Workshop Numerics of the Laplace and Poisson Equation

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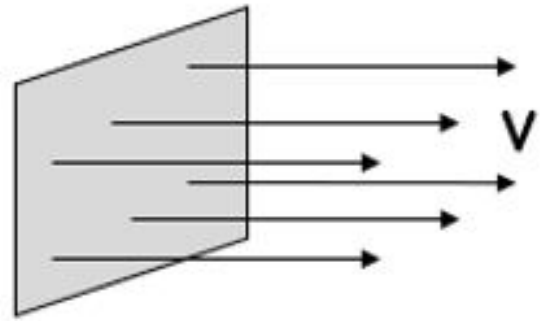
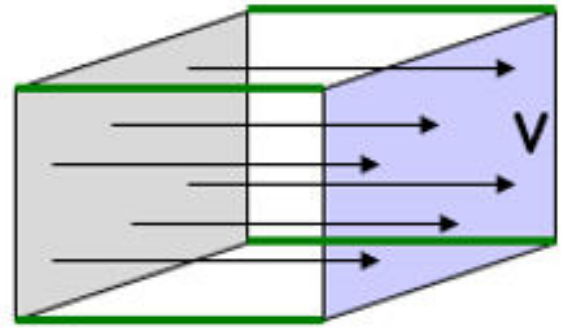
Chapter 1

Flux and divergence



If a physical quantity is being transferred, the **flux** is the amount passing per second trough a window of one unit area perpendicular to the flow.



If the arrows indicate the (local) velocity v of the flow, the flux is just the contents of the box spanned by the window and the velocity vector.

Examples: the mass flux is ρv, the heat energy flux is hv (with h the energy density), and the volume flux is just v.

If the area is not unity, but *A*, the flow per second is the flux times *A*.

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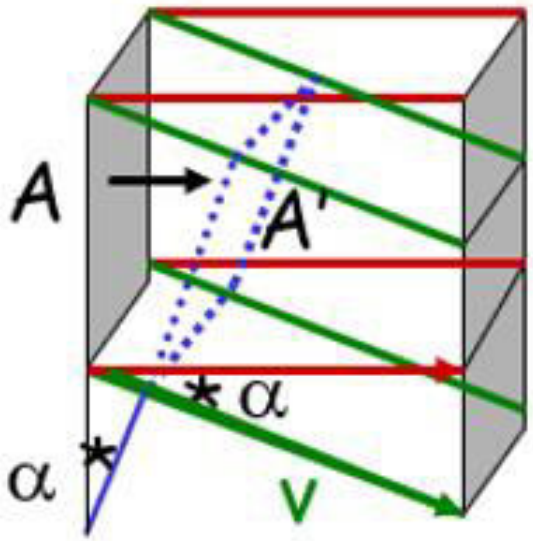
And if the window is not perpendicular to the flow, a factor $\cos\alpha$ enters:



Volume = $A' \times$ length of $v = A \cos\alpha \times |v|$

Volume = $A \times$ perpendicular component of v

$= A \times v \cos\alpha$

$A\, v \cos\alpha = A\ \ \mathbf{v}\cdot\mathbf{n}$, $\mathbf{n}$ normal to the surface

The flux through a general surface is an integral:

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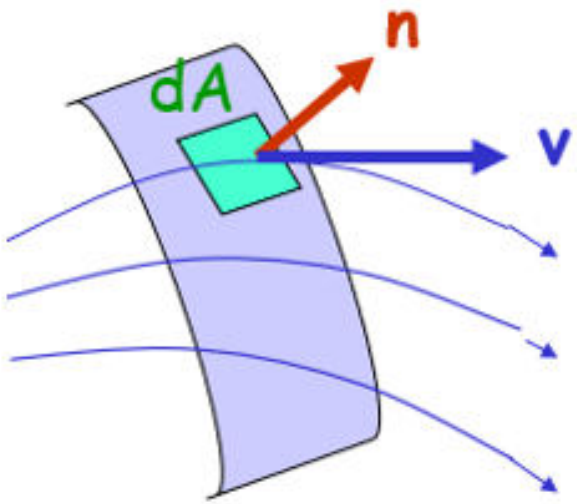
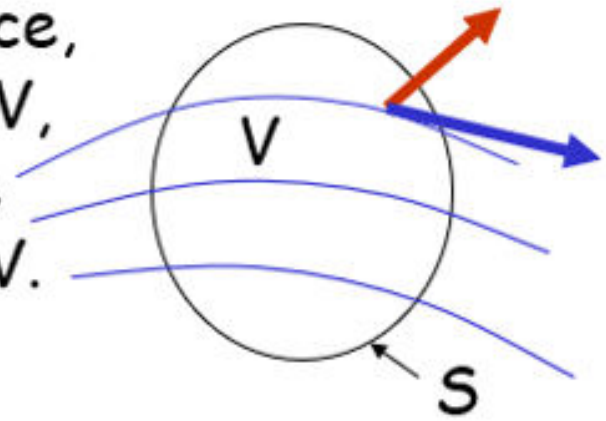


If S is a closed surface, surrounding a volume V, this integral is the net outflux out of V.



When divided by the volume, we get the average outflux density in V.

In the limit for V -> 0, this becomes the local outflux density, and we call it the divergence of the vectorfield **v**:

$$\operatorname{div} \mathbf{v} = \lim_{V \to 0} \frac{\oiint \mathbf{v}\cdot\mathbf{n}\, dA}{V} \qquad (2)$$

If the quantity that is transferred, cannot disappear into nothing, cannot be compressed or expanded, we expect the flux integral over the closed surface S to be zero: “what comes in goes out”, and the net outflow is zero. If this integral would have a positive value, then there is production of the quantity inside the volume, at a rate equal to the net outflux per second, and the production density (production per unit volume) is given by the divergence of the flow field. (see the yellow box)

In a divergence-free field,

the flux integral over any closed surface is zero. (3)

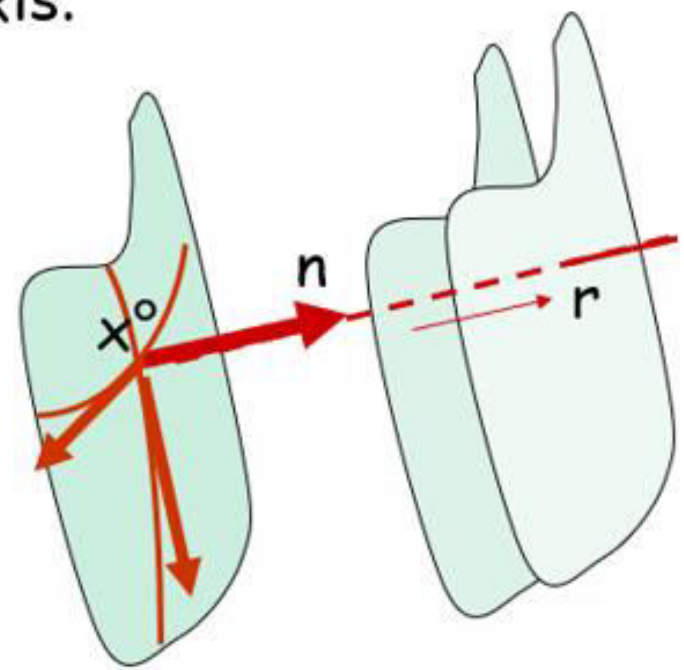
Chapter 2

Gradient and directional derivative

Let f be a scalar function in 3-dim. space, x° a point, and let $f(x^\circ) =: c$. All x with $f(x) = c$ make a surface in space. In x° choose a local coordinate system, two axes tangential to the surface, the third one, the r-axis say, perpendicular. Let n be the unit vector along the r-axis.

Then f is a function of r only: $f=f(r)$, and the first order behavior of f in x° is fully known by the value of df/dr at r=0, [i.e. at x°], and the direction n, that is: by the vector $f'(0)\,n$. This vector is what we call the gradient:

$$\text{grad } f(x^\circ) = f'(r=0)\,n \qquad (4)$$

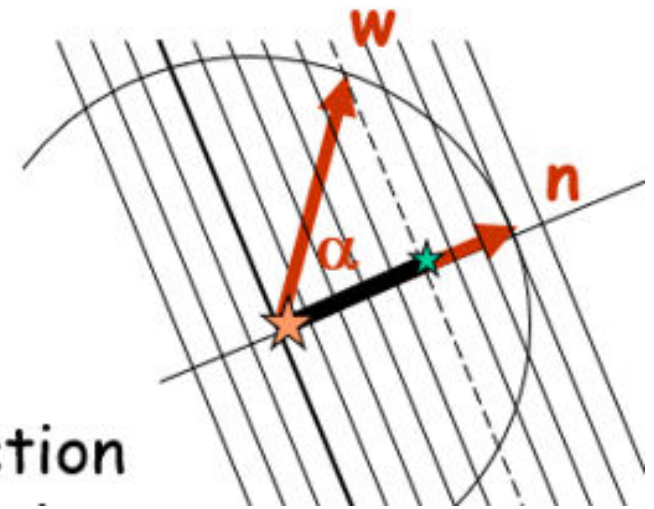


$$\text{grad } f\,(x^\circ) \;=\; f'\,(r=0)\;\mathbf{n} \qquad (4)$$

The gradient of a scalar function f is the vector pointing into the direction of steepest increase with modulus equal to the value of this increase.

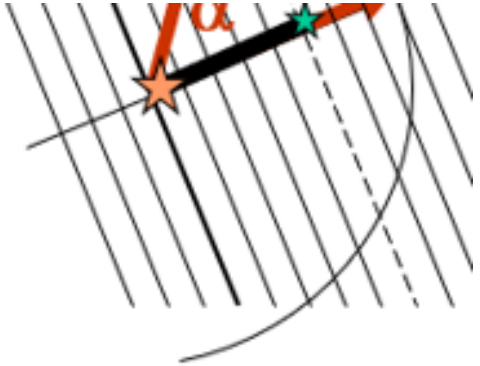
The derivative in any other direction **w** is smaller in modulus, involving the cos of the angle in between **w** and **n** :

$$\partial_{\mathbf{w}} f \;\equiv\; \mathbf{w} \bullet \text{grad } f \qquad (5)$$



In particular, the derivative in the direction

$$\partial_{\boldsymbol{w}} f \equiv \boldsymbol{w} \bullet \operatorname{grad} f \qquad (5)$$



In particular, the derivative in the direction of $\boldsymbol{e}_1$, the first basis vector, denoted by $\boldsymbol{\partial}_1$, is what we get when choosing $\boldsymbol{w} = \boldsymbol{e}_1$:

$$\partial_1 f = \frac{\partial}{\partial x} f = \boldsymbol{e}_1 \bullet \operatorname{grad} f$$

In words: the first component of grad f is $\boldsymbol{\partial}_1 f$. Similar for 2 and 3. So in total:

$$\operatorname{grad} f = \begin{pmatrix} \partial_1 f \\ \partial_2 f \\ \partial_3 f \end{pmatrix} = \begin{pmatrix} \dfrac{\partial f}{\partial x} \\ \dfrac{\partial f}{\partial y} \\ \dfrac{\partial f}{\partial z} \end{pmatrix}$$

Motivations for chapter 1 and 2:

In most textbooks the operators $grad$ and div (and $curl$) are **defined** in terms of partial derivatives with respect to the three cartesian coordinates; and then certain properties of the operators are shown. But in fact, $grad$, $curl$, div are **coordinate-free concepts**, as we have shown: we first defined the concepts, only later we introduced the cartesian coordinates, and we saw that they take the familiar form in terms of partial derivatives.

It is just a different, more physical way of looking at the material.

Chapter 3 Laplace Equation (divergence-free gradient fields) and **stationary heat flow** as a physical example

From now on, all our material (Laplace Equation, physical interpretation of the boundary conditions, discretization formula's and numerical treatment) will be illustrated by the example of stationary heat flow in a thermally conductive medium.

We will work with the following quantities.

The **temperature field** u is a scalar field such that $u(x, y, z)$ denotes the temperature in the point (x, y, z).

The **heat flow field** $\boldsymbol{\varphi}$ is a vector field (therefore we use bold face), such that $\boldsymbol{\varphi}(x, y, z)$ is a vector with the direction of the heat flow in the point (x, y, z), and with length (magnitude) equal to the amount of heat that per second passes through a virtual window of unit area, positioned at (x, y, z) and perpendicular to the direction of the flow (see previous section).
This quantity is called the **flux** at (x, y, z).

