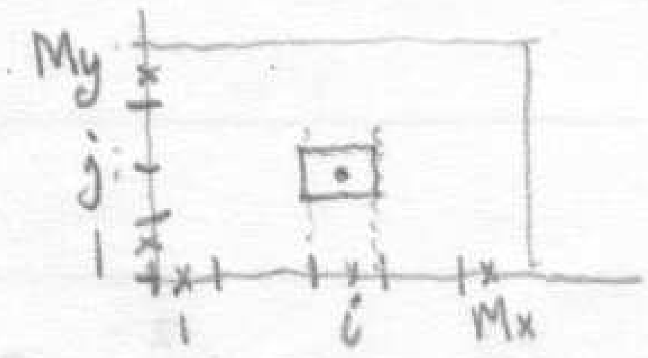
2D diffusion

$$\begin{cases} u_t = \nabla\cdot(D\nabla u) & \text{in } \Omega,\ t>0 \\ u(x,y,0) = u_{init}(x,y) \\ \text{BCs on each bry} \end{cases} \qquad \text{i.e. } u_t + \nabla\cdot\vec{F} = 0,\quad \vec{F} = -D\nabla u$$

Now $\vec{F} = -D\nabla u = (-D_x u_x, -D_y u_y)$ nodes (x_i, y_j), $A_{i-1/2,j} = \Delta y$, $A_{i,j-1/2} = \Delta x$, $Vol_{ij} = \Delta x\,\Delta y$

In Cartesian: $U^{n+1}_{ij} = U^n_{ij} + \frac{\Delta t}{Vol_{ij}}\left[\left(AF_{i-\frac12,j} - AF_{i+1/2,j}\right) + \left(AF_{i,j-1/2} - AF_{i,j+1/2}\right)\right]$

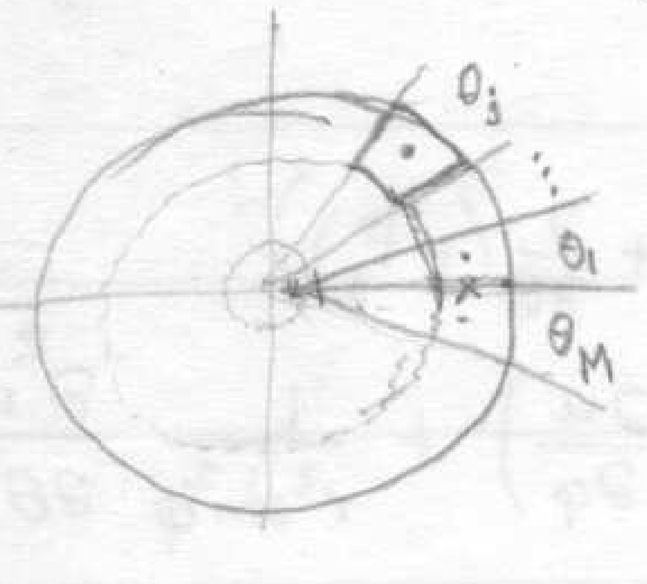


flow rates: $(AF_x)_{i-1/2,j} = A_{i-1/2,j}\cdot\left(-D_x \frac{U_{ij} - U_{i-1,j}}{\Delta x = x_i - x_{i-1}}\right)$, $i = 2,3,\dots,M_x$, $j = 1,2,\dots,M_y$

$(AF_y)_{i,j-1/2} = A_{i,j-1/2}\left(-D_y \frac{U_{ij} - U_{i,j-1}}{\Delta y = y_j - y_{j-1}}\right)$, $i = 1,\dots,M_x$, $j = 2,\dots,M_y$

$F_{1/2,j}$, $F_{M_x+1/2,j}$, $F_{i,\frac12}$, $F_{i,M_y+1/2}$ from BCs

In polar: $u(r,\theta)$ same, now nodes are: (r_i, θ_j)

