#### Exercise 1

1. Formulate the conservation of mass for a two-dimensional infinitesimal volume as shown in the sketch.



- (a) Formulate the conservation equation in integral form and derive its differential form.
- (b) Formulate the differential equation in a non-conservative form.
- 2. Reformulate the conservative form of the 2-D Euler equations in Cartesian coordinates into a form with the variables  $\vec{V} = (\varrho, \vec{v}, E)^{\top}$  and the substantial derivative  $\frac{D\vec{V}}{Dt}$ .
- 3. Derive the potential equation for compressible flow from the Euler equations under the assumption of steady, isoenergetic, and irrotational flow  $(\vec{\zeta} = 0 \Rightarrow ds = 0$  (Crocco's theorem)  $\Rightarrow \nabla p = \frac{\partial p}{\partial \varrho} \Big|_s \nabla \rho \Rightarrow \nabla p = a^2 \nabla \varrho$ ).

# Exercise 1 (solution)

1. (a) conservation of mass:

$$\int_{\tau} \frac{\partial U_1}{\partial t} d\tau + \oint_A \vec{H}_1 \cdot \vec{n} dA = 0 \quad , \qquad \begin{array}{l} U_1 = \varrho \\ \vec{H}_1 = \varrho \vec{v} = \varrho \begin{pmatrix} u \\ v \end{pmatrix} \end{array}$$

$$y, v \qquad (4) \qquad (4)$$

$$\Rightarrow \int_{\Delta \tau} \frac{\partial \varrho}{\partial t} d\tau + \int_{\Delta x} -\varrho v \, dx + \int_{\Delta y} (\varrho u + \frac{\partial (\varrho u)}{\partial x} \Delta x) dy \\ + \int_{\Delta x} (\varrho v + \frac{\partial (\varrho v)}{\partial y} \Delta y) dx + \int_{\Delta y} -\varrho u \, dy = 0 \\ \lim_{\Delta \tau, \Delta x, \Delta y \to d\tau, dx, dy} \Rightarrow \frac{\partial \varrho}{\partial t} d\tau - \varrho v \, dx + (\varrho u + \frac{\partial (\varrho u)}{\partial x} \Delta x) dy + (\varrho v + \frac{\partial (\varrho v)}{\partial y} \Delta y) dx - \varrho u \, dy = 0 \\ \Leftrightarrow \frac{\partial \varrho}{\partial t} + \frac{\partial (\varrho u)}{\partial x} + \frac{\partial (\varrho v)}{\partial y} = \frac{\partial \varrho}{\partial t} + \nabla \cdot \underbrace{\begin{pmatrix} \varrho u \\ \varrho v \end{pmatrix}}_{\varrho \vec{v}} = 0$$

Alternative solution: use Gauss theorem

$$\begin{split} \oint\limits_{A} \varrho \vec{v} \cdot \vec{n} dA &= \int_{\tau} \operatorname{div}(\varrho \vec{v}) d\tau \\ \Rightarrow \int\limits_{\tau} \frac{\partial \varrho}{\partial t} d\tau + \int_{\tau} \operatorname{div}(\varrho \vec{v}) d\tau = 0 \\ \lim_{\Delta \tau \to d\tau} \quad \Rightarrow \frac{\partial \varrho}{\partial t} + \nabla \cdot \varrho \vec{v} = 0 \end{split}$$

(b) conservative form:  

$$\begin{aligned} & \frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \vec{v}) &= 0 \\ & \Rightarrow & \underbrace{\frac{\partial \varrho}{\partial t} + \vec{v} \cdot \nabla \varrho}_{\text{Substantial/material derivative}} & \underline{p_{\varrho}}_{Dt} \end{aligned} \qquad \Rightarrow \end{aligned}$$

non-conservative form:

$$\frac{D\varrho}{Dt} + \varrho \nabla \cdot \vec{v} = 0$$

$$\varrho_t + (\varrho u)_x + (\varrho v)_y = 0 \quad (\text{mass})$$

$$(\varrho u)_t + (\varrho u^2 + p)_x + (\varrho uv)_y = 0 \quad (x - \text{momentum})$$

$$(\varrho v)_t + (\varrho uv)_x + (\varrho v^2 + p)_y = 0 \quad (y - \text{momentum})$$

$$(\varrho E)_t + (\varrho uE + up)_x + (\varrho vE + vp)_y = 0 \quad (\text{energy})$$

$$\varrho_t + u\varrho_x + v\varrho_y + \varrho(u_x + v_y) = 0 \Leftrightarrow \frac{D\varrho}{Dt} + \varrho\nabla \cdot \vec{v} = 0$$

conservation of mass:

$$\Leftrightarrow \quad \frac{Du}{Dt} + \frac{1}{\varrho} p_x = 0$$

energy equation:

$$\varrho E_t + \varrho u E_x + \varrho v E_y + \underbrace{E \varrho_t + E(\varrho u)_x + E(\varrho v)_y}_{= 0 \quad (\text{mass-conservation eq.})} + (up)_x + (vp)_y = 0$$

$$\Leftrightarrow \quad \frac{DE}{Dt} + \frac{1}{\varrho} \left( (up)_x + (vp)_y \right) = 0$$

3. Derivative of pressure can be transformed to derivative of density:

$$\nabla p = \begin{pmatrix} p_x \\ p_y \end{pmatrix} = \begin{pmatrix} \frac{\partial \varrho}{\partial \varrho} \frac{\partial p}{\partial x} \\ \frac{\partial \varrho}{\partial \varrho} \frac{\partial p}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial p}{\partial \varrho} \frac{\partial \varrho}{\partial x} \\ \frac{\partial p}{\partial \varrho} \frac{\partial \varrho}{\partial y} \end{pmatrix} = \frac{\partial p}{\partial \varrho} \nabla \varrho = a^2 \nabla \varrho \qquad a \text{ is speed of sound}$$

Introduce potential  $\Phi$ :

$$\vec{v} = \nabla \Phi$$
  $u = \Phi_x$ ,  $v = \Phi_y$   $dp = a^2 d\varrho$ 

Euler equations (2–D, steady for Cartesian coordinates) :

$$(\varrho u)_x + (\varrho v)_y = 0$$
  

$$(\varrho u^2 + p)_x + (\varrho uv)_y = 0$$
  

$$(\varrho uv)_x + (\varrho v^2 + p)_y = 0$$

$$\varrho u u_x + \underbrace{u(\varrho u)_x + u(\varrho v)_y}_{= 0} + \varrho v u_y + p_x = 0 \qquad | \cdot u \\ \varrho u v_x + \underbrace{v(\varrho u)_x + v(\varrho v)_y}_{= 0} + \varrho v v_y + p_y = 0 \qquad | \cdot v$$

2.

Replace u and v by potential  $\Phi$ :

$$\begin{array}{rcl} \varrho u^2 \Phi_{xx} + \varrho uv \Phi_{xy} + up_x &= 0 \\ \varrho uv \Phi_{xy} + \varrho v^2 \Phi_{yy} + vp_y &= 0 \end{array} & \left| + \right. \\ u^2 \Phi_{xx} + 2uv \Phi_{xy} + v^2 \Phi_{yy} + \frac{1}{\varrho} (\underbrace{up_x + vp_y}_{(\stackrel{u}{v}) \cdot \nabla p = (\stackrel{u}{v}) \cdot a^2 \nabla \varrho} \right) = 0 \\ \Rightarrow \quad u^2 \Phi_{xx} + 2uv \Phi_{xy} + v^2 \Phi_{yy} + ua^2 \frac{1}{\varrho} \varrho_x + va^2 \frac{1}{\varrho} \varrho_y = 0 \end{array}$$

with the conservation of mass  $u\varrho_x + v\varrho_y = -\varrho u_x - \varrho v_y = -\varrho \Phi_{xx} - \varrho \Phi_{yy}$ potential equation:  $(u^2 - a^2)\Phi_{xx} + 2uv\Phi_{xy} + (v^2 - a^2)\Phi_{yy} = 0$ 

### Exercise 2

- 1. (a) Derive the vorticity transport equation and the Poisson equation for the stream function  $\Psi$  for a two dimensional incompressible and viscous flow.
  - (b) Formulate the boundary conditions for the stream function and the vorticity component at the boundaries of the channel flow domain shown in the sketch.



- 2. Formulate for incompressible flows (without taking into account the energy equation)
  - (a) the Euler equations
    - with the velocity vector  $\vec{v}$  and the pressure p
    - with stream function  $\Psi$  and vorticity component  $\omega$
  - (b) the potential equation
    - with the velocity components u, v (Cauchy–Riemann differential equation)
    - with  $\Phi$
    - with  $\Psi$

Determine for a two-dimensional and steady flow the characteristic lines and the type of the equations.

### Exercise 2 (solution)

1. (a) Navier-Stokes equations 2D, incompressible flow ( $\rho = const \Rightarrow \rho_t = 0$ ):

$$\begin{aligned} u_x + v_y &= 0\\ u_t + uu_x + vu_y + \frac{1}{\rho} p_x &= \nu \nabla^2 u\\ v_t + uv_x + vv_y + \frac{1}{\rho} p_y &= \nu \nabla^2 v \end{aligned}$$

The vorticity transport equation is obtained by taking the curl  $(\nabla \times \vec{f})$  of the momentum equations:  $\frac{\partial}{\partial x}$ (y-momentum equation) -  $\frac{\partial}{\partial y}$ (x-momentum equation)

$$\begin{array}{c} v_{xt} + u_x v_x + u v_{xx} + v_x v_y + v v_{xy} + \frac{1}{\rho} p_{xy} \\ - u_{yt} - u_y u_x - u u_{xy} - v_y u_y - v u_{yy} - \frac{1}{\rho} p_{xy} \end{array} = \nu \begin{array}{c} \nabla^2 (v_x \\ - u_y) \end{array}$$

where the pressure terms fall out:

$$(v_x - u_y)_t + \underbrace{u_x(v_x - u_y) + v_y(v_x - u_y)}_{= 0 \quad \text{(mass-conserv. eq.)}} + v(v_x - u_y)_y + u(v_x - u_y)_x = \nu \nabla^2 (v_x - u_y)$$

With the vorticity component  $\omega = v_x - u_y$ :

$$\omega_t + \underbrace{u\omega_x + v\omega_y}_{\text{convection of vorticity}} = \underbrace{\nu\nabla^2\omega}_{\text{diffusion of vorticity}}$$
$$\Rightarrow \frac{D\omega}{Dt} = \nu\nabla^2\omega$$

which is the vorticity- (or eddy-) transport equation. The Poisson equation for the stream function  $\Psi$  is obtained with  $u = \Psi_y, v = -\Psi_x$ :

$$-\omega = -v_x + u_y = \Psi_{xx} + \Psi_{yy} = \nabla^2 \Psi$$

Finally, we have two coupled partial differential equations for the two variables  $\omega$  and  $\Psi$ , the velocities u and v in the vorticity-transport equation can be replaced by  $u = \Psi_y$  and  $v = -\Psi_x$ .

