \\ \vdots \\ r_h^7 \end{bmatrix}$$

3. solve. $A_{2h}\, e_{2h} = r_{2h}$? $R^T = P.$

$$\underset{3\times 3.}{A_{2h}} = R A_h P = \underset{3\times 7}{R}\, \underset{7\times 7}{A_h}\, \underset{7\times 3.}{R^T}$$

4. prolongation.

$$P\, e_{2h} = e_h.$$

5. $x_{10} = x_{10} + e_h$

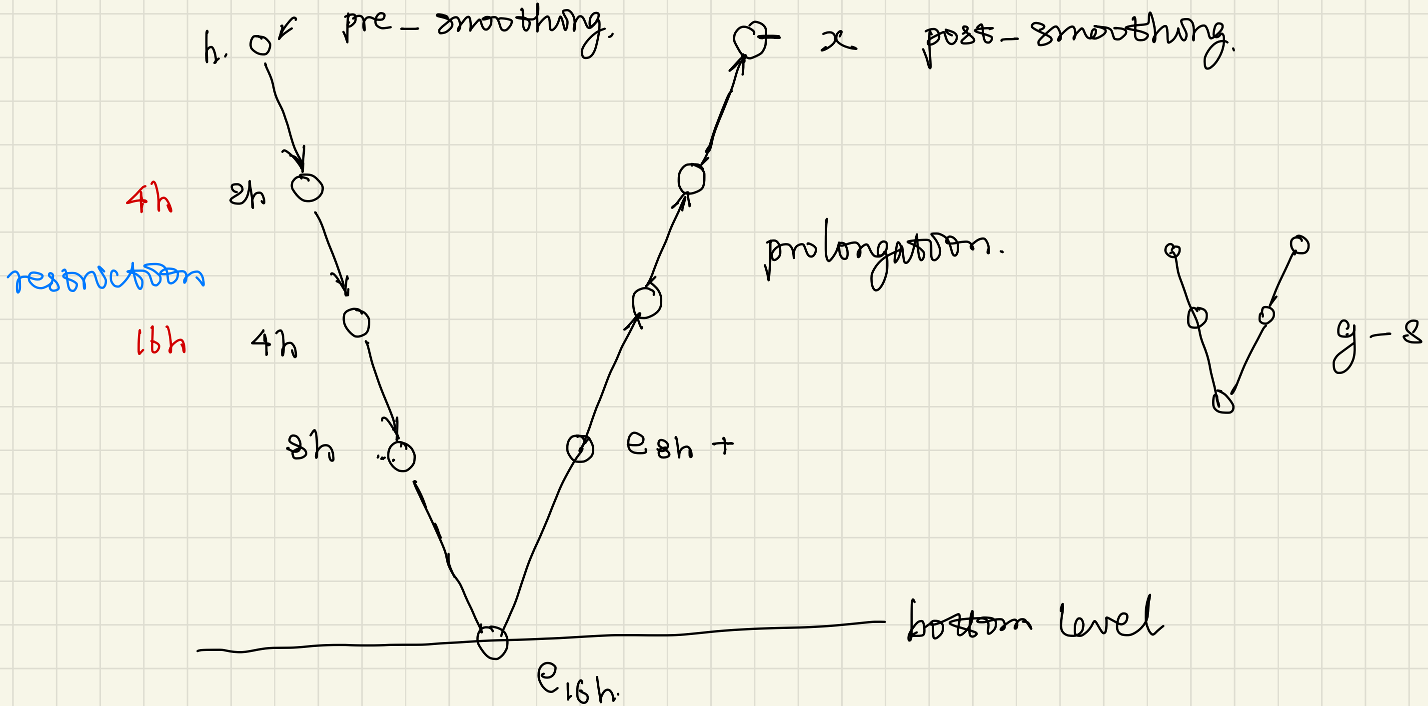
$r = b - A_h x_{10} < \varepsilon.$

$> \varepsilon.$

post_smoothing.

$r = b - A_h x_{20} < \varepsilon.$

1 pre_smoothing $x_{30}.$



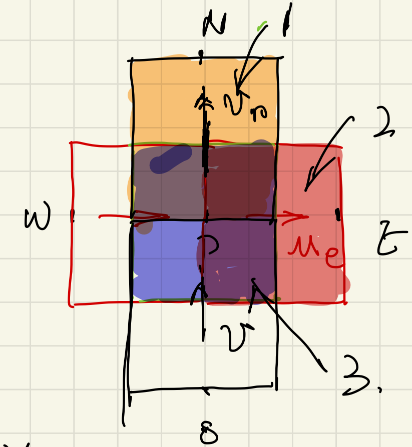
h.
pre_ smoothing.
x
post_ smoothing.
4h
2h
restriction
16h
4h
8h
e8h +
prolongation.
bottom level
e16h.
g-s.

