

(Review finite-diff. and metrics)

Second derivatives: Evaluate $\partial^2\psi/\partial^2x$ as $\partial_x F$ with $F = \partial_x\psi$

Outside, then in, but iterated central would give 5 i -points.

Wrong:


$$\delta_\xi(F) = (F_{i+1} - F_{i-1})/2 \text{ with } F = \delta_\xi\psi \rightarrow [(\psi_{i+2} - \psi_i) - (\psi_i - \psi_{i-2})]/4.$$

Instead use:

$$(F_{i+1/2} - F_{i-1/2})/2 \rightarrow [(\psi_{i+1} - \psi_i) - (\psi_i - \psi_{i-1})]/4.$$

$F_{i+1/2}$ = value on cell face F_{i+1} is data at cell center.

Or recall formulating equations in conservation form: Flux in - Flux out + source = rate of change inside c.v. Recall 1-D diffusion



$$\partial_t T = \partial_x (\kappa \partial_x T) = -\partial_x F \quad \text{where } F = -\kappa \partial_x T$$

$$i-1/2 \leftarrow \Delta x \rightarrow i+1/2$$

Flux in is in $-\mathbf{n}$ direction.

$$\partial_t \int T dx = - (F \cdot \mathbf{n})_{i-1/2} - (F \cdot \mathbf{n})_{i+1/2} = F_{i-1/2} - F_{i+1/2} \text{ is exact conservation.}$$

Finite difference method for curvilinear grids

We have a method for chain rule derivatives:

$$\begin{aligned} \text{Rtxy}(*,1,1) &= \partial \xi / \partial x \quad ; \quad \text{Rtxy}(*,1,2) = \partial \xi / \partial y \\ \text{Rtxy}(*,2,1) &= \partial \eta / \partial x \quad ; \quad \text{Rtxy}(*,2,2) = \partial \eta / \partial y \end{aligned}$$

$$\text{e.g., grid, } x(i,j), y(i,j) \rightarrow \text{Rtxy}(*,1,1) = \delta y / \delta j / (\delta x / \delta i \cdot \delta y / \delta j - \delta x / \delta j \cdot \delta y / \delta i)$$

$$\begin{aligned} \partial \psi / \partial x &= \partial \xi / \partial x \partial \psi / \partial \xi + \partial \eta / \partial x \partial \psi / \partial \eta = \text{Rtxy}(i,j,1,1) [\psi(i+1,j) - \psi(i-1,j)]/2 \\ &\quad + \text{Rtxy}(i,j,2,1) [\psi(i,j+1) - \psi(i,j-1)]/2 \end{aligned}$$

Use this to discretize Poisson equation by centered finite differences.

Second derivatives make it 'messy'; chain rule leads to cross derivatives $\partial^2 \psi / \partial \xi \partial \eta$ (explain how this \rightarrow 9 point stencil)

Gauss-Seidel in Δ -form

Loop over i, j

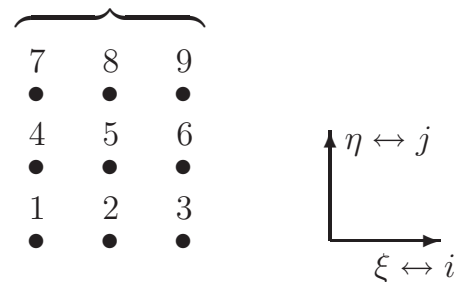
$$R = \omega - \left[\frac{\delta^2}{\delta^2 x} + \frac{\delta^2}{\delta^2 y} \right] \psi \quad (1)$$

$$\Delta \psi = R(i, j) / A_5 \quad (2)$$

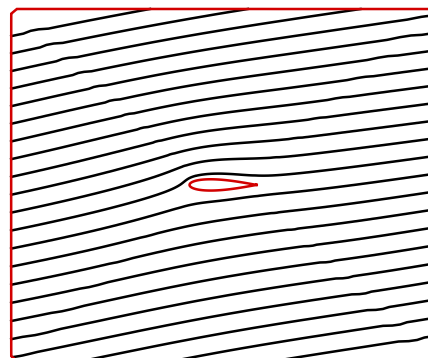
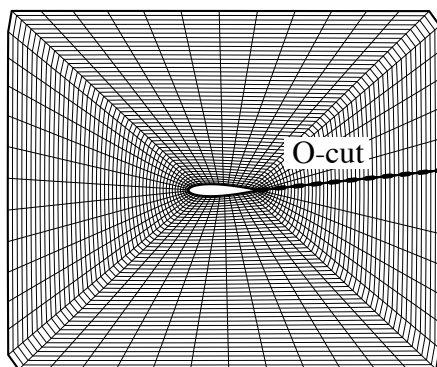
$$\psi^{n+1}(i, j) = \psi^n(i, j) + \lambda \Delta \psi \quad (3)$$

endloop

9 point stencil



R is evaluated with the current values of ψ — a combination of n and $n + 1$.