(b) We have boundary conditions given for u and v, but we need them for  $\omega$  and  $\Psi$ :

#### • In- and outflow boundary:

The velocity profile u(y) is given and we know that  $\Psi_y = \frac{d\Psi}{dy} = u$ , therefore integration of  $d\Psi = u(y)dy$  yields:

$$\Psi_E(y) = \int_{y_{\text{wall}}}^y u_E(y') dy' + \Psi(y_{\text{wall}})$$

where the value at the wall  $\Psi(y_{\text{wall}})$  can be chosen arbitrary as our PDE contains only derivatives of  $\Psi$ . For the vorticity boundary condition we compute the derivatives of u and v:

$$\omega_E = v_x - u_y = -\frac{\partial u_E(y)}{\partial y}$$

#### • Solid wall:

The no slip condition u = v = 0 holds, therefore  $v = \Psi_x = 0 \Rightarrow \Psi_{wall} = const.$ 

From the Poisson function for the stream function  $\Psi_{xx} + \Psi_{yy} = -\omega$  with  $\Psi_{xx} = 0$ :

 $\Rightarrow -\omega_{\text{wall}} = u_y = \Psi_{yy} \text{ and } u_{\text{wall}} = 0 = \Psi_{y,\text{wall}}$ 

Therefore we use a Taylor series expansion for  $y_{\text{wall}}$ :

$$\Psi(y_{\text{wall}} + \Delta y) = \Psi(y_{\text{wall}}) + \underbrace{\Psi_y(y_{\text{wall}})}_{= 0} \Delta y + \Psi_{yy}(y_{\text{wall}}) \frac{\Delta y^2}{2} + \dots$$
  

$$\Rightarrow \Psi_{yy}(y_{\text{wall}}) = 2 \frac{\Psi(y_{\text{wall}} + \Delta y) - \Psi(y_{\text{wall}})}{\Delta y^2}$$
  

$$\Rightarrow \omega(y_{\text{wall}}) = -\Psi_{yy}(y_{\text{wall}}) = -2 \frac{\Psi(y_{\text{wall}} + \Delta y) - \Psi(y_{\text{wall}})}{\Delta y^2}$$

2. (a) Euler equations for incompressible flow  $(\vec{v}, p)$ :

$$\label{eq:varphi} \begin{split} \nabla\cdot\vec{v} &= 0\\ \frac{D\vec{v}}{Dt} + \frac{1}{\rho}\nabla p &= 0 \end{split}$$

characteristic lines (steady 2D flow):

$$\begin{aligned} u_x + v_y &= 0\\ uu_x + vu_y + 1/\rho p_x &= 0 \Leftrightarrow\\ uv_x + vv_y + 1/\rho p_y &= 0 \end{aligned} \qquad \begin{pmatrix} \partial_x & \partial_y & 0\\ u\partial_x + v\partial_y & 0 & \frac{1}{\rho}\partial_x\\ 0 & u\partial_x + v\partial_y & \frac{1}{\rho}\partial_y \end{pmatrix} \begin{pmatrix} u\\ v\\ p \end{pmatrix} = 0 \end{aligned}$$

Use chain rule of PDE  $(u_x = u_\Omega \Omega_x + u_S S_x)$  to transform PDE to

$$\underbrace{\begin{pmatrix} \Omega_x & \Omega_y & 0\\ u\Omega_x + v\Omega_y & 0 & \frac{1}{\rho}\Omega_x\\ 0 & u\Omega_x + v\Omega_y & \frac{1}{\rho}\Omega_y \end{pmatrix} \begin{pmatrix} u_\Omega\\ v_\Omega\\ p_\Omega \end{pmatrix}}_{\text{crosswise derivative}} + \begin{pmatrix} S_x & S_y & 0\\ uS_x + vS_y & 0 & \frac{1}{\rho}S_x\\ 0 & uS_x + vS_y & \frac{1}{\rho}S_y \end{pmatrix} \begin{pmatrix} u_S\\ v_S\\ p_S \end{pmatrix} = 0$$

We need the determinant of the coefficients matrix of the crosswise derivatives to be zero:

$$\begin{vmatrix} \Omega_x & \Omega_y & 0\\ u\Omega_x + v\Omega_y & 0 & \frac{1}{\rho}\Omega_x\\ 0 & u\Omega_x + v\Omega_y & \frac{1}{\rho}\Omega_y \end{vmatrix} = 0 = -(u\Omega_x + v\Omega_y)\frac{1}{\rho}\Omega_x^2 - (u\Omega_x + v\Omega_y)\frac{1}{\rho}\Omega_y^2$$
$$\Leftrightarrow (u\frac{\Omega_x}{\Omega_y} + v)(\frac{\Omega_x^2}{\Omega_y^2} + 1) = 0 \Rightarrow \frac{dy}{dx} = -\frac{\Omega_x}{\Omega_y} = \frac{v}{u} \quad \text{or} \quad \frac{\Omega_x}{\Omega_y} = \pm\sqrt{-1}$$

i. e. 1 real, 2 imaginary characteristic lines  $\Rightarrow$  mixed hyperbolic elliptic type

Euler equations (2D) 
$$\Psi, \omega$$
:  

$$\nabla^2 \Psi = -\omega$$

$$\frac{D\omega}{Dt} = 0$$

characteristic lines (steady flow):

$$\begin{aligned}
\Psi_{xx} + \Psi_{yy} &= -\omega \\
u\omega_x + v\omega_y &= 0
\end{aligned} \Leftrightarrow \left(\begin{array}{cc} \partial_{xx} + \partial_{yy} & 1 \\
0 & u\partial_x + v\partial_y \end{array}\right) \left(\begin{array}{c} \Psi \\
\omega \end{array}\right) = 0
\end{aligned}$$

to solve:

$$\begin{vmatrix} \Omega_x^2 + \Omega_y^2 & 0\\ 0 & u\Omega_x + v\Omega_y \end{vmatrix} = 0 = (u\Omega_x + v\Omega_y)(\Omega_x^2 + \Omega_y^2)$$

 $\Rightarrow$  see Euler equations  $(\vec{v},p)$ 

(b) Euler equations (incompressible, 2D, irrotational:  $\omega = 0$ ):  $(\Psi_y = u, \Psi_x = -v, \Phi_x = u, \Phi_y = v)$ 

$$\nabla^2 \Phi = \Phi_{xx} + \Phi_{yy} = 0 \qquad \text{Potential formulation} \quad \vec{v} = \nabla \Phi$$
$$\nabla^2 \Psi = \Psi_{xx} + \Psi_{yy} = 0 \qquad \text{Stream function formulation}$$

for which the characteristic slopes are computed by

$$Q = \Omega_x^2 + \Omega_y^2 = 0 \Rightarrow \frac{dy}{dx} = \frac{-\Omega_x}{\Omega_y} = \pm \sqrt{-1}$$

which results in two imaginary lines  $\Rightarrow$  the PDE is of elliptic type.

Either of the above second-order PDEs can be transformed to a system of two first-order PDEs:

$$\begin{aligned} u_x + v_y &= 0\\ v_x - u_y &= 0 \end{aligned}$$

which in this case are known as the Cauchy-Riemann differential equation, to compute the characteristic lines solve:

$$\begin{vmatrix} \Omega_x & \Omega_y \\ -\Omega_y & \Omega_x \end{vmatrix} = 0 \Rightarrow \Omega_x^2 + \Omega_y^2 = 0 \Leftrightarrow \frac{dy}{dx} = -\frac{\Omega_x}{\Omega_y} = \pm \sqrt{-1}$$

i. e. 2 imaginary characteristic lines  $\Rightarrow$  elliptic type (same results as above)

### Exercise 3

1. Consider the non-linear, hyperbolic partial differential equation

$$u_t + uu_x = 0$$

- (a) Determine the characteristic line and the characteristic solution.
- (b) The following initial condition is given:

$$u(x, t = 0) = \begin{cases} 0 & \text{for} \quad x \le 0\\ x & \text{for} \quad 0 < x \le 1\\ 1 & \text{for} \quad x > 1 \end{cases}$$

Determine the solution for the time levels  $t=\frac{1}{2}$  and t=1 in the (x,t)-diagram



#### Exercise 3 (solution)

1. (a) PDE:  $u_t + uu_x = 0$ : Use coordinate transformation

$$u_x = u_\Omega \Omega_x + u_S S_x$$
$$u_t = u_\Omega \Omega_t + u_S S_t$$

and fill into PDE:

$$u_{\Omega}\Omega_{t} + u_{S}S_{t} + u(u_{\Omega}\Omega_{x}u_{S}S_{x}) = 0$$
  
$$\Rightarrow \underbrace{(\Omega_{t} + u\Omega_{x})}_{=Q}u_{\Omega} + (S_{t} + uS_{x})u_{S} = 0$$

Set Q = 0 for the cross-wise derivative  $u_{\Omega}$  to be undetermined and determine the slope of the characteristic line:

$$Q = \Omega_t + u\Omega_x = 0 \Leftrightarrow \frac{-\Omega_t}{\Omega_x} = \frac{dx}{dt} = u$$

When assuming u = const. for the slope of the characteristic line, integration from  $x_0$ ,  $t_0$  yields the characteristic line C:

C: 
$$x - x_0 = u (t - t_0)$$
 or  $t = t_0 + \frac{x - x_0}{u}$ 

The characteristic solution is obtained by transforming the PDE from (x, y) to  $(\tau, \xi)$ :  $d\tau = dt$ ,  $d\xi = dx - udt$ :

$$u_t = \xi_t u_{\xi} + \tau_t u_{\tau} = -u u_{\xi} + u_{\tau}$$
$$u_x = \xi_x u_{\xi} + \tau_x u_{\tau} = u_{\xi}$$

apply to PDE  $\Rightarrow$ 

$$-uu_{\xi} + u_{\tau} + uu_{\xi} = u_{\tau} = 0$$

That is, the value of u will be constant in time **on** each individual characteristic curve due to the absence of any source/sink terms in the original PDE. Integration over  $\tau$  with  $\xi = x - ut = const. \Rightarrow$ 

$$u(\tau,\xi) = c(\xi)$$

With the initial condition  $u_0(x_0, t_0)$  on the characteristic line  $\xi = \xi_0 = x_0 - ut_0$ :

$$u(x,t) = u_0(x_0,t_0)$$

i.e. the solution remains constant on the characteristic line.

The general transformation  $(x, y) \rightarrow (\xi, \tau)$  yields an result independent in u, therefore the assumption u = const. for the first integration of the slope of the characteristic line is valid, as long as it does not cross other characteristic lines. In this case the nonlinearity would result in a new slope.