mgpcg

$$u\frac{\partial\phi}{\partial x} + v\frac{\partial\phi}{\partial y} = \Gamma\left(\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2}\right)$$

$$u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$



$$\int_S^N \int_E^P -\frac{\partial p}{\partial x}\,dx\,dy = -(P_E - P_P)\Delta y = (P_P - P_E)\Delta y$$

$$= (P_P - P_E)A_e$$

Δy 2D

$\Delta y \Delta z$ 3D.

$$a_e u_e = \sum a_{nb}u_{nb} + (P_P - P_E)A_e$$

$$u_e = \frac{\sum a_{nb}u_{nb} + b}{a_e} + \frac{A_e}{a_e}(P_P - P_E)$$

$$\boxed{u_e = \frac{\sum a_{nb}u_{nb}}{a_e} + d_e(P_P - P_E)}$$

$$a_e u_e' = \cancel{\sum a_{nb}u_{nb}'}^{\,0} + (P_P' - P_E')$$

$$\boxed{u_e' = d_e(P_P' - P_E')}$$

速度修正 $$\boxed{v_n' = d_n(P_P' - P_N')}$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \Rightarrow [u_e - u_w]\Delta y + [v_n - v_s]\Delta x = 0$$

$$u_e = u_e^* + u' = u_e^* + d_e[P_P' - P_E']$$

$$v_e = v_n^* + d_n[P_P' - P_N']$$

$$\Delta y\,(u_e^* - u_w^*) + (d_e - d_w)\Delta y\, P_P'$$

$$a_e u_e' = \sum a_{nb} u_{nb}' + (P_P^* - P_E^*) A_e$$

$\sum a_{nb} u_{nb}' \to 0$

semi-implicit link

$$a_P P_P' = a_E P_E' + a_W P_W' + a_N P_N' + a_S P_S'$$

u_e' 修正流(速度)

$$\underbrace{\nabla \cdot U}\ = 0 \qquad \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0$$

$$P = P^* + P'$$

1. SIMPLE (不可压) 稳态

$$\begin{cases} \nabla \cdot U = 0 & \text{连续} \\ \nabla \cdot (\underbrace{UU}) = -\frac{\nabla p}{\rho} + \nabla \cdot (\nu \nabla U) & \text{动量} \end{cases}$$

非线性项

个方程 个未知量

$$\begin{cases} u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} + \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) \\ u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = -\frac{\partial p}{\partial y} + \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) \end{cases}$$

1 2

1. → u 网

2. → v 网格

压力梯度 → 对流-扩散方程 → 扩散方程

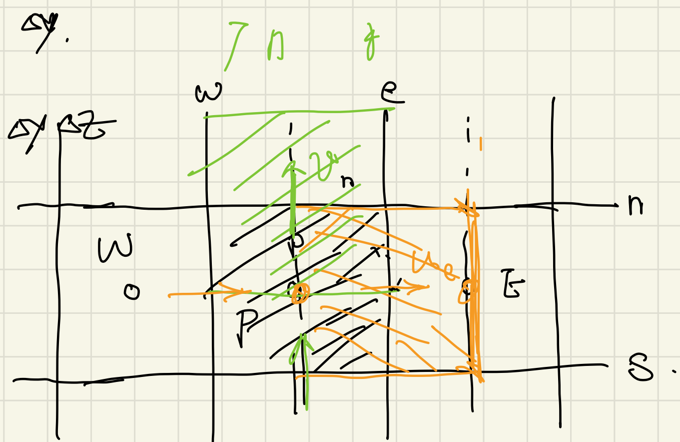
$$a_e u_e = \sum a_{nb} u_{nb} + b + (P_P - P_E) A_e$$

$A_e \leftarrow \Delta y$; $\Delta y \Delta z$

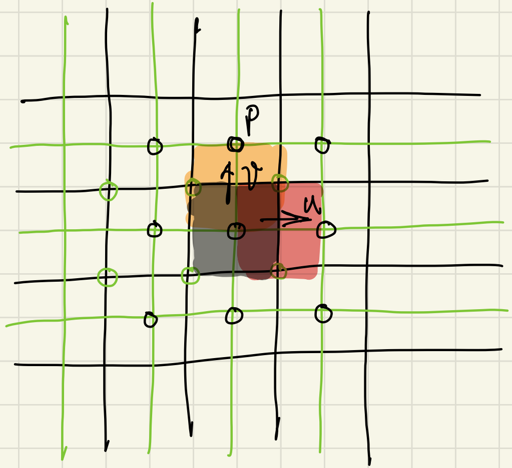
$$u_e = \underbrace{\frac{\sum a_{nb} u_{nb} + b}{a_e}} + d_e (P_P - P_E)$$

$$d_e = \frac{A_e}{a_e}$$

v_n



交错网格.



(u, v, p) 分开存.

网格. 4套网格.

simple

1. 给定一个 p^* (猜)

2. ① ② 算出 u^*, v^*

3. 代入压力修正方程 → p', u', v'

4. 算出 u, v, p

simple