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

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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

$$
\begin{aligned}
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}
\end{aligned}
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and higher order derivatives

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

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f_i''' &= \frac{f_{i+1}'' - f_{i-1}''}{2\Delta x} \\
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$$f_i''' = \frac{f''_{i+1} - f''_{i-1}}{2\Delta x} = \frac{f_{i+2} - 2f_{i+1} + 2f_{i-1} - f_{i-2}}{2\Delta x^3}$$

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

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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}
\end{aligned}
$$

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

Error analysis by Taylor series

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Then

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

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

Similarly,

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

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With $O(\Delta x)$ error

$$\begin{aligned} f_0' &= \frac{f_1 - f_0}{\Delta x} + O(\Delta x), \\ f_0'' &= \frac{f_2 - 2f_1 + f_0}{\Delta x^2} + O(\Delta x), \\ f_0''' &= \frac{f_3 - 3f_2 + 3f_1 - f_0}{\Delta x^3} + O(\Delta x) \end{aligned}$$

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Error analysis by Taylor series

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

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Using the first-order expression above for f_0''

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Similarly

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c. Non-equispaced points

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

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

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

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Splines better than higher order polynomials $\rightarrow$ FEM

Compact 4th order Poisson solver

a. one-dimensional version

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

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

Problems: wide molecule, need special form near boundary

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Error in 2nd order version

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

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

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Hence

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

b. two-dimensional version

Use

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

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Now

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

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

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

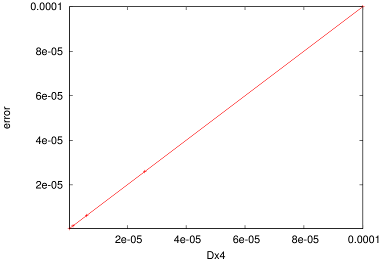
$$\frac{1}{\Delta x^2} \begin{pmatrix} \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \\ \frac{2}{3} & -\frac{10}{3} & \frac{2}{3} \\ \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{pmatrix} \phi = \begin{pmatrix} 0 & \frac{1}{12} & 0 \\ \frac{1}{12} & \frac{2}{3} & \frac{1}{12} \\ 0 & \frac{1}{12} & 0 \end{pmatrix}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

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



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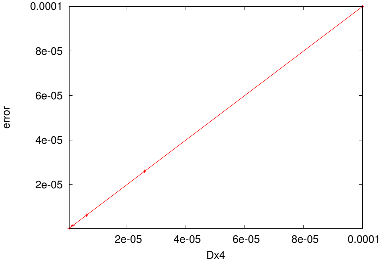

Error decreasing as $0.27\Delta x^4$,
i.e $N = 20$ gives $2\,10^{-6}$ cf $2\,10^{-3}$ for 2nd order.

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.

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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.

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

Upwinding

Advection $\mathbf{u} \cdot \nabla\phi$ propagates information in direction $\mathbf{u}$.

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

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Correct flow of info by upwinding

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

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

Higher order

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

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

But wide molecule.

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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,

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Increased resolution of important small regions

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

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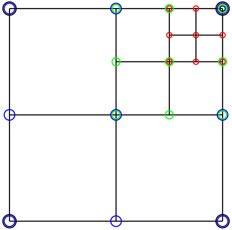
Difficult to match different resolutions



but stability

Time-step stability controlled by smallest grid block

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Time-step stability controlled by smallest grid block
Diffusive numerical stability

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

Advection stability

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

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In infinite domains, bring infinity nearer with stretch such as

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

Conservative forms

Two ideas

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

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Recast Navier-Stokes to

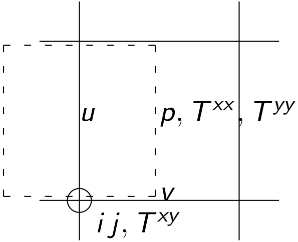
$$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \boldsymbol{\nabla} \cdot \mathbf{T} = 0$$

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



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

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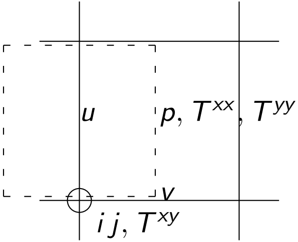

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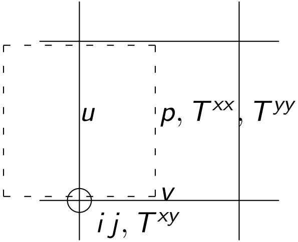

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When integrate over a large volume, internal momentum fluxes cancel.

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

$$
\begin{aligned}
T^{xx}_{i+\frac{1}{2}\,j+\frac{1}{2}} &= \rho\left(\frac{u_{i+1\,j+\frac{1}{2}}+u_{i\,j+\frac{1}{2}}}{2}\right)^2 + p_{i+\frac{1}{2}\,j+\frac{1}{2}} - 2\mu\frac{u_{i+1\,j+\frac{1}{2}}-u_{i\,j+\frac{1}{2}}}{\Delta x} \\
T^{xy}_{i\,j} &= \rho\left(\frac{u_{i\,j+\frac{1}{2}}+u_{i\,j-\frac{1}{2}}}{2}\right)\left(\frac{v_{i+\frac{1}{2}\,j}+v_{i-\frac{1}{2}\,j}}{2}\right) \\
&\quad -2\mu\left(\frac{u_{i\,j+\frac{1}{2}}-u_{i\,j-\frac{1}{2}}}{\Delta x}+\frac{v_{i+\frac{1}{2}\,j}-v_{i-\frac{1}{2}\,j}}{\Delta x}\right) \\
T^{yy}_{i+\frac{1}{2}\,j+\frac{1}{2}} &= \rho\left(\frac{v_{i+\frac{1}{2}\,j+1}+v_{i+\frac{1}{2}\,j}}{2}\right)^2 + p_{i+\frac{1}{2}\,j+\frac{1}{2}} - 2\mu\frac{v_{i+\frac{1}{2}\,j+1}-v_{i+\frac{1}{2}\,j}}{\Delta x}.
\end{aligned}
$$

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

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

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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

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

Two-phase flows

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

Alternative forms of nonlinear term

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

Last called "skew-symmetric" form.

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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