(b) graphical solution, e.g. for time level t = 1:



### Exercise 3 Appendix

Given is the PDE  $\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u}{\partial x} = 1.$ 

- 1. Determine the characteristic slope and the characteristic solution.
- 2. Determine the solution at time level t = 1 for the initial condition  $u(t = 0, x) = sin(\pi x)$ .

$$u_t + \frac{1}{2}u_x = 1$$
  
$$\Rightarrow \Omega_t + \frac{1}{2}\Omega_x = 0$$
  
$$\Rightarrow -\frac{\Omega_t}{\Omega_x} = \frac{dx}{dt}|_c = \frac{1}{2}$$

$$d\xi = 2dx - dt \qquad d\tau = dt$$
$$u_x = u_{\xi} \cdot 2 \qquad u_t = u_{\xi} \cdot (-1) + u_{\tau}$$

$$\Rightarrow -u_{\xi} + u_{\tau} + \frac{1}{2} \cdot 2u_{\xi} = 1$$
$$\Rightarrow u_{\tau} = 1$$
$$\Rightarrow u(\xi, \tau) = \tau + c(\xi)$$

b)

a)

$$u\left(t=0,x\right)=\sin\left(\pi x\right)$$

 $t = \tau$ :

$$\Rightarrow u (\tau = 0, \xi) = \sin\left(\frac{\pi}{2}\xi\right) \qquad \xi = 2x - t$$
$$= c (\xi)$$
$$\Rightarrow u (\xi, \tau) = \tau + \sin\left(\frac{\pi}{2}\xi\right)$$
$$\Rightarrow u (x, t) = t + \sin\left(\pi\left(x - \frac{1}{2}t\right)\right)$$
$$u (x, t = 1) = 1 + \sin\left(\pi\left(x - \frac{1}{2}t\right)\right)$$

t = 1

#### Exercise 4

1. The vorticity transport equation for unsteady one-dimensional flow is given:

$$\omega_t + u\omega_x = \nu\omega_{xx}$$

The viscosity  $\nu$  ( $\nu > 0$ ) and the velocity u = u(x, t) are assumed to be known. The equation should discretised for constant time and spatial steps  $\Delta t, \Delta x$ :

 $x_i = i\Delta x, \quad t^n = n\Delta t, \quad \omega(x_i, t^n) = \omega_i^n$ 

- (a) Determine with the help of Taylor series:
  - $\omega_t$  for  $t^n$ , resp.  $t^{n+1}$  (forward, resp. backward difference)
  - $\omega_x$  and  $\omega_{xx}$  around  $x_i$  (central differences)
- (b) Formulate an explicit and an implicit solution scheme for the PDE and check the consistency.

### Exercise 4 (solution)

#### 1. (a) Discretisation of the time derivative:

Formulate Taylor series expansion for  $\omega^{n+1}$  around  $\omega^{n}$ :

$$\omega_i^{n+1} = \omega_i^n + \omega_t |_i^n \Delta t + \omega_{tt} |_i^n \frac{\Delta t^2}{2!} + \dots$$

and reformulate to get forward difference:

$$\omega_t |_i^n = \frac{\omega_i^{n+1} - \omega_i^n}{\Delta t} - \omega_{tt} |_i^n \frac{\Delta t}{2} + \dots$$

Formulate Taylor series expansion for  $\omega^{\mathbf{n}}$  around  $\omega^{\mathbf{n+1}}$ :

$$\omega_{i}^{n} = \omega_{i}^{n+1} - \omega_{t}|_{i}^{n+1} \Delta t + \omega_{tt}|_{i}^{n+1} \frac{\Delta t^{2}}{2!} + \dots$$

and reformulate to get **backward difference**:

$$\omega_t|_i^{n+1} = \frac{\omega_i^{n+1} - \omega_i^n}{\Delta t} + \omega_{tt}|_i^{n+1} \frac{\Delta t}{2} + \dots$$

#### Discretisation of the spatial derivative:

Formulate Taylor series expansion for  $\omega_{i+1}$  and  $\omega_{i-1}$  around  $\omega_i$ :

$$\omega_{i\pm 1}^n = \omega_i^n \pm \omega_x |_i^n \Delta x + \omega_{xx} |_i^n \frac{\Delta x^2}{2!} \pm \omega_{xxx} |_i^n \frac{\Delta x^3}{3!} + \omega_{xxxx} |_i^n \frac{\Delta x^4}{4!} + \dots$$

Subtract  $\omega_{i-1}^n$  from  $\omega_{i+1}^n$  to get finite difference expression for  $\omega_x$ :

$$\omega_{x}|_{i}^{n} = \frac{\omega_{i+1}^{n} - \omega_{i-1}^{n}}{2\,\Delta x} - \omega_{xxx}|_{i}^{n}\frac{\Delta x^{2}}{6} + \dots$$

Add  $\omega_{i+1}^n$  and  $\omega_{i-1}^n$  to get finite difference expression for  $\omega_{xx}$ :

$$\omega_{xx}|_{i}^{n} = \frac{\omega_{i+1}^{n} - 2\omega_{i}^{n} + \omega_{i-1}^{n}}{\Delta x^{2}} - \omega_{xxxx}|_{i}^{n} \frac{\Delta x^{2}}{12} + \dots$$

#### (b) • Explicit solution scheme:

$$\underbrace{\frac{\omega_i^{n+1} - \omega_i^n}{\Delta t}}_{\text{forward} \quad \omega_t} + u_i^n \underbrace{\frac{\omega_{i+1}^n - \omega_{i-1}^n}{2\,\Delta x}}_{\text{central} \quad \omega_x} - \nu \underbrace{\frac{\omega_{i+1}^n - 2\omega_i^n + \omega_{i-1}^n}{\Delta x^2}}_{\text{central} \quad \omega_{xx}} = 0$$

Explicit, since only one term  $\omega_i^{n+1}$  is defined at the highest time level (n+1), thus the equation can be explicitly solved.

$$\Rightarrow \quad \omega_i^{n+1} = f_i(\omega^n, u^n, \nu, \Delta t, \Delta x)$$

truncation error

$$\tau = L(\omega) - L_{\Delta}(\omega)$$
  
=  $-\omega_{tt}|_{i}^{n} \frac{\Delta t}{2} - u \,\omega_{xxx}|_{i}^{n} \frac{\Delta x^{2}}{6} + \nu \,\omega_{xxxx}|_{i}^{n} \frac{\Delta x^{2}}{12} + \text{terms of higher order}$   
=  $\mathcal{O}(\Delta t, \Delta x^{2})$  consistent, since  $\lim_{\Delta t, \Delta x \to 0} \tau = 0$ 

#### • Implicit solution scheme:

$$\underbrace{\frac{\omega_i^{n+1} - \omega_i^n}{\Delta t}}_{\text{backward } \omega_t} + u_i^{n+1} \underbrace{\frac{\omega_{i+1}^{n+1} - \omega_{i-1}^{n+1}}{2\Delta x}}_{\text{central } \omega_x} - \nu \underbrace{\frac{\omega_{i+1}^{n+1} - 2\omega_i^{n+1} + \omega_{i-1}^{n+1}}{\Delta x^2}}_{\text{central } \omega_{xx}} = 0$$

Several terms  $\omega_i^{n+1}$ ,  $\omega_{i-1}^{n+1}$ , and  $\omega_{i+1}^{n+1}$  are defined at the highest time level (n+1), therefore the equation can not be explicitly solved. The unknowns at the highest time level are implicitly coupled and build a tridiagonal system of equations:

$$\Rightarrow \text{ tridiagonal system of equations} \qquad a_i \omega_{i-1}^{n+1} + b_i \omega_i^{n+1} + c_i \omega_{i+1}^{n+1} = f_i(\omega^n, u^n, \nu, \Delta t, \Delta x)$$

truncation error

$$\tau = \omega_{tt} |_{i}^{n+1} \frac{\Delta t}{2} - u \,\omega_{xxx} |_{i}^{n+1} \frac{\Delta x^{2}}{6} + \nu \,\omega_{xxxx} |_{i}^{n+1} \frac{\Delta x^{2}}{12} + \text{ terms of higher order} = \mathcal{O}(\Delta t, \Delta x^{2}) \qquad \text{consistent, since } \lim_{\Delta t, \Delta x \to 0} \tau = 0$$

### Exercise 5

1. The heat conduction equation is given:

$$T_t = \alpha T_{xx}, \quad \alpha = const. > 0$$

The equation is discretised with a 3-time level scheme (Dufort-Frankel scheme):

$$L_{\Delta}(T) = \frac{T_i^{n+1} - T_i^{n-1}}{2\Delta t} - \alpha \frac{T_{i+1}^n - (T_i^{n+1} + T_i^{n-1}) + T_{i-1}^n}{\Delta x^2} = 0$$

Check the consistency of this scheme.

- 2. Discretise the above equation with an explicit scheme. Check the stability of this scheme with
  - (a) the discrete perturbation theory.
  - (b) the help of a periodical test function,

$$T(x,t) = V(t) \cos(kx)$$
 resp.  $T_i^n = V^n \cos(\Theta i)$ 

with  $t = n\Delta t$ ,  $x = i\Delta x$ ,  $\Theta = k\Delta x$ , by analysing, whether the amplitude V(t) is in- or decreasing with the time level.