At this moment it seems we have *two* unknown fields: the scalar field u, and the vector field $\boldsymbol{\varphi}$, which is equivalent to *three* scalar fields, so in total we have four unknown scalar fields. Fortunately this complexity is immediately reduced to only *one scalar field*, by **Fourier**'s Law, which says that in stationary situations

$$\boldsymbol{\varphi}(x,y,z) = -\lambda \; grad \; u(x,y,z) \qquad (6)$$

that is:

- in magnitude, the heat flux vector is proportional to the local gradient of the temperature field
- while the direction of the heat flux is opposite to the direction of the temperature gradient, that is: in de direction of steepest descent.

where λ is a positive factor, a material constant, called the **conductivity**.

Referring to earlier discussion of divergence we have:

$$div\big(\boldsymbol{\varphi}(x,y,z)\big) = f(x,y,z), \tag{7}$$

where $f(x,y,z)$ is the **production density**, that is: the amount of heat that is produced per second in a unit volume at the position (x,y,z). If there is no heat production, i.e. $f = 0$, then the divergence (7) is zero, and we say that $\boldsymbol{\varphi}$ is a *divergence-free* flow field.

To illustrate the concept of heat production we can think of a block of material, in the interior of which an electrical wire is producing heat. This is not an ideal example: due to the presence of the wire the assumption of a homogeneous medium is no longer satisfied. Another example: consider a heap of mowed grass (e.g. meant as food storage for cattle), in which a fermentation process takes place everywhere, creating heat. This heat will find a way out through the surface of the heap, and in stationary situation we have equation (7).

$$\boldsymbol{\varphi}(x,y,z) = -\lambda\ grad\ u(x,y,z) \tag{6}$$

$$div\big(\boldsymbol{\varphi}(x,y,z)\big) = f(x,y,z), \tag{7}$$

Now combining eqs (6) and (7) we get

$$div\big(\lambda\ grad\ u(x,y,z)\big) = -f(x,y,z), \tag{8}$$

that is: $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = -\frac{1}{\lambda} f(x,y,z)$ **Poisson Equation** (9)

In case of no heat production inside the domain, the right hand side is zero, and we have:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} = 0 \qquad \textbf{Laplace Equation} \tag{10}$$

Definition: a second order PDE in n coordinates: $\sum_{i,j=1}^{n} a_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} u + \text{lower order terms} = f$, is

elliptic if the matrix A formed by the coefficients $\{a_{i,j}\}$, $i,j = 1, \dots, n$, is positive definite

When these coefficients $\{a_{i,j}\}$ are functions of the coordinates, ellipticity of the equation may be confined to only a subset of R^n. We will not go further in this matter, but we just note that for the Poisson or Laplace equation the matrix A is the identity matrix, which is clearly positive definite.

Chapter 4 Boundary conditions

In boundary value problems for second order *ordinary* differential equations we know that we need conditions at the boundaries (that is: at both ends of the interval, one condition at each end) and these conditions may involve the value and/or the derivative of the unknown function. Similarly, for two- or three-dimensional second order partial differential equations of elliptic type we need conditions all along the boundaries of the domain, and these conditions may involve the unknown function u itself and/or its first order partial derivatives.

For the first boundary condition: u is given at the boundary, we can imagine that we keep the boundary at a fixed temperature, by pouring water over it from a container that is maintained at that temperature.

Concerning derivatives occurring in boundary conditions we can distinguish between derivatives in tangential directions and in normal direction. The latter, $\frac{\partial u}{\partial n}$, the derivative in the direction of the outward normal n, is the most occurring one. In the first place, because $\frac{\partial u}{\partial n} = 0$ is the condition for perfect insulation: no flow through the boundary implies that the normal component of $\boldsymbol{\varphi}$ is zero, and then, by (6), we have $\frac{\partial u}{\partial n} = 0$. In the second place, because if the *tangential* derivative(s) would have been given as boundary condition, we can simply integrate them along the boundary to find a condition for the function u itself. For instance, if in a two-dimensional problem the tangential derivative is given to be zero at the boundary, it means that u is a constant all along the boundary. (The value of this constant seems to be unknown, but generally it follows from another condition, e.g. from conservation of some overall quantity.)

From the above, we can expect that there are three standard types of boundary conditions: one about u, one about $\frac{\partial u}{\partial n}$, and one about a (linear) combination of u and $\frac{\partial u}{\partial n}$. All three can occur in one problem, but each one along *different* parts of the boundary, and every part of the boundary must have *one* boundary condition.

These three types have the following names:

1. **Dirichlet** boundary condition: the value of u is given in all points of that part of the boundary. Along the boundary a function g_1 is given (e.g. an expression in terms of coordinates defined along the boundary), and along the boundary the solution u is required to coincide with this function:

$$u = g_1. \tag{11}$$

2. **Neumann** boundary condition: the value of the outward normal derivative $\frac{\partial u}{\partial n}$ is set equal to a given function g_2 of coordinates along the boundary:

$$\frac{\partial u}{\partial n} = g_2. \qquad (12$$

3. **Robin** boundary condition: a certain linear combination of u and its norma derivative $\frac{\partial u}{\partial n}$ must be equal to a given function g_3 along the boundary:

$$\frac{\partial u}{\partial n} + \alpha\, u = g_3\,, \qquad (13$$

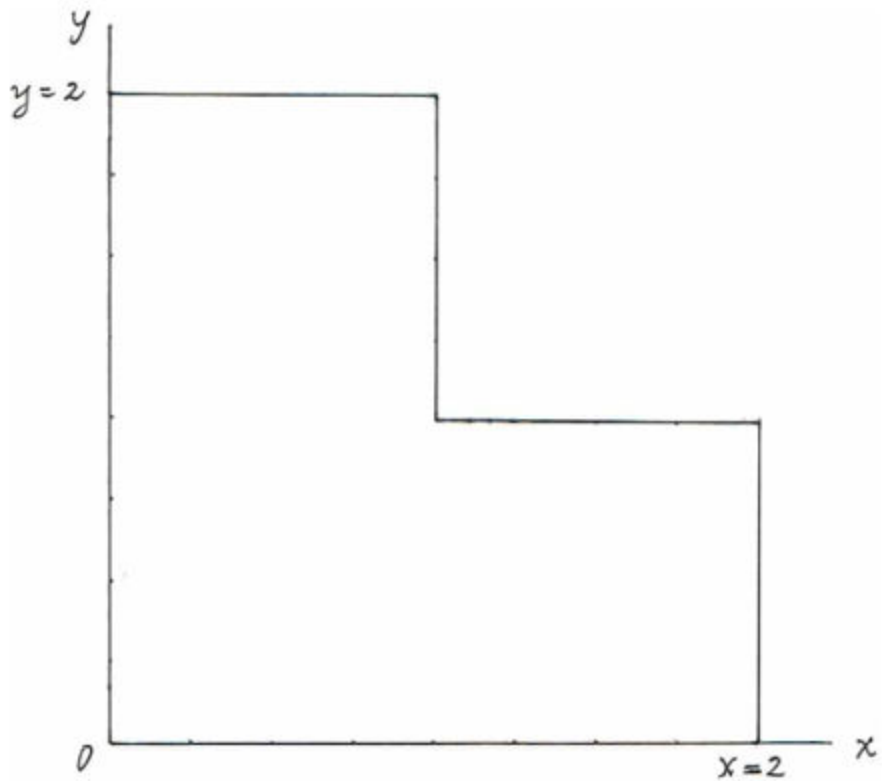
where the factor α is positive and may also be function of the coordinates along the boundary.

A detailed derivation of this condition by modeling the physical situation will be given later.

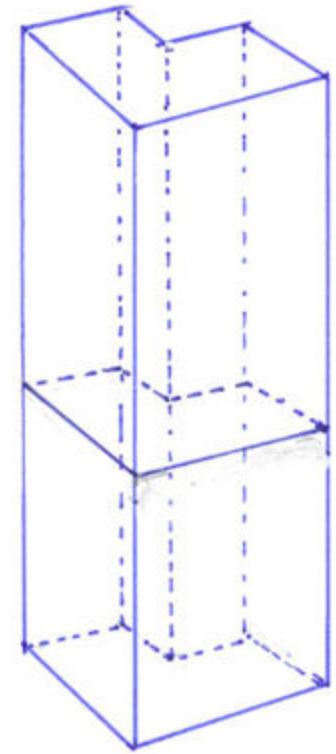
Chapter 5 The heat conduction problem in a two-dimensional L-shaped domain

In the x, y-plane we consider an L-shaped domain as in figure F1

The physical reality may be a thin flat heat conducting plate having this geometry, lying on an insulating sheet and also covered with an insulating sheet, such that heat flow can only be in x- and y-direction.



Alternatively, we can think of an infinitely long beam with this L-shaped cross section, with z-invariant boundary conditions: then the solution is also z-invariant and can be studied in any cross section.



We assume no internal heat production: $f(x, y) = 0$, so we have the Laplace Equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \qquad (14)$$

We apply the following **boundary conditions**.

On top, at $y = 2$, the temperature is given to be a constant, and higher than the room temperature. Let us say

$$u(x, 2) = 100℃. \qquad (15)$$

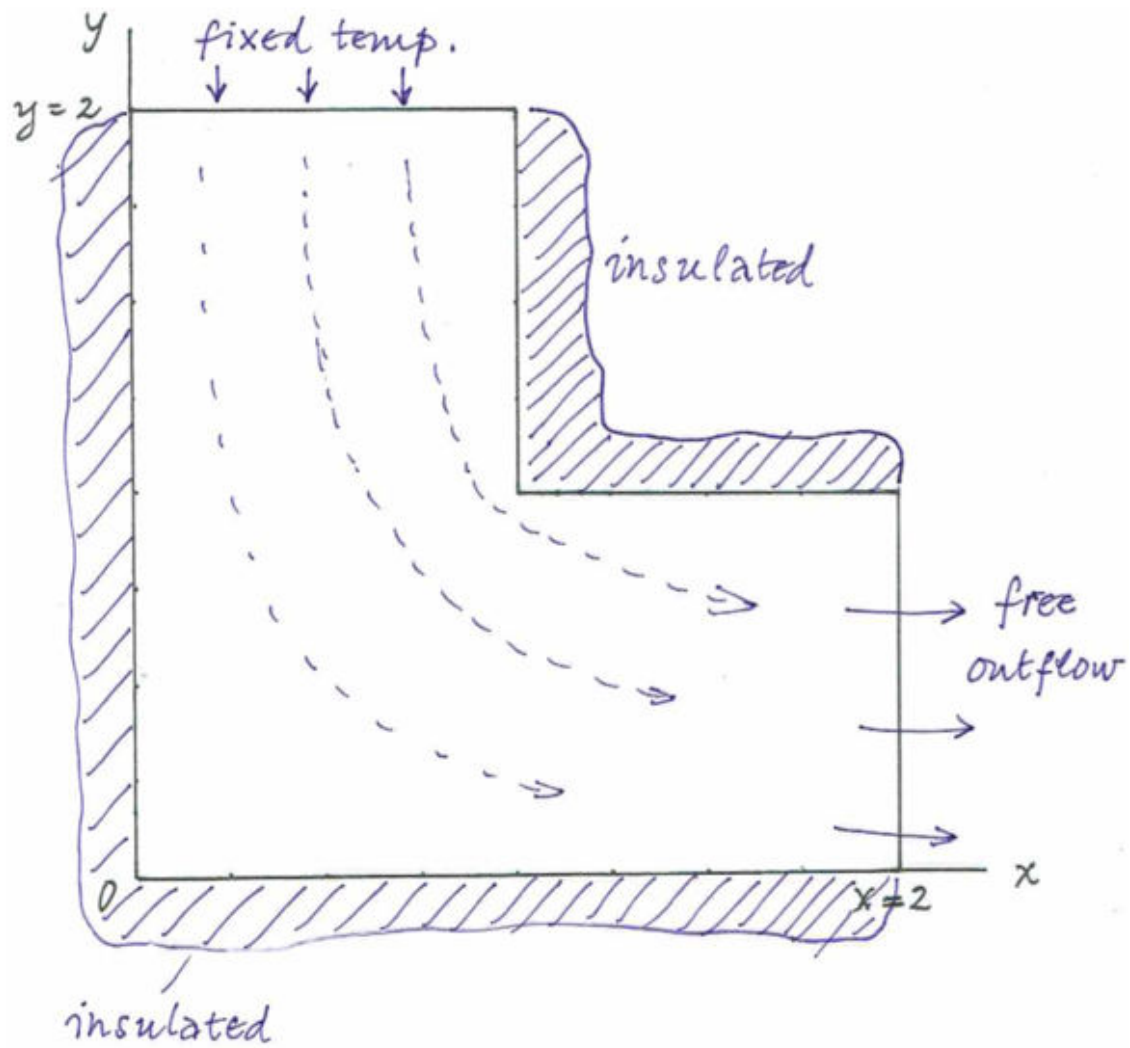
This boundary condition is of **Dirichlet** type.

