Chair DYNAMICS, CONTROL AND NUMERICS FAU

Department of DATA SCIENCE

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
NATURWISSENSCHAFTLICHE FAKULTÄT

Practical Course: Modeling, Simulation, Optimization

Week 2

Daniël Veldman
Chair in Dynamics, Control, and Numerics, Friedrich-Alexander-University Erlangen-Nürnberg

Contents

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2.A 2-D Conservation laws

Recap: Conservation of mass in 1-D

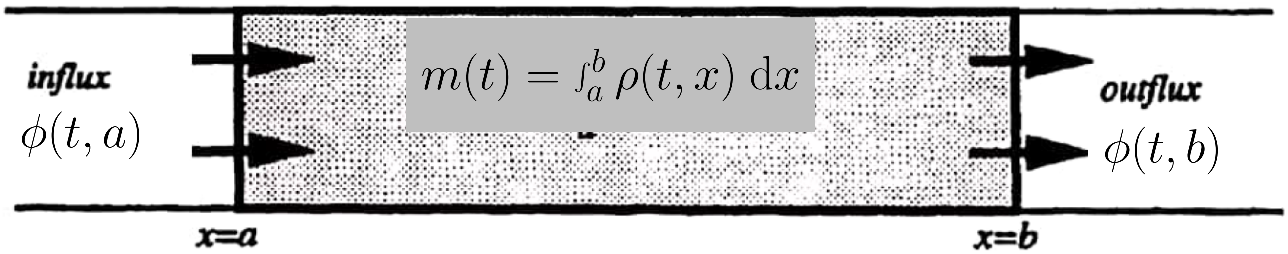


Figure: A slice of a 1-D continuum to investigate the conservation of mass (from [Roberts, 1994] but edited)

The mass $m(t)$ [kg] in $[a,b]$ changes only because of the mass fluxes $\phi(\cdot,a)$ and $\phi(\cdot,b)$ [kg/s]:

$$\frac{\partial m}{\partial t} = \phi(t,a) - \phi(t,b).$$

Using the fundamental theorem of calculus, we find

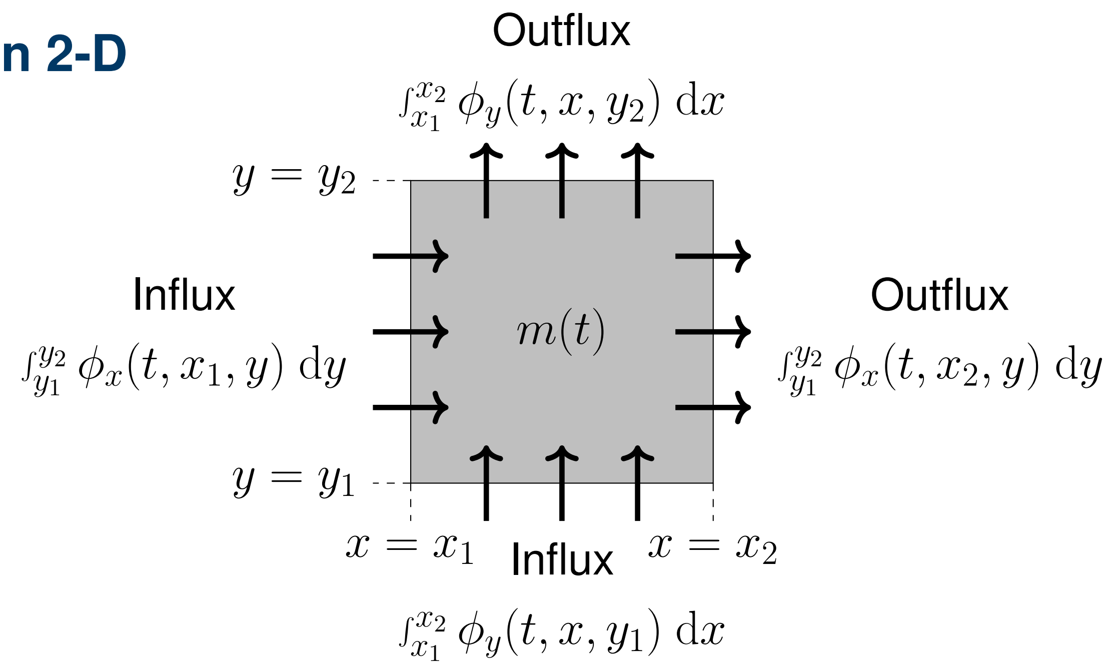
$$\int_a^b \frac{\partial \rho}{\partial t}(t,x)\,\mathrm{d}x = -\int_a^b \frac{\partial \phi}{\partial x}(t,x)\,\mathrm{d}x.$$

Because this holds for any interval $[a,b]$ in the domain $\Omega = [0,L]$:

Conservation of mass in 1-D

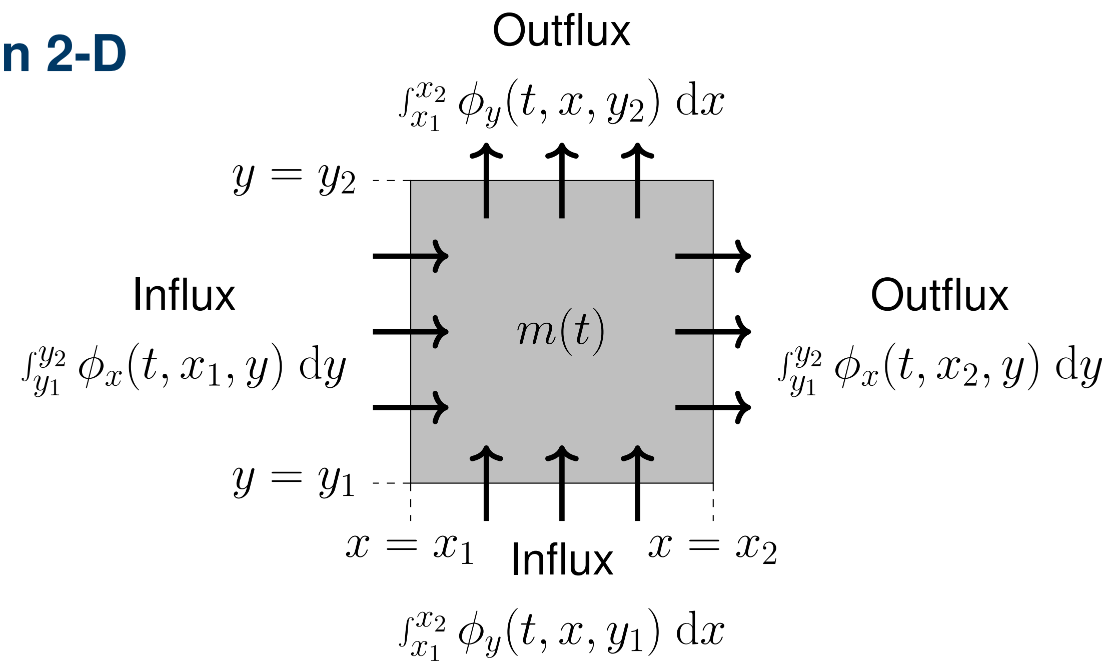
$$\frac{\partial \rho}{\partial t}(t,x) = -\frac{\partial \phi}{\partial x}(t,x).$$

Conservation of mass in 2-D



$$\begin{aligned}\frac{\partial m}{\partial t}(t,x,y) &= \int_{y_1}^{y_2} \left(\phi_x(t,x_1,y) - \phi_x(t,x_2,y)\right)\, \mathrm{d}y + \int_{x_1}^{x_2} \left(\phi_y(t,x,y_1) - \phi_y(t,x,y_2)\right)\, \mathrm{d}x \\ &= -\int_{y_1}^{y_2} \int_{x_1}^{x_2} \left(\frac{\partial \phi_x}{\partial x}(t,x,y) + \frac{\partial \phi_y}{\partial y}(t,x,y)\right)\, \mathrm{d}x\, \mathrm{d}y\end{aligned}$$