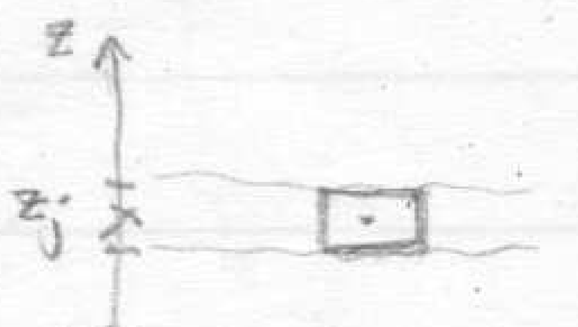


$Ar_{i-\frac12,j} = r_{i-1/2}\,\Delta\theta$, $A\theta_{i,j-1/2} = \Delta r$, $Vol_{ij} = r_i\,\Delta\theta\,\Delta r$

BC at axis: $Fr_{1/2,j} = 0$ if full disc $(0 \le r \le R_{out})$

Axisymmetric in (r,z) coordinates:

$u(r,z)$

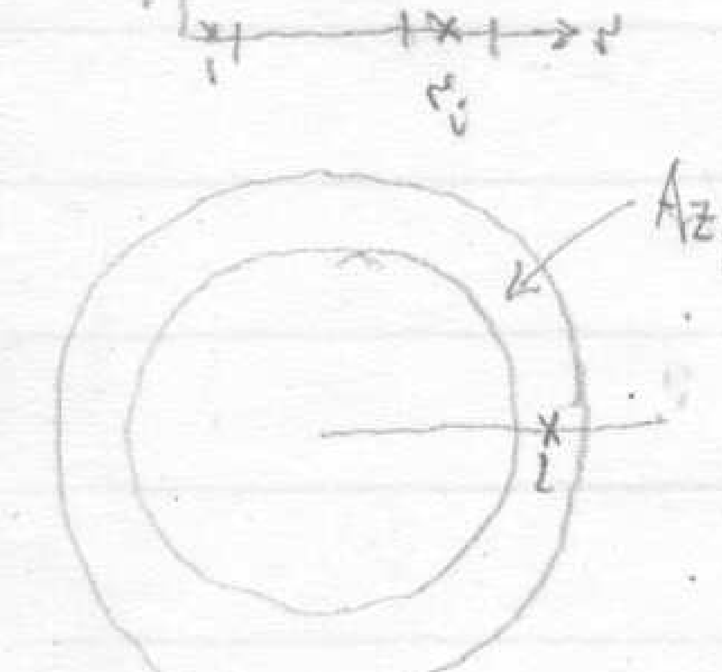


V_{ij} rotated all around

$Ar_{i-\frac12,j} = 2\pi r_{i-\frac12}\,\Delta z$

$Az_{i,j-\frac12} = \pi r^2_{i+\frac12} - \pi r^2_{i-\frac12} = 2\pi\left(\frac{r_{i+\frac12} + r_{i-\frac12}}{2}\right)\Delta r = 2\pi r_i\,\Delta r$ $\forall_j$ for uniform mesh or nodes midway of faces

$\Delta V_{i,j} = Az_{i,j-\frac12}\cdot\Delta z = 2\pi r_i\,\Delta r\,\Delta z$

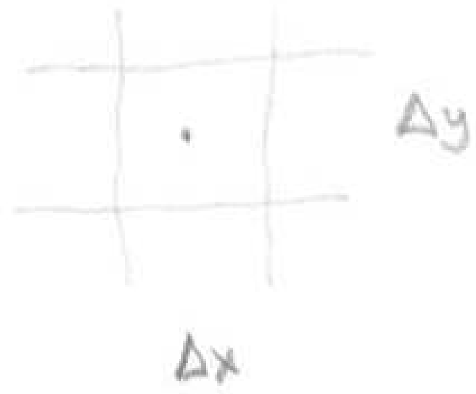


$Fr_{i-\frac12,j} = -D\frac{U_{ij} - U_{i-1,j}}{\Delta r}$, $Fz_{i,j-\frac12} = -D\frac{U_{i,j} - U_{i,j-1}}{\Delta z}$

$$U^{n+1}_{ij} = U^n_{ij} + \frac{\Delta t}{\Delta V_{ij}}\left[(AFr)_{i-\frac12,j} - (AFr)_{i+\frac12,j} + (AFz)_{i,j-\frac12} - (AFz)_{i,j+\frac12}\right]$$

for $u_t = \nabla\cdot(D\nabla u) = \frac{1}{r}\frac{\partial}{\partial r}\left(r D_r \frac{\partial u}{\partial r}\right) + \frac{\partial}{\partial z}\left(D_z\frac{\partial u}{\partial z}\right)$

