Numerical Methods
in Engineering and Applied Science

Lecture 17. Partial differential equation.

A *partial differential equation* is an equation of the form

$$F(u, t, x, ...; u'_t, u'_x, ...; u''_{tt}, u''_{xx}, ...; ...) = 0 \tag{1}$$

where$u = u(t, x, ...)$ is the unknown function of the variables $t, x, ...$ and F is a given function. In general, we require that the sought solution u satisfy the equation for the values of $t, x, ...$ in a given domain Ω and that u satisfies other conditions called *initial conditions* and/or *boundary conditions*.
The equation is linear if F is a linear function.
The order of the highest partial derivative determines *the order of the equation.*
We speak of a *homogeneous* equation if the all terms contain the function and/or its partial derivatives. Otherwise, this is a *non-homogeneous* equation.

There is a classification of second order linear partial differential equations. Consider for example a partial differential equation written in the form:

$$Au_{xx} + Bu_{yy} + Cu_{xy} + Du_x + Eu_y + F = 0.$$

The "*elliptic*", "*parabolic*" or "*hyperbolic*" types correspond to the nature of the conical section described by the corresponding characteristic equation, i.e.:

$$Ax^2 + By^2 + Cxy + Dx + Ey + F = 0.$$

These names are also used for certain equations of order different from 2.
The *elliptic* equations often describe phenomena that do not depend on time. *Parabolic* equations correspond to diffusive phenomena. *Hyperbolic* equations correspond to wave propagation with finite velocity.

The model elliptic equation is the *Poisson equation*,

$$-\Delta u = f.$$

This equation models for example the phenomenon of heat conduction in steady state. In two-dimensional Cartesian coordinates, the Laplacian is

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

In polar coordinates ($x = r\cos\theta$, $y = r\sin\theta$) the Laplacian is

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}.$$

In elasticity, we also encounter the *bi-Laplacian* and the biharmonic equation,

$$\Delta^2 u = f.$$

The model parabolic equation is *the heat equation*,

$$u_t - \Delta u = f,$$

where $u_t = \partial_t u = \partial u / \partial t$ denotes the partial derivative of u with respect to time (u is therefore a function of x, space variable, and of t, time variable). This equation models the *diffusion* of quantities such as heat or salinity. This parabolic equation has two operators: the derivative of order 1 in time is a differential operator of order 2 (Laplace operator).
For a initial value problem defined by this equation and the initial condition u_0, it is easy to calculate the exact solution. For example, in 1D, $\Omega = \mathbb{R}$,

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\xi x - \xi^2 t} \hat{u}_0(\xi) d\xi = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{\infty} e^{-(x-s)^2/4t} u_0(s) ds.$$

The component of the initial condition which corresponds to the wavenumber ξ decreases as $e^{-\xi^2 t}$.

Hyperbolic type equations are often obtained by neglecting diffusion phenomena in the conservation equations of mechanics. The most classical example of a linear hyperbolic equation is *the transport* (or *advection* equation),

$$u_t = u_x \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}. \tag{2}$$

If the initial condition

$$u(x, 0) = u_0(x) \tag{3}$$

is sufficiently smooth, it is easy to see that the function

$$u(x, t) = u_0(x + t) \tag{4}$$

is a solution of (2)-(3). If u_0 is not regular (for example discontinuous), there is still a way to show that the function defined by (4) is a solution in a “ weak” sense.

If the equation is nonlinear, i.e.

$$u_t = (f(u))_x \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}. \tag{5}$$

with for example $f(u) = u^2$, and initial condition (3), we can still define weak solutions, but their computation is more difficult.