Conservation of mass in 2-D



$$\frac{\partial m}{\partial t}(t,x,y) = \int_{y_1}^{y_2} \left(\phi_x(t,x_1,y) - \phi_x(t,x_2,y)\right)\,\mathrm{d}y + \int_{x_1}^{x_2} \left(\phi_y(t,x,y_1) - \phi_y(t,x,y_2)\right)\,\mathrm{d}x$$

$$= -\int_{y_1}^{y_2}\int_{x_1}^{x_2} \left(\frac{\partial \phi_x}{\partial x}(t,x,y) + \frac{\partial \phi_y}{\partial y}(t,x,y)\right)\,\mathrm{d}x\,\mathrm{d}y$$

Because $m(t) = \int_{y_1}^{y_2}\int_{x_1}^{x_2} \rho(t,x,y)\,\mathrm{d}x\,\mathrm{d}y$ and $[x_1,x_2]\times[y_1,y_2]$ is arbitrary:

Conservation of mass in 2-D

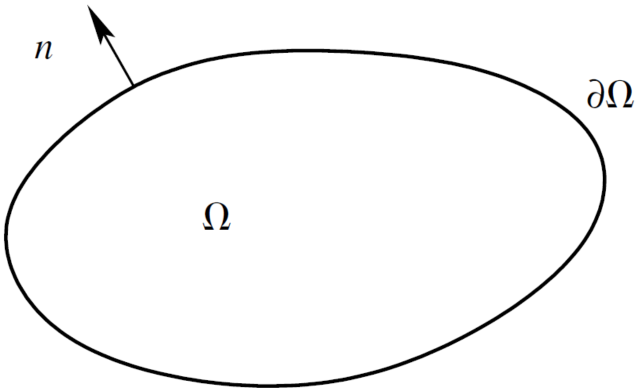
$$\frac{\partial \rho}{\partial t}(t,x,y) = -\frac{\partial \phi_x}{\partial x}(t,x,y) - \frac{\partial \phi_y}{\partial y}(t,x,y).$$

Another derivation

Mass flux vector $\boldsymbol{\phi} = [\phi_x, \phi_y]^\top$ [kg/m/s]
Outward pointing unit normal $n = [n_1, n_2]^\top$ [-]
Coordinate vector $\mathbf{x} = [x, y]^\top$ [m].

Mass flux through $\partial\Omega$ into Ω [kg/s]

$$-\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s$$



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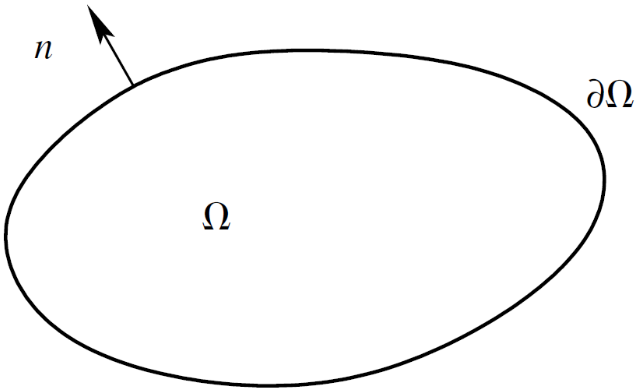

Mass flux through $\partial\Omega$ into Ω [kg/s]

$$-\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s$$

Conservation of mass in Ω and Gauss theorem:

$$\frac{\partial m}{\partial t} = -\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s = -\int_{\Omega} \nabla \cdot \boldsymbol{\phi} \, \mathrm{d}\mathbf{x}.$$

Because $m(t) = \int_\Omega \rho \, \mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Another derivation

Mass flux vector $\boldsymbol{\phi} = [\phi_x, \phi_y]^\top$ [kg/m/s]
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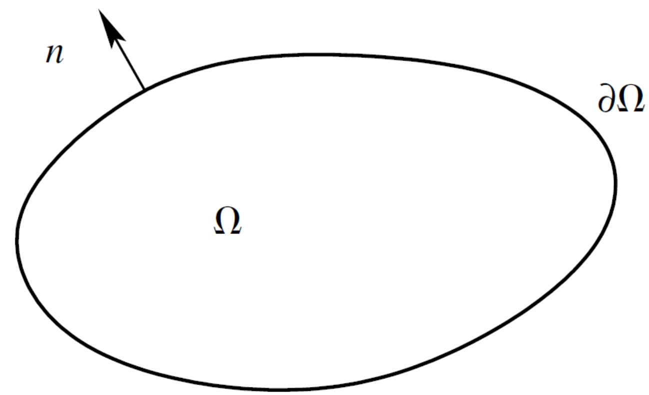

Mass flux through $\partial\Omega$ into Ω [kg/s]

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Conservation of mass in Ω and Gauss theorem:

$$\frac{\partial m}{\partial t} = -\int_{\partial\Omega} \boldsymbol{\phi} \cdot n \, \mathrm{d}s = -\int_{\Omega} \nabla \cdot \boldsymbol{\phi} \, \mathrm{d}\mathbf{x}.$$

Because $m(t) = \int_\Omega \rho \, \mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Conservation of mass

$$\frac{\partial \rho}{\partial t}(t, \mathbf{x}) = -\nabla \cdot \boldsymbol{\phi}(t, \mathbf{x}).$$

Completing the model

$$\frac{\partial \rho}{\partial t}(t, \mathbf{x}) = -\nabla \cdot \boldsymbol{\phi}(t, \mathbf{x}) \qquad \left(\frac{\partial \rho}{\partial t}(t, x, y) = -\frac{\partial \phi_x}{\partial x}(t, x, y) - \frac{\partial \phi_y}{\partial y}(t, x, y)\right).$$

To complete the model, we need a *constitutive relation*
that relates the mass flux $\boldsymbol{\phi}(t, \mathbf{x})$ to the mass density $\rho(t, \mathbf{x})$.

Two commonly used constitutive relations:

Fick's law

$$\boldsymbol{\phi}(t, \mathbf{x}) = -\kappa(t, \mathbf{x}) \nabla \rho(t, \mathbf{x}) \qquad \left(\begin{bmatrix} \phi_x(t, x, y) \\ \phi_y(t, x, y) \end{bmatrix} = -\kappa(t, x, y) \begin{bmatrix} \frac{\partial \rho}{\partial x}(t, x, y) \\ \frac{\partial \rho}{\partial y}(t, x, y) \end{bmatrix}\right).$$

The coefficient $\kappa(t, \mathbf{x})$ [m^2/s] is called the diffusivity.
'Mass flows from locations with high concentrations to locations with low concentrations'

Advective transport

$$\boldsymbol{\phi}(t, \mathbf{x}) = \rho(t, \mathbf{x}) \mathbf{v}(t, \mathbf{x}) \qquad \left(\begin{bmatrix} \phi_x(t, x, y) \\ \phi_y(t, x, y) \end{bmatrix} = \begin{bmatrix} \rho(t, x, y) v_x(t, x, y) \\ \rho(t, x, y) v_y(t, x, y) \end{bmatrix}\right).$$

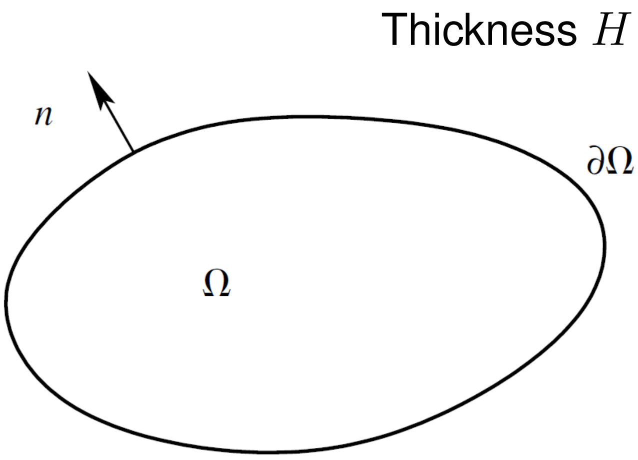
The velocity field $\mathbf{v}(t, \mathbf{x})$ [m/s] is given.
'Mass flows along the velocity field $\mathbf{v}(t, \mathbf{x})$'

Energy conservation

Heat flux vector $\mathbf{q} = [q_x, q_y]^\top$ [W/m^2].
Outward pointing unit normal $n = [n_1, n_2]^\top$ [-].
Coordinate vector $\mathbf{x} = [x, y]^\top$ [m].