So R can be evaluated in aggregate. A_5 is needed too.

Basic idea: Let $F = \partial_x \psi$ and $G = \partial_y \psi$. Then $\nabla^2 \psi = \partial_x F + \partial_y G$.

(Recall the heat equation and gradient diffusion.) Term-by-term evaluation

A) $\partial_x F_{i,j} = (\partial \xi / \partial x)_{i,j} \delta_\xi F_{i,j} + (\partial \eta / \partial x)_{i,j} \partial_\eta F_{i,j}$

Use centered formulas; consider first term. Note that ξ and η directions stencils differ.

B) $\delta_\xi F_{i,j} = \delta_\xi [\partial_x \psi]_{i,j} = \delta_\xi [\partial \xi / \partial x \partial \psi / \partial \xi + \partial \eta / \partial x \partial \psi / \partial \eta]_{i,j}$

$$= (\partial \xi / \partial x)_{i+1/2,j} \partial_\xi \psi_{i+1/2,j} + \frac{1}{2} (\partial \eta / \partial x \partial_\eta \psi)_{i+1,j}$$

$$- (\partial \xi / \partial x)_{i-1/2,j} \partial_\xi \psi_{i-1/2,j} - \frac{1}{2} (\partial \eta / \partial x \partial_\eta \psi)_{i-1,j}$$

Where $2(\partial \xi / \partial x)_{i+1/2,j} = (\partial \xi / \partial x)_{i+1,j} + (\partial \xi / \partial x)_{i,j}$ etc.

For the derivatives in computational space:

- 1) $\delta_\xi \psi_{i+1/2,j} = \psi_{i+1,j} - \psi_{i,j}$
- 2) $\frac{1}{2} (\partial \eta / \partial x \partial_\eta \psi)_{i+1,j} = \frac{1}{4} \partial \eta / \partial x_{i+1,j} [\psi_{i+1,j+1} - \psi_{i+1,j-1}]$

Note that metric terms are at grid points.

Repeat with i -index shifted down to obtain second line of B:

- 3) $\partial_\xi \psi_{i-1/2,j} = \psi_{i,j} - \psi_{i-1,j}$
- 4) $\frac{1}{2} (\partial \eta / \partial x \partial_\eta \psi)_{i-1,j} = \frac{1}{4} \partial \eta / \partial x_{i-1,j} [\psi_{i-1,j+1} - \psi_{i-1,j-1}]$

Stencil contains $\psi_{i+1,j+1}$, $\psi_{i+1,j-1}$, $\psi_{i-1,j+1}$, $\psi_{i-1,j-1}$ in addition to the 5-point stencil; so now it is a **9-point** stencil.

This can be coded as: evaluate 1,2,3,4 ; use them to evaluate B, then evaluate A.

Same for $\partial_y G_{i,j}$.

Gauss-Seidel requires diagonal element (A_5). Can work it out, or apply the above with

$$\psi_{1-4} = 0 = \psi_{6-9}, \psi_5 = 1: \text{ which can be described as } A_5 = \sum_{i=1-5} A_i \delta_{i5}$$

General geometry: From

$$\frac{\partial F}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial F}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial F}{\partial \eta} \quad \text{and} \quad \frac{\partial G}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial G}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial G}{\partial \eta}$$

with $F = \partial_x \psi$ and $G = \partial_y \psi$,

$$\text{and } \frac{\partial \psi}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta}$$

$$\begin{aligned} R &= \overbrace{\frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} \left[\frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta} \right]}^{\partial_x \psi} + \frac{\partial \eta}{\partial x} \frac{\partial}{\partial \eta} \left[\frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta} \right] \\ &+ \frac{\partial \xi}{\partial y} \frac{\partial}{\partial \xi} \left[\frac{\partial \xi}{\partial y} \frac{\partial \psi}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial \psi}{\partial \eta} \right] + \frac{\partial \eta}{\partial y} \frac{\partial}{\partial \eta} \left[\frac{\partial \xi}{\partial y} \frac{\partial \psi}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial \psi}{\partial \eta} \right] \end{aligned}$$