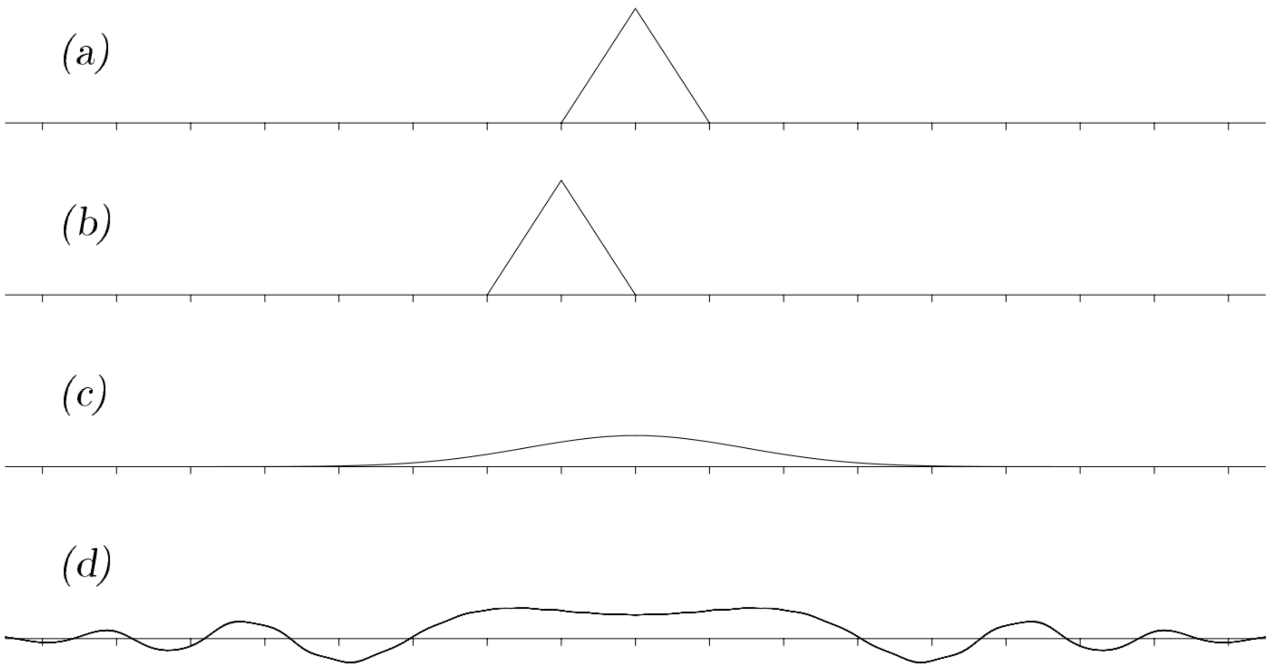
Another example of a hyperbolic equation is the *Schrödinger equation*. In 1D,

$$u_t = iu_{xx}, \qquad t \in \mathbb{R}_+, \quad x \in \mathbb{R}. \tag{6}$$

The exact solution is

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{i\xi x - i\xi^2 t}\hat{u}_0(\xi)d\xi = \frac{1}{\sqrt{4\pi i t}}\int_{-\infty}^{\infty} e^{i(x-s)^2/4t}u_0(s)ds.$$

This equation is *dispersive*: the solution forms wave packets.



(a) : initial condition; (b) : solution at $t = 1$, advection equation; (c) : solution at $t = 1$, heat equation; (d) : solution at $t = 1$, Schrödinger equation.

Advection, diffusion and dispersion mechanisms characterize many linear phenomena. The equations above are model equations useful for analyzing more complex PDEs as well as numerical methods.
These generalities can be extended to PDE systems where we need to determine several unknown functions u_1, u_2, ... of variables $t, x, ...$; in this case, F of (1) is a vector function of the vector unknown function $u = (u_1, u_2, ...)$ and its partial derivatives.

Main methods of discretization.
Finite difference methods.
The essence of finite difference methods consists in taking a certain number of points of the domain which we will note $(x_1, ..., x_N)$. We approximate the differential operator at every point x_i by finite differences.