<u>advice:</u>  $cos(\alpha \pm \beta) = cos\alpha \ cos\beta \mp sin\alpha \ sin\beta$ 

### Exercise 5 (solution)

1. We are given a finite difference equation without the truncation error, it can be determined by developing Taylor series for time level "n" and location "i"

$$T^{n\pm 1} = T^n \pm T^n_t \Delta t + T^n_{tt} \frac{\Delta t^2}{2} \pm T^n_{ttt} \frac{\Delta t^3}{6} + \text{terms of higher order}$$

$$\implies \frac{T^{n+1} - T^{n-1}}{2\Delta t} = T^n_t + T^n_{ttt} \frac{\Delta t^2}{6} + \text{tho}$$

$$T^{n+1} + T^{n-1} = 2T^n + 2T^n_{tt} \frac{\Delta t^2}{2} + \text{tho}$$

apply in  $L_{\Delta}(T)$ :

$$T_{ti}^{n} + T_{ttti}^{n} \frac{\Delta t^{2}}{6} + \dots - \alpha \left( \underbrace{\frac{T_{i+1}^{n} - 2T_{i}^{n} + T_{i-1}^{n}}{\Delta x^{2}}}_{= T_{xxi} + T_{xxxxi} \frac{\Delta x^{2}}{12} + \dots} - T_{tti}^{n} \frac{\Delta t^{2}}{\Delta x^{2}} + \dots \right) = 0$$

The truncation error of the spatial discretization  $T_{xxi} + T_{xxxi}\frac{\Delta x^2}{12} + \ldots$  can be either determined by knowledge (second-order accurate approximation of second-order derivative, see script pp. 3-3) or also via spatial Taylor series expansions. Finally, the **original PDE** (left hand side) and the **truncation error** (right hand side) is

recovered 
$$\Longrightarrow$$
  $(T_t - \alpha T_{xx})_i^n = \underbrace{-T_{ttt} \frac{\Delta t^2}{6} + \alpha T_{xxxx} \frac{\Delta x^2}{12} - \alpha T_{tt} \frac{\Delta t^2}{\Delta x^2} + \text{tho}}_{\tau}$ 

which together is the **modified PDE**.

consistency:

$$\lim_{\Delta x, \Delta t \to 0} \tau = 0 ? \qquad \text{only fulfilled, if } \lim_{\Delta x, \Delta t \to 0} \frac{\Delta t^2}{\Delta x^2} = 0$$

i.e.  $\Delta t$  has to vanish faster than  $\Delta x$ 

- for finite  $\Delta x$ ,  $\Delta t$  choose:  $\frac{\Delta t}{\Delta x} \ll 1$ , e.g.  $\frac{\Delta t}{\Delta x} = O(\Delta x)$
- irrelevant for steady solution, since in this case  $T_t = T_{tt} = \ldots = 0$

2. discretisation:

$$\delta_t T = \frac{T_i^{n+1} - T_i^n}{\Delta t} \qquad \qquad \delta_{xx} T = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

explicit scheme:

$$T_i^{n+1} = T_i^n + \sigma \left( T_{i+1}^n - 2T_i^n + T_{i-1}^n \right) \qquad \text{with} \quad \sigma = \frac{\alpha \Delta t}{\Delta x^2}$$

(a) **Discrete perturbation theory:** For linear equations a perturbation  $\varepsilon$  (error) satisfies the same difference equation as the solution, therefore

$$\varepsilon_i^{n+1} = \sigma \varepsilon_{i-1}^n + (1-2\sigma)\varepsilon_i^n + \sigma \varepsilon_{i+1}^n \quad \text{mit} \quad \sigma = \nu \frac{\Delta t}{\Delta x^2}$$
 (\*)

The analysis of the error behaviour yields the following results:



• Time step n = 1 compute solution of equation \* with values from n = 0:

$$\begin{split} \varepsilon_{is}^{1} &= \sigma \varepsilon_{is-1}^{0} + (1-2\sigma) \varepsilon_{is}^{0} + \sigma \varepsilon_{is+1}^{0} = (1-2\sigma) \varepsilon \\ \varepsilon_{is+1}^{1} &= \sigma \varepsilon_{is}^{0} + (1-2\sigma) \varepsilon_{is+1}^{0} + \sigma \varepsilon_{is+2}^{0} = \sigma \varepsilon \\ \varepsilon_{is-1}^{1} &= \sigma \varepsilon_{is-2}^{0} + (1-2\sigma) \varepsilon_{is-1}^{0} + \sigma \varepsilon_{is}^{0} = \sigma \varepsilon \end{split}$$

solution at all other points i < is - 1 and i > is + 1 is zero. from  $\frac{\max|\varepsilon^1|}{\max|\varepsilon^0|} \le 1$  folgt  $|\sigma| \le 1$  bzw.  $|1 - 2\sigma| \le 1$  $\rightarrow 0 < \sigma \le 1$ 

Repeat procedure for following time steps (see script, p. 3-8ff), for  $n \to \infty$  the asymptotical stability limit is  $0 < \sigma \leq 1/2$ .

#### (a) von Neumann stability analysis:

A periodic error function

$$T_{i,j}^{n} = V^{n} \cdot e^{Ik_{x}x}$$
$$= V^{n} \cdot e^{Ik_{x}i\Delta x}$$
$$= V^{n} \cdot e^{I\Theta i}$$

is applied to the original PDE

$$T_i^{n+1} = T_i^n + \sigma \left( T_{i+1}^n - 2T_i^n + T_{i-1}^n \right)$$

such that

$$V^{n+1}e^{I\Theta i} = V^n e^{I\Theta i} + \sigma \left( V^n e^{I\Theta(i+1)} - 2V^n e^{I\Theta i} + V^n e^{I\Theta(i-1)} \right)$$

divide by  $V^n e^{I\Theta i}$ 

$$\frac{V^{n+1}}{V^n} = 1 + \sigma \left( e^{I\Theta} - 2 + e^{-I\Theta} \right)$$

use  $e^{\pm I\Theta} = \cos(\Theta) \pm I \sin(\Theta)$  and  $G = \frac{V^{n+1}}{V^n}$ 

$$G = 1 + \sigma \left( \cos(\Theta) + I \sin(\Theta) - 2 + \cos(\Theta) - I \sin(\Theta) \right)$$
  

$$G = 1 - 2\sigma \left( 1 - \cos(\Theta) \right)$$

stable, if  $|G| \le 1 \rightarrow -1 \le G \le 1$  for  $-\pi \le \Theta \le \pi$ 

$$\implies \sigma \leq \frac{1}{2}$$
 resp.  $\Delta t \leq \frac{\Delta x^2}{2\alpha}$ 

### Exercise 6

1. For the convection equation

$$u_t + a u_x = 0, \quad a = const. \neq 0$$

the following general scheme will be used:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\left(1 - \Theta\right)\delta_x u_i^n + a\Theta\,\delta_x u_i^{n+1} = 0$$

where  $\delta_x u_i = \frac{u_{i+1} - u_{i-1}}{2\Delta x}$  and  $0 \le \Theta \le 1$  ( $\Theta = 0$ : explicit scheme,  $\Theta = 1$ : implicit

scheme).

- (a) Show with the help of the analysis of Hirt for which values of the parameter  $\Theta$  the scheme above will be stable.
- (b) Check the result with the von Neumann analysis.

### Exercise 6 (solution)

#### 1. (a) Hirt's analysis:

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + a\left(1 - \Theta\right)\delta_x u_i^n + a\Theta\,\delta_x u_i^{n+1} = 0$$

with

$$\delta_x u_i = \frac{u_{i+1} - u_{i-1}}{2\,\Delta x}$$

becomes

$$\Rightarrow \frac{u_i^{n+1} - u_i^n}{\Delta t} + a \left(1 - \Theta\right) \frac{u_{i+1}^n - u_{i-1}^n}{2 \,\Delta x} + a \,\Theta \, \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2 \,\Delta x} = 0$$

To recover the truncation error formulate a Taylor series expansion for the variable u:

$$u_{i}^{n+1} = u_{i}^{n} + u_{t}|_{i}^{n}\Delta t + u_{tt}|_{i}^{n}\frac{\Delta t^{2}}{2} + u_{ttt}|_{i}^{n}\frac{\Delta t^{3}}{6} + \dots$$
$$u_{i\pm1}^{n} = u_{i}^{n} \pm u_{x}|_{i}^{n}\Delta x + u_{xx}|_{i}^{n}\frac{\Delta x^{2}}{2} + u_{xxx}|_{i}^{n}\frac{\Delta x^{3}}{6} + \dots$$

and rearrange to get expressions for finite difference expressions:

$$\frac{u^{n+1} - u^n}{\Delta t} = u^n_t + \frac{\Delta t}{2} u^n_{tt} + \frac{\Delta t^2}{6} u^n_{ttt} + \cdots$$

$$\frac{u^n_{i+1} - u^n_{i-1}}{2\Delta x} = u^n_x + \frac{\Delta x^2}{6} u^n_{xxx} + \cdots$$

$$\frac{u^{n+1}_{i+1} - u^{n+1}_{i-1}}{2\Delta x} = u^{n+1}_x + \frac{\Delta x^2}{6} u^{n+1}_{xxx} + \cdots$$

$$= \underbrace{u^n_x + \Delta t u^n_{xt} + \frac{\Delta t^2}{2} u^n_{xtt}}_{xtt} + \cdots + O(\Delta x^2)$$

temporal Taylor series expansion for  $u_x^{n+1}$ 

follows

$$u_t^n + \frac{\Delta t}{2} u_{tt}^n + a \left( (1 - \Theta) u_x^n + \Theta \left( u_x^n + \Delta t u_{xt}^n \right) \right) + O(\Delta x^2, \Delta t^2) = 0$$
  
$$\implies u_t^n + a u_x + \frac{\Delta t}{2} u_{tt}^n + a \Theta \Delta t u_{xt}^n + O(\Delta x^2, \Delta t^2) = 0$$

Index n for the time layer will be omitted:

$$\implies u_t + au_x = -\frac{\Delta t}{2}u_{tt} - a\Theta\Delta tu_{xt} + O(\Delta x^2, \Delta t^2),$$

which is the **modified PDE**. Using the original PDE  $u_t + au_x = 0$ :

$$\implies u_{tt} = -au_{xt}, \qquad u_{tx} = -au_{xx}, \qquad u_{tt} = a^2 u_{xx}$$

we can transform temporal derivatives to spatial ones:

$$\iff u_t + au_x = \underbrace{a^2 \Delta t(\Theta - \frac{1}{2})}_{\text{numerical viscosity}} u_{xx} + O(\Delta x^2, \Delta t^2)$$

from the condition, that only a positive (numerical) viscosity has a damping or stabilizing effect, it follows:

$$\frac{1}{2} \le \Theta \le 1$$

#### (b) von Neumann analysis:

Approach for the error function  $\epsilon$ :

$$\epsilon_i^n = \sum_{\phi = -\pi}^{\phi = \pi} V^n(\Phi) e^{i\Phi I} , \quad \Phi = \frac{2\pi\Delta x}{\lambda} , \quad t = n\Delta t , \quad I = \sqrt{-1}$$

Inserting the approach into the finite difference equation, omitting the sums and requiring the equation is satisfied for every discrete wave angle  $\Phi$  (see script, p. 3-10 to 3-12) yields:

$$\frac{V^{n+1}e^{i\Phi I} - V^{n}e^{i\Phi I}}{\Delta t} + a(1-\Theta)\frac{V^{n}\left(e^{(i+1)\Phi I} - e^{(i-1)\Phi I}\right)}{2\Delta x} + a\Theta\frac{V^{n+1}\left(e^{(i+1)\Phi I} - e^{(i-1)\Phi I}\right)}{2\Delta x} = 0$$
$$\iff \frac{\frac{V^{n+1}}{V^{n}} - 1}{\Delta t} + a(1-\Theta)\frac{\left(e^{\Phi I} - e^{-\Phi I}\right)}{2\Delta x} + a\Theta\frac{V^{n+1}}{V^{n}}\frac{\left(e^{\Phi I} - e^{-\Phi I}\right)}{2\Delta x} = 0$$

with  $e^{\Phi I} = \cos(\Phi) + I\sin(\Phi)$  one receives a term for the amplification factor G:

$$\iff G = \frac{V^{n+1}}{V^n} = \frac{1 - (1 - \Theta)a\frac{\Delta t}{\Delta x}Isin(\Phi)}{1 + \Theta a\frac{\Delta t}{\Delta x}Isin(\Phi)}$$