Discretize with central differences, using $\Delta \xi=1$ etc. Look at first two terms

1) Diagonal term

$$\begin{aligned} \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} \left[\frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} \right] &= \frac{\partial \xi}{\partial x} \left\{ \frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} \Big|_{i+1/2} - \frac{\partial \xi}{\partial x} \frac{\partial \psi}{\partial \xi} \Big|_{i-1/2} \right\} \\ &= \frac{\partial \xi}{\partial x}(i, j) \left\{ \frac{\partial \xi}{\partial x}(i+1/2, j) \left(\psi(i+1, j) - \psi(i, j) \right) - \frac{\partial \xi}{\partial x}(i-1/2, j) \left(\psi(i, j) - \psi(i-1, j) \right) \right\} \end{aligned}$$

$$\text{Using } Rxy_{11} = \frac{\partial \xi}{\partial x}$$

$$= Rxy_{11}(i, j) \left[Rxy_{11}(i+1/2, j) \left(\psi(i+1, j) - \psi(i, j) \right) - Rxy_{11}(i-1/2, j) \left(\psi(i, j) - \psi(i-1, j) \right) \right]$$

2) cross term

$$\begin{aligned} \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} \left[\frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta} \right] &= \frac{\partial \xi}{\partial x} \left\{ \frac{1}{2} \left(\frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta} \Big|_{i+1} - \frac{\partial \eta}{\partial x} \frac{\partial \psi}{\partial \eta} \Big|_{i-1} \right) \right\} \\ &= \frac{\partial \xi}{\partial x}(i, j) \frac{1}{4} \left(\frac{\partial \eta}{\partial x}(i+1, j) (\psi(i+1, j+1) - \psi(i+1, j-1)) - \frac{\partial \eta}{\partial x}(i-1, j) (\psi(i-1, j+1) - \psi(i-1, j-1)) \right) \end{aligned}$$

$$\text{If } R_{21}^{xy} = \frac{\partial \eta}{\partial x}(i, j)$$

$$= R_{11}^{xy}(i, j) \left[R_{21}^{xy}(i+1, j) \left(\psi(i+1, j+1) - \psi(i+1, j-1) \right) - R_{21}^{xy}(i-1, j) \left(\psi(i-1, j+1) - \psi(i-1, j-1) \right) \right]$$

Note: $\psi(i+1, j+1)$ etc. fill in a 9-point stencil

The residual can be evaluated in this form, without writing the coefficients $A_{[1-9]}$; but A_5 is needed also.

Summing the coefficients of $\psi(i,j)$ in the discretization of R gives the diagonal element

$$A_5 = - \frac{\partial \xi}{\partial x}(i, j) \left[\frac{\partial \xi}{\partial x}(i - 1/2, j) + \frac{\partial \xi}{\partial x}(i + 1/2, j) \right] - \frac{\partial \eta}{\partial x}(i, j) \left[\frac{\partial \eta}{\partial x}(i, j - 1/2) + \frac{\partial \eta}{\partial x}(i, j + 1/2) \right] \\ - \frac{\partial \xi}{\partial y}(i, j) \left[\frac{\partial \xi}{\partial y}(i - 1/2, j) + \frac{\partial \xi}{\partial y}(i + 1/2, j) \right] - \frac{\partial \eta}{\partial y}(i, j) \left[\frac{\partial \eta}{\partial y}(i, j + 1/2) + \frac{\partial \eta}{\partial y}(i, j - 1/2) \right]$$

In these formulas $\partial \eta / \partial x(i + 1/2, j) = \frac{1}{2} [\partial \eta / \partial x(i, j) + \partial \eta / \partial x(i + 1, j)]$, etc.

Recall what is stored in the 'metric tensor'

$$T_{Rxy}(*,1,1) = \partial \xi / \partial x ; \quad T_{Rxy}(*,1,2) = \partial \xi / \partial y ; \quad T_{Rxy}(*,2,1) = \partial \eta / \partial x ; \quad T_{Rxy}(*,2,2) = \partial \eta / \partial y$$

!-- 1,1 -----

$$\partial \xi / \partial x_{1/2} \cdot \partial \psi / \partial \xi_{1/2}$$

$$xy1p = (rtxy(i,j,1,1) + rtxy(i+1,j,1,1))/2 * (\psi_{ij}(i+1,j) - \psi_{ij}(i,j))$$

$$\partial \xi / \partial x_{-1/2} \cdot \partial \psi / \partial \xi_{-1/2}$$

$$xy1m = (rtxy(i,j,1,1) + rtxy(i-1,j,1,1))/2 * (\psi_{ij}(i,j) - \psi_{ij}(i-1,j))$$

