Resumé of Part 1

Solve driven cavity at $Re = 10$

Physics, maths of PDE

$\psi - \omega$ and $u - v - p$ formulations: Pressure

Finite Differences

Poisson solver, SOR

Time stepping, numerical instability

Accuracy, no bugs?, results

Part II – more details on general issues

Discretisation – FD, FE, Spectral

Time-stepping – implicit, pressure

Solving large sparse linear equations

Part III – collection of special topics

Finite Differences
Higher order derivatives

a. central differencing

With $O(\Delta x^2)$ errors

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x}$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}$$

and higher order derivatives

$$f_i''' = \frac{f_{i+1}'' - f_{i-1}''}{2\Delta x}$$

$$= \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2\Delta x^3}$$

$$f_i'''' = \frac{f_{i+1}'' - 2f_i'' + f_{i-1}''}{\Delta x^2}$$

$$= \frac{f_{i+2} - 4f_{i+1} + 6f_i - 4f_{i-1} + f_{i-2}}{\Delta x^4}$$

even $\rightarrow$ Pascal Δ, odd $\rightarrow$ 2$\times$ Pascal with shift

Error analysis by Taylor series

$$f_{i+1} = f(x = i\Delta x + \Delta x)$$
$$= f_i + \Delta x f_i' + \tfrac{1}{2}\Delta x^2 f_i'' + \tfrac{1}{6}\Delta x^3 f_i''' + \tfrac{1}{24}\Delta x^4 f_i'''' + \dots.$$

Then

$$f_{i+1} - f_{i-1} = 2\Delta x f_i' + \tfrac{1}{3}\Delta x^3 f_i''' + O(\Delta x^5).$$

But have f_i''' to second order. Substitute for

$$f_i' = \frac{-\frac{1}{12}f_{i+2} + \frac{2}{3}f_{i+1} - \frac{2}{3}f_{i-1} + \frac{1}{12}f_{i-2}}{\Delta x} + O(\Delta x^4).$$

Check expression with $f = 1, x, x^2, x^3, x^4 \rightarrow$ correct $0, 1, 0, 0, 0$

Similarly,

$$f_i'' = \frac{-\frac{1}{12}f_{i+2} + \frac{4}{3}f_{i+1} - \frac{5}{2}f_i + \frac{4}{3}f_{i-1} - \frac{1}{12}f_{i-2}}{\Delta x^2} + O(\Delta x^4).$$

b. One-side differencing – used in BC

With $O(\Delta x)$ error

$$f_0' = \frac{f_1 - f_0}{\Delta x} + O(\Delta x),$$

$$f_0'' = \frac{f_2 - 2f_1 + f_0}{\Delta x^2} + O(\Delta x),$$

$$f_0''' = \frac{f_3 - 3f_2 + 3f_1 - f_0}{\Delta x^3} + O(\Delta x)$$

Error analysis by Taylor series

$$f_1 = f_0 + \Delta x f_0' + \tfrac{1}{2}\Delta x^2 f_0'' + O(\Delta x^3).$$

Using the first-order expression above for f_0''

$$f_0' = \frac{-\frac{1}{2}f_2 + 2f_1 - \frac{3}{2}f_0}{\Delta x} + O(\Delta x^2).$$

Similarly

$$f_0'' = \frac{-f_3 + 4f_2 - 5f_1 + 2f_0}{\Delta x^2} + O(\Delta x^2).$$

c. Non-equispaced points

To find kth derivative $f^{(k)}(x_0)$ to $O(\Delta x^l)$
fit polynomial of degree $k + l$ through $k + l + 1$ points $x_0 + \Delta x_i$,

$$f(x_0 + \Delta x_i) = a_0 + a_1 \Delta x_i + a_2 \Delta x_i^2 + \ldots a_{k+l} \Delta x_i^{k+l}.$$

Solve for polynomial coefficients a_j, e.g. by MAPLE, then

$$f^{(k)}(x_0) = k! a_k$$

Central differencing on equispaced points $\rightarrow$ one degree accuracy better