CFL for 2D advection-diffusion in Cartesian coordinates



$$U_{ij}^{n+1} = U_{ij}^{n} + \frac{\Delta t}{\Delta V_{ij}}\left[(AF)^n_{i-1/2,j} - (AF)^n_{i+1/2,j} + (AF)_{i,j-1/2} - (AF)_{i,j+1/2} \right]$$

upwind $v_{i-1/2,j} > 0$, $v_{i,j-1/2} > 0$

$$F_{i-1/2,j} = v_{i-1/2,j} U_{i-1,j} - D\frac{U_{ij} - U_{i-1,j}}{\Delta x}$$

$$F_{i,j-1/2} = v_{i,j-1/2} U_{i,j-1} - D\frac{U_{ij} - U_{i,j-1}}{\Delta y}$$

x face $A_{i\mp 1/2,j} = \Delta y$

y face $A_{i,j\mp 1/2} = \Delta x$

$\Delta V_{ij} = \Delta x \, \Delta y$

$$\Rightarrow U_{ij}^{n+1} = U_{ij}^{n} + \frac{\Delta t}{\Delta x}\left[v_{i-1/2,j} U_{i-1,j} - v_{i+1/2,j} U_{ij} - D\frac{U_{ij} - U_{i-1,j}}{\Delta x} + D\frac{U_{i+1,j} - U_{i,j}}{\Delta x} \right]$$
$$+ \frac{\Delta t}{\Delta y}\left[v_{i,j-1/2} U_{i,j-1} - v_{i,j+1/2} U_{ij} - D\frac{U_{ij} - U_{i,j-1}}{\Delta y} + D\frac{U_{i,j+1} - U_{ij}}{\Delta y} \right]$$

$$= \left[1 - \left(\frac{\Delta t}{\Delta x} v_{i+1/2,j} + \frac{2D\Delta t}{\Delta x^2} \right) - \left(\frac{\Delta t}{\Delta y} v_{i,j+1/2} + \frac{2D\Delta t}{\Delta y^2} \right) \right] U_{ij}$$
$$+ \frac{\Delta t}{\Delta x} v_{i-1/2,j} U_{i-1,j} + \frac{D\Delta t}{\Delta x^2} U_{i-1,j} + \frac{D\Delta t}{\Delta x^2} U_{i+1,j} + \frac{\Delta t}{\Delta y} v_{i,j-1/2} U_{i,j-1} + \frac{D\Delta t}{\Delta y^2} U_{i,j-1} + \frac{D\Delta t}{\Delta y^2} U_{i,j+1}$$

positive coeffs: $\Delta t \left(\frac{v_{i+1/2,j}}{\Delta x} + \frac{v_{i,j+1/2}}{\Delta y} + \frac{2D}{\Delta x^2} + \frac{2D}{\Delta y^2} \right) \leq 1$

$$\Rightarrow \boxed{\Delta t \leq \frac{1}{\max(\quad)} = \frac{1}{\max|v| \left(\frac{1}{\Delta x} + \frac{1}{\Delta y} \right) + 2D\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} \right)}}$$

So if $\Delta x = \Delta y =: h$ then need $\Delta t \leq \dfrac{1}{\dfrac{2\max|v|}{h_{min}} + \dfrac{4D}{h^2_{min}}} = \dfrac{1}{\dfrac{1}{\Delta t_{adv}} + \dfrac{1}{\Delta t_{diff}}}$

or $h = \min\{\Delta x_i, \Delta y_j\}$

For pure advection ($D=0$): $\Delta t_{adv} \leq \dfrac{h}{2 v_{max}}$, For pure diffusion ($v \equiv 0$): $\Delta t_{diff} \leq \dfrac{h^2}{4D}$

Is it enough to take $\Delta t = \min\{\Delta t_{adv}, \Delta t_{diff}\}$? NO! $0 < \min\{a,b\} \not< \dfrac{1}{\frac{1}{a} + \frac{1}{b}}$

e.g. if $a<b$ then $\min\{a,b\} = a \overset{?}{<} \dfrac{1}{\frac{1}{a}+\frac{1}{b}} = \dfrac{ab}{a+b} \Leftrightarrow a+b \overset{?}{<} b$ false (for $a,b>0$)!