In the laboratory it can be realized by pouring boiling water over this top surface. In fact we can realize any other value of the boundary temperature if we pour the water from a container which is monitored and controlled at that temperature.

Along the L-shaped boundaries we have an insulated wall: there is no heat flowing through it, so the flow is tangent to the boundary. Mathematically: the flux $\boldsymbol{\varphi}$ has zero normal component. Then, in view of Fourier's Law (6), the normal derivative of u is zero:

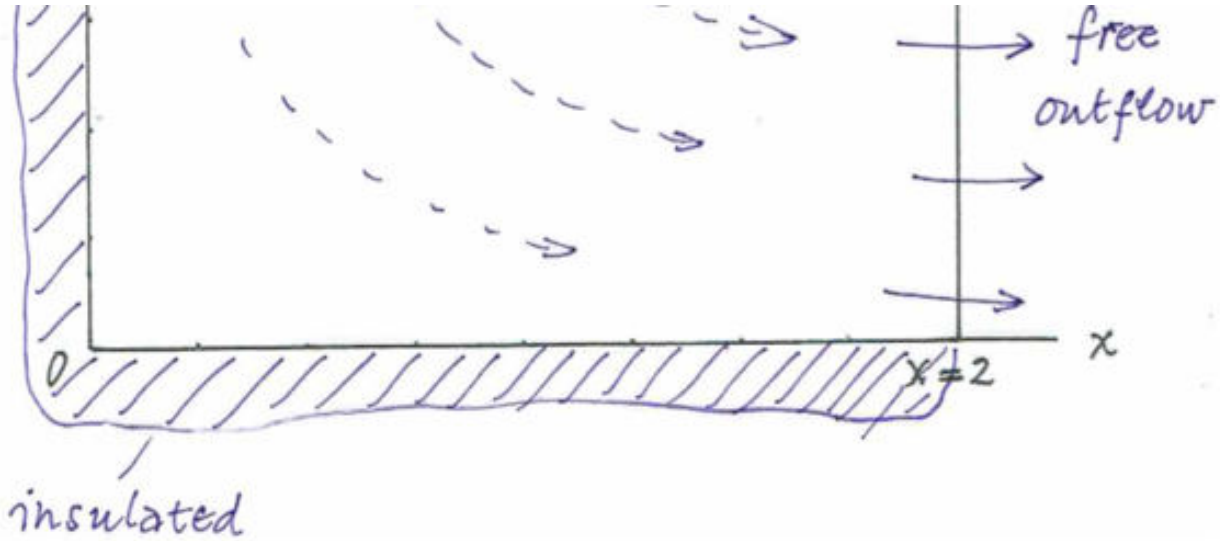
$$\frac{\partial u}{\partial n} = 0. \tag{16}$$

(On the vertical parts of these two boundaries the normal derivative is the x-derivative, and on horizontal parts it is the y-derivative.) This condition (16) is the most simple and most frequently occurring example of **Neumann** boundary condition (12).



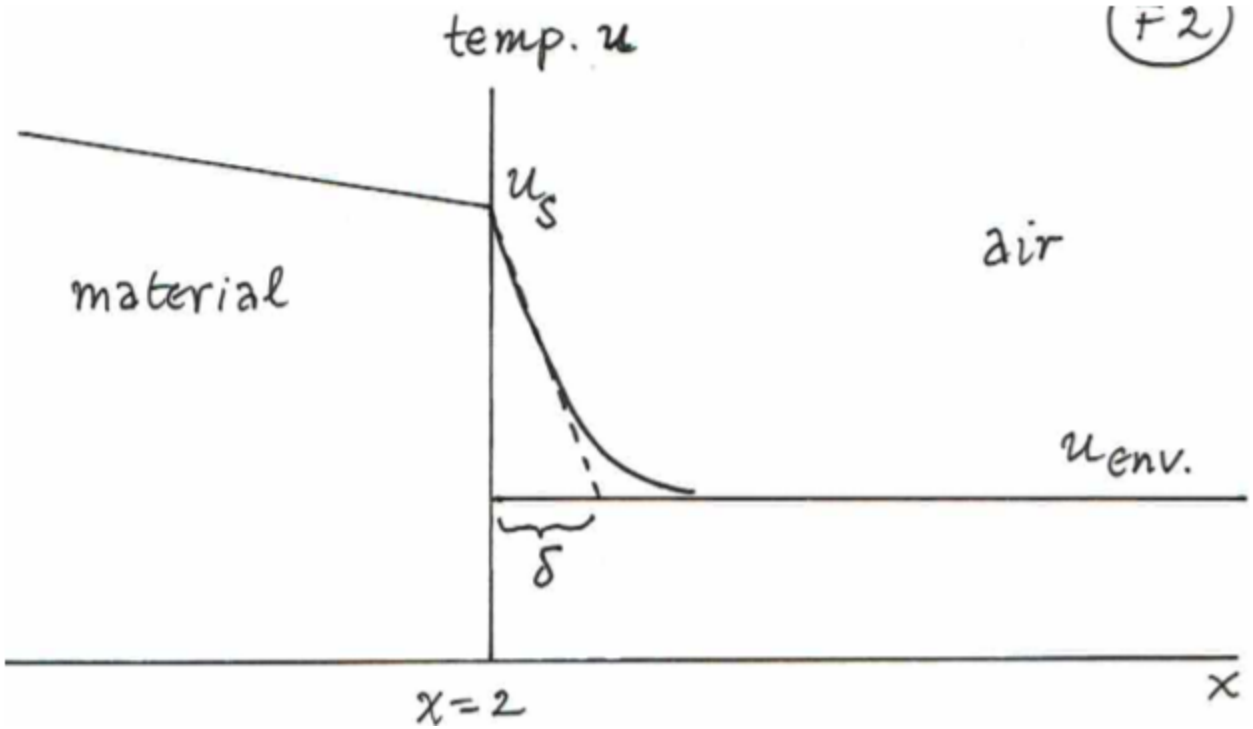
The Neumann boundary condition $\frac{\partial u}{\partial n} = g_2$ with $g_2 \neq 0$ does not occur so frequently; and also it is harder to imagine how it is realized in the laboratory. This is certainly so for $g_2 < 0$, in which case a certain *outflux* is prescribed. For positive g_2, i.e. when an certain *influx* is specified,

The Neumann boundary condition $\frac{\partial u}{\partial n} = g_2$ with $g_2 \neq 0$ does not occur so frequently; and also it is harder to imagine how it is realized in the laboratory. This is certainly so for $g_2 < 0$, in which case a certain *outflux* is prescribed. For positive g_2, i.e. when an certain *influx* is specified, we can be more successful. E.g. we may think of operating the boundary with heaters and radiators with known power, sending focused heat towards the boundary. However, part of this heat will be reflected at the surface, and how do you know how much has really gone into the material? Maybe the following alternative is more effective. On the boundary surface we lay a fine wire netting (kawat kasa) and we make it glow by an electrical current. The electrical power can of course be controlled, and if we cover this netting with an insulating layer, the heat that is produced will totally be conducted away from the boundary into the material, and in stationary situation this heat influx is equal to the power per unit area.

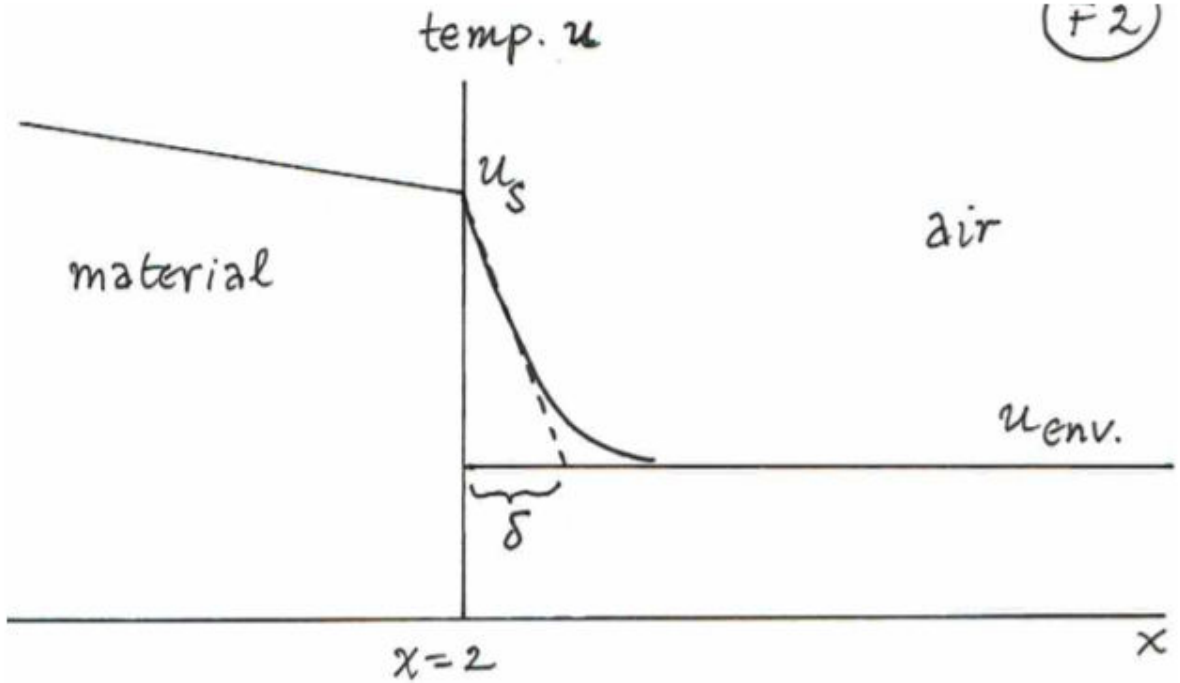


At the right hand boundary we have free outflow of heat to the environment.

In order to come to a mathematical form of this boundary condition we imagine that the heat is taken away from the boundary by air molecules colliding with surface molecules: during collision they exchange heat energy. With this new energy the air molecules move away from the surface, having further collisions in a stochastic way known as *Brownian motion*, thus contributing to a temperature profile that more or less looks like in figure F2.



The steady outflow of heat into the environment will cause a slow but never ending increase of this profile. We are not going to calculate this process in detail; we only seek a way to incorporate the outcome of the process into the boundary condition.



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A standard way to model this profile is *thin film theory*: along the boundary there is a thin film of air, in which the temperature decays from u_s down to u_{env}, while the environment outside the film, called the *bulk*, absorbs all heat that is transferred across the film (and we are not interested in what exactly happens there).

So over the film there is diffusive heat transfer, it is stationary and constant over the film, and is governed by the (still unknown) physical data: conductivity of the air, say μ, and film thickness, say δ. The heat flux, say ψ (scalar: only an x-component), is by Fourier (6):

$$\psi = -\mu \frac{u_{env} - u_s}{\delta} \qquad (17)$$

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(check: positive). Now this ψ must be equal to the heat flux arriving at the surface from inside the material, which is, also by Fourier:

$$\varphi = -\lambda \frac{\partial u}{\partial x} \tag{18}$$

Equating (17) and (18) we get:

$$\lambda \frac{\partial u}{\partial x} + \frac{\mu}{\delta} u_s = \frac{\mu}{\delta} u_{env} \tag{19}$$