Heat flux through $\partial\Omega$ into Ω [W]

$$-H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s$$



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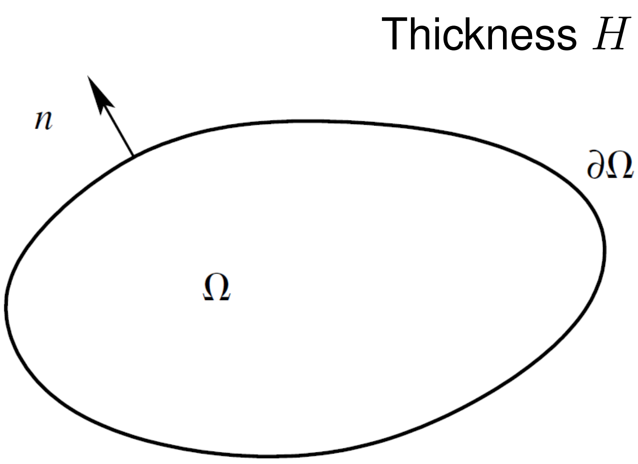


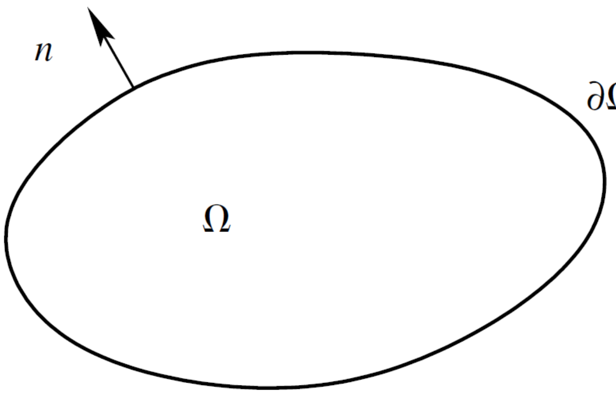
Heat flux through $\partial\Omega$ into Ω [W]

$$-H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s$$

Heat generated in Ω is $\int_\Omega Q(t, \mathbf{x}) \, \mathrm{d}\mathbf{x}$.
Conservation of energy in Ω and Gauss theorem:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = \int_\Omega Q(t, \mathbf{x}) \, \mathrm{d}\mathbf{x} - H \int_{\partial\Omega} \mathbf{q} \cdot n \, \mathrm{d}s = \int_\Omega Q \, \mathrm{d}\mathbf{x} - H \int_\Omega \nabla \cdot \mathbf{q} \, \mathrm{d}\mathbf{x}.$$

Energy conservation



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Because $U(t) = \int_\Omega \rho_u(t, \mathbf{x}) \, \mathrm{d}\mathbf{x}$ and Ω is arbitrary:

Conservation of mass

$$\frac{\partial \rho_u}{\partial t}(t, \mathbf{x}) = -H \nabla \cdot \mathbf{q}(t, \mathbf{x}) + Q(t, \mathbf{x}).$$

Completing the model

$$\frac{\partial \rho_u}{\partial t}(t, \mathbf{x}) = -H\nabla \cdot \mathbf{q}(t, \mathbf{x}) + Q(t, \mathbf{x}).$$

We again need constitutive relations to complete the model.

Fourier's law of heat conduction in 2-D

$$\mathbf{q}(t, \mathbf{x}) = -k\nabla T(t, \mathbf{x}).$$

The coefficient k^* [W/m/K] is the thermal conductivity and $T(t, \mathbf{x})$ [K] is the temperature.
'Heat flows from locations with high temperatures to locations with low temperatures'

Internal energy in 2-D

$$\rho_u(t, \mathbf{x}) = cHT(t, \mathbf{x}).$$

The coefficient c [J/K/m^3] heat capacity per unit volume.

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2.B 2-D Finite differences

2-D Finite differences

Suppose we want to approximate the solution $u(x,y)$ of the boundary value problem

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) + f(x,y) = 0, \qquad (x,y) \in (0, L_x) \times (0, L_y),$$

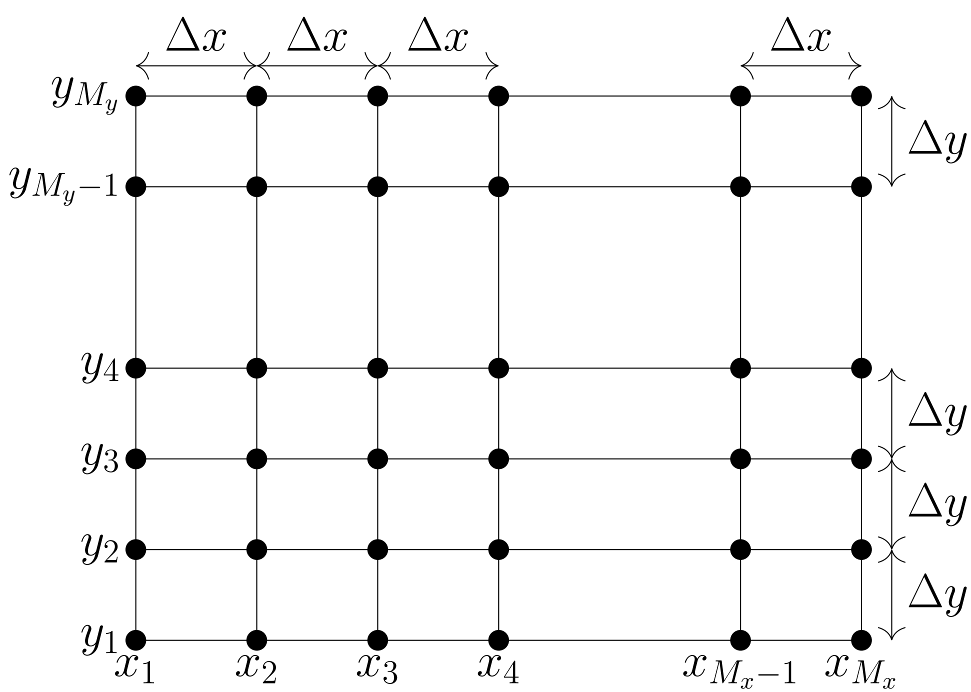
+boundary conditions.

2-D Finite differences

Suppose we want to approximate the solution $u(x, y)$ of the boundary value problem

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) + f(x,y) = 0, \qquad (x,y) \in (0, L_x) \times (0, L_y),$$

+boundary conditions.
Introduce an $M_x \times M_y$-point grid in $(0, L_x) \times (0, L_y)$ with a grid spacings $\Delta x = L_x/(M_x - 1)$ and $\Delta y = L_y/(M_y - 1)$.



Finite difference approximation

Find a system of equations in terms of $f_{m\ell}$ $(= f(x_m, y_\ell))$ and $u_{m\ell}$ $(\approx u(x_m, y_\ell))$.