CFL for 2D polar advection-diffusion

$$U_{ij}^{n+1} = U_{ij}^{n} + \frac{\Delta t}{Vol_{ij}}\left[\left(AF_{i-1/2,j} - AF_{i+1/2,j}\right) + \left(AF_{i,j-1/2} - AF_{i,j+1/2}\right)\right]$$

polar: $A_{i-1/2,j} = r_{i-1/2}\Delta\theta$, $A\theta_{i,j-1/2} = \Delta r$, $Vol_{ij} = r_i \Delta\theta \Delta r$

for $v > 0$:

$$F_{i-1/2,j} = v_{i-1/2,j} U_{i-1,j} - D\frac{U_{ij} - U_{i-1,j}}{\Delta r}, \quad F_{i,j-1/2} = v_{i,j-1/2} U_{i,j-1} - D\frac{U_{ij} - U_{i,j-1}}{\Delta r}$$

$$\Rightarrow U_{ij}^{n+1} = U_{ij} + \frac{\Delta t}{r_i \Delta r \Delta\theta}\left[r_{i-1/2}\Delta\theta\left(v_{i-1/2,j} U_{i-1,j} - D\frac{U_{ij} - U_{i-1,j}}{\Delta r}\right) - r_{i+1/2}\Delta\theta\left(v_{i+1/2,j} U_{ij} - D\frac{U_{i+1,j} - U_{ij}}{\Delta r}\right)\right.$$

$$\left. + \Delta r\left(v_{i,j-1/2} U_{i,j-1} - D\frac{U_{ij} - U_{i,j-1}}{\Delta r}\right) - \Delta r\left(v_{i,j+1/2} U_{ij} - D\frac{U_{i,j+1} - U_{ij}}{\Delta r}\right)\right]$$

$$= U_{ij}\left[1 - \frac{D\Delta t\, r_{i-1/2}}{r_i \Delta r^2} - \frac{\Delta t\, r_{i+1/2} v_{i+1/2,j}}{r_i \Delta r} - \frac{D\Delta t\, r_{i+1/2}}{r_i \Delta r^2} - \frac{D\Delta t}{r_i \Delta\theta \Delta r} - v_{i,j+1/2}\frac{\Delta t}{r_i \Delta\theta} - \frac{D\Delta t}{r_i \Delta\theta \Delta r}\right] + \dots$$

$$\Rightarrow \Delta t\left[D\frac{r_{i-1/2} + r_{i+1/2}}{r_i \Delta r^2} + 2D\frac{1}{r_i \Delta r \Delta\theta} + v\left(\frac{r_{i+1/2}}{r_i \Delta r} + \frac{1}{r_i \Delta\theta}\right)\right] \le 1$$

$$\Delta t\left[\frac{2D}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{r_i \Delta\theta}\right) + \frac{v}{r_i}\left(\frac{r_{i+1/2}}{\Delta r} + \frac{1}{\Delta\theta}\right)\right] \le 1$$

$$\Delta t \le \frac{1}{\max \frac{2D}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{r_i \Delta\theta}\right) + \max\left(\frac{v}{r_i}\left(\frac{r_{i+1/2}}{\Delta r} + \frac{1}{\Delta\theta}\right)\right)}$$

$$= \frac{1}{\frac{2D}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{\Delta\theta \cdot \min r_i}\right) + v\left(\max\frac{r_{i+1/2}}{r_i \Delta r} + \frac{1}{\Delta\theta \cdot \min r_i}\right)}$$

$$= \frac{1}{\frac{2D}{\Delta r}\left(\frac{1}{\Delta r} + \frac{2}{\Delta\theta \Delta r}\right) + v\left(\frac{2}{\Delta r} + \frac{2}{\Delta\theta \Delta r}\right)}$$