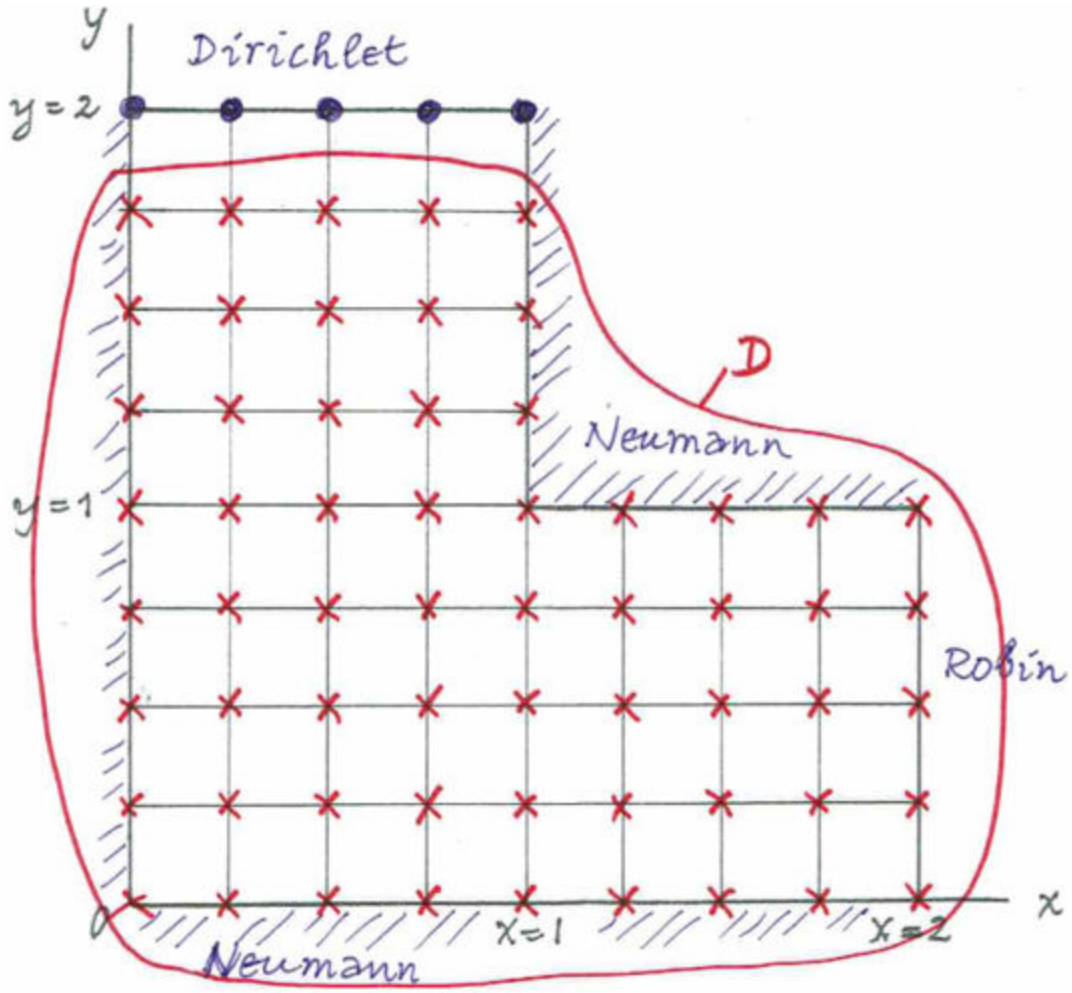
This boundary condition is of type **Robin**, (13) with $\alpha = \frac{\mu}{\lambda\delta}$ and $g_3 = \alpha\, u_{env}$.

Remark. Both δ and μ are (very) small, when compared to the corresponding quantities in the material, but only their ratio μ/δ plays a role, and its value is not necessarily very small or very large. It has to be determined experimentally.

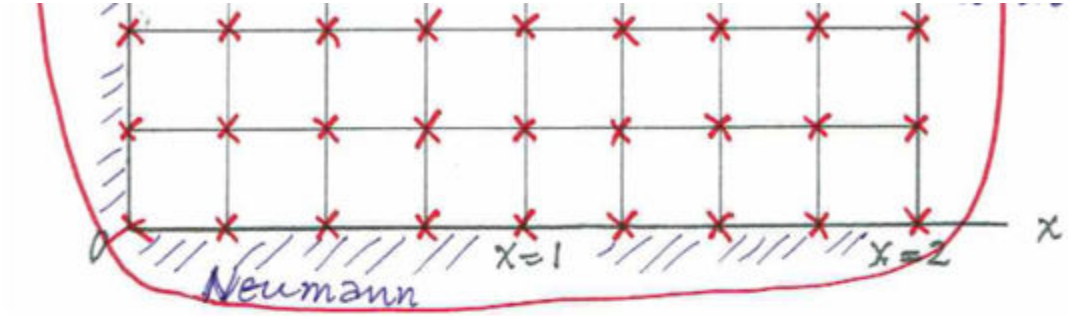
Remark. Eq (17), stating that the outflow is proportional to the temperature difference between material and environment, has already been proposed by Newton and is known as Newton's Law of cooling.

Chapter 6 Discretization of the Laplace Equation

Discretization of a problem that is formulated for a continuous function $u(x, y)$ of two variables x and y on a certain domain, means that we will be satisfied if we can find an approximation of its function values in a finite number of points in that domain. So we first define these points, and in two dimensions it is an obvious choice to take them as the nodal points of a rectangular grid; to keep it simple, we take a uniform grid, that is: all steps in x-direction have the same length, say h_x, and all steps in y-direction have the same length, say h_y; finally we even take $h_x = h_y = h$. So the x-values of the nodal points are $x_i = i\,h$, the y-values are $y_j = j\,h$, and the *approximations* that we are going to find for the solution $u(x_i, y_j)$ in these points, we denote with subscripts: $u_{i,j}$.



These $u_{i,j}$ are the unknowns of the so-called *discretized problem* that we now will derive: we construct a set of **algebraic** equations involving the discrete variables $u_{i,j}$, such that the solution of this set reflects the behavior of the solution $u(x,y)$ of the continuous problem. These algebraic equations can be written in matrix form, and from Linear Algebra we know that (a) it is wise to have as many equations as we have unknowns, and that (b) we will have a unique solution if the matrix of the system has nonzero determinant.



form, and from Linear Algebra we know that (a) it is wise to have as many equations as we have unknowns, and that (b) we will have a unique solution if the matrix of the system has nonzero determinant.

Therefore, to satisfy (a), we start by identifying the unknowns; or rather: identifying all nodal points (x_i, y_j) where the value of u is unknown. These are: all interior nodal points, and quite some of the nodal points on the boundaries: in fact, all nodal points except those on the Dirichlet boundary $y_j = 2$ (because Dirichlet means: their values are known.) This set of nodal points we name D.

Secondly, we count the points in D: $1, 2, \dots, n$.

Thirdly, in each of these nodal points in D we now construct one equation.

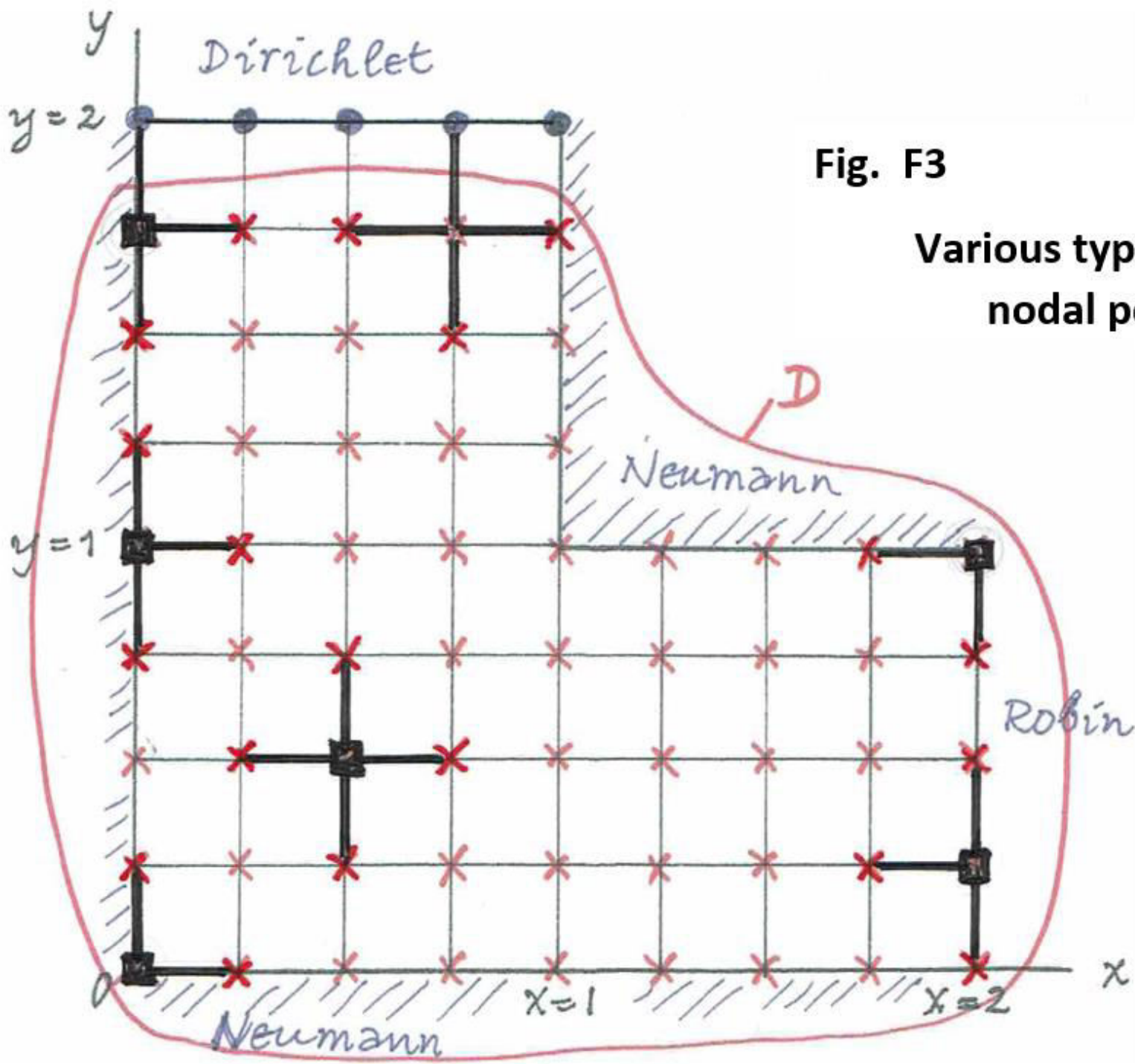
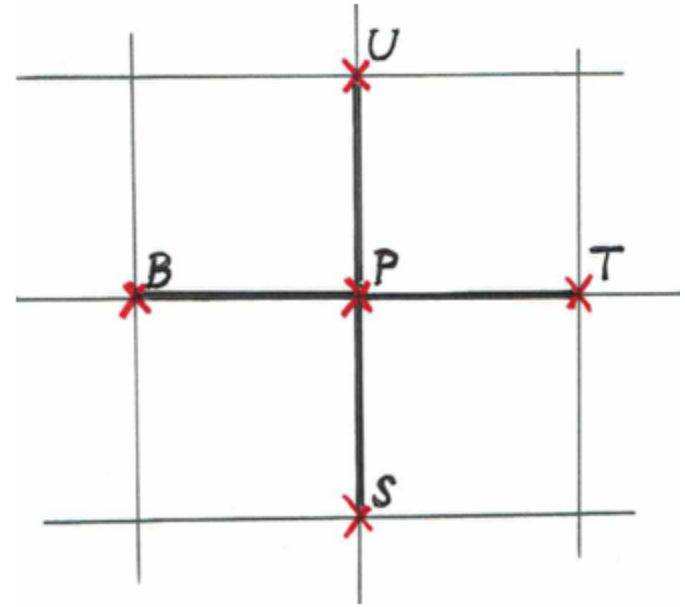


Fig. F3

Various types of nodal points

Interior nodal points



By interior nodal point we mean a point $P = (x_i, y_j)$ in D such that each of its four closest neighbors $T = (x_{i+1}, y_j)$, $U = (x_i, y_{j+1})$, $B = (x_{i-1}, y_j)$ and $S = (x_i, y_{j-1})$ are also in D. See figure(5). Using the Taylor expansion in the center point P, we can write for $u(T)$:

$$u(T) = u(P) + h\frac{\partial u}{\partial x}(P) + \frac{1}{2}h^2\frac{\partial^2 u}{\partial x^2}(P) + \frac{1}{6}h^3\frac{\partial^3 u}{\partial x^3}(P) + \frac{1}{24}h^4\frac{\partial^4 u}{\partial x^4}(P) + \ldots \quad (20)$$

and similar for $u(B)$:

$$u(B) = u(P) - h\frac{\partial u}{\partial x}(P) + \frac{1}{2}h^2\frac{\partial^2 u}{\partial x^2}(P) - \frac{1}{6}h^3\frac{\partial^3 u}{\partial x^3}(P) + \frac{1}{24}h^4\frac{\partial^4 u}{\partial x^4}(P) - \ldots \quad (21)$$

Adding up we get:

$$u(T) + u(B) = 2u(P) + h^2\frac{\partial^2 u}{\partial x^2}(P) + \frac{1}{12}h^4\frac{\partial^4 u}{\partial x^4}(P) + \ldots\ldots \quad (22)$$

$$u(T) + u(B) = 2u(P) + h^2 \frac{\partial^2 u}{\partial x^2}(P) + \frac{1}{12} h^4 \frac{\partial^4 u}{\partial x^4}(P) + \ldots\ldots \quad (22)$$

Similarly in y-direction:

$$u(U) + u(S) = 2u(P) + h^2 \frac{\partial^2 u}{\partial y^2}(P) + \frac{1}{12} h^4 \frac{\partial^4 u}{\partial y^4}(P) + \ldots\ldots \quad (23)$$

Adding up (22) and (23) we find:

$$u(T) + u(U) + u(B) + u(S) - 4\,u(P) = h^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(P) + \mathcal{O}(h^4) \quad (24)$$

This leads to the important conclusion, the basis of elliptic numerics:

the linear combination $\frac{1}{h^2}[u(T) + u(U) + u(B) + u(S) - 4\,u(P)]$ (25)

is an $\mathcal{O}(h^2)$ accurate approximation of $\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(P)$

$$u(T) + u(U) + u(B) + u(S) - 4\,u(P) = h^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(P) + \mathcal{O}(h^4) \quad (24)$$

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Applying (24) to the Poisson Equation $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\frac{1}{\lambda} f(x, y)$ we see that u satisfies $\frac{1}{h^2}[u(T) + u(U) + u(B) + u(S) - 4\,u(P)] = -\frac{1}{\lambda} f(P)$

within $\mathcal{O}(h^2)$ *accuracy*. (26)

Now we come up with the unknowns of the discretized problem. First a matter of notation: instead of indices $i, i \pm 1, j, j \pm 1$ in subscript, we can as well use a letter index referring to east, north, west and south: for the central point $u_{i,j}$ or u_P , the point east of it: $u_{i+1,j}$ or u_T , north: $u_{i,j+1}$ or u_U , west: $u_{i-1,j}$ or u_B , and south: $u_{i,j-1}$ or u_S .