Observe that (for $u \in C^4([0, L])$)

$$u(x + \Delta x, y) = u(x, y) + \Delta x \frac{\mathrm{d}u}{\mathrm{d}x}(x, y) + \frac{(\Delta x)^2}{2} \frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x, y) + \frac{(\Delta x)^3}{6} \frac{\mathrm{d}^3 u}{\mathrm{d}x^3}(x, y) + O((\Delta x)^4),$$

$$u(x - \Delta x, y) = u(x, y) - \Delta x \frac{\mathrm{d}u}{\mathrm{d}x}(x, y) + \frac{(\Delta x)^2}{2} \frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x, y) - \frac{(\Delta x)^3}{6} \frac{\mathrm{d}^3 u}{\mathrm{d}x^3}(x, y) + O((\Delta x)^4).$$

Adding these two equations:

$$u(x + \Delta x, y) + u(x - \Delta x, y) = 2u(x, y) + (\Delta x)^2 \frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x, y) + O((\Delta x)^4).$$

Rearranging and dividing by $(\Delta x)^2$ yields

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x, y) = \frac{u(x + \Delta x, y) - 2u(x, y) + u(x - \Delta x, y)}{(\Delta x)^2} + O((\Delta x)^2).$$

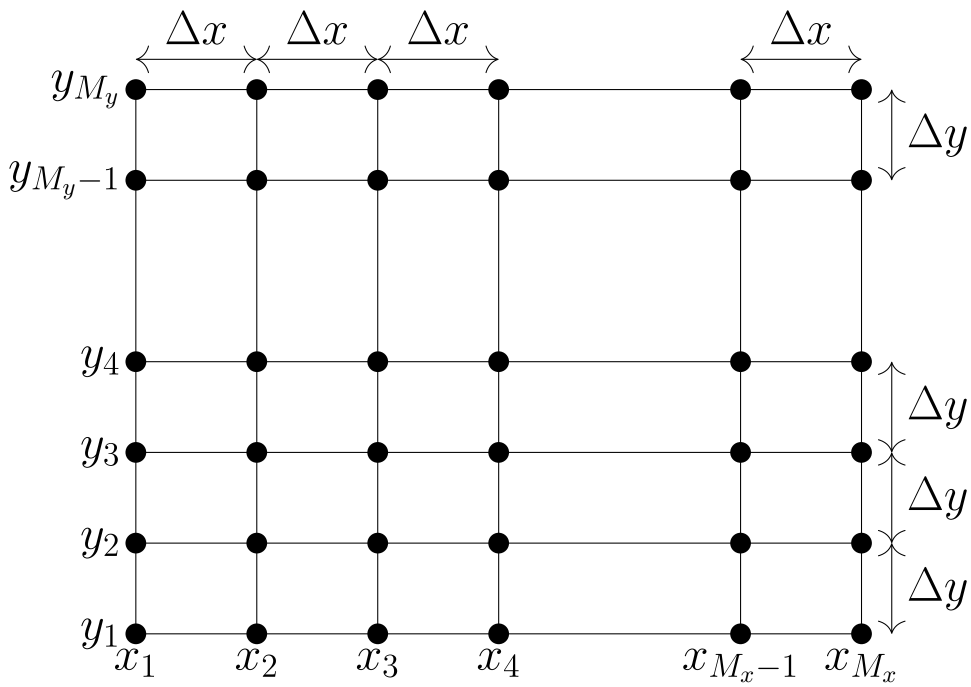
We can do a similar computation for the y-direction.

Finite difference approximation (for the 2nd derivatives)

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x_m, y_\ell) \approx \frac{u_{m+1,\ell} - 2u_{m\ell} + u_{m-1,\ell}}{(\Delta x)^2}, \qquad \frac{\mathrm{d}^2 u}{\mathrm{d}y^2}(x_m, y_\ell) \approx \frac{u_{m,\ell+1} - 2u_{m\ell} + u_{m,\ell-1}}{(\Delta y)^2}$$

Equations for internal nodes

$$\frac{\partial^2 u}{\partial x^2}(x,y) + \frac{\partial^2 u}{\partial y^2}(x,y) + f(x,y) = 0, \qquad (x,y) \in (0,L_x) \times (0,L_y),$$

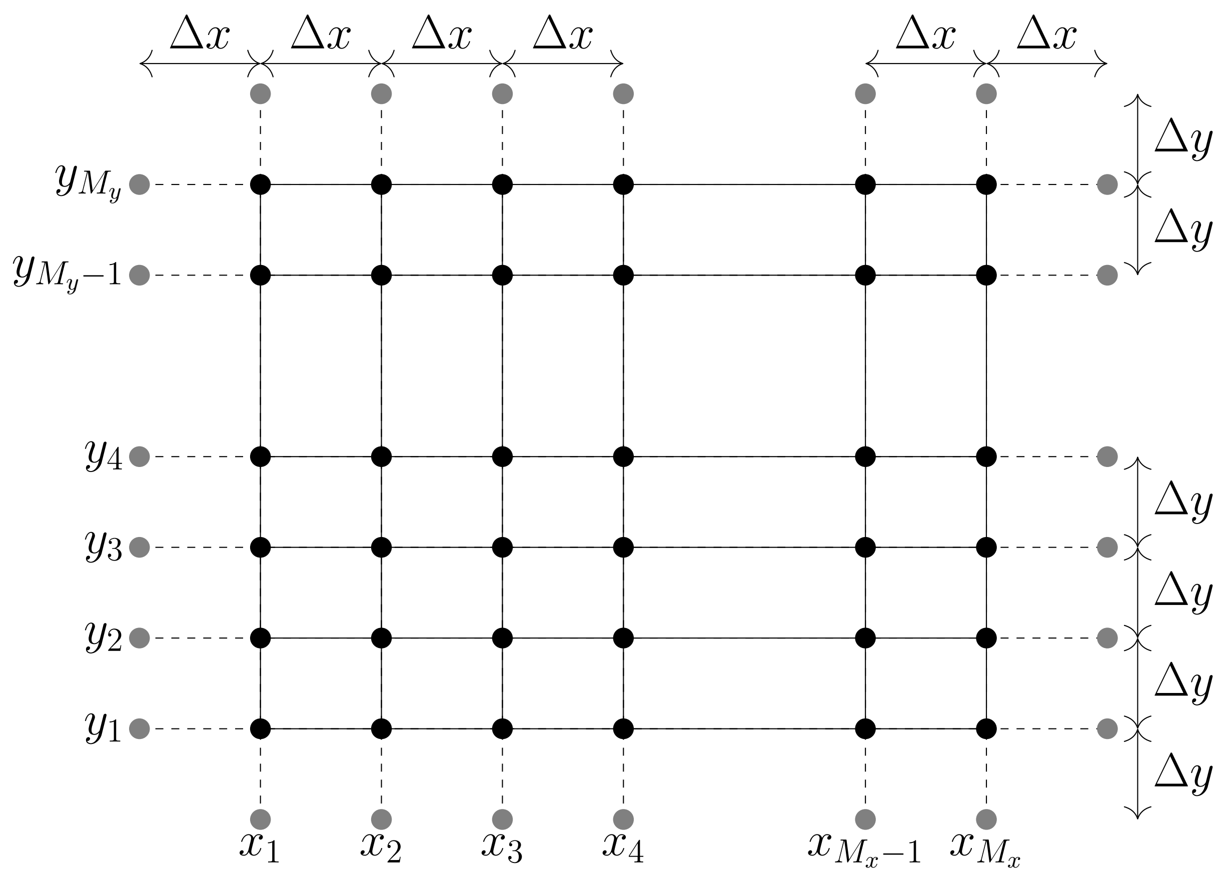


$$\frac{u_{m+1,\ell} - 2u_{m\ell} + u_{m-1,\ell}}{(\Delta x)^2} + \frac{u_{m,\ell+1} - 2u_{m\ell} + u_{m,\ell-1}}{(\Delta y)^2} + f_{m\ell} = 0.$$

with $m \in \{1,2,\ldots,M_x\}$ and $\ell \in \{1,2,\ldots,M_y\}$.

Ghost points

Note: we need $2M_x + 2M_y$ ghost points!



$$\frac{u_{m+1,\ell} - 2u_{m\ell} + u_{m-1,\ell}}{(\Delta x)^2} + \frac{u_{m,\ell+1} - 2u_{m\ell} + u_{m,\ell-1}}{(\Delta y)^2} + f_{m\ell} = 0.$$

with $m \in \{1, 2, \dots, M_x\}$ and $\ell \in \{1, 2, \dots, M_y\}$.

Resulting equations (implicit formulation for the BCs)

$M_x M_y$ internal nodes:

$$\frac{u_{m+1,\ell} - 2u_{m\ell} + u_{m-1,\ell}}{\Delta x^2} + \frac{u_{m,\ell+1} - 2u_{m\ell} + u_{m,\ell-1}}{\Delta y^2} + f_{m\ell} = 0,$$

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with $m \in \{1, 2, \dots, M_x\}$ and $\ell \in \{1, 2, \dots, M_y\}$.