Finite volume method.
Finite volume methods have been adapted to conservation equations and have been used in fluid mechanics for several decades. The principle consists of dividing the domain Ω into "control volumes"; we integrate the conservation equation over the control volumes; we then approach the fluxes on the faces of the control volume by finite differences.
Variational methods, finite element methods
We put the problem of partial differential equations in a variational form:

$$\begin{cases} a(u,v) = (f,v)_H, \quad \forall v \in H, \\ u \in H \end{cases}$$

where H is a suitably chosen Hilbert space (for example because there is existence and uniqueness of the solution in this space), $(\cdot,\cdot)_H$ the scalar product on H and a a bilinear form. The discretization consists in replacing H by a finite dimensional subspace H_k, constructed for example using finite element basis functions:

$$\begin{cases} a(u_k, v_k) = (f, v_k)_H, & \forall v_k \in H_k, \\ u_k \in H_k. \end{cases}$$

For example, consider the Poisson equation

$$-\Delta u = f$$

With a homogeneous Dirichlet boundary condition. Let v be arbitrary, zero on the boundary. Multiply both parts of the previous equation by v then sum over the domain Ω,

$$-\int_\Omega v\Delta u \; d\omega = \int_\Omega vf \; d\omega.$$

We use Green's formula to obtain the weak formulation of the problem:

$$\int_\Omega \nabla v \cdot \nabla u \; d\omega = \int_\Omega vf \; d\omega.$$

Spectral methods.

The idea of these methods is to seek an approximate solution in the form of an expansion on a certain family of functions. We choose the basis so that the derivatives are easy to calculate. These latter methods are reputed to be expensive, but accurate. They are most often used as an aid to understanding physical phenomena.

Finite difference methods, elliptic problems.

Consider the Poisson equation in 1D,

$$-u''(x) = f(x), \quad 0 < x < 1, \tag{7}$$

with the boundary conditions

$$u(0) = \alpha, \quad u(1) = \beta. \tag{8}$$

We are looking for $U_0, U_1, ..., U_m, U_{m+1}$, where U_j is an approximation of $u(x_j)$, $x_j = jh$, $h = 1/(m+1)$ is the discretization step. The boundary conditions give $U_0 = \alpha$ and $U_{m+1} = \beta$. The unknowns are $U_1, ..., U_m$. The second-order central finite difference method gives

$$-\frac{1}{h^2}(U_{j-1} - 2U_j + U_{j+1}) = f(x_j), \quad j = 1, 2, ..., m.$$

We obtain a linear system with the tridiagonal matrix which we solve with a direct method.

Now consider the Poisson equation in 2D, in Cartesian coordinates,

$$-(u_{xx} + u_{yy}) = f. \tag{9}$$

It is necessary to specify boundary conditions at the boundary of the domain. For example, Robin boundary condition,

$$au + b\frac{\partial u}{\partial n} = g \quad \text{sur} \quad \partial\Omega,$$

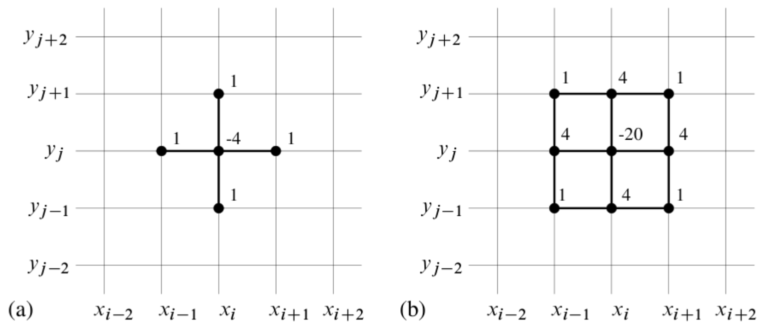
where a, b and g are functions on $\partial\Omega$ and $\partial u/\partial n$ denotes the derivative with respect to the outer normal on the boundary. If $b = 0$, we obtain the Dirichlet condition. If $a = 0$, we obtain the Neumann condition.
Suppose that Ω is the square $0 \leq x \leq 1$, $0 \leq y \leq 1$ and that the boundary conditions are those of Dirichlet. We define the grid (x_i, y_j), where $x_i = i\Delta x$ and $y_j = j\Delta y$. If we replace u_{xx} and u_{yy} by their approximations by second order finite differences, we obtain

$$-\left(\frac{1}{(\Delta x)^2}(u_{i-1,j} - 2u_{ij} + u_{i+1,j}) + \frac{1}{(\Delta y)^2}(u_{i,j-1} - 2u_{ij} + u_{i,j+1})\right) = f_{ij}.$$

This is the 5-point Laplacian. In the case $\Delta x = \Delta y \equiv h$, we can rewrite it as

$$-\frac{1}{h^2}(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}) = f_{ij},$$

where $i = 1, 2, ..., m$, $j = 1, 2, ..., m$ and $h = 1/(m+1)$. We have m^2 unknowns u_{ij} and m^2 equations.