$\min r_i = \frac{\Delta r}{2}$

$\max \frac{r_{i+1/2}}{r_i \Delta r} = \max \frac{r_i + \frac{\Delta r}{2}}{r_i \Delta r} = $

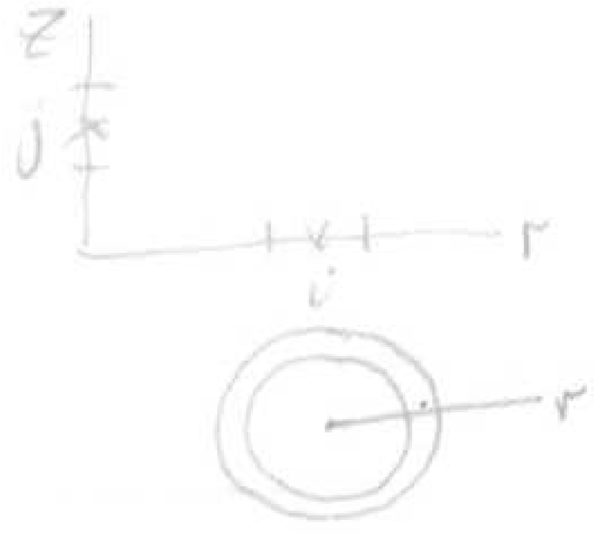
$= \frac{1}{\Delta r} + \frac{1}{2 \min r_i} = \frac{1}{\Delta r} + \frac{1}{\cancel{2}\frac{\Delta r}{\cancel{2}}}$

$= \frac{2}{\Delta r}$

$$\boxed{\Delta t \le \frac{1}{\frac{2D}{\Delta r^2}\left(1 + \frac{2}{\Delta\theta}\right) + \frac{2|v|}{\Delta r}\left(1 + \frac{1}{\Delta\theta}\right)}}$$

$|v| = \max |v_{i-1/2,j},\ v_{i,j-1/2}|$

CFL for axisymmetric advection-diffusion (r, z)



$$U_{ij}^{n+1} = U_{ij}^{n} + \frac{\Delta t}{Vol_{ij}}\left[\left(ArF_{i-1/2,j} - ArF_{i+1/2,j}\right) + \left(AzF_{i,j-1/2} - AzF_{i,j+1/2}\right)\right]$$

$$Ar_{i-1/2,j} = 2\pi r_{i-1/2}\Delta z\,, \quad Az_{i,j-1/2} = 2\pi r_i \Delta r\,, \quad V_{ij} = 2\pi r_i \Delta r \Delta z$$

For $\vec{v} > 0$: $F_{i-1/2,j} = v U_{i-1,j} - D\dfrac{U_{ij} - U_{i-1,j}}{\Delta r}$, $\quad F_{i,j-1/2} = v U_{i,j-1} - D\dfrac{U_{ij} - U_{i,j-1}}{\Delta z}$

$$\Rightarrow U_{ij}^{n+1} = U_{ij}^{n} + \frac{\Delta t}{2\pi r_i \Delta r \Delta z}\left[2\pi r_{i-1/2}\Delta z\left(v U_{i-1,j} - D\frac{U_{ij} - U_{i-1,j}}{\Delta r}\right) - 2\pi r_{i+1/2}\Delta z\left(v U_{ij} - D\frac{U_{i+1,j} - U_{ij}}{\Delta r}\right)\right.$$

$$\left. + 2\pi r_i \Delta r\left(v U_{i,j-1} - D\frac{U_{ij} - U_{i,j-1}}{\Delta z}\right) - 2\pi r_i \Delta r\left(v U_{i,j} - D\frac{U_{i,j+1} - U_{ij}}{\Delta z}\right)\right]$$

