Computational Fluid Dynamics I

Exercise 9

1. The Poisson equation
$$\nabla^2 u = f(x,y)$$
is to be solved in general coordinates.

   (a) Transform the equation from Cartesian to curvilinear coordinates $(x,y) \to (\xi,\eta)$.

   (b) Check the results of the general coordinate transformation with the formulation for polar coordinates ($x = r\cos\theta, y = r\sin\theta$), where
$$\nabla^2 \quad = \quad \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} \quad .$$

   (c) Discretize the transformed equation with central differences and formulate a point Gauß-Seidel method for the solution. Explain the solution procedure with red-black ordering.

Computational Fluid Dynamics I

Exercise 9 (solution)

1. (a) The Poisson equation

$$\nabla^2 u = f(x,y)$$

in Cartesian coordinates reads:

$$u_{xx} + u_{yy} = f(x,y)$$

Transformation into curvilinear coordinates $(x,y) \rightarrow (\xi,\eta)$:

$$\begin{aligned}
u_x &= \xi_x u_\xi + \eta_x u_\eta \\
u_{xx} &= (u_x)_x = (\xi_x u_\xi + \eta_x u_\eta)_x \\
&= \xi_x u_{\xi x} + \xi_{xx} u_\xi + \eta_x u_{\eta x} + \eta_{xx} u_\eta \\
&= \xi_x(\xi_x u_{\xi\xi} + \eta_x u_{\xi\eta}) + \xi_{xx} u_\xi + \eta_x(\xi_x u_{\eta\xi} + \eta_x u_{\eta\eta}) + \eta_{xx} u_\eta \\
&= \xi_{xx} u_\xi + \xi_x^2 u_{\xi\xi} + 2\xi_x \eta_x u_{\xi\eta} + \eta_x^2 u_{\eta\eta} + \eta_{xx} u_\eta
\end{aligned}$$

yields the Poisson equation in curvilinear coordinates:

$$\xi_x^2 u_{\xi\xi} + 2\xi_x\eta_x u_{\xi\eta} + \eta_x^2 u_{\eta\eta} + \xi_{xx} u_\xi + \eta_{xx} u_\eta + \xi_y^2 u_{\xi\xi} + 2\xi_y\eta_y u_{\xi\eta} + \eta_y^2 u_{\eta\eta} + \xi_{yy} u_\xi + \eta_{yy} u_\eta = f(\xi,\eta)$$

$\Leftrightarrow$

$$(\xi_x^2+\xi_y^2)u_{\xi\xi} + 2(\xi_x\eta_x+\xi_y\eta_y)u_{\xi\eta} + (\eta_x^2+\eta_y^2)u_{\eta\eta} + (\xi_{xx}+\xi_{yy})u_\xi + (\eta_{xx}+\eta_{yy})u_\eta = f(\xi,\eta) \quad (*)$$

(b) From

$$\nabla^2 u = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}u\right) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}u = u_{rr} + \frac{1}{r}u_r + \frac{1}{r^2}u_{\theta\theta}$$

and $r = \xi$ and $\theta = \eta$ it follows

$$\nabla^2 u = u_{\xi\xi} + \frac{1}{r}u_\xi + \frac{1}{r^2}u_{\eta\eta} \qquad (**)$$

Relation between polar and Cartesian coordinates:

$$x = \xi\cos\eta \qquad y = \xi\sin\eta$$

$$\Rightarrow \qquad \xi = \sqrt{x^2+y^2} \qquad \eta = \arctan\frac{y}{x}$$

The partial derivatives of ξ and η with respect to x and y for the polar coordinates are:

$$\begin{aligned} \xi_x &= \frac{x}{\sqrt{x^2+y^2}} & \eta_x &= -\frac{y}{x^2+y^2} \\ \xi_y &= \frac{y}{\sqrt{x^2+y^2}} & \eta_y &= \frac{x}{x^2+y^2} \end{aligned}$$

$$\begin{aligned} \xi_{xx} &= \frac{y^2}{(x^2+y^2)^{\frac{3}{2}}} & \eta_{xx} &= \frac{2xy}{(x^2+y^2)^2} \\ \xi_{yy} &= \frac{x^2}{(x^2+y^2)^{\frac{3}{2}}} & \eta_{yy} &= -\frac{2xy}{(x^2+y^2)^2} \end{aligned}$$

Equation $(*)$ must be identical to equation $(**)$, comparison of coefficients for $u_{\xi\xi}, u_{\xi\eta}, u_{\eta\eta}, u_\xi$ and u_η yields:

$$\begin{aligned} 1 = (\xi_x^2 + \xi_y^2) &= \left(\frac{x}{\sqrt{x^2+y^2}}\right)^2 + \left(\frac{y}{\sqrt{x^2+y^2}}\right)^2 = \frac{x^2}{x^2+y^2} + \frac{y^2}{x^2+y^2} = \frac{x^2+y^2}{x^2+y^2} \\ &= 1 \end{aligned}$$