Splines better than higher order polynomials $\rightarrow$ FEM

b. two-dimensional version

Use
$$\nabla^2 \rho = \nabla^2 \nabla^2 \phi = \frac{\partial^4 \phi}{\partial x^4} + 2\frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{\partial^4 \phi}{\partial y^4}.$$

Now
$$\begin{pmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{pmatrix} \phi = \Delta x^2 \nabla^2 \phi + \frac{1}{12}\Delta x^4 \left(\frac{\partial^4 \phi}{\partial x^4} + \frac{\partial^4 \phi}{\partial y^4} \right).$$

and
$$\begin{pmatrix} 1 & & 1 \\ & -4 & \\ 1 & & 1 \end{pmatrix} \phi = 2\Delta x^2 \nabla^2 \phi + \frac{1}{6}\Delta x^4 \left(\frac{\partial^4 \phi}{\partial x^4} + 6\frac{\partial^4 \phi}{\partial x^2 \partial y^2} + \frac{\partial^4 \phi}{\partial y^4} \right).$$

Hence $\frac{2}{3}$ of first $+ \frac{1}{6}$ of second

$$\frac{1}{\Delta x^2} \begin{pmatrix} \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \frac{2}{3} & -\frac{10}{3} & \frac{2}{3} \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{pmatrix} \phi = \begin{pmatrix} 0 & \frac{1}{12} & 0 \\ \frac{1}{12} & \frac{2}{3} & \frac{1}{12} \\ 0 & \frac{1}{12} & 0 \end{pmatrix} \rho + O(\Delta x^4).$$

Compact 4th order Poisson solver

a. one-dimensional version

Fourth-order differencing for $\phi_i'' = \rho$

$$-\tfrac{1}{12}\phi_{i+2} + \tfrac{4}{3}\phi_{i+1} - \tfrac{5}{2}\phi_i + \tfrac{4}{3}\phi_{i-1} - \tfrac{1}{12}\phi_{i-2} = \Delta x^2 \rho_i.$$

Problems: wide molecule, need special form near boundary

Error in 2nd order version

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = \phi_i'' + \tfrac{1}{6}\Delta x^2 \phi_i'''' + O(\Delta x^4).$$

Now $\phi_i'' = \rho_i$ and so

$$\phi_i'''' = \rho_i'' = \frac{\rho_{i+1} - 2\rho_i + \rho_{i+1}}{\Delta x^2} + O(\Delta x^2).$$
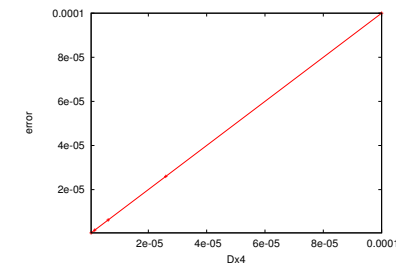
Hence

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta x^2} = \tfrac{1}{6}\rho_{i+1} + \tfrac{2}{3}\rho_i + \tfrac{1}{6}\rho_{i-1} + O(\Delta x^4).$$

Test

Analytic solution

$$\rho = 2\pi^2 \sin \pi x \sin \pi y \quad \text{and} \quad \phi = -\sin \pi x \sin \pi y.$$

with $N = 10, 14, 20, 40$ and 56

Error decreasing as $0.27\Delta x^4$,
i.e $N = 20$ gives $2\,10^{-6}$ cf $2\,10^{-3}$ for 2nd order.

Crandall 4th order for diffusion equation

Similar trick, with cancellation of $\Delta t^2 \frac{\partial^2 u}{\partial t^2}$ with $\frac{1}{6}\Delta x^4 \frac{\partial^4 u}{\partial x^4}$ errors.

$$u_i^{n+1} + \left(\frac{1}{12} - \frac{\Delta t}{2\Delta x^2}\right)\left(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}\right)$$
$$= u_i^n + \left(\frac{1}{12} + \frac{\Delta t}{2\Delta x^2}\right)\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right).$$

Upwinding

Advection $\mathbf{u}\cdot\nabla\phi$ propagates information in direction $\mathbf{u}$.
Violated by central differencing

$$u_i \frac{\phi_{i+1} - \phi_{i-1}}{2\Delta x}$$

where if $u_i > 0$ downstream ϕ_{i+1} influences ϕ_i.