$2(M_x + M_y)$ ghost points:

- For a Dirichlet BC $u(x, y) = 0$ at $(x, y) = (x_m, y_\ell)$:

$$u_{m\ell} = 0.$$

- For a Neumann BC $\partial u / \partial x = 0$ (at $x = 0$ or $x = L_x$) or $\partial u / \partial y = 0$ (at $y = 0$ or $y = L_y$):

$$\frac{u_{m+1,\ell} - u_{m-1,\ell}}{2\Delta x} = 0, \qquad (m \in \{1, M_x\}),$$

or

$$\frac{u_{m,\ell+1} - u_{m,\ell-1}}{2\Delta y} = 0, \qquad (\ell \in \{1, M_y\}).$$

This set of equations gives an implicit formulation for the BCs.

Resulting equations (explicit formulation for the BCs)

To obtain the explicit formulation for the BCs, we eliminate the values at the ghost points.

$(M_x - 2)(M_y - 2)$ equations for nodes in the interior:

$$\frac{u_{m+1,\ell} - 2u_{m\ell} + u_{m-1,\ell}}{\Delta x^2} + \frac{u_{m,\ell+1} - 2u_{m\ell} + u_{m,\ell-1}}{\Delta y^2} + f_{m\ell} = 0,$$

with $m \in \{2, 3, \ldots, M_x - 1\}$ and $\ell \in \{2, 3, \ldots, M_y - 1\}$.

Resulting equations (explicit formulation for the BCs)

To obtain the explicit formulation for the BCs, we eliminate the values at the ghost points.

$(M_x - 2)(M_y - 2)$ equations for nodes in the interior:

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with $m \in \{2, 3, \ldots, M_x - 1\}$ and $\ell \in \{2, 3, \ldots, M_y - 1\}$.

$2(M_x + M_y)$ ghost points:

- For a Dirichlet BC $u(x, y) = 0$ at $(x, y) = (x_m, y_\ell)$:
  We omit the $u_{m\ell} = 0$ from the vector DOFs.
  (The neighboring ghost point is also omitted.)
- For a Neumann BC $\partial u/\partial x = 0$ (at $x = 0$ or $x = L_x$) or $\partial u/\partial y = 0$ (at $y = 0$ or $y = L_y$):

$$\frac{2u_{2,\ell} - 2u_{1,\ell}}{\Delta x^2} = 0, \qquad \frac{-2u_{M_x,\ell} + 2u_{M_x-1,\ell}}{\Delta x^2} = 0,$$

$$\frac{2u_{m,2} - 2u_{m,1}}{\Delta x^2} = 0, \qquad \frac{-2u_{m,M_y} + 2u_{m,M_y-1}}{\Delta x^2} = 0,$$

This set of equations gives an implicit formulation for the BCs.

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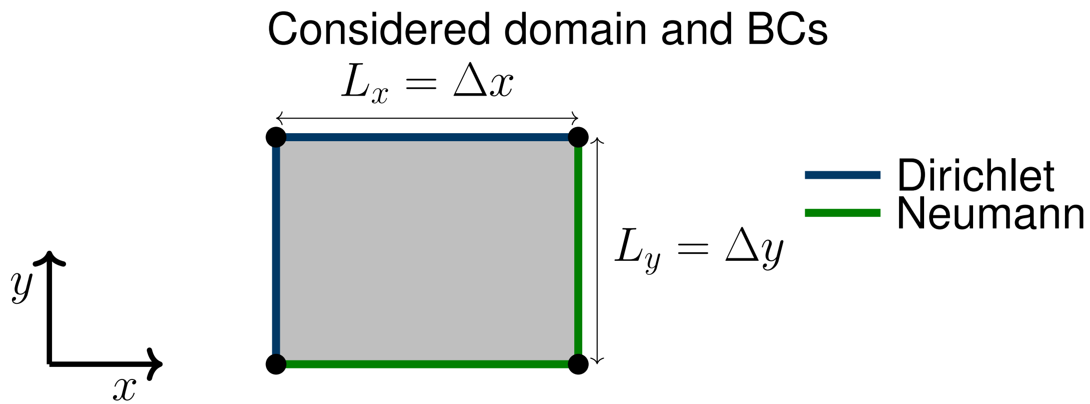
2.C Writing the equations in matrix form

An example with the implicit formulation of the BCs

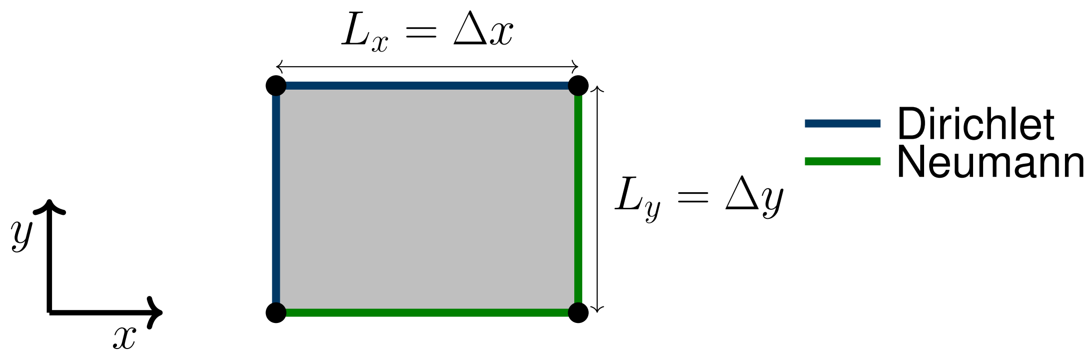
To illustrate this idea, we consider a (very) small example with $N_x = N_y = 2$.



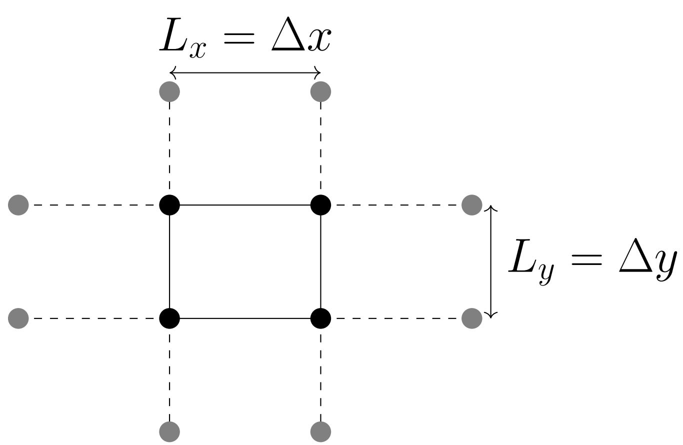
An example with the implicit formulation of the BCs

To illustrate this idea, we consider a (very) small example with $N_x = N_y = 2$.

Considered domain and BCs

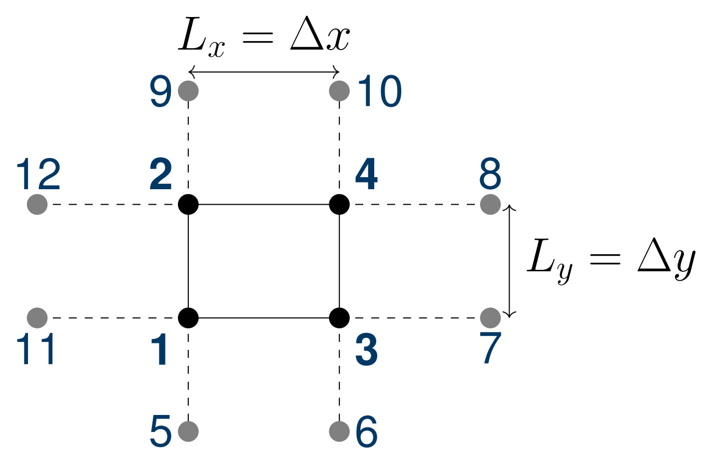


Grid with ghost points



Matrix form for the implicit formulation of the BCs: step 1

Step 1: Assign numbers to all nodes in the grid (including the ghost points).



Note: we can obtain the correct system of equations for any choice for the numbering.