Now, in view of (25) we require these five unknowns to satisfy the equation

$$\frac{1}{h^2}[u_T + u_U + u_B + u_S - 4\,u_P] = -\frac{1}{\lambda}\,f(P) \quad \textit{exactly}. \tag{27}$$

$$\frac{1}{h^2}[u(T)+u(U)+u(B)+u(S)-4\,u(P)] = -\frac{1}{\lambda}\,f(P) \quad \textit{within } \mathcal{O}(h^2) \textit{ accuracy.} \quad (26)$$

$$\frac{1}{h^2}[u_T+u_U+u_B+u_S-4\,u_P] = -\frac{1}{\lambda}\,f(P) \quad \textit{exactly.} \quad (27)$$

Applied to the Laplace Equation $\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}=0$, we will have instead of (26) and (27):

$$\frac{1}{h^2}[u(T)+u(U)+u(B)+u(S)-4\,u(P)] = 0 \quad \textit{within } \mathcal{O}(h^2) \textit{ accuracy.} \quad (28)$$

and the numerical unknowns *exactly* satisfy

$$\frac{1}{h^2}[u_T+u_U+u_B+u_S-4\,u_P] = 0 \quad (29)$$

In case of the Laplace equation (like our model problem) we can omit the factor $\frac{1}{h^2}$. Finally, we will change the minus sign to have a positive coefficient in the center point, so we will work with the equation:

$$4\,u_P - u_T - u_U - u_B - u_S = 0 \quad (30)$$

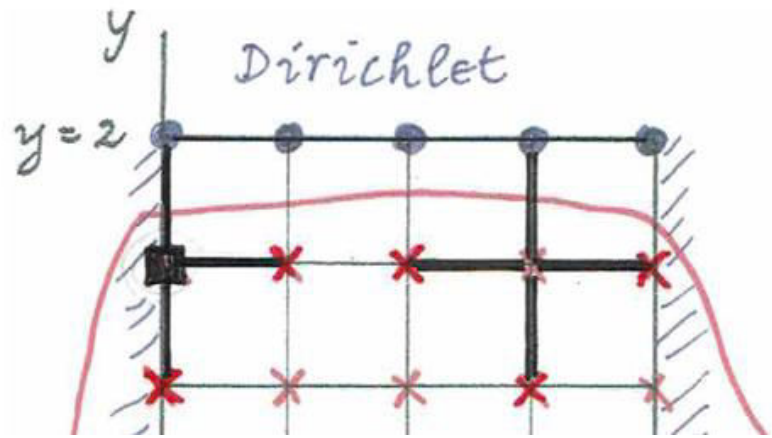
An often seen representation, referring to the geometry of the connection, is the following

$$\begin{bmatrix} \cdot & -1 & \cdot \\ -1 & 4 & -1 \\ \cdot & -1 & \cdot \end{bmatrix} u = h^2 f \quad \text{or } 0, \text{ respectively} \tag{31}$$

and is called: *stencil*, or *molecule*.

The equation (30), as we already said, can be applied in each **interior point** of D. Written in a matrix, all these equations have 4 on the diagonal, and four entries -1 elsewhere in the row. Where exactly, depends on the order in which we number the points. Commonly we follow the way we read a text: starting in the upper line, going from left the right, then one line down, again left to right, etc. For interior points that have one neighbor on the **Dirichlet** boundary, the value in that neighboring point is given, so it moves to the right hand side, and the equation now relates the central unknown with only three neighboring unknowns:

$$4\,u_P - u_T - u_B - u_S = g_1(U) = 100°\mathrm{C} \qquad (30)$$



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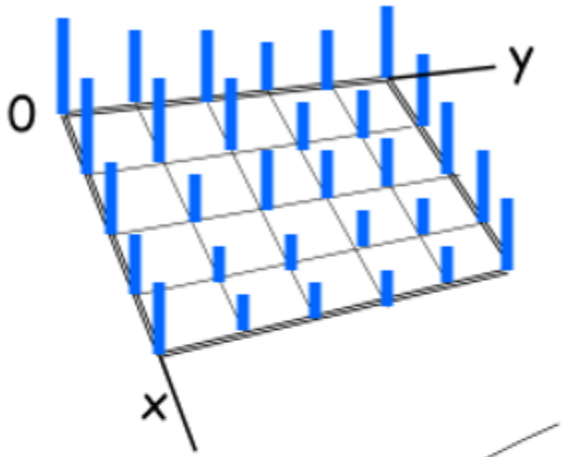

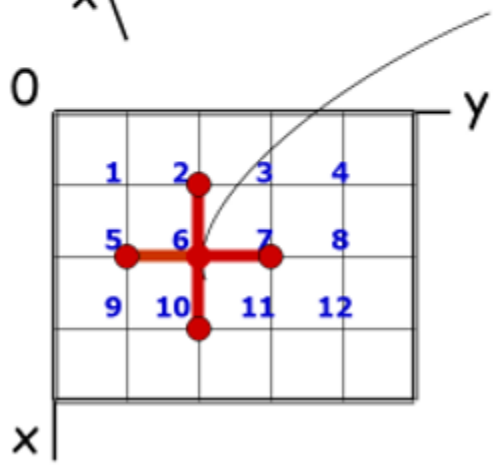

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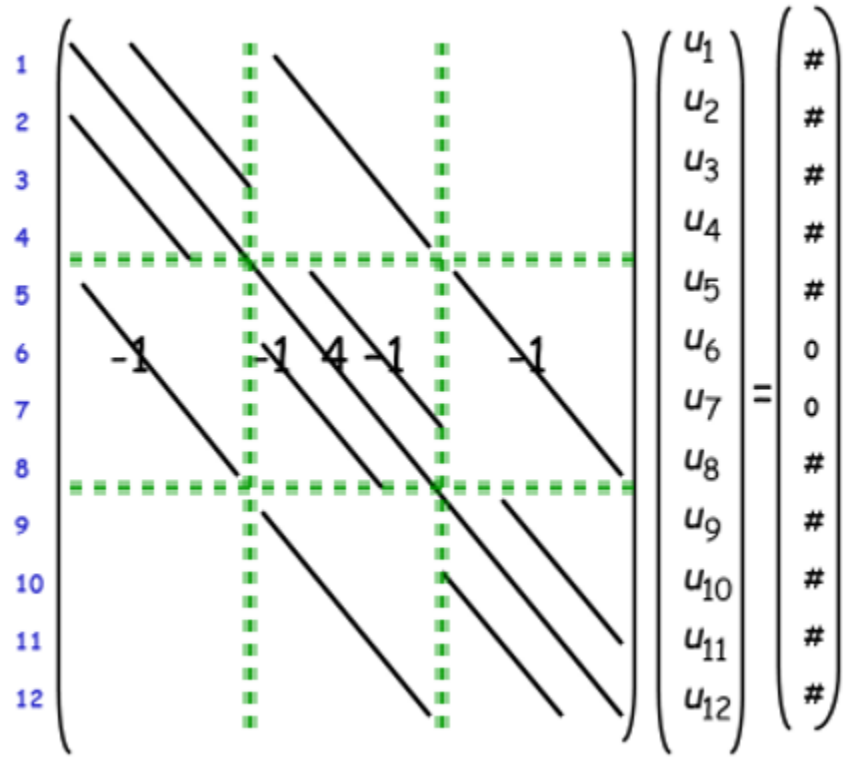
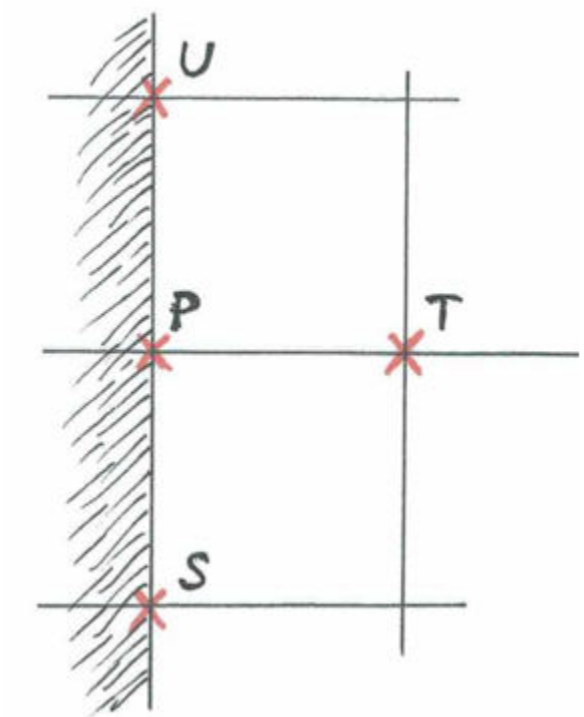


Now for nodal points **on the insulated boundaries** we implement the **Neumann** boundary condition (12) in the molecule. Note that the Neumann boundary condition is about the (normal) derivative, and not about the value of the temperature itself. So the value in a Neumann boundary point is an *unknown*, and we need to construct an equation for it.



Let P be a nodal point on the left boundary. The continuous solution u is in this point P still perfectly differentiable in y-direction, so (23) applies also here.

But differentiability with respect to x is only in *positive* x-direction, so we have (20) but we cannot use (21) for eliminating the first derivative $\frac{\partial u}{\partial x}(P)$. However, this is precisely the derivative that is given by the Neumann condition; in our case it is 0. Therefore, besides (23):

$$u(U) + u(S) = 2u(P) + h^2 \frac{\partial^2 u}{\partial y^2}(P) + \frac{1}{12} h^4 \frac{\partial^4 u}{\partial y^4}(P) + \ldots\ldots \qquad (23)$$

we have:

$$u(T) = u(P) + \frac{1}{2} h^2 \frac{\partial^2 u}{\partial x^2}(P) + \frac{1}{6} h^3 \frac{\partial^3 u}{\partial x^3}(P) + \frac{1}{24} h^4 \frac{\partial^4 u}{\partial x^4}(P) + \ldots\ldots \qquad (32)$$

Multiplying the last equation with 2 and adding it to (y2 23) we find

$$\frac{1}{h^2}[2u(T) + u(U) + u(S) - 4u(P)] = (\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})(P) + \frac{1}{12} h^2 \frac{\partial^4 u}{\partial y^4}(P) + \ldots \quad (33)$$

where we have already used that $\frac{\partial^3 u}{\partial x^3}(P) = 0$ (why is this?), so that the accuracy is still $\mathcal{O}(h^2)$.

$$\frac{1}{h^2}[2u(T) + u(U) + u(S) - 4u(P)] = (\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2})(P) + \frac{1}{12}h^2\frac{\partial^4 u}{\partial y^4}(P) + \ldots \quad (33)$$

where we have already used that $\frac{\partial^3 u}{\partial x^3}(P) = 0$ (why is this?), so that the accuracy is still $\mathcal{O}(h^2)$.

The equation for the numerical unknowns becomes:

$$4\,u_P - 2u_T - u_U - u_S = 0 \quad (34)$$

Written as a molecule:

$$\begin{bmatrix} \cdot & -1 & \cdot \\ \cdot & 4 & -2 \\ \cdot & -1 & \cdot \end{bmatrix} u = 0 \quad (35)$$

Comparing with (31) it looks like the missing point at the left is “folded” over to the right (mirroring symmetry).