$$= U_{ij}\left[1 + \frac{\Delta t}{2\pi r_i \Delta r \Delta z}\left(-2\pi r_{i-1/2}\Delta z\frac{D}{\Delta r} - 2\pi r_{i+1/2}\Delta z\, v - 2\pi r_{i+1/2}\Delta z\frac{D}{\Delta r}\right.\right.$$

$$\left.\left. - 2\pi r_i \Delta r\frac{D}{\Delta z} - 2\pi r_i \Delta r\, v - 2\pi r_i \Delta r\frac{D}{\Delta z}\right)\right] + \cdots$$

$$\Rightarrow \Delta t\left[\frac{r_{i-1/2}}{r_i}\frac{D}{\Delta r^2} + \frac{r_{i+1/2}}{r_i}\frac{v}{\Delta r} + \frac{r_{i+1/2}}{r_i}\frac{D}{\Delta r^2} + \frac{D}{\Delta z^2} + \frac{v}{\Delta z} + \frac{D}{\Delta z^2}\right] \leq 1$$

$$\Rightarrow \Delta t\left[\frac{r_{i-1/2} + r_{i+1/2}}{r_i}\frac{D}{\Delta r^2} + \frac{2D}{\Delta z^2} + v\left(\frac{r_{i+1/2}}{r_i \Delta r} + \frac{1}{\Delta z}\right)\right] \leq 1$$

$$\Rightarrow \Delta t\left[2D\left(\frac{1}{\Delta r^2} + \frac{1}{\Delta z^2}\right) + v\left(\frac{2}{\Delta r} + \frac{1}{\Delta z}\right)\right] \leq 1$$

$$\max\frac{r_{i+1/2}}{r_i \Delta r} = \max\frac{r_i + \frac{\Delta r}{2}}{r_i \Delta r} = \frac{1}{\Delta r} + \frac{1}{2\min r_i} = \frac{1}{\Delta r} + \frac{1}{2\frac{\Delta r}{2}} = \frac{2}{\Delta r}$$

$$\Rightarrow \Delta t \leq \frac{1}{\max(\;)} = \frac{1}{2D\left(\frac{1}{\Delta r^2} + \frac{1}{\Delta z^2}\right) + |v|\left(\frac{2}{\Delta r} + \frac{1}{\Delta z}\right)}$$

CFL condition for 2D advection - diffusion

As before, plugging fluxes into scheme and applying Positive Coeff. Rule

in Cartesian: $$\Delta t \leqslant \frac{1}{\frac{|v_{i-\frac{1}{2},j}|}{\Delta x_i} + \frac{|v_{i,j-\frac{1}{2}}|}{\Delta y_j} + 2D\left(\frac{1}{\Delta x_i^2} + \frac{1}{\Delta y_j^2}\right)}$$

For uniform mesh $\Delta x = \Delta y = h$ or $h = \min\{\Delta x_i, \Delta y_j\}$

$$\Delta t \leqslant \frac{1}{2\frac{\max|v|}{h} + 4\frac{D}{h^2}}$$

in polar: $$\Delta t \leqslant \frac{1}{\max|v|\left(\frac{r_{i+1/2}}{r_i \Delta r} + \frac{1}{r_i \Delta\theta}\right) + \frac{2D}{\Delta r}\left(\frac{1}{\Delta r} + \frac{1}{r_i \Delta\theta}\right)}$$

$$\boxed{\max\frac{r_{i+\frac{1}{2}}}{r_i} = \max\frac{r_i + \frac{\Delta r}{2}}{r_i} = 1 + \frac{\Delta r}{2\cdot\min r_i} = 1 + \frac{\Delta r}{2\cdot\frac{\Delta r}{2}} = 2}$$

$$\leqslant \frac{1}{\frac{2|v|}{\Delta r}\left(1 + \frac{1}{\Delta\theta}\right) + \frac{2D}{\Delta r^2}\left(1 + \frac{2}{\Delta\theta}\right)}$$