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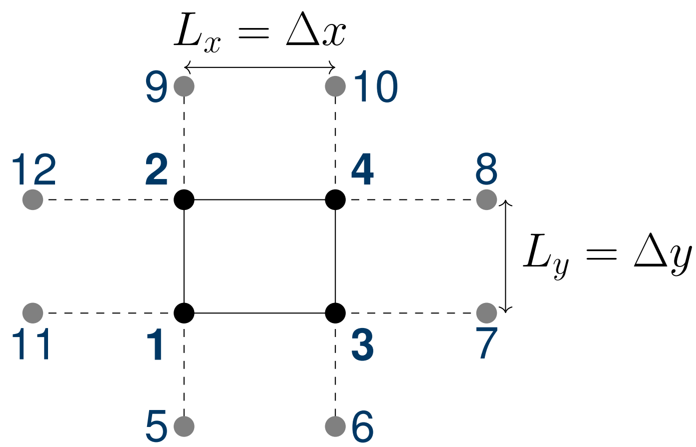


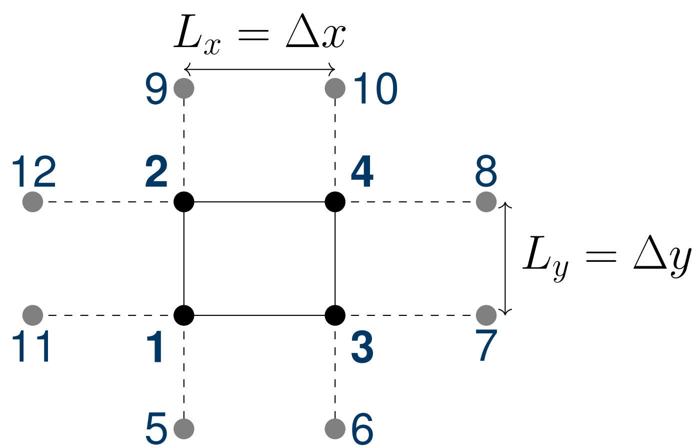
Note: we can obtain the correct system of equations for any choice for the numbering.

We can encode this numbering in the matrix `node_nbmrs`

$$\texttt{node\_nmbrs} = \begin{bmatrix} 0 & 11 & 12 & 0 \\ 5 & 1 & 2 & 9 \\ 6 & 3 & 4 & 10 \\ 0 & 7 & 8 & 0 \end{bmatrix}.$$

This is a very useful tool in the numerical implementation because one obtains the node number of the node at (x_i, y_j) as `node_nmbrs(i+1, j+1)`.
Note: we place zero at the locations for which there is no corresponding node.

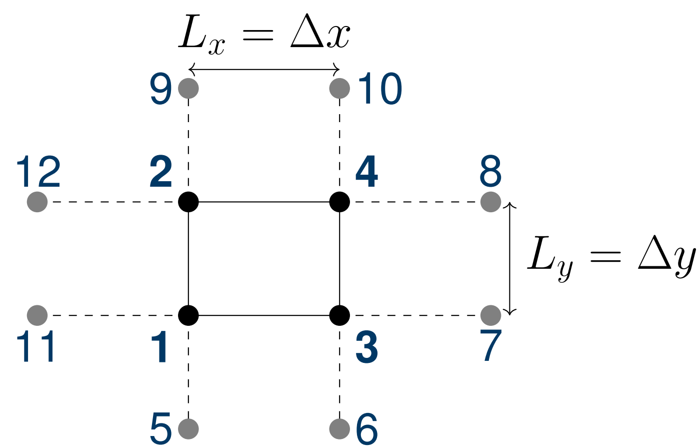
Matrix form for the implicit formulation of the BCs: step 2



Step 2: Define the number of nodes $\mathtt{nn} = N_x N_y + 2(N_x + N_y)$.
Set up a zero $\mathtt{nn} \times \mathtt{nn}$-matrix $\mathbf{A}$ and a zero $\mathtt{nn}$-(column)vector $\mathbf{f}$:

$$\underbrace{\begin{bmatrix} 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0&0&0&0 \end{bmatrix}}_{\mathbf{A}} \begin{bmatrix} u_1\\u_2\\u_3\\u_4\\u_5\\u_6\\u_7\\u_8\\u_9\\u_{10}\\u_{11}\\u_{12} \end{bmatrix} + \underbrace{\begin{bmatrix} 0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}}_{\mathbf{f}} = \begin{bmatrix} 0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0\\0 \end{bmatrix}.$$

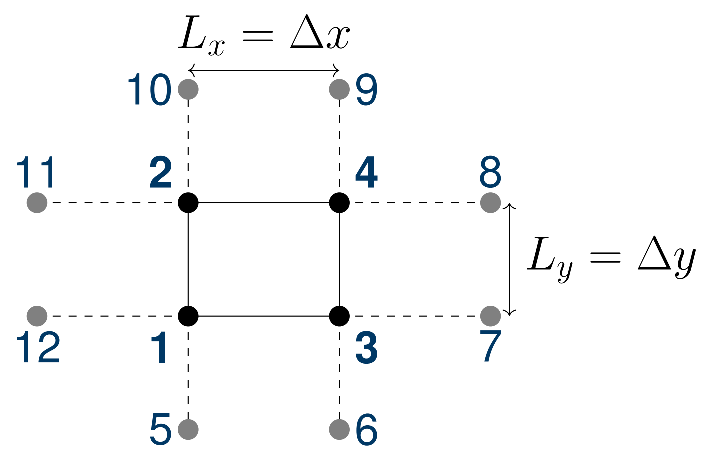
Matrix form for the implicit formulation of the BCs: step 3



Step 3: Write the equations for the internal nodes.

$$\begin{bmatrix}
\frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & 0 & 0 & 0 & 0 & 0 & \frac{1}{(\Delta x)^2} & 0 \\
\frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & \frac{1}{(\Delta y)^2} & 0 & 0 & \frac{1}{(\Delta x)^2} \\
\frac{1}{(\Delta x)^2} & 0 & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{(\Delta x)^2} & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & 0 & 0 & 0 & \frac{1}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix}
+
\begin{bmatrix} f_{11} \\ f_{12} \\ f_{21} \\ f_{22} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

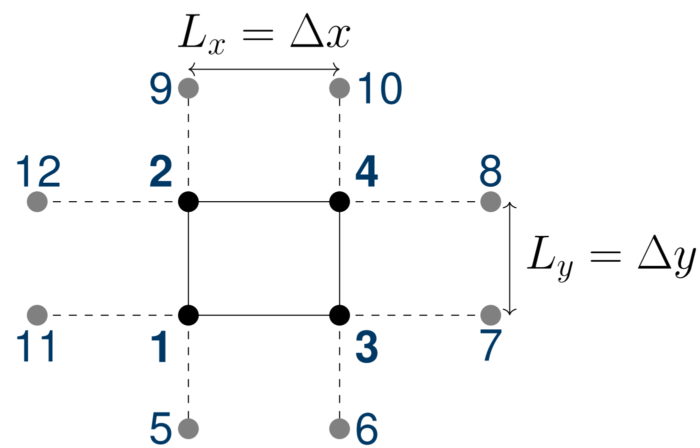
Matrix form for the implicit formulation of the BCs: step 4



Step 4: Write the equations for the Neumann boundary conditions.
(also for the edges on which Dirichlet BCs are applied).

$$
\begin{bmatrix}
\frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{(\Delta x)^2} \\
\frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & 0 & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 \\
\frac{1}{(\Delta x)^2} & 0 & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{(\Delta x)^2} & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2}+\frac{-2}{(\Delta y)^2} & 0 & 0 & 0 & \frac{1}{(\Delta x)^2} & \frac{1}{(\Delta y)^2} & 0 & 0 & 0 \\
0 & \frac{-1}{2\Delta y} & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{-1}{2\Delta y} & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{-1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 \\
\frac{-1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 \\
0 & 0 & 0 & \frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 \\
0 & 0 & \frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x}
\end{bmatrix}
\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix}
+
\begin{bmatrix} f_{11} \\ f_{12} \\ f_{21} \\ f_{22} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
=
\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}
$$