The matrix if this system is of size $m^2 \times m^2$. It is sparse. Each row has no more than 5 non-zero elements. This matrix is less compact than in 1d. There are two ways to regroup elements. The natural way is to compose the vector u from $u_{11}, u_{21}, u_{31}, ..., u_{m1}$ followed by $u_{12}, u_{22}, u_{32}, ..., u_{m2}$, etc. So we get

$$u = \begin{pmatrix} u^{[1]} \\ u^{[2]} \\ \vdots \\ u^{[m]} \end{pmatrix}, \quad \text{where} \quad u^{[j]} = \begin{pmatrix} u_{1j} \\ u_{2j} \\ \vdots \\ u_{mj} \end{pmatrix}.$$

The elements of the vector f_{ij} are reordered accordingly. We obtain the system

$$Au = f$$

where the matrix A consists of blocks.

$$A = -\frac{1}{h^2}\begin{pmatrix} T & I & & & \\ I & T & I & & \\ & I & T & I & \\ & & \ddots & \ddots & \ddots \\ & & & I & T \end{pmatrix}$$

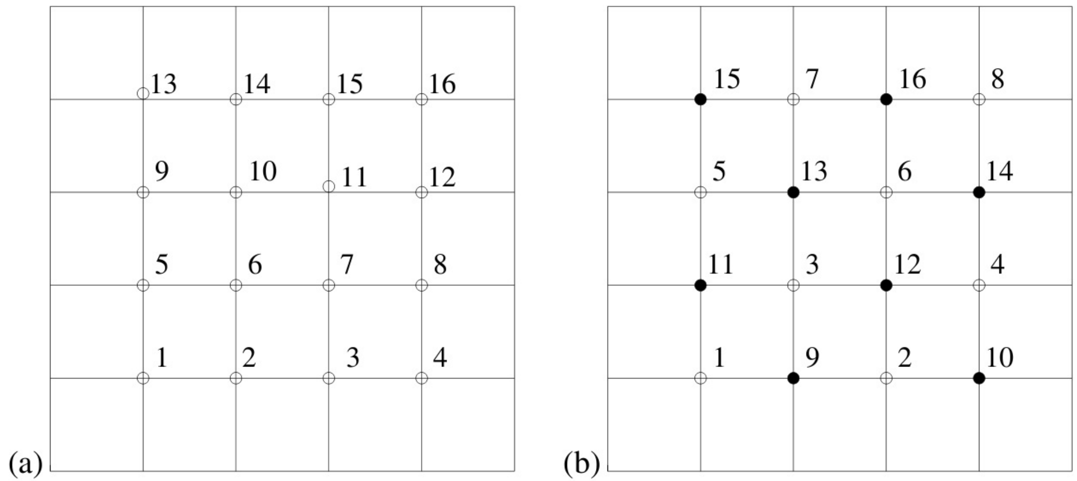
where the blocks T and I are of size $m \times m$, I is the identity matrix and

$$T = \begin{pmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & 1 & -4 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -4 \end{pmatrix}$$

Another effective structure is checkerboard, which gives the system

$$\begin{pmatrix} D & H \\ H^T & D \end{pmatrix} \begin{pmatrix} u_A \\ u_B \end{pmatrix} = \begin{pmatrix} f_A \\ -f_B \end{pmatrix}$$

with $D = \frac{4}{h^2} I$ being a diagonal matrix of size $m^2/2$ and H a band matrix with 4 nonzero diagonals.