Correct flow of info by upwinding

$$u\frac{\partial\phi}{\partial x} = \begin{cases} u_i \dfrac{\phi_i - \phi_{i-1}}{\Delta x} & \text{if } u_i > 0 \\[2mm] u_i \dfrac{\phi_{i+1} - \phi_i}{\Delta x} & \text{if } u_i < 0, \end{cases}$$

But only 1st order accurate, $O(\Delta x)$ errors.

Higher order

One-sided differencing at $O(\Delta x^2)$

$$u\frac{\partial\phi}{\partial x} = \begin{cases} u_i \dfrac{\frac{3}{2}\phi_i - 2\phi_{i-1} + \frac{1}{2}\phi_{i-2}}{\Delta x} & \text{if } u_i > 0 \\[3mm] u_i \dfrac{-\frac{1}{2}\phi_{i+2} + 2\phi_{i+1} - \frac{3}{2}\phi_i}{\Delta x} & \text{if } u_i < 0, \end{cases}$$

But wide molecule.

More compact and nearly upwinding

$$\frac{u}{\Delta x}\begin{pmatrix} 0 & 0 & 0 \\ -1 & 1 & 0 \\ -\frac{1}{2} & 1 & \frac{1}{2} \end{pmatrix}\phi + \frac{v}{\Delta x}\begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 1 & 1 & 0 \\ -\frac{1}{2} & -1 & 0 \end{pmatrix}\phi.$$

$u > 0$ and $v > 0$

Other grids

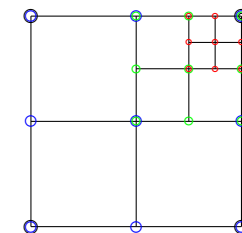Geometry of problem $\rightarrow$ polars, other OG coods, non–OG bad idea

Increased resolution of important small regions

stretched grid $\quad x(\xi)\quad$ and/or $\quad y(\eta)$

NB OG. Central differencing on ξ and η better than non-equispaced
Can give unnecessary coverage, e.g. away from important corner.

Difficult to match
different resolutions

but stability

Time-step stability controlled by smallest grid block

Diffusive numerical stability

$$\Delta t < \tfrac{1}{4} Re\, \Delta x_{\min}^2,$$

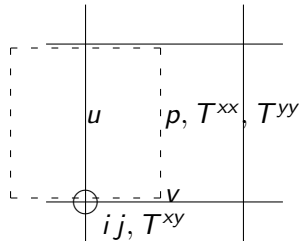Advection stability

$$\Delta t < (\Delta x / U)_{\min}.$$

Restriction acute for polars

$$\Delta x_{\min} = r_{\min} \Delta \theta_{\min} \quad \text{with} \quad r_{min} = \Delta r$$

In infinite domains, bring infinity nearer with stretch such as

$$x = e^\xi \quad \text{or} \quad x = \frac{\xi}{1 - \xi}.$$

Conservative forms

- conservative formulation of governing equation
- apply to a Finite Volume of Fluids (VoF)

Recast Navier-Stokes to

$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \mathbf{T} = 0$$

with total momentum flux

$$\mathbf{T} = \rho \mathbf{u}\mathbf{u} + p\mathbf{I} - 2\mu \mathbf{E}$$

Reynolds stresses, isotropic pressure and viscous stresses

apply to Volume of Fluid on staggered grid

$$\rho u_{i\,j+\frac{1}{2}}^{n+1} = \rho u_{i\,j+\frac{1}{2}}^{n} - \Delta t \left(\frac{T^{xx}_{i+\frac{1}{2}\,j+\frac{1}{2}} - T^{xx}_{i-\frac{1}{2}\,j+\frac{1}{2}}}{\Delta x} + \frac{T^{xy}_{i\,j+1} - T^{xy}_{i\,j}}{\Delta x} \right).$$

When integrate over a large volume, internal momentum fluxes cancel.