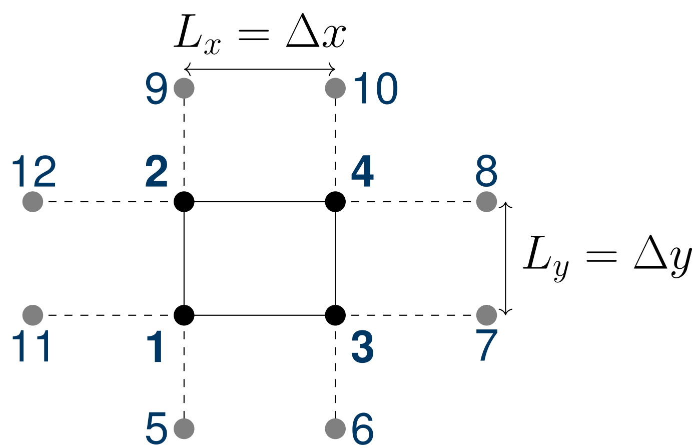
Matrix form for the implicit formulation of the BCs: step 5



Step 5: Delete the rows and columns of the nodes with *zero* Dirichlet BCs.

$$\begin{bmatrix} \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 \\ \frac{-1}{2\Delta y} & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 \\ \frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} \end{bmatrix} \begin{bmatrix} u_3 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix} + \begin{bmatrix} f_{21} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Matrix form for the implicit formulation of the BCs: step 5



Step 5: Delete the rows and columns of the nodes with *zero* Dirichlet BCs.

$$\begin{bmatrix} \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 & 0 & 0 & 0 \\ \frac{-1}{2\Delta y} & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta y} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} & 0 \\ \frac{-1}{2\Delta x} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2\Delta x} \end{bmatrix} \begin{bmatrix} u_3 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \\ u_{10} \\ u_{11} \\ u_{12} \end{bmatrix} + \begin{bmatrix} f_{21} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

For this (pathologically small) example we thus find that $u_3 = \frac{f_{21}}{\frac{2}{(\Delta x)^2} + \frac{2}{(\Delta y)^2}}$.

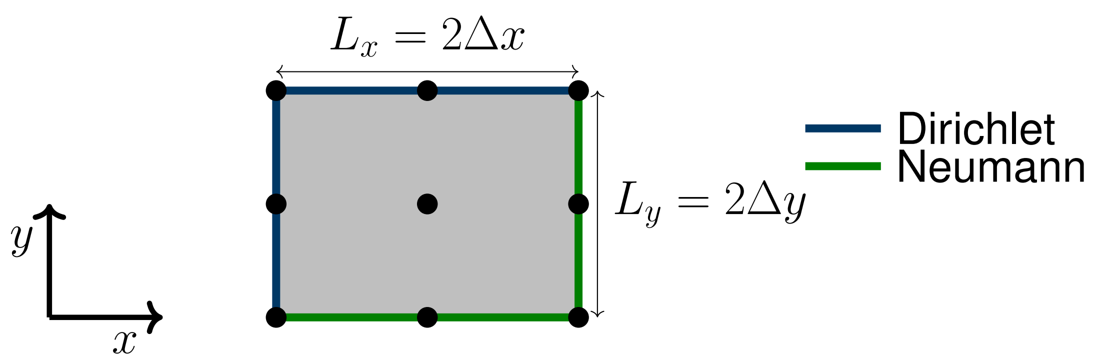
(The values in the ghost points are not of interest.)

An example with the explicit formulation of the BCs

With the explicit formulation, the involved matrices are slightly smaller.
We can therefore present on the slides an example with $N_x = N_y = 3$.

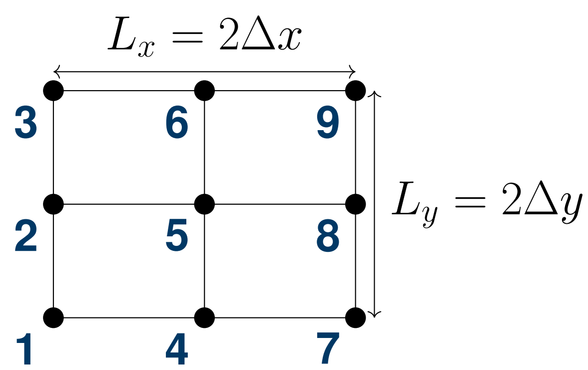
Note: for larger N_x and N_y, the difference between the $N_x N_y + 2(N_2 + N_y)$ nodes in the implicit formulation and the $N_x N_y$ nodes in the explicit formulation is neglegible.

Considered domain and BCs



Matrix form for the explicit formulation of the BCs: step 1

Step 1: Assign numbers to all nodes
(do not introduce and number ghost points!)

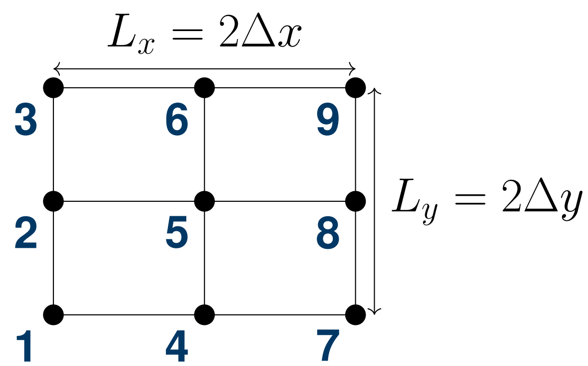


We can again construct the corresponding a matrix `node_nmbrs`

$$\texttt{node\_nmbrs} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}.$$

This matrix is very useful in the numerical implementation because we can find the number of the node at (x_i, y_j) as `node_nmbrs(i,j)`.

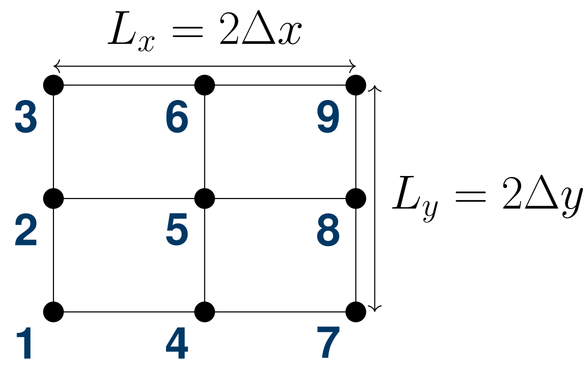
Matrix form for the explicit formulation of the BCs: step 2



Step 2: Define the number of nodes $\texttt{nn} = N_x N_y$.
Set up a zero $\texttt{nn} \times \texttt{nn}$-matrix $\mathbf{A}$ and a zero $\texttt{nn}$-(column)vector $\mathbf{f}$:

$$\underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}}_{\mathbf{A}} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \end{bmatrix} + \underbrace{\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}}_{\mathbf{f}} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

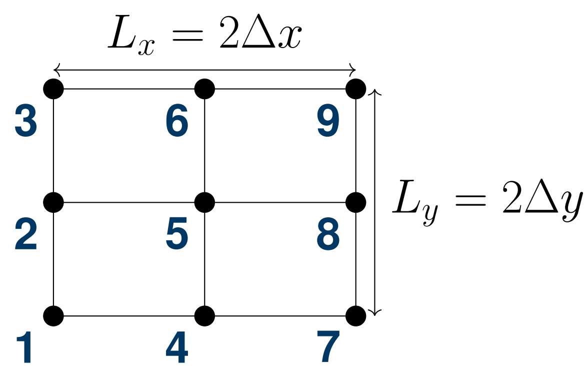
Matrix form for the explicit formulation of the BCs: step 3



Step 3: Write the equations for nodes not on the boundary.