The absolute value of a complex number is  $\left|\frac{a+b*I}{c+d*I}\right| = \sqrt{\frac{a^2+b^2}{c^2+d^2}}$ :

$$\implies |G|^2 = \frac{1 + (1 - 2\Theta + \Theta^2) \left(a\frac{\Delta t}{\Delta x}sin(\Phi)\right)^2}{1 + \left(\Theta a\frac{\Delta t}{\Delta x}sin(\Phi)\right)^2}$$

for a stable difference scheme it is required that:  $|G|^2 \leq 1$  for  $-\pi \leq \Phi \leq \pi$ :

$$(1 - 2\Theta)\sin^2(\Phi) \le 0$$

according to the problem is  $\Theta \leq 1$ :

$$\Longrightarrow \frac{1}{2} \le \Theta \le 1$$

### Exercise 7

1. Given is the PDE (convection-diffusion equation):

$$L(u) = u_t + a u_x - \nu u_{xx} = 0$$
 with  $a = const., \quad \nu = const. \ge 0$ 

Check the convergence of the following generalised difference scheme with central differences:

$$L_{\Delta}(u) = \frac{u_i^{n+1} - u_i^n}{\Delta t} + (1 - \Theta)Res_{\Delta}(u^n) + \Theta Res_{\Delta}(u^{n+1}) = 0$$

with  $Res_{\Delta}(u) = \frac{a}{2\Delta x} (u_{i+1} - u_{i-1}) - \frac{\nu}{\Delta x^2} (u_{i+1} - 2u_i + u_{i-1})$ 

and the discretisation factor  $\Theta$ :

$$\Theta = 0 \quad \text{explicit scheme } \mathcal{O}(\Delta t, \Delta x^2) \qquad \qquad \stackrel{n+1}{\underset{\text{(Crank-Nicholson)}}{}} \qquad \qquad \stackrel{n+1}{\underset{\text{(Crank-nicholson)}}{} \qquad \quad \stackrel{n+1}{\underset{\text{(Crank-nicholson)}}{} \qquad \quad \stackrel{n+1}{\underset{\text{(Crank-nicholson)}}{}} \qquad \quad \stackrel{n+1}{\underset{\text{(Crank-nicholson)}}{} \qquad \quad \stackrel{n+1}{\underset{\text{(Crank-nicholson)}}$$

Check with the general solution for  $L_{\Delta}(u)$  the special cases  $\Theta = 0, \frac{1}{2}, 1$  and the

convection-diffusion equation	:	$a \neq 0$	$\nu \neq 0$
convection equation	:	$a \neq 0$	$\nu = 0$
diffusion equation	:	a = 0	$\nu \neq 0$

### Exercise 7 (solution)

1. (a) From Lax's theorem the convergence of a finite difference equation for an initial value problem requires consistency and stability.

consistency (see as well exercise 4):

separate checking time and space using Taylor series expansion in x- and t-direction:

$$\begin{aligned} t: & \frac{u^{n+1}-u^n}{\Delta t} &= u_t |^n + \frac{\Delta t}{2} u_{tt} |^n + \frac{\Delta t^2}{6} u_{ttt} |^n + \dots \\ x: & Res_{\Delta}(u) &= au_x |_i - \nu u_{xx} |_i + a(\frac{\Delta x^2}{6} u_{xxx} |_i + \dots) - \nu(\frac{\Delta x^2}{12} u_{xxxx} |_i + \dots) \\ &= Res(u) + \mathcal{O}(\Delta x^2) \\ t: & Res_{\Delta}(u^{n+1}) &= Res_{\Delta}(u^n) + (Res_{\Delta}(u^n))_t |^n \Delta t + (Res_{\Delta}(u^n))_{tt} |^n \frac{\Delta t^2}{2} + \dots \\ &= Res(u^n) + (Res(u^n))_t |^n \Delta t + \mathcal{O}(\Delta t^2, \Delta x^2) \\ \text{apply to the difference scheme (with  $u_t = -Res(u) \iff u_{tt} = -(Res(u))_t$ ):  $u_t + Res(u) &= (\Theta - \frac{1}{2}) \Delta t u_{tt} + \mathcal{O}(\Delta t^2, \Delta x^2) \implies \text{consistent for } \Delta x, \Delta t \to 0 \end{aligned}$$$

$$u_t + Res(u) = (\Theta - \frac{1}{2})\Delta t u_{tt} + \mathcal{O}(\Delta t^2, \Delta x^2) \implies \text{consistent for } \Delta x, \Delta t \rightarrow 0$$

accuracy: 
$$\mathcal{O}(\Delta t, \Delta x^2), \text{ if } \Theta \neq \frac{1}{2}$$
  
 $\mathcal{O}(\Delta t^2, \Delta x^2), \text{ if } \Theta = \frac{1}{2}$ 

stability: von Neumann analysis (approach see exercise 6):

$$\frac{V^{n+1}e^{i\Phi I} - V^{n}e^{i\Phi I}}{\Delta t} + (1-\Theta)V^{n}\left(\frac{a}{2\Delta x}\left(e^{(i+1)\Phi I} - e^{(i-1)\Phi I}\right) - \frac{\nu}{\Delta x^{2}}\left(e^{(i+1)\Phi I} - 2e^{i\Phi I} + e^{(i-1)\Phi I}\right)\right) + \Theta V^{n+1}\left(\frac{a}{2\Delta x}\left(e^{(i+1)\Phi I} - e^{(i-1)\Phi I}\right) - \frac{\nu}{\Delta x^{2}}\left(e^{(i+1)\Phi I} - 2e^{i\Phi I} + e^{(i-1)\Phi I}\right)\right) = 0$$

with  $c = \frac{a\Delta t}{\Delta x}$  and  $\sigma = \frac{\nu\Delta t}{\Delta x^2}$  follows:

$$G = \frac{V^{n+1}}{V^n} = \frac{1 - (1 - \Theta)(2\sigma(1 - \cos(\Phi)) + cI\sin(\Phi))}{1 + \Theta(2\sigma(1 - \cos(\Phi)) + cI\sin(\Phi))}$$

stability condition:

$$\implies |G|^{2} = \frac{(1 - (1 - \Theta)2\sigma(1 - \cos(\Phi)))^{2} + ((1 - \Theta)c\sin(\Phi))^{2}}{(1 + \Theta 2\sigma(1 - \cos(\Phi)))^{2} + (\Theta c\sin(\Phi))^{2}} \le 1$$
  
$$\iff (1 - 2\Theta)\underbrace{(4\sigma^{2}(1 - \cos(\Phi))^{2} + c^{2}\sin^{2}(\Phi))}_{\ge 0} - \underbrace{4\sigma(1 - \cos(\Phi))}_{\ge 0} \le 0$$

 $\implies$  scheme is unconditionally stable for  $\Theta \geq \frac{1}{2}$ 

 $\underbrace{ \text{analysis for } 0 \le \Theta < \frac{1}{2} : }_{\text{with } \sin^2(\Phi) = 1 - \cos^2(\Phi) = (1 + \cos(\Phi))(1 - \cos(\Phi)) : }_{\ge 0}$  $\Longrightarrow \underbrace{(1 - 2\Theta)(c^2 + 4\sigma^2)}_{\ge 0} + \underbrace{(1 - 2\Theta)}_{>0}(c^2 - 4\sigma^2)\cos(\Phi) - \underbrace{4\sigma}_{\ge 0} \le 0$ 

for  $c^2 - 4\sigma^2 > 0$  is  $\cos(\Phi) = 1$  the adverse case:

$$\implies (1 - 2\Theta)c^2 \le 2\sigma$$

for  $c^2 - 4\sigma^2 \le 0$  is  $\cos(\Phi) = -1$  the adverse case:

$$\implies (1 - 2\Theta)\sigma \le \frac{1}{2}$$

the outcome of this is the following stability range: stability range for  $0 \le \Theta \le 1$ 



summary:

From consistency and stability follows convergence (theorem of Lax).

- consistency of the difference approximation is obtained for all parameters  $(\Theta, \nu, a)$
- stability is obtained

 $\star \ \frac{1}{2} \leq \Theta \leq 1$  for all values of  $(\nu,a)$ 

 $\star 0 \le \Theta < \frac{1}{2}$  see diagram

• instability is obtained for

★ 0 ≤ Θ <  $\frac{1}{2}$  for the pure convection equation ( $\nu = 0$  or  $\sigma = 0$ ) ★ 0 ≤ Θ <  $\frac{1}{2}$  and  $\sigma > \frac{1}{2(1-2\Theta)}$  for the pure diffusion equation (a = 0 or c = 0)



### Exercise 8

1. Formulate for the discretised Poisson equation

$$u_{i,j} - \Theta_x(u_{i-1,j} + u_{i+1,j}) - \Theta_y(u_{i,j-1} + u_{i,j+1}) = \delta^2 f_{i,j},$$
$$\Theta_x = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)}, \quad \Theta_y = \frac{\Delta x^2}{2(\Delta x^2 + \Delta y^2)}$$

- (a) the Jacobi–method
- (b) the method of Gauß–Seidel point iteration with overrelaxation
- (c) the method of Gauß–Seidel line iteration with overrelaxation

Check the stability of these methods with the help of the von Neumann analysis.