$\min r_i = \frac{\Delta r}{2}$

axisymmetric: $$\Delta t \leqslant \frac{1}{|v|\left(\frac{2}{\Delta r} + \frac{1}{\Delta z}\right) + 2D\left(\frac{1}{\Delta r^2} + \frac{1}{\Delta z^2}\right)}$$

$$u_t + \nabla\cdot(\vec{v}u) = 0,\ \nabla\cdot v = 0 \Rightarrow u_t + \vec{v}\cdot\nabla u = 0$$
$$\vec{v} = \langle v, w\rangle$$

Consistency of 2D advection

2D: $u_t + v u_x + w u_y = 0$

expansion about (x_i, y_j, t_n): $u(x_i, y_j, t_n+\Delta t) = u + \Delta t\, u_t + \frac{\Delta t^2}{2} u_{tt} + \cdots$

$u(x_i-\Delta x, y_j, t_n) = u - \Delta x\, u_x + \frac{\Delta x^2}{2} u_{xx} + \cdots$

$y_j - \Delta y$: $\quad -\Delta y\, u_y + \frac{\Delta y^2}{2} u_{yy} + \cdots$

$$U_{ij}^{n+1} = U_{ij}^n - \frac{\Delta t}{\Delta x \Delta y}\left[\Delta y\left(v U_{i-1,j} - v U_{ij}\right) + \Delta x\left(w U_{i,j-1} - w U_{ij}\right)\right]$$

$$\Rightarrow \mathrm{FDE}[U] = \frac{U^{n+1} - U^n}{\Delta t} - v\frac{U_{i-1,j} - U_{ij}}{\Delta x} - w\frac{U_{i,j-1} - U_{ij}}{\Delta y}$$

$$\mathrm{FDE}[u] = u_t + \frac{\Delta t}{2}u_{tt} + \cdots - v\left[-u_x + \frac{\Delta x}{2}u_{xx} + \cdots\right] - w\left[-u_y + \frac{\Delta y}{2}u_{yy} + \cdots\right]$$

$$= \underbrace{\left[u_t + v u_x + w u_y\right]}_{\mathrm{PDE}=0} + \frac{1}{2}\left[\Delta t\cdot u_{tt} - v\Delta x\, u_{xx} - w\Delta y\, u_{yy}\right] + \cdots$$

and $u_t = -v u_x - w u_y \Rightarrow u_{tt} = -v(u_t)_x - w(u_t)_y = -v\left[-v u_{xx} - w u_{xy}\right] - w\left[-v u_{xy} - w u_{yy}\right]$

$$= \mathrm{PDE}[u] + \frac{\Delta t}{2}\left[v^2 u_{xx} + vw\left(u_{xy} + u_{yx}\right) + w^2 u_{yy}\right] - \frac{v\Delta x}{2}u_{xx} - \frac{w\Delta y}{2}u_{yy} + \cdots$$

$$= \mathrm{PDE}[u] + \frac{1}{2}\left[v^2\Delta t - v\Delta x\right]u_{xx} + \frac{1}{2}\left[w^2\Delta t - w\Delta y\right]u_{yy} + \frac{\Delta t\, vw}{\cancel{2}}\cancel{2}(u_{xy}) + \cdots$$

$$= \mathrm{PDE}[u] + \frac{v}{2}\left[v\Delta t - \Delta x\right]u_{xx} + \frac{w}{2}\left[w\Delta t - \Delta y\right]u_{yy} + \Delta t\, vw\, u_{xy} + \cdots$$

CFL: $\Delta t \le \dfrac{1}{\frac{v}{\Delta x} + \frac{w}{\Delta y}} \Rightarrow \dfrac{v\Delta t}{\Delta x} + \dfrac{w\Delta t}{\Delta y} = \mu \le 1$

$\mu_1 + \mu_2 =: \mu \le 1$

$$= \mathrm{PDE}[u] - \underbrace{\frac{v}{2}\Delta x\left[1-\mu_1\right]u_{xx}}_{\text{num. diffusion in x-dir}} - \underbrace{\frac{w\Delta y}{2}\left[1-\mu_2\right]u_{yy}}_{\text{num. diffusion in y-dir}} + \underbrace{\Delta t\, vw\, u_{xy}}_{\text{num. dispersion}} + \cdots$$

There is no choice of Δt that will eliminate both diffusion terms and dispersion term