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ f_{22} \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

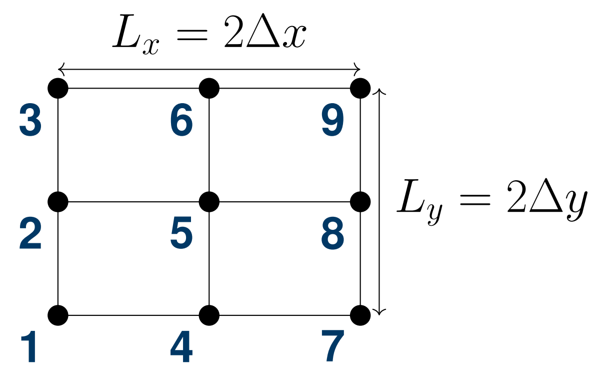
Matrix form for the explicit formulation of the BCs: step 4



Step 4: Write the equations for the Neumann boundary conditions.
(You can omit the nodes at which a Dirichlet BC is applied)

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{(\Delta x)^2} & 0 & 0 & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} & 0 & 0 \\ 0 & \frac{1}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{2}{(\Delta x)^2} & 0 & 0 & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{2}{(\Delta y)^2} & 0 \\ 0 & 0 & 0 & 0 & \frac{2}{(\Delta x)^2} & 0 & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{1}{(\Delta y)^2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \\ u_9 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ f_{21} \\ f_{22} \\ 0 \\ f_{31} \\ f_{32} \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Matrix form for the explicit formulation of the BCs: step 5



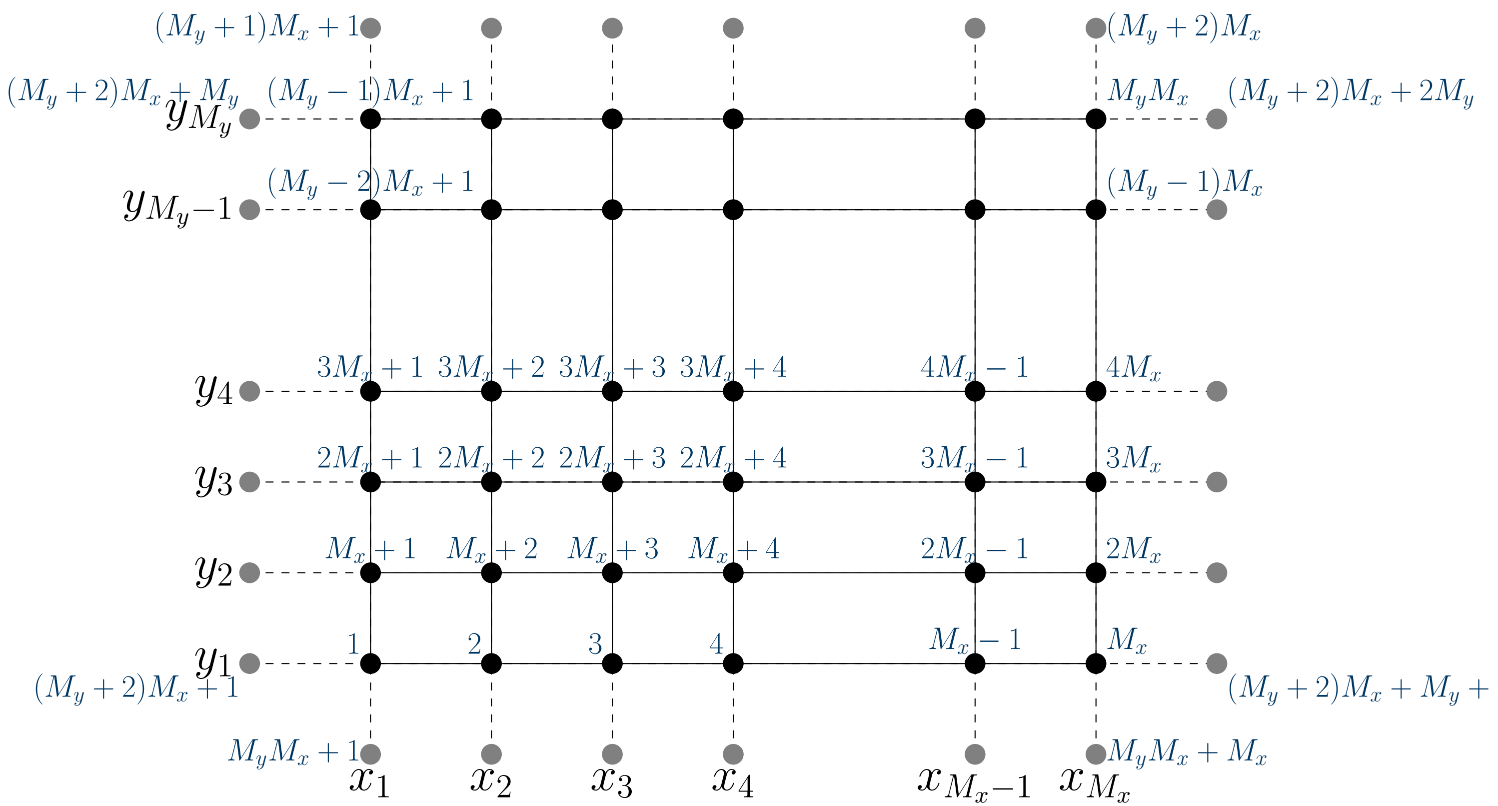
Step 5: Remove the rows and columns of nodes with *zero* Dirichlet BCs.

$$\begin{bmatrix} \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{2}{(\Delta y)^2} & \frac{1}{(\Delta x)^2} & 0 \\ \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & 0 & \frac{1}{(\Delta x)^2} \\ \frac{2}{(\Delta x)^2} & 0 & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} & \frac{2}{(\Delta y)^2} \\ 0 & \frac{2}{(\Delta x)^2} & \frac{1}{(\Delta y)^2} & \frac{-2}{(\Delta x)^2} + \frac{-2}{(\Delta y)^2} \end{bmatrix} \begin{bmatrix} u_4 \\ u_5 \\ u_7 \\ u_8 \end{bmatrix} + \begin{bmatrix} f_{21} \\ f_{22} \\ f_{31} \\ f_{32} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

This system can now be solved for u_4, u_5, u_7, and u_8.
Because of the Dirichlet BCs, we also know that $u_1 = u_2 = u_3 = u_6 = u_9 = 0$.

More general: numbering of the grid points

At which position do we store the element $u_{m\ell}$ in the vector $\mathbf{u}$?



Note: In principle, any numbering can be used.
But the numbering affects the structure of the matrix $\mathbf{A}$,
and may thus also affect how fast the system $\mathbf{Au}+\mathbf{f}=0$ can be solved.

Matrix with node numbers

```
node_nmbrs = zeros(Mx+2,My+2);
counter = 0;
for ll = 1:My
    for mm = 1:Mx
        counter = counter + 1;
        node_nmbrs(mm+1,ll+1) = counter;
    end
end
```

Note: for the implicit formulation of the BCs you also need to number the ghost points.

Matrix with node numbers

```
node_nmbrs = zeros(Mx+2,My+2);
counter = 0;
for ll = 1:My
    for mm = 1:Mx
        counter = counter + 1;
        node_nmbrs(mm+1,ll+1) = counter;
    end
end
```

Note: for the implicit formulation of the BCs you also need to number the ghost points. With this numbering, you can write the finite difference equations in matrix form.

$$\mathbf{A}\mathbf{u} + \mathbf{f} = 0.$$

Note: in principle the ordering of the rows/equations does not matter, but it is natural to use the ordering of the nodes/columns also for the rows/equations.

2.D Convergence analysis

Convergence analysis

Convergence analysis can be done similarly as for the 1-D problem in the previous lecture.
We can thus again show that

$$\|\mathbf{u} - u(\mathbf{x})\|_\infty \leq KC(\Delta x)^2.$$

The proof consists of two steps:

- Consistency $\|\mathbf{A}(\mathbf{u} - u(\mathbf{x}))\|_\infty = C(\Delta x)^2$
- Stability $\|\mathbf{u} - u(\mathbf{x})\|_\infty \leq K\|\mathbf{A}(\mathbf{u} - u(\mathbf{x}))\|_\infty$ (where K is independent of Δx)

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Two remarks:

- The stability argument is based on the discrete maximum principle
- The constant is C is proportional to

$$\max\left\{\left|\frac{\partial^4 u}{\partial x^4}\right|_{L^\infty}, \left|\frac{\partial^4 u}{\partial y^4}\right|_{L^\infty}\right\}.$$

(the solution of the continuous problem u should thus be sufficiently smooth)