For momentum conservation on whole domain, need e.g. on $x = 0$

$$T^{xx}_{-\frac{1}{2}\,j+\frac{1}{2}} = T^{xx}_{\frac{1}{2}\,j+\frac{1}{2}} + T^{xy}_{0,j+1} - T^{xy}_{0,j},$$

fluxes on staggered grid

Some averaging for inertia terms, but not for pressure and viscous terms

$$T^{xx}_{i+\frac{1}{2}\,j+\frac{1}{2}} = \rho \left(\frac{u_{i+1\,j+\frac{1}{2}} + u_{i\,j+\frac{1}{2}}}{2} \right)^2 + p_{i+\frac{1}{2}\,j+\frac{1}{2}} - 2\mu \frac{u_{i+1\,j+\frac{1}{2}} - u_{i\,j+\frac{1}{2}}}{\Delta x}$$

$$T^{xy}_{i\,j} = \rho \left(\frac{u_{i\,j+\frac{1}{2}} + u_{i\,j-\frac{1}{2}}}{2} \right) \left(\frac{v_{i+\frac{1}{2}\,j} + v_{i-\frac{1}{2}\,j}}{2} \right)$$
$$\quad -2\mu \left(\frac{u_{i\,j+\frac{1}{2}} - u_{i\,j-\frac{1}{2}}}{\Delta x} + \frac{v_{i+\frac{1}{2}\,j} - v_{i-\frac{1}{2}\,j}}{\Delta x} \right)$$

$$T^{yy}_{i+\frac{1}{2}\,j+\frac{1}{2}} = \rho \left(\frac{v_{i+\frac{1}{2}\,j+1} + v_{i+\frac{1}{2}\,j}}{2} \right)^2 + p_{i+\frac{1}{2}\,j+\frac{1}{2}} - 2\mu \frac{v_{i+\frac{1}{2}\,j+1} - v_{i+\frac{1}{2}\,j}}{\Delta x}.$$

Use conservative form in non-Cartesian coods

$$\nabla^2\phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2}$$

better numerically than theoretically equivalent

$$\frac{\partial^2\phi}{\partial r^2} + \frac{2}{r}\frac{\partial\phi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2}$$

Discretisation

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\phi}{\partial r}\right) \approx \frac{\left(r^2\frac{\partial\phi}{\partial r}\right)_{i+\frac{1}{2}} - \left(r^2\frac{\partial\phi}{\partial r}\right)_{i-\frac{1}{2}}}{r_i^2\Delta r}$$

with

$$\left(r^2\frac{\partial\phi}{\partial r}\right)_{i+\frac{1}{2}} \approx r_{i+\frac{1}{2}}^2\frac{\phi_{i+1} - \phi_i}{\Delta r}.$$

Alternative forms of nonlinear term

$$
\begin{aligned}
\mathbf{u}\cdot\nabla\mathbf{u} &= \nabla\cdot\mathbf{u}\,\mathbf{u} & &\text{conserves momentum} \\
&= \nabla\tfrac{1}{2}u^2 - \mathbf{u}\wedge\boldsymbol{\omega} & &\text{rotational form} \\
&= \tfrac{1}{2}\mathbf{u}\cdot\nabla\mathbf{u} + \tfrac{1}{2}\nabla\cdot\mathbf{u}\,\mathbf{u} & &\text{conserves energy.}
\end{aligned}
$$

Last called "skew-symmetric" form.
Scalar product with $\mathbf{u}$

$$\left(u_i u_j(u_i^{j+1} - u_i^{j-1}) + u_i(u_j^{j+1}u_i^{j+1} - u_j^{j-1}u_i^{j-1})\right)/2\Delta x,$$

subscripts for components and superscripts for location.
On summing across domain, cancellations first–fourth,
second–third

Two-phase flows

Volume-of-Fluid or One-Fluid Method
= conservative scheme with $\rho(x)$ and $\mu(x)$