### Exercise 8 (solution)

#### 1. (a) Jacobi-method ( $\nu$ is iteration counter):

$$u_{i,j}^{\nu+1} = \Theta_x \left( u_{i-1,j}^{\nu} + u_{i+1,j}^{\nu} \right) + \Theta_y \left( u_{i,j-1}^{\nu} + u_{i,j+1}^{\nu} \right) + \delta^2 f_{i,j}$$

stability, approach:  $u_{i,j}^{\nu} = u_{exact,i,j}^{\nu} + V^{\nu}e^{I\alpha i + I\beta j}$ , where  $u_{exact,i,j}$  is the exact solution of this equation, therefore

$$u_{exact,i,j}^{\nu+1} + V^{\nu+1}e^{I\alpha i + I\beta j} = \Theta_x \quad \left(u_{exact,i-1,j}^{\nu} + V^{\nu}e^{I\alpha(i-1) + I\beta j} + u_{exact,i+1,j}^{\nu} + V^{\nu}e^{I\alpha(i+1) + I\beta j}\right) + \Theta_y \quad \left(u_{exact,i,j-1}^{\nu} + V^{\nu}e^{I\alpha i + I\beta(j-1)} + u_{exact,i,j+1}^{\nu} + V^{\nu}e^{I\alpha i + I\beta(j+1)}\right) + \delta^2 f_{i,j}$$

where for the given definitions of  $\Theta_x$  and  $\Theta_y$  the terms  $u_{exact,i,j}^{\nu}$  and  $\delta^2 f_{i,j}$  fulfill the original FDE and thus falls out, dividing by  $V^{\nu}e^{I\alpha i+I\beta j}$  then yields:

$$G = \frac{V^{\nu+1}}{V^{\nu}} = \Theta_x \left( e^{-I\alpha} + e^{I\alpha} \right) + \Theta_y \left( e^{-I\beta} + e^{I\beta} \right) = 2 \left( \Theta_x \cos\left(\alpha\right) + \Theta_y \cos\left(\beta\right) \right)$$

with  $\Theta_x = \frac{\Delta y^2}{2(\Delta x^2 + \Delta y^2)}$ ,  $\Theta_y = \frac{\Delta x^2}{2(\Delta x^2 + \Delta y^2)}$  and  $-\pi \le \alpha \le \pi$ ,  $-\pi \le \beta \le \pi$  consider two cases:

$$2\left(\Theta_x \cos\left(\alpha\right) + \Theta_y \cos\left(\beta\right)\right) \le 2\left(\Theta_x + \Theta_y\right) = 2\left(\frac{\Delta x^2 + \Delta y^2}{2\left(\Delta x^2 + \Delta y^2\right)}\right) = 1$$
  
$$2\left(\Theta_x \cos\left(\alpha\right) + \Theta_y \cos\left(\beta\right)\right) \ge 2\left(-\Theta_x - \Theta_y\right) = 2\left(\frac{-\Delta x^2 - \Delta y^2}{2\left(\Delta x^2 + \Delta y^2\right)}\right) = -1$$
  
$$-1 \le G \le 1$$

Thus the Jacobi–method is stable.

(b) Gauß–Seidel point iteration with overrelaxation

 $(\tilde{u} \text{ is intermediate value})$ :

$$\tilde{u}_{i,j} - \Theta_x \left( u_{i-1,j}^{\nu+1} + u_{i+1,j}^{\nu} \right) - \Theta_y \left( u_{i,j-1}^{\nu+1} + u_{i,j+1}^{\nu} \right) = \delta^2 f_{i,j}$$
$$u_{i,j}^{\nu+1} = u_{i,j}^{\nu} + \omega \left( \tilde{u}_{i,j} - u_{i,j}^{\nu} \right)$$

or

$$u_{i,j}^{\nu+1} = u_{i,j}^{\nu} + \omega \left( \Theta_x \left( u_{i-1,j}^{\nu+1} + u_{i+1,j}^{\nu} \right) + \Theta_y \left( u_{i,j-1}^{\nu+1} + u_{i,j+1}^{\nu} \right) + \delta^2 f_{i,j} - u_{i,j}^{\nu} \right)$$

with  $\omega > 0$  and the order of calculation  $i = 1, \cdots, im$  and  $j = 1, \cdots, jm$  for  $u_{i,j}^{\nu+1}$ 

stability, approach see above:

$$\frac{V^{\nu+1}}{V^{\nu}} = 1 + \omega \left(\Theta_x \left(\frac{V^{\nu+1}}{V^{\nu}}e^{-I\alpha} + e^{I\alpha}\right) + \Theta_y \left(\frac{V^{\nu+1}}{V^{\nu}}e^{-I\beta} + e^{I\beta}\right) - 1\right)$$

with  $c = \Theta_x \cos(\alpha) + \Theta_y \cos(\beta)$  and  $s = \Theta_x \sin(\alpha) + \Theta_y \sin(\beta)$ 

$$\Leftrightarrow G = \frac{V^{\nu+1}}{V^{\nu}} = \frac{\frac{1}{\omega} - 1 + c + I s}{\frac{1}{\omega} - c + I s}$$

$$\Rightarrow |G|^{2} = \frac{\left(\frac{1}{\omega} - 1 + c\right)^{2} + s^{2}}{\left(\frac{1}{\omega} - c\right)^{2} + s^{2}} = \frac{\frac{1}{\omega^{2}} - \frac{2}{\omega} + 1 + \frac{2}{\omega}c - 2c + c^{2} + s^{2}}{\frac{1}{\omega^{2}} - \frac{2}{\omega}c + c^{2} + s^{2}}$$

with the condition  $|G|^2 \leq 1$ :

$$\Rightarrow 1 - \frac{2}{\omega} + \frac{4}{\omega}c - 2c \le 0 \quad \Leftrightarrow \quad \omega - 2 - 2c(\omega - 2) \le 0$$
$$\Leftrightarrow (1 - 2c)(\omega - 2) \le 0$$

because of  $\Theta_x + \Theta_y = \frac{1}{2}$  the value of c is between  $-\frac{1}{2} \leq c \leq \frac{1}{2}$ , therefore the expression in the first bracket is  $0 \leq 1 - 2c \leq 2$ , consider the adverse case (1 - 2c) = 2, then

 $\Rightarrow \omega \leq 2$ 

Thus the Gauß–Seidel point iteration with overrelaxation is stable for  $0 < \omega \leq 2$ .

#### (c) Gauß–Seidel line iteration with overrelaxation:

$$-\Theta_x \tilde{u}_{i-1,j} + \tilde{u}_{i,j} - \Theta_x \tilde{u}_{i+1,j} = \Theta_y \left( u_{i,j-1}^{\nu+1} + u_{i,j+1}^{\nu} \right) + \delta^2 f_{i,j}$$
$$u_{i,j}^{\nu+1} = u_{i,j}^{\nu} + \omega \left( \tilde{u}_{i,j} - u_{i,j}^{\nu} \right)$$

with  $\omega > 0$  and a line iteration in *i*-direction and the order of calculation j = $1, \cdots, jm$  for  $u_{i,j}^{\nu+1}$ .

stability, approach for  $u_{i,j}^{\nu}$  see above,  $\tilde{u}_{i,j} = u_{exact} + \tilde{V}e^{I\alpha i + I\beta j}$ :

$$\Rightarrow -\Theta_x \tilde{V} e^{-I\alpha} + \tilde{V} - \Theta_x \tilde{V} e^{I\alpha} = \Theta_y \left( V^{\nu+1} e^{-I\beta} + V^{\nu} e^{I\beta} \right)$$
$$\frac{V^{\nu+1}}{V^{\nu}} = 1 + \omega \left( \frac{\tilde{V}}{V^{\nu}} - 1 \right)$$
$$\Leftrightarrow \frac{\tilde{V}}{V^{\nu}} \left( 1 - \Theta_x \left( e^{-I\alpha} + e^{I\alpha} \right) \right) = \Theta_y \left( \frac{V^{\nu+1}}{V^{\nu}} e^{-I\beta} + e^{I\beta} \right)$$
$$\frac{\tilde{V}}{V^{\nu}} = \frac{1}{\omega} \left( \frac{V^{\nu+1}}{V^{\nu}} - 1 \right) + 1$$
$$\Leftrightarrow G = \frac{V^{\nu+1}}{V^{\nu}} = \frac{\left( \frac{1}{\omega} - 1 \right) \left( 1 - 2\Theta_x \cos\left(\alpha\right) \right) + \Theta_y \cos\left(\beta\right) + I\Theta_y \sin\left(\beta\right)}{\frac{1}{\omega} \left( 1 - 2\Theta_x \cos\left(\alpha\right) \right) - \Theta_y \cos\left(\beta\right) + I\Theta_y \sin\left(\beta\right)}{\left( \frac{1}{\omega} \left( 1 - 2\Theta_x \cos\left(\alpha\right) \right) - \Theta_y \cos\left(\beta\right) \right)^2 + \Theta_y^2 \sin^2\left(\beta\right)}$$
$$\Rightarrow |G|^2 = \frac{\left( \left( \frac{1}{\omega} - 1 \right) \left( 1 - 2\Theta_x \cos\left(\alpha\right) \right) - \Theta_y \cos\left(\beta\right) \right)^2 + \Theta_y^2 \sin^2\left(\beta\right)}{\left( \frac{1}{\omega} \left( 1 - 2\Theta_x \cos\left(\alpha\right) \right) - \Theta_y \cos\left(\beta\right) \right)^2 + \Theta_y^2 \sin^2\left(\beta\right)}$$

with the condition  $|G|^2 \leq 1$  it follows:

$$\Rightarrow \left(\frac{1}{\omega^2} - \frac{2}{\omega} + 1\right) \left(1 - 2\Theta_x \cos\left(\alpha\right)\right)^2 + \left(\frac{2}{\omega} - 2\right) \left(1 - 2\Theta_x \cos\left(\alpha\right)\right) \Theta_y \cos\left(\beta\right)$$
$$\leq \frac{1}{\omega^2} \left(1 - 2\Theta_x \cos\left(\alpha\right)\right)^2 - \frac{2}{\omega} \left(1 - 2\Theta_x \cos\left(\alpha\right)\right) \Theta_y \cos\left(\beta\right)$$
with  $\alpha = \Theta_x \cos\left(\alpha\right) + \Theta_x \cos\left(\beta\right)$ 

with  $c = \Theta_x \cos(\alpha) + \Theta_y \cos(\beta)$ 

$$\Rightarrow \left(\frac{2}{\omega} - 1\right) \underbrace{\left(\underbrace{2\Theta_x \cos\left(\alpha\right) - 1}_{\leq 1}\right)}_{\leq 0} \underbrace{\underbrace{(1 - 2c)}_{\geq 0}}_{\leq 0} \leq 0$$

With  $2\Theta_x \cos(\alpha) - 1 \le 0$  and  $0 \le 1 - 2c \le 2$ , the expression in the first bracket has to be  $\frac{2}{\omega} - 1 \ge 0$ Thus the Gauß–Seidel line iteration with overrelaxation is stable for  $0 < \omega \le 2$ .

### 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

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

(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.