For the **Neumann point just under the Dirichlet boundary**, see Fig. F3 top left, the value of $u(U)$ is given and goes to the right hand side; so that the stencil becomes:

$$\begin{bmatrix} \cdot & \cdot & \cdot \\ \cdot & 4 & -2 \\ \cdot & -1 & \cdot \end{bmatrix} u = u(U) \tag{36}$$

and in the **lower left corner**, see again Fig. F3, we have double symmetry:

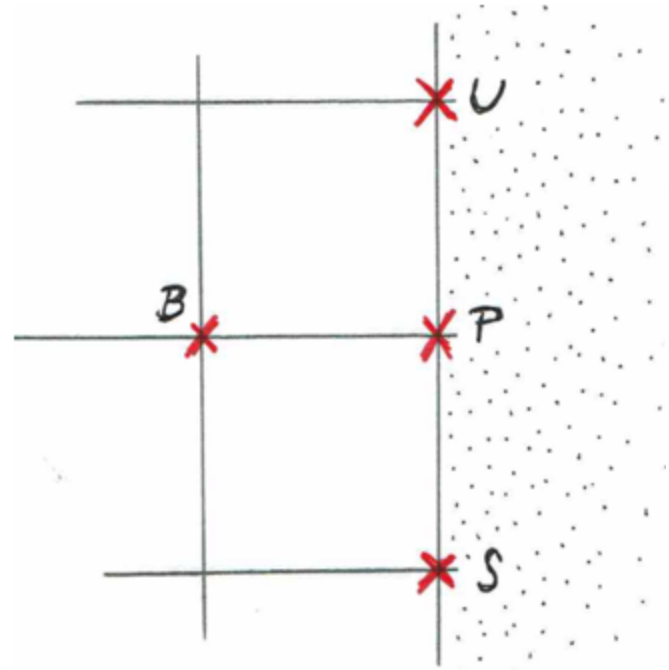
$$\begin{bmatrix} \cdot & -2 & \cdot \\ \cdot & 4 & -2 \\ \cdot & \cdot & \cdot \end{bmatrix} u = 0 \tag{37}$$

In the point $(x, y) = (1,1)$ we meet a difficulty: the solution u of the continuous problem is not differentiable in that point, so we cannot use Taylor expansions. We will discuss this later. If you want to write a computer program now, then for the moment you may just simply assume that in this corner point P the value of u_P is the average of u_T and u_U .

Finally we implement the **Robin** condition at the right boundary (the outward normal is in positive x-direction). We write (19) in the form

$$\frac{\partial u}{\partial x} + \alpha\, u = \alpha\, u_{env} \qquad \text{with} \quad \alpha = \frac{\mu}{\lambda\delta} > 0 \tag{38}$$

This may look like the most difficult condition of the three, but after what we have already seen about the numerics of the Neumann condition, it will go smoothly, as follows.



We start in a nodal point P, not being a corner point, that is: its coordinates are $(2, y)$ with $0 \neq y \neq 1$. In y-direction we then still have (23), and in x-direction we only have (21) from which we eliminate the first derivative by substituting the boundary condition (38):

$$u(U) + u(S) = 2u(P) + h^2 \frac{\partial^2 u}{\partial y^2}(P) + \frac{1}{12} h^4 \frac{\partial^4 u}{\partial y^4}(P) + \ldots\ldots \qquad (23)$$

$$u(B) = u(P) - h \frac{\partial u}{\partial x}(P) + \frac{1}{2} h^2 \frac{\partial^2 u}{\partial x^2}(P) - \frac{1}{6} h^3 \frac{\partial^3 u}{\partial x^3}(P) + \frac{1}{24} h^4 \frac{\partial^4 u}{\partial x^4}(P) - \ldots \quad (21)$$

$$\frac{\partial u}{\partial x} + \alpha\, u = \alpha\, u_{env} \qquad \text{with} \quad \alpha = \frac{\mu}{\lambda \delta} > 0 \qquad (38)$$

$$u(B) = u(P) - h(-\alpha\, u(P) + \alpha\, u_{env}) + \frac{1}{2} h^2 \frac{\partial^2 u}{\partial x^2}(P) +$$

$$= (1 + h\alpha) u(P) - h\alpha\, u_{env} + \frac{1}{2} h^2 \frac{\partial^2 u}{\partial x^2}(P) +$$

Multiplying with 2 and adding up to (23) we find:

$$2u(B) + u(U) + u(S) - (4u + 2h\alpha)\, u(P) =$$

$$-2h\alpha\, u_{env} + h^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(P) + \mathcal{O}(h^4).$$

(Exercise: is the exponent 4 in $\mathcal{O}(h^4)$ correct?)

$$2u(B) + u(U) + u(S) \; - (4u + 2h\alpha)\, u(P) =$$

$$-2h\alpha\, u_{env} \; + \; h^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)(P) \; + \; \mathcal{O}(h^4).$$

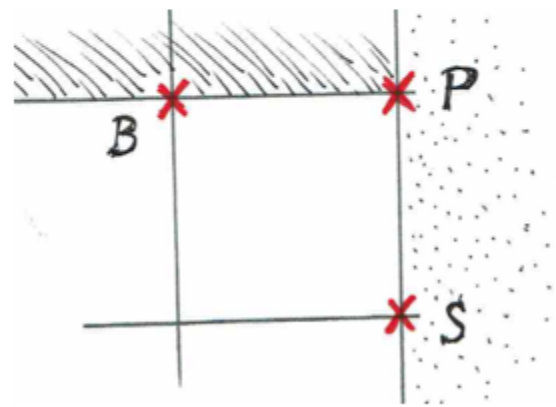
and the equation for the numerical unknowns becomes:

$$(4 + 2h\alpha)\, u_P - \; u_U - 2u_B - u_S = 2h\alpha\, u_{env} \tag{40}$$

In stencil:

$$\begin{bmatrix} \cdot & -1 & \cdot \\ -2 & 4 + 2h\alpha & \cdot \\ \cdot & -1 & \cdot \end{bmatrix} u = \; 2h\alpha\, u_{env} \tag{41}$$

In both **corner points of the outlet** we have to implement the insulation: one of the two entries -1 in the molecule will be folded (or mirrored) on to the other, so making it -2 , like in (35), but there the mirror was vertical, now horizontal. For the case as in the adjacent figure we find:



$$(4 + 2h\alpha)\, u_P - \; 2u_B - 2u_S = 2h\alpha\, u_{env} \tag{41a}$$

A note to make here is that the central coefficient $4 + 2h\alpha$ is, in modulus, larger than the sum of the moduli of the other coefficients in the molecule. Then the matrix is so-called *diagonally dominant*, which ensures a unique solution. (We will not further discuss now.)

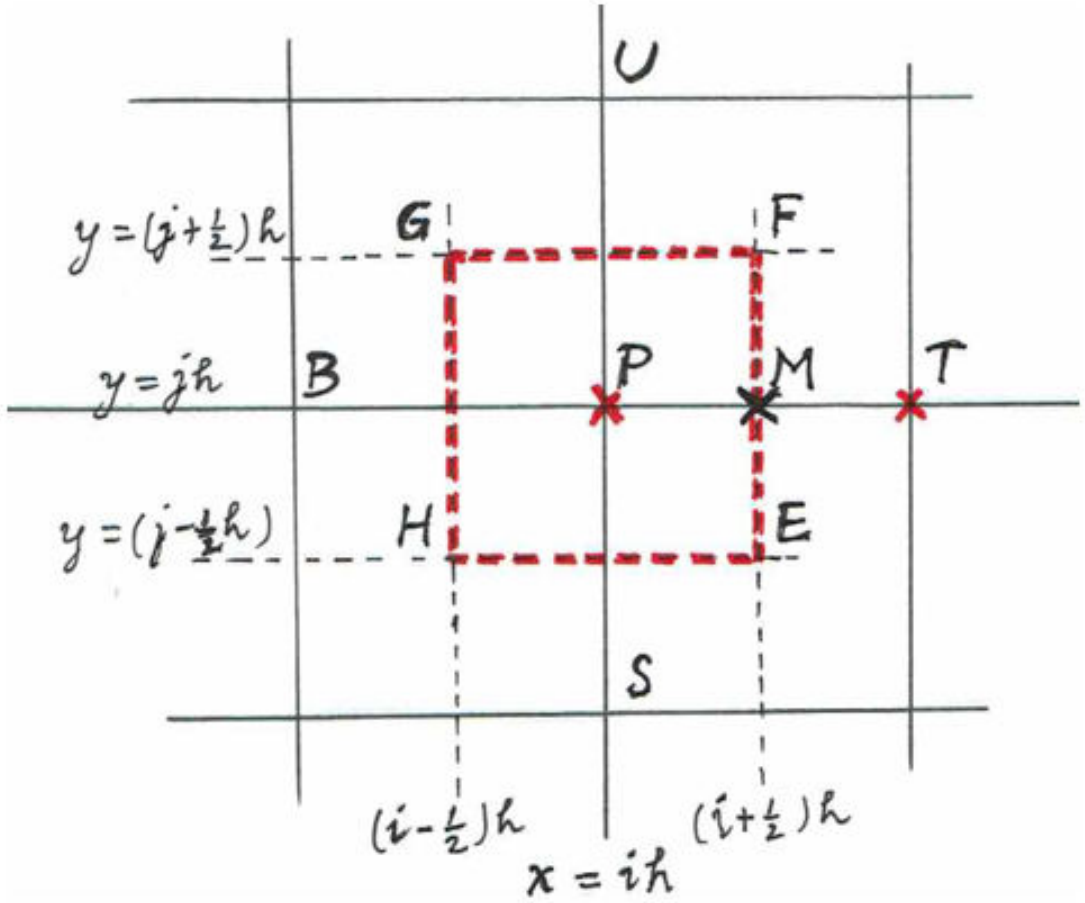
Chapter 7 Discretization derived through box-integration

In the previous chapter we have derived the discrete problem by approximating the second order derivatives by linear combinations of neighboring temperature values, to the best possible accuracy (given that only four neighboring points participate; if we allow for bigger "molecules" the accuracy can of course be higher). In doing so, the focus of our analysis was on pointwise behavior. But what can we say about the behavior or accuracy in between the nodal points?

And what is the relation with the physics? E.g. what will we answer when we are asked: how much is the total heat flow through a cross section? We might do a calculation at the outlet: the heat flow through the outlet is an y-integral of the x-derivative of temperature, so having the solution of the discrete problem we may apply numerical differentiation and then numerical integration. But will we get the same answer when we do these calculations at the inlet? Or over any cross section in the interior? Ya, we know that if we take finer and finer grids, more and more nodal points, more and more work, the accuracy will become higher (mathematically speaking: the truncation error will decrease).

Instead of deriving discrete formulas for a problem formulated in second order derivatives, we now go back to the formulation in first order derivatives, which is **closer to the physics**. The physical **law of Conservation of Heat** says that the net outflow of heat from any closed surface in the domain is zero. Here, in 2D, it is of course about contours instead of surfaces:

The net outflow of heat from any closed contour in the domain is zero, where the net outflow from the contour is the integral of the normal flux, and the normal flux is $-\lambda$ times the normal derivative of the temperature u. (42)



Like in Chapter 6, we start with a nodal point $P = (ih, jh)$ in the **interior** of the domain D. Now in order to derive an equation for the discrete unknown u_P in relation to its neighbors, we apply this physical law on a contour around P, a square contour with its edges along the four lines $x = \left(i \pm \frac{1}{2}\right)h$ and $y = \left(j \pm \frac{1}{2}\right)h$. So the contour integral consists of four parts; we start with the eastern part: the line EF. The integral of the normal flux is, in second order accuracy, approximated by the flux in the midpoint M, multiplied with the length of the edge, which is h. And then: the normal flux in M is in second order accuracy approximated by $\lambda(u_P - u_T)/h$. So this first quarter of the integral is just: $\lambda(u_P - u_T)$.