$$\begin{aligned} 0 = 2(\xi_x\eta_x + \xi_y\eta_y) &= 2\left(\left(\frac{x}{\sqrt{x^2+y^2}}\right)\left(-\frac{y}{x^2+y^2}\right) + \left(\frac{y}{\sqrt{x^2+y^2}}\right)\left(\frac{x}{x^2+y^2}\right)\right) \\ &= 0 \end{aligned}$$

$$\begin{aligned} \frac{1}{r^2} = (\eta_x^2 + \eta_y^2) &= \left(-\frac{y}{x^2+y^2}\right)^2 + \left(\frac{x}{x^2+y^2}\right)^2 = \frac{x^2+y^2}{(x^2+y^2)^2} = \frac{1}{x^2+y^2} \\ &= \frac{1}{r^2\cos^2\theta + r^2\sin^2\theta} \\ &= \frac{1}{r^2} \end{aligned}$$

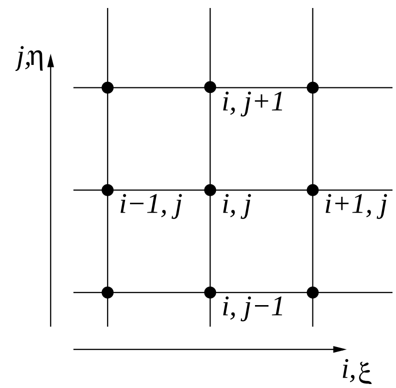
$$\begin{aligned} \frac{1}{r} = (\xi_{xx} + \xi_{yy}) &= \frac{y^2}{(x^2+y^2)^{\frac{3}{2}}} + \frac{x^2}{(x^2+y^2)^{\frac{3}{2}}} = \frac{x^2+y^2}{(x^2+y^2)^{\frac{3}{2}}} = \frac{1}{\sqrt{(x^2+y^2)}} \\ &= \frac{1}{\sqrt{r^2\cos^2\theta + r^2\sin^2\theta}} \\ &= \frac{1}{r} \end{aligned}$$

$$\begin{aligned} 0 = (\eta_{xx} + \eta_{yy}) &= \frac{2xy}{(x^2+y^2)^2} + \left(-\frac{2xy}{(x^2+y^2)^2}\right) \\ &= 0 \end{aligned}$$

(c) **Discretization of metric terms:**

Discretize metric terms with central differences $\mathcal{O}(\Delta x^2, \Delta y^2)$, using $\xi_x = \frac{1}{J} y_\eta,\ \xi_y = -\frac{1}{J} x_\eta,\ \eta_x = -\frac{1}{J} y_\xi,\ \eta_y = \frac{1}{J} x_\xi,\ J = x_\xi y_\eta - y_\xi x_\eta,\ \Delta\xi = \Delta\eta = 1$:

$$
\begin{aligned}
y_\eta &= \frac{y_{i,j+1} - y_{i,j-1}}{2} \\
x_\eta &= \frac{x_{i,j+1} - x_{i,j-1}}{2} \\
y_\xi &= \frac{y_{i+1,j} - y_{i-1,j}}{2} \\
x_\xi &= \frac{x_{i+1,j} - x_{i-1,j}}{2}
\end{aligned}
$$



How to compute second-order metrics terms, e.g., ξ_{xx}, assume we already have computed all first-order metrics $(y_\eta, x_\eta, y_\xi, x_\xi)$:

$$
\begin{aligned}
\xi_{xx} &= (\xi_x)_x = \left(\frac{1}{J} y_\eta\right)_x \\
\frac{\partial}{\partial x}(\xi_x) &= \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}(\xi_x) + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta}(\xi_x) \\
&= \xi_x \xi_{x\xi} + \eta_x \xi_{x\eta} \\
&= \frac{1}{J} y_\eta \left(\frac{1}{J} y_\eta\right)_\xi - \frac{1}{J} y_\xi \left(\frac{1}{J} y_\eta\right)_\eta
\end{aligned}
$$

Now discretize also second-order metrics:

$$
\xi_{xx} = \frac{1}{J} y_\eta \left[\frac{\left(\frac{1}{J} y_\eta\right)_{i+1,j} - \left(\frac{1}{J} y_\eta\right)_{i-1,j}}{2\Delta\xi}\right] - \frac{1}{J} y_\xi \left[\frac{\left(\frac{1}{J} y_\eta\right)_{i,j+1} - \left(\frac{1}{J} y_\eta\right)_{i,j-1}}{2\Delta\eta}\right]
$$

Discretization of partial derivatives/PDE:

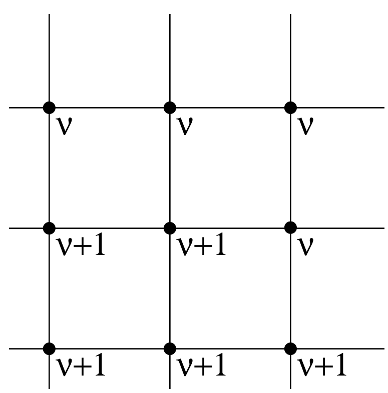
$$
\begin{aligned}
\left(\frac{\partial u}{\partial \xi}\right)_{i,j} &= \frac{u_{i+1,j} - u_{i-1,j}}{2\Delta\xi} + O(\Delta\xi)^2 \\
\left(\frac{\partial^2 u}{\partial \xi^2}\right)_{i,j} &= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta\xi^2} + O(\Delta\xi)^2
\end{aligned}
$$