! *First term of Residual* $\omega - \partial^2 \psi / \partial x^2$

$$! \quad \partial \xi / \partial x \left\{ \quad \partial / \partial \xi \left[\partial \xi / \partial x \cdot \partial \psi / \partial \xi \right] \right.$$

$$R = \omega - rtxy(i,j,1,1) * (xy1p - xy1m \&$$

$$! \quad \left. \partial / \partial \xi \left[\partial \eta / \partial x \cdot \partial \psi / \partial \eta \right] \right\}$$

$$+ .25 * rtxy(i+1,j,2,1) * (\psi_{ij}(i+1,j+1) - \psi_{ij}(i+1,j-1)) \&$$

$$- .25 * rtxy(i-1,j,2,1) * (\psi_{ij}(i-1,j+1) - \psi_{ij}(i-1,j-1)))$$

! *coef of ij from red terms*

$$A5 = - rtxy(i,j,1,1) * (rtxy(i,j,1,1) + rtxy(i+1,j,1,1)/2 + rtxy(i-1,j,1,1)/2)$$

!-- 1,2 -----

$$xy2p = (rtxy(i,j,1,2) + rtxy(i+1,j,1,2))/2 * (\psi_{ij}(i+1,j) - \psi_{ij}(i,j))$$

$$xy2m = (rtxy(i,j,1,2) + rtxy(i-1,j,1,2))/2 * (\psi_{ij}(i,j) - \psi_{ij}(i-1,j))$$

$$R = R - rtxy(i,j,1,2) * (xy2p - xy2m \&$$

$$+ .25 * rtxy(i+1,j,2,2) * (\psi_{ij}(i+1,j+1) - \psi_{ij}(i+1,j-1)) \&$$

$$- .25 * rtxy(i-1,j,2,2) * (\psi_{ij}(i-1,j+1) - \psi_{ij}(i-1,j-1)))$$

$$A5 = A5 - rtxy(i,j,2,1) * (rtxy(i,j,2,1) + rtxy(i,j+1,2,1)/2 + rtxy(i,j-1,2,1)/2)$$

!-- 2,1 -----

$$xy3p = (rtxy(i,j,2,1) + rtxy(i,j+1,2,1))/2 * (\psi_{ij}(i,j+1) - \psi_{ij}(i,j))$$

$$xy3m = (rtxy(i,j,2,1) + rtxy(i,j-1,2,1))/2 * (\psi_{ij}(i,j) - \psi_{ij}(i,j-1))$$

$$R = R - rtxy(i,j,2,1) * (xy3p - xy3m \&$$

$$+ .25 * rtxy(i,j+1,1,1) * (\psi_{ij}(i+1,j+1) - \psi_{ij}(i-1,j+1)) \&$$

$$- .25 * rtxy(i,j-1,1,1) * (\psi_{ij}(i+1,j-1) - \psi_{ij}(i-1,j-1)))$$

$$A5 = A5 - rtxy(i,j,1,2) * (rtxy(i,j,1,2) + rtxy(i+1,j,1,2)/2 + rtxy(i-1,j,1,2)/2)$$

!-- 2,2 -----

$$xy4p = (rtxy(i,j,2,2) + rtxy(i,j+1,2,2))/2 * (\psi_{ij}(i,j+1) - \psi_{ij}(i,j))$$

$$xy4m = (rtxy(i,j,2,2) + rtxy(i,j-1,2,2))/2 * (\psi_{ij}(i,j) - \psi_{ij}(i,j-1))$$

$$R = R - rtxy(i,j,2,2) * (xy4p - xy4m \&$$

$$+ .25 * rtxy(i,j+1,1,2) * (\psi_{ij}(i+1,j+1) - \psi_{ij}(i-1,j+1)) \&$$

$$\begin{aligned}
 & - .25 * r_{txy}(i, j-1, 1, 2) * (\psi_{ij}(i+1, j-1) - \psi_{ij}(i-1, j-1))) \\
 A5 & = A5 - r_{txy}(i, j, 2, 2) * (r_{txy}(i, j, 2, 2) + r_{txy}(i, j+1, 2, 2)/2 + r_{txy}(i, j-1, 2, 2)/2)
 \end{aligned}$$