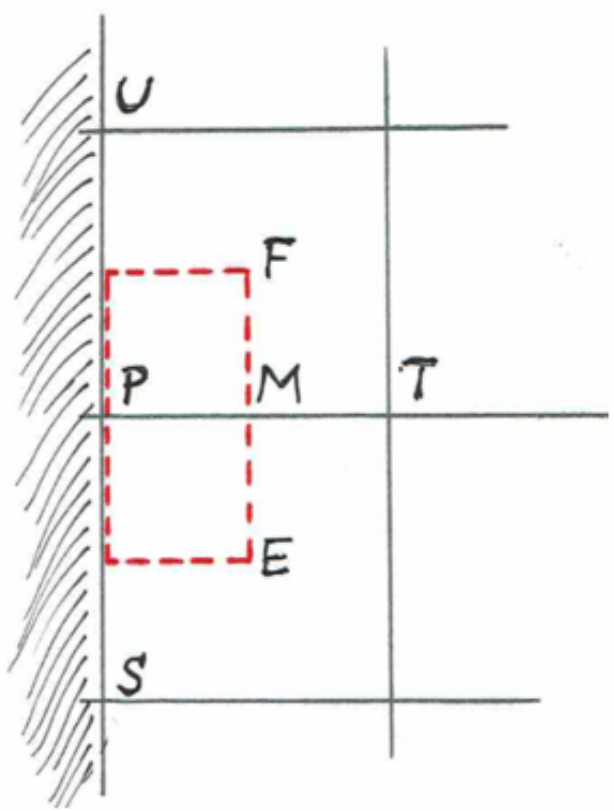
Similarly, the outflow to the north is in second order approximated by $\lambda(u_P - u_U)$, to the west by $\lambda(u_P - u_B)$, and to the south by $\lambda(u_P - u_S)$. And the sum must be zero, so (omitting the factor λ) we simply arrive at the well know relation:

$$4\,u_P - u_T - u_U - u_B - u_S = 0 \qquad (43)$$

Now, in **an interior point just under the Dirichlet boundary**, the value of u_U is given and will be moved to the right hand side, as we already saw in chapter 6, formula (30):

$$4\,u_P - u_T - u_B - u_S = g_1(U) = 100°\mathrm{C} \qquad (30)$$

Now we will go over to nodal points on the insulated boundaries. Here the homogeneous **Neumann condition** applies: $\frac{\partial u}{\partial n} = 0.$ (16)



We choose the point P to lie on the boundary $x = 0$, and we draw a rectangular contour around it: we cannot make it a full square, as half of it would lie outside the domain; so we have only half a square: three edges along the three lines $x = \left(i + \frac{1}{2}\right)h$ and $y = \left(j \pm \frac{1}{2}\right)h$, and the forth edge is along the boundary. This last edge the outflow is zero, by definition: it is insulated. The east edge has, as we saw earlier, an outflow equal to $\lambda(u_P - u_T)$. The outflux integral over the northern edge is the length of the edge $\frac{1}{2}h$ multiplied with the flux which is $-\lambda(u_U - u_P)/h$, so the contribution to the integral is $\frac{1}{2}\lambda(u_P - u_U)$. Similarly for the southern edge: is $\frac{1}{2}\lambda(u_P - u_S)$. In total, omitting the factor λ, we find the relation:

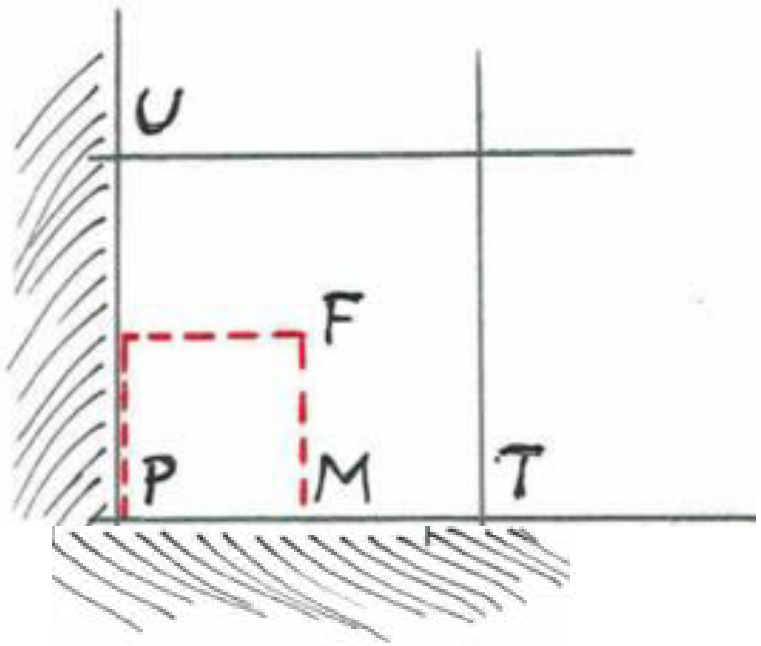
$$2\,u_P - u_T - \tfrac{1}{2}u_U - \tfrac{1}{2}u_S = 0 \qquad (44)$$

This is equivalent to (34), they only differ by a factor 2.

And if we have P in the corner $(x = 0, y = 0)$ then the contour is only a quarter of the original square. Two of its edges are insulated: the west and south edge; over the east edge the outflow is $-\frac{1}{2}h\,\lambda(u_T - u_P)/h = .\frac{1}{2}\lambda(u_P - u_T)$, and similarly over the northern edge $\frac{1}{2}\lambda(u_P - u_U)$, so in total we find the relation

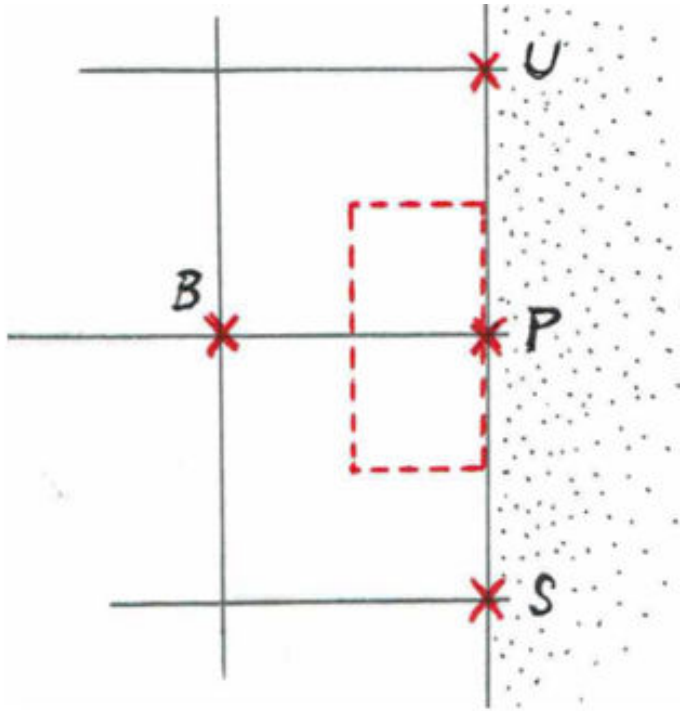
$$u_P - \tfrac{1}{2}u_T - \tfrac{1}{2}u_U = 0. \tag{45}$$

This is equivalent to (37), but for a factor 4.



Finally we consider the **outlet boundary**. Here we have the **Robin condition**

$$\lambda \frac{\partial u}{\partial x} + \frac{\mu}{\delta} u_s = \frac{\mu}{\delta} u_{env} \qquad (19)$$



Consider the rectangle in the adjacent figure. The outflow over the western edge is, just like for interior boxes: $\lambda(u_P - u_B)$, over the northern edge: $\frac{1}{2}\lambda(u_P - u_U)$, and over the southern edge: $\frac{1}{2}\lambda(u_P - u_S)$. Of course the most interesting thing is the expression for what is going out over the eastern edge. The outward normal derivative there is in positive x-direction, so the outflow is approximated by the length h multiplied with the flux at P : $-h\,\lambda \frac{\partial u}{\partial x}(P) =$ [by (19)] $= -h \frac{\mu}{\delta}(-u_P + u_{env})$. The total over the four edges is:

$$\lambda\left(2u_P - \tfrac{1}{2}u_U - u_B - \tfrac{1}{2}u_S\right) + h \frac{\mu}{\delta}(u_P - u_{env}) = 0$$

Or, dividing by λ and writing $\frac{\mu}{\lambda\delta} = \alpha$, we get:

$$(2 + \alpha h)\, u_P - \tfrac{1}{2}u_U - u_B - \tfrac{1}{2}u_S = \alpha h\, u_{env} \qquad (46)$$

which is equivalent to (40) but for a factor 2.

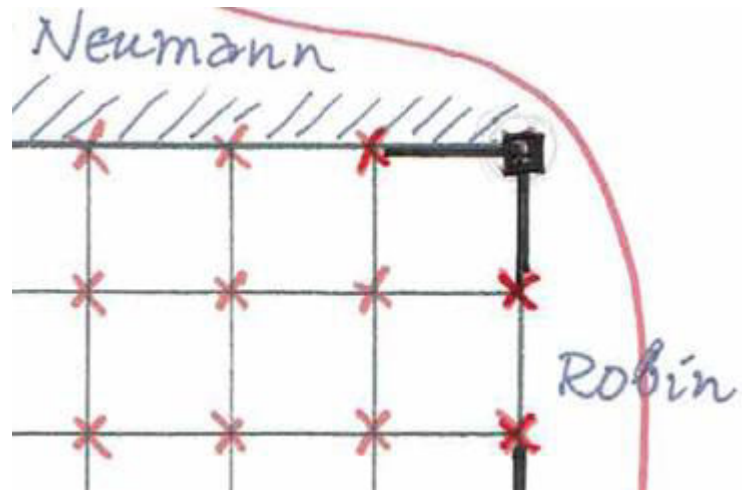
In corners with the insulated wall, we have only one quarter of the standard box. Let us consider the corner $(x, y) = (2,1)$. Compared to the previous box (last figure), the point U is absent, and the vertical edges are only half. So along the boundary BP we have no contribution, over the half west edge we get: $\frac{1}{2}\lambda(u_P - u_B)$, over the southern edge: $\frac{1}{2}\lambda(u_P - u_S)$, and over the (half) outflow edge: $-\frac{1}{2}h\,\lambda\,\frac{\partial u}{\partial x}(P) = -\frac{1}{2}h\,\frac{\mu}{\delta}(-u_P + u_{env})$.

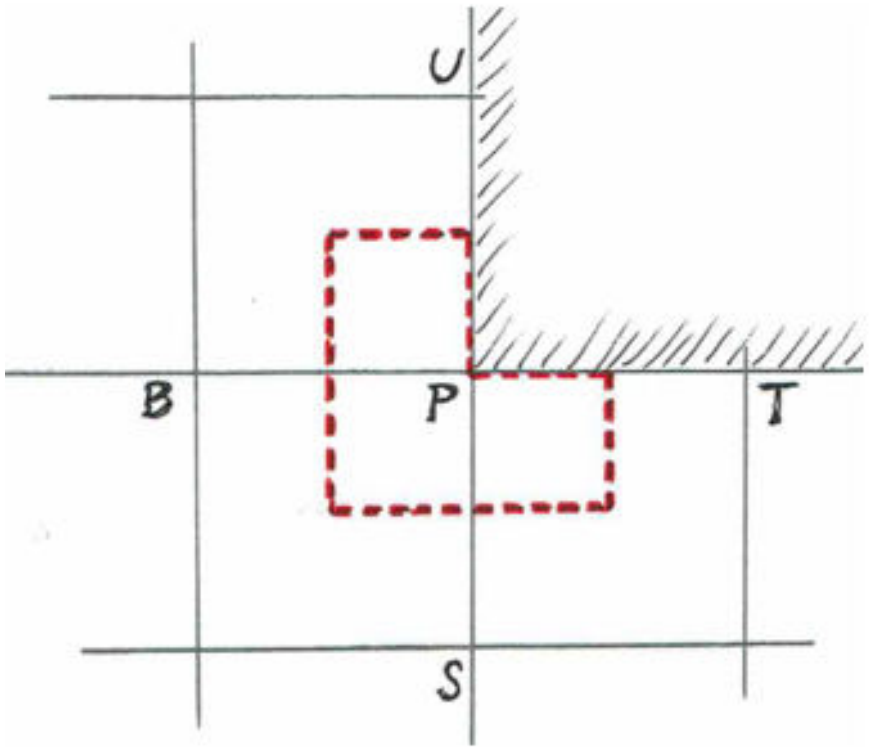
Altogether:

$$\lambda\left(u_P - \tfrac{1}{2}u_B - \tfrac{1}{2}u_S\right) + \tfrac{1}{2}h\,\frac{\mu}{\delta}(u_P - u_{env}) = 0 \quad \text{or:}$$

$$(1 + \tfrac{1}{2}\alpha h)\,u_P - \tfrac{1}{2}u_B - \tfrac{1}{2}u_S = \tfrac{1}{2}\alpha h\,u_{env} \qquad (47)$$

Compare with (41a): again only a factor difference, now factor 4.





Finally we address the **inward corner**.