To do the error analysis, we define the local truncation error,

$$\tau_{ij} = -\frac{1}{h^2}(u(x_{i-1}, y_j)+u(x_{i+1}, y_j)+u(x_i, y_{j-1})+u(x_i, y_{j+1})-4u(x_i, y_j))-f(x_i, y_j)$$

and we get, by Taylor expansion,

$$\tau_{ij} = -\frac{1}{12}h^2(u_{xxxx} + u_{yyyy}) + \mathcal{O}(h^4).$$

The global error $E_{ij} = u_{ij} - u(x_i, y_j)$ is the solution of a system

$$A^h E^h = -\tau_{ij}$$

where A^h is the discretization matrix with step h. Convergence is of order 2 if it is stable, i.e. $||(A^h)^{-1}||$ is uniformly bounded in limit $h \to 0$. We know how to calculate the norm 2 of this matrix. The eigenvectors are

$$u_{ij}^{p,q} = \sin(p\pi ih)\sin(q\pi jh)$$

and the eigenvalues are

$$\lambda_{p,q} = \frac{2}{h^2}((\cos(p\pi h) - 1) + (\cos(q\pi h) - 1))$$

for the parameters $p, q = 1, 2, ..., m$ which correspond to the wavenumbers in the two directions.
The eigenvalues are all negative and the value closest to zero is

$$\lambda_{1,1} = -2\pi^2 + \mathcal{O}(h^2).$$

The spectral radius of $(A^h)^{-1}$ is

$$\rho((A^h)^{-1}) = 1/\lambda_{1,1} \approx -1/2\pi^2.$$

and the method is stable in second norm. Moreover, we see that

$$\kappa_2(A) \approx \frac{4}{\pi^2 h^2} = \mathcal{O}(1/h^2) \quad \text{in the limit of} \quad h \to 0.$$

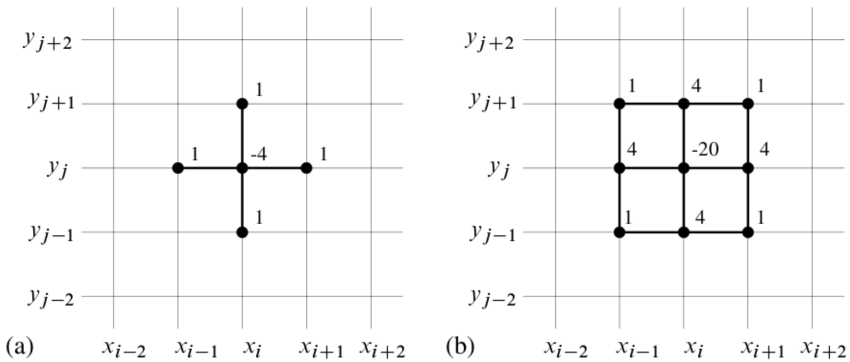
Consider again the Laplacian in 2D, in Cartesian coordinates,

$$\nabla^2 u = u_{xx} + u_{yy} \tag{10}$$

In the case $\Delta x = \Delta y \equiv h$, we write the 5-point scheme as

$$\nabla_5^2 u_{ij} = \frac{1}{h^2}(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}).$$

where $i = 1, 2, ..., m$, $j = 1, 2, ..., m$ et $h = 1/(m + 1)$.



For the Poisson equation with the homogeneous Dirichlet boundary condition we obtain the system

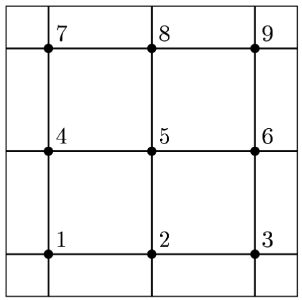
$$Au = f$$

with the block matrix A,

$$A = -\frac{1}{h^2}\begin{pmatrix} T & I & & & \\ I & T & I & & \\ & I & T & I & \\ & & \ddots & \ddots & \ddots \\ & & & I & T \end{pmatrix} \quad \text{où} \quad T = \begin{pmatrix} -4 & 1 & & & \\ 1 & -4 & 1 & & \\ & 1 & -4 & 1 & \\ & & \ddots & \ddots & \ddots \\ & & & 1 & -4 \end{pmatrix},$$

I is the identity matrix,

$u = (u_{11}, u_{21}, ..., u_{m1}, u_{12}, u_{22}, ..., u_{m2}, ..., u_{1m}, u_{2m}, ..., u_{mm})$ et $f = (f_{11}, f_{21}, ..., f_{m1}, f_{12}, f_{22}, ..., f_{m2}, ..., f_{1m},$