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

$$u_{x} = \xi_{x}u_{\xi} + \eta_{x}u_{\eta}$$

$$u_{xx} = (u_{x})_{x} = (\xi_{x}u_{\xi} + \eta_{x}u_{\eta})_{x}$$

$$= \xi_{x}u_{\xi x} + \xi_{xx}u_{\xi} + \eta_{x}u_{\eta x} + \eta_{xx}u_{\eta}$$

$$= \xi_{x}(\xi_{x}u_{\xi\xi} + \eta_{x}u_{\xi\eta}) + \xi_{xx}u_{\xi} + \eta_{x}(\xi_{x}u_{\eta\xi} + \eta_{x}u_{\eta\eta}) + \eta_{xx}u_{\eta}$$

$$= \xi_{xx}u_{\xi} + \xi_{x}^{2}u_{\xi\xi} + 2\xi_{x}\eta_{x}u_{\xi\eta} + \eta_{x}^{2}u_{\eta\eta} + \eta_{xx}u_{\eta}$$

yields the Poisson equation in curvilinear coordinates:

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

(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:

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

The partial derivatives of  $\xi$  and  $\eta$  with respect to x and y for the polar coordinates are:

$\xi_x$	=	$\frac{x}{\sqrt{x^2 + y^2}}$	$\eta_x = -\frac{y}{x^2 + y^2}$
$\xi_y$	=	$\frac{y}{\sqrt{x^2 + y^2}}$	$\eta_y = \frac{x}{x^2 + y^2}$
$\xi_{xx}$	=	$\frac{y^2}{(x^2+y^2)^{\frac{3}{2}}}$	$\eta_{xx} = \frac{2xy}{(x^2 + y^2)^2}$
$\xi_{yy}$	=	$\frac{x^2}{(x^2 + y^2)^{\frac{3}{2}}}$	$\eta_{yy} = -\frac{2xy}{(x^2 + y^2)^2}$

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

$$1 = (\xi_x^2 + \xi_y^2) = \left(\frac{x}{\sqrt{x^2 + y^2}}\right)^2 + \left(\frac{y}{\sqrt{x^2 + y^2}}\right)^2 = \frac{x^2}{x^2 + y^2} + \frac{y^2}{x^2 + y^2} = \frac{x^2 + y^2}{x^2 + y^2}$$
  
= 1  
$$0 = 2(\xi_x \eta_x + \xi_y \eta_y) = 2\left(\left(\frac{x}{\sqrt{x^2 + y^2}}\right)\left(-\frac{y}{x^2 + y^2}\right) + \left(\frac{y}{\sqrt{x^2 + y^2}}\right)\left(\frac{x}{x^2 + y^2}\right)\right)$$
  
= 0  
$$\frac{1}{r^2} = (\eta_x^2 + \eta_y^2) = \left(-\frac{y}{x^2 + y^2}\right)^2 + \left(\frac{x}{x^2 + y^2}\right)^2 = \frac{x^2 + y^2}{(x^2 + y^2)^2} = \frac{1}{x^2 + y^2}$$
  
=  $\frac{1}{r^2}$   
$$\frac{1}{r} = (\xi_{xx} + \xi_{yy}) = \frac{y^2}{(x^2 + y^2)^{\frac{3}{2}}} + \frac{x^2}{(x^2 + y^2)^{\frac{3}{2}}} = \frac{x^2 + y^2}{(x^2 + y^2)^{\frac{3}{2}}} = \frac{1}{\sqrt{(x^2 + y^2)}}$$
  
=  $\frac{1}{r^2}$   
$$0 = (\eta_{xx} + \eta_{yy}) = \frac{2xy}{(x^2 + y^2)^2} + \left(-\frac{2xy}{(x^2 + y^2)^2}\right)$$
  
= 0

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

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



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

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

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:

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

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

$$u_{\xi} = \frac{u_{i+1,j} - u_{i-1,j}}{2}$$

$$u_{\eta} = \frac{u_{i,j+1} - u_{i,j-1}}{2}$$

$$u_{\xi\xi} = u_{i+1,j} - 2u_{i,j} + u_{i-1,j}$$

$$u_{\eta\eta} = u_{i,j+1} - 2u_{i,j} + u_{i,j-1}$$

$$u_{\xi\eta} = \frac{u_{i+1,j+1} - u_{i-1,j+1} - u_{i+1,j-1} + u_{i-1,j-1}}{4}$$

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:



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.

## Exercise 9 (appendix)

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

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x} \frac{\partial}{\partial \eta} 
\frac{\partial}{\partial y} = \frac{\partial \xi}{\partial y} \frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial y} \frac{\partial}{\partial \eta} 
\Rightarrow \left( \begin{pmatrix} \xi_x & \eta_x \\ \xi_y & \eta_y \end{pmatrix} \left( \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial \eta} \right) = \left( \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \right) \tag{1}$$

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

$$\frac{\partial}{\partial\xi} = \frac{\partial x}{\partial\xi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial\xi} \frac{\partial}{\partial y} 
\frac{\partial}{\partial\eta} = \frac{\partial x}{\partial\eta} \frac{\partial}{\partial x} + \frac{\partial y}{\partial\eta} \frac{\partial}{\partial y} 
\Rightarrow \begin{pmatrix} x_{\xi} & y_{\xi} \\ x_{\eta} & y_{\eta} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{pmatrix} = \begin{pmatrix} \frac{\partial}{\partial\xi} \\ \frac{\partial}{\partial\eta} \end{pmatrix}$$
(2)
a) compute the inverse of equation 2:

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

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

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

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

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

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

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

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

#### Exercise 10

1. The Laplace equation

 $\nabla\cdot\vec{f}=0 \quad , \qquad \text{with} \quad \vec{f}=\nabla u$ 

is to be solved on a curvilinear structured grid.

- (a) Transform the equation for  $\vec{f}$  into curvilinear coordinates  $(x, y) \to (\xi, \eta)$  (conservative form) and discretize the equation for an equidistant grid in curvilinear space.
- (b) Formulate a discretization based on a finite volume method for the solution of the equation for  $\vec{f}$ . Reformulate the equation as a surface integral, define a meaningful control volume and discretize the equation.
- (c) Show that the formulation obtained with the transformation in cuvilinear coordinates is identical to the finite volume formulation.

# Exercise 10 (solution)

1. (a)

$$\nabla \cdot \vec{f} = 0 \qquad \qquad \vec{f} = \nabla u = \begin{pmatrix} u_x \\ u_y \end{pmatrix} = \begin{pmatrix} g \\ h \end{pmatrix}$$
$$(x, y) \Rightarrow (\xi, \eta) \qquad \qquad \nabla \cdot \vec{f} = g_x + h_y = 0$$

with

$$g_x = \xi_x g_{\xi} + \eta_x g_{\eta}$$
$$h_y = \xi_y h_{\xi} + \eta_y h_{\eta}$$

follows for the terms in the square brackets

$$\xi_x g_{\xi} + \eta_x g_{\eta} + \xi_y h_{\xi} + \eta_y h_{\eta} = 0 \qquad | \cdot J$$
  
$$J\xi_x g_{\xi} + J\eta_x g_{\eta} + J\xi_y h_{\xi} + J\eta_y h_{\eta} = 0$$

product rule

$$\frac{\partial}{\partial\xi}\left(J\xi_xg + J\xi_yh\right) + \frac{\partial}{\partial\eta}\left(J\eta_xg + J\eta_yh\right) - g\left[\frac{\partial}{\partial\xi}(J\xi_x) + \frac{\partial}{\partial\eta}(J\eta_x)\right] - h\left[\frac{\partial}{\partial\xi}(J\xi_y) + \frac{\partial}{\partial\eta}(J\eta_y)\right] = 0$$

with metric terms

$$\xi_x = \frac{y_\eta}{J}$$
  $\xi_y = -\frac{x_\eta}{J}$   $\eta_x = -\frac{y_\xi}{J}$   $\eta_y = \frac{x_\xi}{J}$ 

follows

$$\frac{\partial}{\partial\xi}(J\xi_x) + \frac{\partial}{\partial\eta}(J\eta_x) = +\frac{\partial}{\partial\xi}y_\eta - \frac{\partial}{\partial\eta}y_\xi = 0$$
$$\frac{\partial}{\partial\xi}(J\xi_y) + \frac{\partial}{\partial\eta}(J\eta_y) = -\frac{\partial}{\partial\xi}x_\eta + \frac{\partial}{\partial\eta}x_\xi = 0$$

final formulation in curvilinear coordinates

$$[J(\xi_x g + \xi_y h)]_{\xi} + [J(\eta_x g + \eta_y h)]_{\eta} = (y_\eta g - x_\eta h)_{\xi} + (-y_{\xi} g + x_{\xi} h)_{\eta} = 0$$

discretisation

$$(y_{\eta}g - x_{\eta}h)_{i+\frac{1}{2},j} - (y_{\eta}g - x_{\eta}h)_{i-\frac{1}{2},j} + (-y_{\xi}g + x_{\xi}h)_{i,j+\frac{1}{2}} - (-y_{\xi}g + x_{\xi}h)_{i,j-\frac{1}{2}} = 0$$



procedure for the computation (example) for an element

$$y_{\eta}g = y_{\eta}u_x \longrightarrow (y_{\eta}u_x)_{i+\frac{1}{2},j} = (y_{\eta})_{i+\frac{1}{2},j} \cdot (\xi_x u_{\xi} + \eta_x u_{\eta})_{i+\frac{1}{2},j}$$

For this we need the metric terms at the point  $i + \frac{1}{2}$ , j, we can compute these for example by second-order accurate central differences (other formulations possible)

$$y_{\eta,i+\frac{1}{2},j} = \frac{y_B - y_A}{\Delta \eta} = \frac{y_B - y_A}{1}$$

where  $y_A$  and  $y_B$  are the averages of the surrounding 4 grid points

$$y_A = \frac{1}{4} \left( y_{i,j} + y_{i+1,j} + y_{i,j-1} + y_{i+1,j-1} \right)$$
$$y_B = \frac{1}{4} \left( y_{i,j} + y_{i+1,j} + y_{i,j+1} + y_{i+1,j+1} \right)$$

The other metric terms, e.g.,  $\xi_x, \eta_x$ , etc, can also be first transformed to the inverse metric terms and then be discretized at  $i + \frac{1}{2}, j$  in a similar manner. The terms  $u_{\xi}$  and  $u_{\eta}$  can be computed as simple central differences on the computational mesh, e.g.

$$u_{\xi,i+\frac{1}{2},j} = \frac{u_{i+1,j} - u_{i,j}}{1}$$

(b) finite volume formulation

$$\int_{\tau} \nabla \cdot \vec{f} d\tau = \oint_{A} \vec{f} \cdot \vec{n} dA \qquad \qquad \vec{f} = \begin{pmatrix} g \\ h \end{pmatrix} \qquad \qquad \vec{n} dA = \begin{pmatrix} dy \\ -dx \end{pmatrix}$$
$$\rightarrow \qquad \oint_{A} g dy - h dx = 0$$

Possible discretization with node-centered formulation (for mathematical positive direction)



$$(g\Delta y)_{i+\frac{1}{2},j} - (h\Delta x)_{i+\frac{1}{2},j} + (g\Delta y)_{i,j+\frac{1}{2}} - (h\Delta x)_{i,j+\frac{1}{2}} + (g\Delta y)_{i-\frac{1}{2},j} - (h\Delta x)_{i-\frac{1}{2},j} + (g\Delta y)_{i,j-\frac{1}{2}} - (h\Delta x)_{i,j-\frac{1}{2}} = 0$$

where the corresponding signs (+ for flux entering the volume, - for flux leaving the volume) are contained in the  $\Delta$  terms:

$$\begin{aligned} \Delta x_{i+\frac{1}{2},j} &= x_B - x_A & \Delta y_{i+\frac{1}{2},j} &= y_B - y_A \\ \Delta x_{i-\frac{1}{2},j} &= x_D - x_C & \Delta y_{i-\frac{1}{2},j} &= y_D - y_C \\ \Delta x_{i,j+\frac{1}{2}} &= x_C - x_B & \Delta y_{i,j+\frac{1}{2}} &= y_C - y_B \\ \Delta x_{i,j-\frac{1}{2}} &= x_A - x_D & \Delta y_{i,j-\frac{1}{2}} &= y_A - y_D \end{aligned}$$

give the surface over which the flux is integrated and the correct sign. The coordinates at points A, B, C, and D are computed by averages of the surrouding four grid points, as shown before.