After all types of boxes that we have seen already, we easily read the formula from the figure:

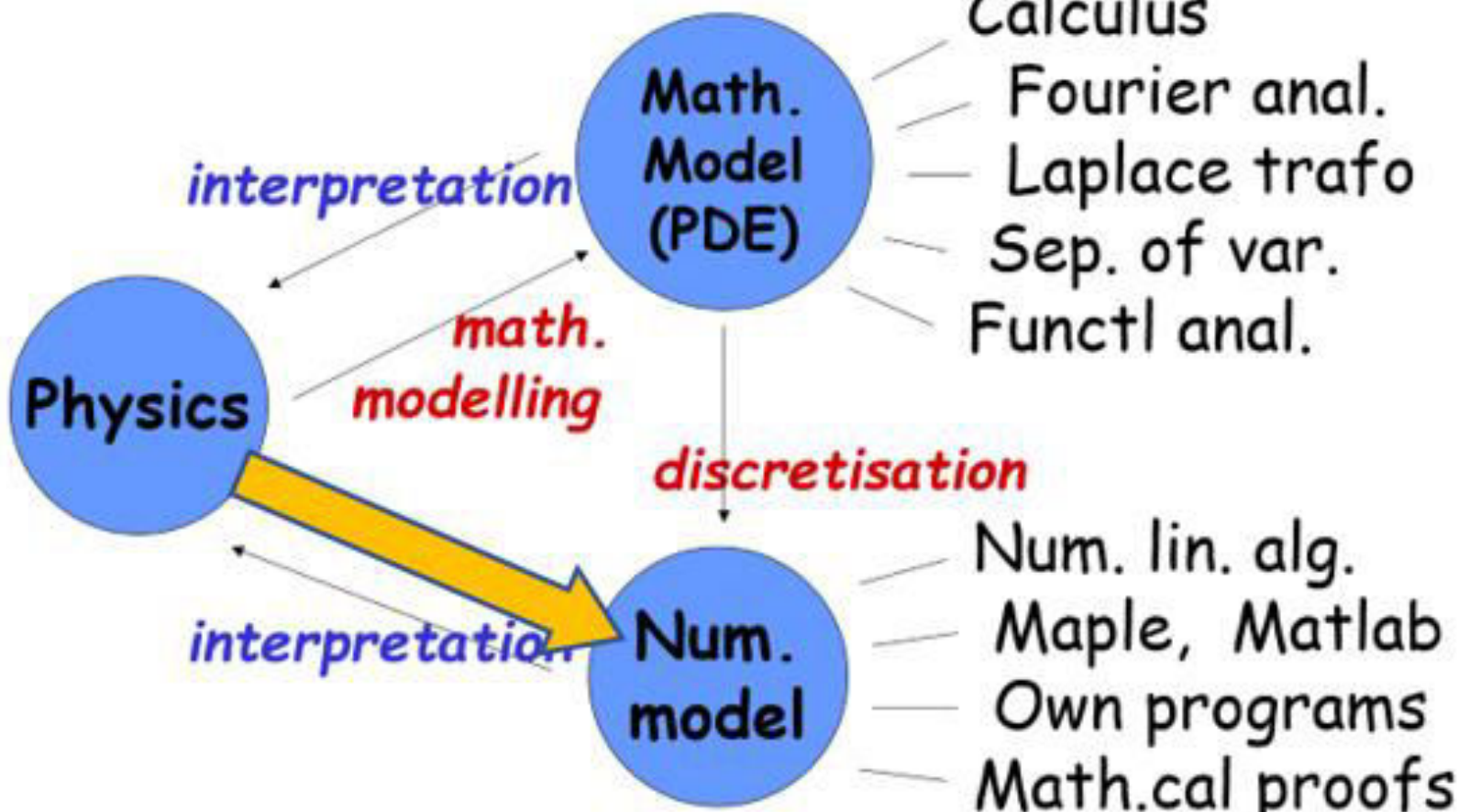
$$\tfrac{1}{2}u_U + u_B + u_S + \tfrac{1}{2}u_T - 3u_P = 0 \qquad (48)$$

Chapter 8 Discussion of the box integration

Here we look back on what we have done (we “reflect”), and we share a few thoughts.

A **mathematical** aspect: for the approach using Taylor expansions, our functions must be twice differentiable in the interior; in the box-integration they need only be differentiable *once;* and even less: it is sufficient if their derivatives are integrable.
A **physical** aspect: in box-integration we in fact have a ***direct*** *numerical model of the physics* (the yellow line in the figure below; I remembered this figure from earlier workshops, but the yellow line I added just now, as I realize this representation precisely describes what I want to say).

Physics, Mathematics and Numerics



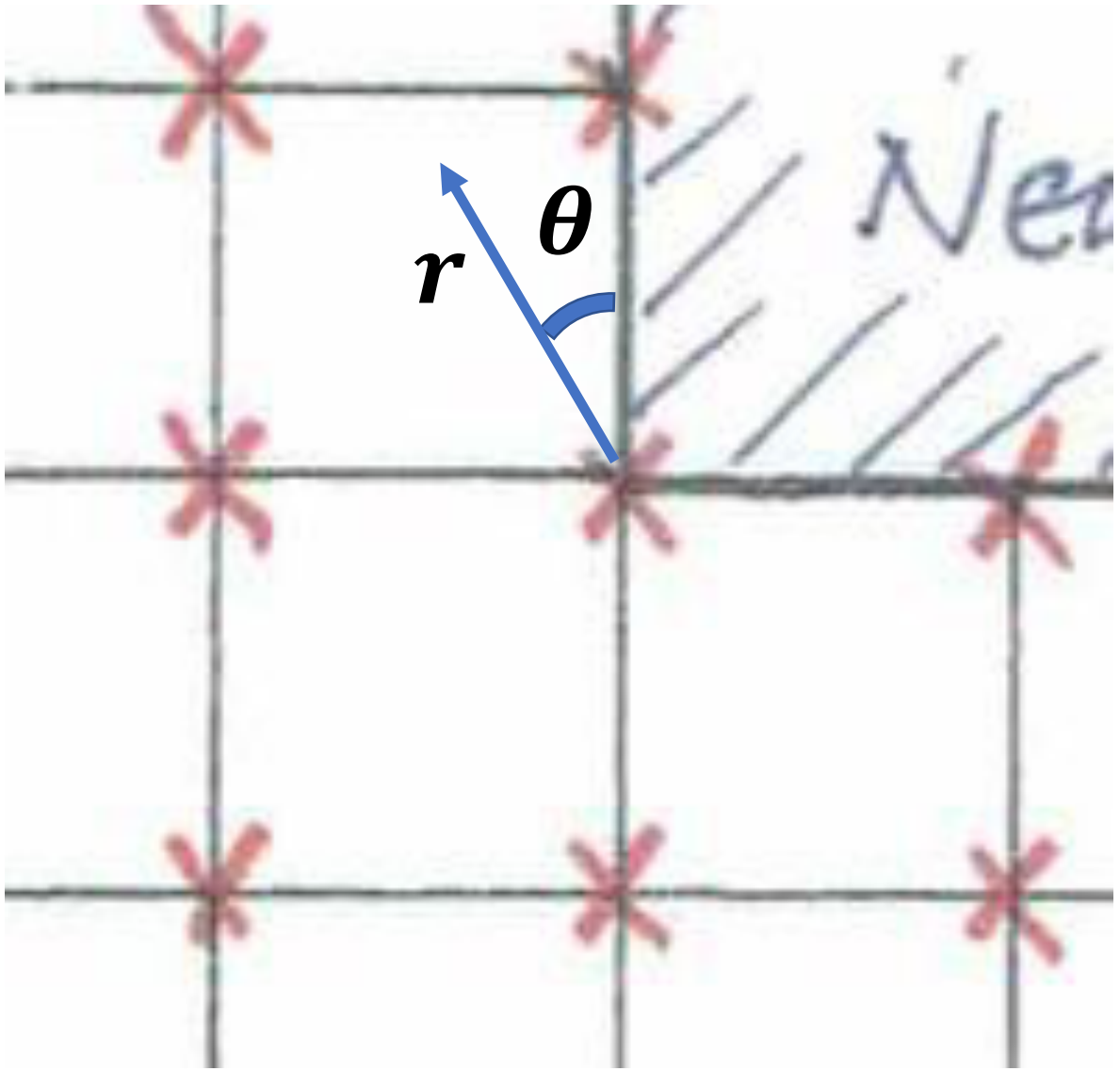
Yes, a ***direct*** *numerical model of the physics,* because in fact we redefine the physical quantities: we have *defined* the outflow over an edge as the normal flux in the midpoint times the length of the edge; we have *defined* the normal flux in the midpoint as the temperature difference between two points on the normal vector, on either side of the edge, at $\frac{1}{2}h$ distance, and then multiplied by λ. Adopting these definitions, our model satisfies conservation of heat in every square or half square or other type of box, and as a consequence, the total flow through any cross section is the same, and this holds not only for straight cross sections, but for any path that is made up from box edges, and that is running from one insulated boundary to the other. And of course we have conservation of heat within any domain made up of a collection of (adjacent) boxes, and ultimately we have heat conservation over the total domain.

A **numerical** aspect: when deriving the box-integration formula for each type of nodal point, we have seen that they were equivalent to the result by Taylor expansions: sometimes they differed by just a factor 2 or 4. Following Taylor expansions we more or less automatically arrived at formulas with coefficient 4 in the central entry point P, and it has some charm to see a matrix diagonal having all entries equal. However, the matrix built up by box-integration is automatically **symmetric**, which is a welcome property in computer work: it not only saves storage (in this case some 40%), but procedures for matrix solving are often quite faster for symmetric than for non-symmetric matrices.

Chapter 9 Analysis of the singularity at the inward corner

To analyze the behavior of the solution around the corner point $(x, y) = (1,1)$, we use polar coordinates r and θ. Let θ be counted from the line $x = 1, y > 1$. The Laplace Equation takes the form: $r\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\,u(r,\theta)\right) + \frac{\partial}{\partial\theta}\frac{\partial}{\partial\theta}\,u(r,\theta) = 0$. By separation of variables, that is: by trying a solution of the form $u(r,\theta) = R(r)\cdot\Theta(\theta)$, we find $R(r) = r^m$ and $\Theta(\theta) = \cos m\theta$ for real $m > 0$, where we do not include $\sin m\theta$, so that $u(r,\theta)$ already satisfies the Neumann condition $\frac{\partial u}{\partial n} = 0$ along the boundary $\theta = 0$. The Neumann condition along the boundary $\theta = \frac{3}{2}\pi$ selects the admissible values of m: $m \times \frac{3}{2}\pi$ must be a multiple of π and so: $m = \frac{2}{3}k$ for $k = 0, 1, 2, 3, \ldots$, so that $m = 0,\ \frac{2}{3},\ \frac{4}{3}, 2, \ldots$ In this way we find the first four terms of the Fourier expansion:

$$u_1(r,\theta) = 1, \quad u_2(r,\theta) = r^{2/3}\cos\tfrac{2}{3}\theta\,, \quad u_3(r,\theta) = r^{4/3}\cos\tfrac{4}{3}\theta\,, \quad u_4(r,\theta) = r^2\cos 2\theta$$


r
θ

Now we fit the first four terms of the expansion

$$u(r,\theta) = a_1 + a_2\, r^{2/3} \cos\tfrac{2}{3}\theta + a_3\, r^{4/3} \cos\tfrac{4}{3}\theta + a_4\, r^2 \cos 2\theta$$

to the five nodal values, the values in P, U, B, S, T:

$$u_P = u(0,\theta) = a_1$$

$$u_U = u(h,0) = a_1 + a_2\, h^{2/3} + a_3\, h^{4/3} + a_4\, h^2$$

$$u_B = u\left(h,\tfrac{\pi}{2}\right) = a_1 + \tfrac{1}{2} a_2\, h^{2/3} - \tfrac{1}{2} a_3\, h^{4/3} - a_4\, h^2$$

$$u_S = u\,(h,\pi) = a_1 - \tfrac{1}{2}\, a_2\, h^{2/3} - \tfrac{1}{2} a_3\, h^{4/3} + a_4\, h^2$$

$$u_T = u\left(h,\tfrac{3}{2}\pi\right) = a_1 - a_2\, h^{2/3} + a_3\, h^{4/3} - a_4\, h^2$$

We see that $u_U + u_T = 2a_1 + 2a_3\, h^{4/3}$

and $u_B + u_S = 2a_1 - a_3\, h^{4/3}$

so that by eliminating a_3 we find $u_U + u_T + 2u_B + 2u_S = 6a_1 = 6\, u_P$

To our surprise this is identical to (48), the result of the simple box-integration.