To obtain matrices of the operators with differences in 2d, one can use the Kronecker matrix product $A \otimes B$. If A is of size $p \times q$ and B is of size $r \times s$, the matrix $A \otimes B$ is of size $pr \times pq$ with $p \times q$ block, and block i, j is $a_{ij}B$. For example,

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \otimes \begin{pmatrix} a & b \\ c & d \end{pmatrix} = \left(\begin{array}{cc|cc} a & b & 2a & 2b \\ c & d & 2c & 2d \\ \hline 3a & 3b & 4a & 4b \\ 3c & 3d & 4c & 4d \end{array}\right).$$

For example, if $m = 3$, the matrix of the Laplacian in 1D is

$$D^2 = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & \\ 1 & -2 & 1 \\ & 1 & -2 \end{pmatrix}$$

Then in 2D, the derivative with respect to x is calculated by the matrix

$$I \otimes D^2 = \frac{1}{h^2}\left(\begin{array}{ccc|ccc|ccc} -2 & 1 & & & & & & & \\ 1 & -2 & 1 & & & & & & \\ & 1 & -2 & & & & & & \\ \hline & & & -2 & 1 & & & & \\ & & & 1 & -2 & 1 & & & \\ & & & & 1 & -2 & & & \\ \hline & & & & & & -2 & 1 & \\ & & & & & & 1 & -2 & 1 \\ & & & & & & & 1 & -2 \end{array}\right)$$

The derivative with respect to y is calculated by the matrix

$$D^2 \otimes I = \frac{1}{h^2}\left(\begin{array}{ccc|ccc|ccc} -2 & & & 1 & & & & & \\ & -2 & & & 1 & & & & \\ & & -2 & & & 1 & & & \\ \hline 1 & & & -2 & & & 1 & & \\ & 1 & & & -2 & & & 1 & \\ & & 1 & & & -2 & & & 1 \\ \hline & & & 1 & & & -2 & & \\ & & & & 1 & & & -2 & \\ & & & & & 1 & & & -2 \end{array}\right)$$

The discrete Laplacian is

$$A = I \otimes D^2 + D^2 \otimes I.$$

The Matlab program to generate this matrix:

```
I = eye(m);
e = ones(m,1);
D2 = spdiags([e -2*e e],[-1 0 1],m,m);
A = (kron(I,D2) + kron(D2,I))/h^2;
```

We can construct a 9-point scheme, very accurate for harmonic functions.

$$\nabla_9^2 u_{ij} = \frac{1}{6h^2}(4u_{i-1,j} + 4u_{i+1,j} + 4u_{i,j-1} + 4u_{i,j+1} + u_{i-1,j-1} + u_{i-1,j+1} + u_{i+1,j-1} + u_{i+1,j+1} - 20u_{ij}).$$

We use Taylor series to show that

$$\nabla_9^2 u - \nabla^2 u = \frac{1}{12}h^2\nabla^4 u + \frac{2}{6!}h^4\left[\nabla^6 u + 2\frac{\partial^4(\nabla^2 u)}{\partial x^2 \partial y^2}\right] + \mathcal{O}(h^6).$$

If u satisfies $-\nabla^2 u = f$ with f harmonic, i.e. $\nabla^2 f = 0$, then $\nabla^4 u = 0$ and we get

$$\nabla_9^2 u - \nabla^2 u = \mathcal{O}(h^4).$$

If $f \equiv 0$, i.e., if u is harmonic ($\nabla^2 u = 0$) then we see that

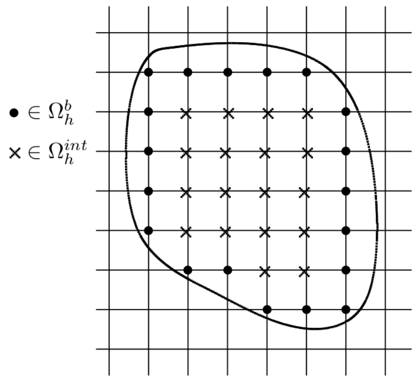
$$\nabla_9^2 u - \nabla^2 u = \mathcal{O}(h^6). \qquad (11)$$