(c) curvilinear form

finite volume formulation

$$(\Delta y \cdot g)_{i+\frac{1}{2},j} - (\Delta x \cdot h)_{i+\frac{1}{2},j} + (\Delta y \cdot g)_{i-\frac{1}{2},j} - (\Delta x \cdot h)_{i-\frac{1}{2},j} + (\Delta y \cdot g)_{i,j+\frac{1}{2}} - (\Delta x \cdot h)_{i,j+\frac{1}{2}} + (\Delta y \cdot g)_{i,j-\frac{1}{2}} - (\Delta x \cdot h)_{i,j-\frac{1}{2}} = 0$$

$$(2)$$

the metric coefficients, e.g.,  $x_{\eta}$ ,  $y_{\xi}$ , etc, are then equal to the lengths from the finite volume approach  $\Delta x$  and  $\Delta y$ . For example for surface  $i + \frac{1}{2}$ , j we have the metric terms

$$\begin{aligned} x_{\eta,i+\frac{1}{2},j} &= \frac{x_B - x_A}{\Delta \eta} = \frac{\Delta x_{i+\frac{1}{2},j}}{1} \\ y_{\eta,i+\frac{1}{2},j} &= \frac{y_B - y_A}{\Delta \eta} = \frac{\Delta y_{i+\frac{1}{2},j}}{1} \end{aligned}$$

The opposite signs in eqs. 1 and 2 are caused by opposite signs in metric terms in comparison with the lengths, for example

$$-(y_{\eta} \cdot g)_{i-\frac{1}{2},j} = -\frac{y_C - y_D}{\Delta \eta} (g)_{i-\frac{1}{2},j} = \frac{y_D - y_C}{\Delta \eta} (g)_{i-\frac{1}{2},j} = \Delta y_{i-\frac{1}{2},j} (g)_{i-\frac{1}{2},j}$$

as we compute the metric terms going into positive  $\xi$  and  $\eta$  direction, but for the lengths in the finite volume approach we follow the surface in positive rotation direction, here counterclockwise.

#### Exercise 11

1. The Laplace equation  $\nabla^2 u = 0$  is discretized on a Cartesian grid, where the variables are stored at the cell centers. The discretization is carried out with a finite volume method, the values on the surface of the cell are reconstructed with the assumption of a linear function, i.e., applying a first-order Taylor-series expansion around the surface centroid located at (0, 0):

$$u(x,y) = u(0,0) + u_x(0,0)x + u_y(0,0)y$$
  
=  $a_0 + a_1x + a_2y$ 

For the reconstruction on the cell surface the cell centered values of points 1-6, see Figure, are used.



This yields a overdetermined,  $6 \times 3$  linear equation system

$$\underline{A}\begin{pmatrix}a_0\\a_1\\a_2\end{pmatrix} = \begin{pmatrix}1&x_1&y_1\\1&x_2&y_2\\\vdots&\vdots&\vdots\\1&x_6&y_6\end{pmatrix}\begin{pmatrix}a_0\\a_1\\a_2\end{pmatrix} = \begin{pmatrix}u_1\\u_2\\\vdots\\u_6\end{pmatrix}$$

The constants  $a_0, a_1, a_2$  can be determined by a least-squares approach. Thereby, the constants are chosen such that the sum of squared errors,  $\sum_i (a_0 + a_1x_i + a_2y_i - u_i)^2$ , is minimal. This is achieved by solving

$$\underline{A}^{T}\underline{A}\left(\begin{array}{c}a_{0}\\a_{1}\\a_{2}\end{array}\right) = \underline{A}^{T}\left(\begin{array}{c}u_{1}\\\vdots\\u_{6}\end{array}\right)$$

which yields the  $3 \times 3$  system

$$\begin{pmatrix} n & \sum x_i & \sum y_i \\ \sum x_i & \sum x_i^2 & \sum x_i y_i \\ \sum y_i & \sum x_i y_i & \sum y_i^2 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \sum u_i \\ \sum u_i \cdot x_i \\ \sum u_i \cdot y_i \end{pmatrix}$$

Determine the truncation error of the finite volume method.

## Exercise 11 (solution)

1. From

$$\begin{pmatrix} n & \sum x_i & \sum y_i \\ \sum x_i & \sum x_i^2 & \sum x_i y_i \\ \sum y_i & \sum x_i y_i & \sum y_i^2 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \sum u_i \\ \sum u_i \cdot x_i \\ \sum u_i \cdot y_i \end{pmatrix}$$

For an equidistant grid (n = number of points):

$$\begin{pmatrix} 6 & 0 & 0 \\ 0 & \frac{3}{2}\Delta x^2 & 0 \\ 0 & 0 & 4\Delta y^2 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \sum u_i \\ \sum u_i \cdot x_i \\ \sum u_i \cdot y_i \end{pmatrix}$$

$$\Rightarrow a_{0} = \frac{1}{6}(u_{1} + u_{2} + u_{3} + u_{4} + u_{5} + u_{6})$$

$$a_{1} = \frac{2}{3\Delta x^{2}} \cdot \frac{\Delta x}{2}(u_{2} + u_{1} + u_{6} - u_{3} - u_{4} - u_{5}) = \frac{1}{3\Delta x}(u_{2} + u_{1} + u_{6} - u_{3} - u_{4} - u_{5})$$

$$a_{2} = \frac{1}{4\Delta y^{2}} \cdot \Delta y(u_{3} + u_{2} - u_{5} - u_{6}) = \frac{1}{4\Delta y}(u_{3} + u_{2} - u_{5} - u_{6})$$

From  $u(x, y) = a_0 + a_1 x + a_2 y$ 

$$\nabla u = \left(\begin{array}{c} u_x \\ u_y \end{array}\right) = \left(\begin{array}{c} a_1 \\ a_2 \end{array}\right)$$

Using Gauß' theorem for  $\nabla^2 u = 0$ 

$$\int_{\tau} \nabla \cdot \vec{f} \, d\tau = \oint_{A} \vec{f} \cdot \vec{n} \, dA = \oint_{A} \begin{pmatrix} u_{x} \\ u_{y} \end{pmatrix} \cdot \vec{n} \, dA = 0 \quad \text{with} \quad \vec{f} = \nabla u = \begin{pmatrix} u_{x} \\ u_{y} \end{pmatrix}$$
Compute 
$$\int \begin{pmatrix} u_{x} \\ u_{y} \end{pmatrix} \cdot \vec{n} \, dA :$$

normal vector  $\vec{n}$  for side 1 to 4:

side 1: 
$$\vec{n} = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$
 side 2:  $\vec{n} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  side 3:  $\vec{n} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$  side 4:  $\vec{n} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ 

$$\int \left( \begin{array}{c} u_x \\ u_y \end{array} \right) \cdot \vec{n} \, dA = -a_1(\text{side 1}) \cdot \Delta y + a_1(\text{side 2}) \cdot \Delta y - a_2(\text{side 3}) \cdot \Delta x + a_2(\text{side 4}) \cdot \Delta x = 0$$
$$= (u_{xx} + u_{yy}) \Delta x \Delta y$$

Use  $u_{xx}$  to evaluate the truncation error (same procedere for  $u_{yy}$ ):

$$u_{xx} = \frac{a_1(\text{side } 2) - a_1(\text{side } 1)}{\Delta x}$$

$$a_1(\text{side } 1) = \frac{1}{3\Delta x}(u_{i,j+1} + u_{i,j} + u_{i,j-1} - u_{i-1,j+1} - u_{i-1,j} - u_{i-1,j-1})$$

$$a_1(\text{side } 2) = \frac{1}{3\Delta x}(u_{i+1,j+1} + u_{i+1,j} + u_{i+1,j-1} - u_{i,j+1} - u_{i,j} - u_{i,j-1})$$

$$= \frac{1}{3\Delta x^2}(u_{i+1,j+1} + u_{i+1,j} + u_{i+1,j-1} - 2u_{i,j+1} - 2u_{i,j} - 2u_{i,j-1} + u_{i-1,j+1} + u_{i-1,j} + u_{i-1,j-1}) (*)$$



Taylor series (multidimensional):

$$f(x,y) = \sum_{\substack{s=0\\t=0}}^{\infty} \frac{1}{s! \cdot t!} \cdot \frac{\partial^{s+t} f}{\partial x^s \partial y^t} (x - x_0)^s (y - y_0)^t$$

Here for  $u_{i+1,j+1}$  (similar for the remaining terms...):

$$\begin{split} u(x + \Delta x, y + \Delta y) &= u(x, y) + \Delta x \cdot u_x + \Delta y \cdot u_y + \Delta x \Delta y \cdot u_{xy} + \frac{\Delta x^2}{2} \cdot u_{xx} + \frac{\Delta y^2}{2} \cdot u_{yy} \\ &+ \frac{\Delta x^2 \Delta y}{2} \cdot u_{xxy} + \frac{\Delta y^2 \Delta x}{2} \cdot u_{xyy} + \frac{\Delta x^3}{6} \cdot u_{xxx} + \frac{\Delta y^3}{6} \cdot u_{yyy} \\ &+ \frac{\Delta x^3 \Delta y}{6} \cdot u_{xxxy} + \frac{\Delta y^3 \Delta x}{6} \cdot u_{xyyy} + \frac{\Delta x^2 \Delta y^2}{4} \cdot u_{xxyy} \\ &+ \frac{\Delta x^4}{24} \cdot u_{xxxx} + \frac{\Delta y^4}{24} \cdot u_{yyyy} + \dots \end{split}$$

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Inserting Taylor series in (\*) yields:

$$u_{xx} = \frac{1}{3\Delta x^2} \left( 3\Delta x^2 \cdot u_{xx} + \Delta x^2 \Delta y^2 \cdot u_{xxyy} + \frac{\Delta x^4}{4} \cdot u_{xxxx} \right)$$
$$= \left( u_{xx} + \frac{\Delta y^2}{3} \cdot u_{xxyy} + \frac{\Delta x^2}{12} \cdot u_{xxxx} \right)$$

 $\Rightarrow \quad \text{Truncation error for } u_{xx}: \quad \tau = \mathcal{O}(\Delta x^2, \Delta y^2)$ Similar for  $u_{yy}$ , therefore truncation error  $\tau = \mathcal{O}(\Delta x^2, \Delta y^2)$