With a uniform computational mesh with $\Delta\xi = \Delta\eta = 1$ follows:

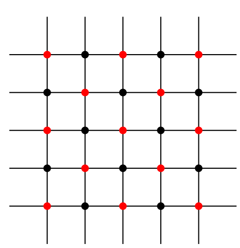
$$
\begin{aligned}
u_\xi &= \frac{u_{i+1,j} - u_{i-1,j}}{2} \\
u_\eta &= \frac{u_{i,j+1} - u_{i,j-1}}{2} \\
u_{\xi\xi} &= u_{i+1,j} - 2u_{i,j} + u_{i-1,j} \\
u_{\eta\eta} &= u_{i,j+1} - 2u_{i,j} + u_{i,j-1} \\
u_{\xi\eta} &= \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4}
\end{aligned}
$$

This leads to a linear system of equations where the constant coefficients $(a, b, c, d, e, f, g, h, i)$ contain the geometrical information from the metric terms, solution with Gauß-Seidel:

$$
\begin{gathered}
a \cdot u^{\nu+1}_{i-1,j-1} + b \cdot u^{\nu+1}_{i,j-1} + c \cdot u^{\nu+1}_{i+1,j-1} + d \cdot u^{\nu+1}_{i-1,j} + e \cdot u^{\nu+1}_{i,j} \\
+f \cdot u^{\nu}_{i+1,j} + g \cdot u^{\nu}_{i-1,j+1} + h \cdot u^{\nu}_{i,j+1} + i \cdot u^{\nu}_{i+1,j+1} = f(x,y)
\end{gathered}
$$

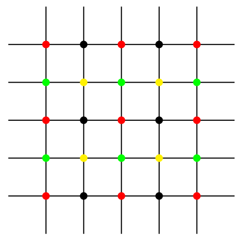


Generally, for a solution procedure with red-black ordering the mesh points are split up into "red" and "black" points, like a checkerboard:



In the first stage of each iteration step the values at all red points are computed with a Gauss-Seidel method, taking into account the surrounding black points but no other red points. In the second stage the values are computed on the black points, taking into consideration the red points that were computed in the first stage. This allows for a vectorization of the solution procedure, as the solution at different points can be computed simultaneously as they are not recursively dependent on each other, as in a standard Gauss-Seidel method.

However, due to the computational stencil in this problem that uses all eight surrounding points to compute the solution we have to use a larger seperation, thus requiring more colors. The ordering for this problem here could look like this:



Thus we have four different stages in each iteration step. For example, in the first stage the values on the yellow points could be computed using the information on the black, red, and green points. In the second stage the values on the green points are computed using the values on the red, black, and the ones on the already updated yellow points. This procedures is then performed for all colors and allows for a vectorization of the given discretization equation.

Computational Fluid Dynamics I

Exercise 9 (appendix)

Transformation $(x, y) \rightarrow (\xi, \eta)$:

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta}$$
$$\frac{\partial}{\partial y} = \frac{\partial \xi}{\partial y}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y}\frac{\partial}{\partial \eta}$$

$$\Rightarrow \quad \begin{pmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \tag{1}$$

Inverse transformation $(\xi, \eta) \rightarrow (x, y)$:

$$\frac{\partial}{\partial \xi} = \frac{\partial x}{\partial \xi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial \xi}\frac{\partial}{\partial y}$$
$$\frac{\partial}{\partial \eta} = \frac{\partial x}{\partial \eta}\frac{\partial}{\partial x} + \frac{\partial y}{\partial \eta}\frac{\partial}{\partial y}$$

$$\Rightarrow \quad \begin{pmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} \tag{2}$$

To set equations 1 and 2 equal compute the inverse of equation 2:

$$\begin{pmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \tag{3}$$

$$\Leftrightarrow \frac{\begin{pmatrix} y_\eta & -y_\xi \\ -x_\eta & x_\xi \end{pmatrix}}{\begin{vmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{vmatrix}} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \tag{4}$$

$$\Leftrightarrow \frac{1}{J} \begin{pmatrix} y_\eta & -y_\xi \\ -x_\eta & x_\xi \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} \tag{5}$$

Now we can set the matrix in 1 and the matrix in 5 equal, such that

$$\begin{pmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{pmatrix} = \frac{1}{J} \begin{pmatrix} y_\eta & -y_\xi \\ -x_\eta & x_\xi \end{pmatrix} \tag{6}$$

where the so-called Jacobian J is computed by $J = x_\xi y_\eta - x_\eta y_\xi$. Finally, the conversion of each term is given by

$$\xi_x = \frac{1}{J} y_\eta \qquad \xi_y = -\frac{1}{J} x_\eta \tag{7}$$

$$\eta_x = -\frac{1}{J} y_\xi \qquad \eta_y = \frac{1}{J} x_\xi \tag{8}$$