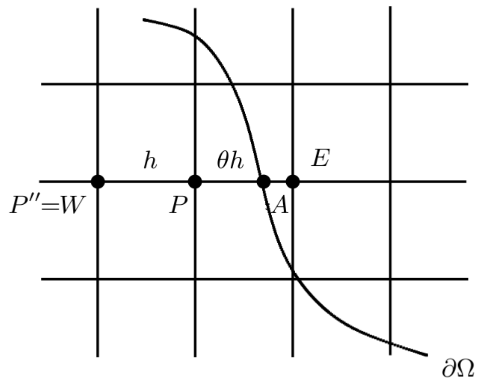
For any other function f sufficiently derivable, we get $||u(x_i, y_j) - u_{ij}|| + \mathcal{O}(h^4)$ by introducing a correction,

$$-\nabla_9^2 u_{ij} = f(x_i, y_j) - \frac{h^2}{12}\nabla_5^2 f(x_i, y_j).$$

Non-rectangular case.

Care must be taken to discrete the operator near the edge of a non-rectangular domain, so as not to lose the order of consistency.





We use the 5-point scheme for points surrounded by interior points. For the other points close to the boundary, we proceed by linear interpolation,

$$u(P) = \frac{1}{\theta+1}u(A) + \frac{\theta}{\theta+1}u(P'') + \mathcal{O}(h^2).$$

given the boundary condition of the problem which gives $u(A) = 0$ we obtain the approximate problem

$$-Lu(P) = \tilde{f}(P)$$

with

$$Lu(P) = \begin{cases} \nabla_5^2 u(P) & \text{si} \quad P \in \Omega_h^{int} \\ u(P) - \frac{\theta}{\theta+1}u(P'') & \text{if} \quad P \in \Omega_h^b. \end{cases}$$

and

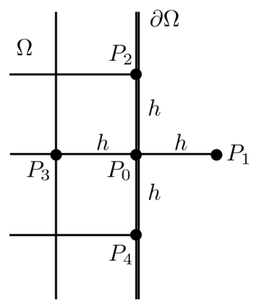
$$\tilde{f}(P) = \begin{cases} f(P) & \text{si} \quad P \in \Omega_h^{int} \\ 0 & \text{si} \quad P \in \Omega_h^b. \end{cases}$$

Non-homogeneous Dirichlet condition. We impose $u|_{\partial\Omega} = g$. Compared to the Dirichlet condition homogeneous ($u|_{\partial\Omega} = 0$), the number of unknowns remains the same and the matrix A is unchanged. Only the second term is changed.

Neumann condition for the Laplacian on a square. We impose

$$\frac{\partial u}{\partial \boldsymbol{n}} := \nabla u \cdot \boldsymbol{n} = g \quad \text{sur} \quad \partial\Omega$$

where is the unit exterior normal to the boundary $\partial\Omega$. A 'mirror imaging' technique is used.



Let P_0 be a mesh node belonging to edge $\partial\Omega$. We have

$$g(P_0) = \frac{\partial u}{\partial \boldsymbol{n}}(P_0) = \frac{u(P_1) - u(P_3)}{2h} + \mathcal{O}(h^2).$$

We write for the approximation of u:

$$u(P_1) = 2hg(P_0) + u(P_3)$$

and we substitute this expression in ∇_5^2,

$$\begin{aligned}\nabla_5^2 u(P_0) &= \tfrac{1}{h^2}\left[-4u(P_0) + u(P_1) + u(P_2) + u(P_3) + u(P_4)\right] \\ &= \tfrac{1}{h^2}\left[-4u(P_0) + (2hg(P_0) + u(P_3)) + u(P_2) + u(P_3) + u(P_4)\right]\end{aligned}$$

The equation $-\nabla_5^2 u(P_0) = f(P_0)$ becomes

$$-\frac{1}{h^2}\left[-4u(P_0) + 2u(P_3) + u(P_2) + u(P_4)\right] = -\frac{2}{h}g(P_0) + f(P_0).$$

Neumann's condition for the Laplacian on a non-rectangular domain. We use the same technique and linear interpolation.