

Numerical methods for Partial Differential Equations

Adriano Festa
Politecnico of Turin, Italy
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Let us consider a fluid which occupies a thin volume in space

$$\mathcal{V} = \overline{\Omega} \times [-\varepsilon, \varepsilon] ,$$

where Ω is a bounded region in the plane.

Let us suppose that the fluid motion is *bi-dimensional*, namely, that its variations in the z -direction are negligible. In this case, the flow can be described by functions defined in Ω .

Let us adopt the *Eulerian* point of view: if ϕ is a physical variable (velocity, pressure, temperature, ...), the expression $\phi(\mathbf{x}, t)$ indicates the value of ϕ associated with the fluid particle that at time t is at the point $\mathbf{x} \in \Omega$.

Let us denote the velocity of the fluid by $\mathbf{a} = \mathbf{a}(\mathbf{x}, t)$, and its temperature by $u = u(\mathbf{x}, t)$. Let us assume that the flow is *incompressible*: this is expressed by the condition

$$\nabla \cdot \mathbf{a} = 0 \quad \text{in } \Omega \quad \text{for each } t ,$$

which implies that the density ρ is constant (in space and time).

Let us also assume that the specific heat c and the thermal conductivity κ are constant.

- If the fluid is at rest, its temperature obeys the heat equation

$$c \rho \frac{\partial u}{\partial t} - \kappa \Delta u = \rho q .$$

- If the fluid is in motion, the partial derivative $\frac{\partial u}{\partial t}$ in this equation must be replaced by the *total derivative* (also known as *Lagrangian derivative*, or *particle derivative*)

$$\frac{Du}{Dt} = \frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u , \quad (69)$$

which represents the time derivative of the temperature of a particle followed along its motion.

Thus, we obtain the equation

$$c \rho \left(\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u \right) - \kappa \Delta u = \rho q .$$

In order to justify this statement, let us recall that particles move along *streamlines* $\mathbf{x} = \mathbf{x}(t)$, defined as the solutions of the differential system

$$\frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}, t)$$

(hence, the velocity vectors are tangent to the streamlines at each point); in particular, the particle that at a certain time t_0 passes through the point \mathbf{x}_0 moves along the streamline defined by the Cauchy problem

$$\begin{cases} \frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}, t) \\ \mathbf{x}(t_0) = \mathbf{x}_0 ; \end{cases}$$

let us indicate such a solution by $\mathbf{x} = \mathbf{x}(t, \mathbf{x}_0)$. Then, the function

$$t \mapsto u(\mathbf{x}(t, \mathbf{x}_0), t)$$

describes the time evolution of the temperature of the particle that at time t_0 passes through \mathbf{x}_0 . Let us set

$$\frac{Du}{Dt}(\mathbf{x}_0, t_0) = \frac{d}{dt}u(\mathbf{x}(t, \mathbf{x}_0), t) \Big|_{t=t_0} .$$

By applying the chain rule (differentiation of a composite function), we have

$$\frac{Du}{Dt}(\mathbf{x}_0, t_0) = \left(\nabla u(\mathbf{x}(t, \mathbf{x}_0), t) \cdot \frac{d}{dt} \mathbf{x}(t, \mathbf{x}_0) + \frac{\partial u}{\partial t}(\mathbf{x}(t, \mathbf{x}_0), t) \right) \Big|_{t=t_0},$$

and since by definition of $\mathbf{x} = \mathbf{x}(t)$

$$\frac{d\mathbf{x}}{dt} = \mathbf{a}(\mathbf{x}, t),$$

we obtain

$$\frac{Du}{Dt}(\mathbf{x}_0, t_0) = \nabla u(\mathbf{x}_0, t_0) \cdot \mathbf{a}(\mathbf{x}_0, t_0) + \frac{\partial u}{\partial t}(\mathbf{x}_0, t_0),$$

namely, formula (69).

Going back to the equation

$$c \rho \left(\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u \right) - \kappa \Delta u = \rho q ,$$

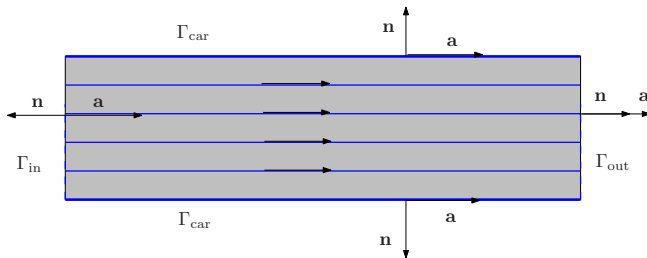
it is convenient to divide both sides by $c \rho$, and set

$$\nu = \frac{\kappa}{c \rho} \quad (\text{coefficient of thermal diffusion}) , \quad f = \frac{q}{c} ;$$

we thus obtain the *convection-diffusion equation*

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u - \nu \Delta u = f \quad \text{in } \Omega , \quad 0 < t \leq T . \quad (70)$$

It requires to specify, in addition to the initial condition $u(0) = u_0$, one condition on u at each point of the boundary of Ω , for each time t .



To this end, it is appropriate to partition the boundary $\partial\Omega$ in

$$\partial\Omega = \Gamma_{\text{in}} \cup \Gamma_{\text{car}} \cup \Gamma_{\text{out}} ,$$

where, denoting as usual by $\mathbf{n} = \mathbf{n}(\mathbf{x})$ the normal unit vector to $\partial\Omega$ pointing outward Ω , we set:

$$\Gamma_{\text{in}} = \{\mathbf{x} \in \partial\Omega : \mathbf{a} \cdot \mathbf{n} < 0\} \quad (\text{inflow boundary, the fluid enters } \Omega) ,$$

$$\Gamma_{\text{car}} = \{\mathbf{x} \in \partial\Omega : \mathbf{a} \cdot \mathbf{n} = 0\} \quad (\text{characteristic boundary, the fluid is flowing along it}) ,$$

$$\Gamma_{\text{out}} = \{\mathbf{x} \in \partial\Omega : \mathbf{a} \cdot \mathbf{n} > 0\} \quad (\text{outflow boundary, the fluid is leaving } \Omega) .$$

Note that, since \mathbf{a} may depend upon time, such a partition may itself vary in time.

- It is reasonable to assume that we know the temperature of the fluid entering Ω , i.e., we enforce the Dirichlet condition

$$u = g \quad \text{on } \Gamma_{\text{in}}, \quad 0 < t \leq T.$$

- At the outflow, the fluid temperature is usually unknown, whereas it is reasonable to make assumptions on the outgoing heat flux; for instance, one may enforce the Neumann condition

$$\frac{\partial u}{\partial n} = 0 \quad \text{on } \Gamma_{\text{out}}, \quad 0 < t \leq T,$$

meaning that we assume therein that the heat flux

$$\Phi = (\mathbf{a} \cdot \mathbf{n}) \rho c u - \kappa \frac{\partial u}{\partial n}$$

takes the value $\Phi = (\mathbf{a} \cdot \mathbf{n}) \rho c u$, i.e., it is fully of convective nature.

- At last, on Γ_{car} one may assign the temperature value (if the wall is a thermostat), or the heat flux (if, for instance, the wall is thermally insulated).

The convection-diffusion equation

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u - \nu \Delta u = f \quad \text{in } \Omega, \quad 0 < t \leq T,$$

also describes the temporal evolution of a mass dispersed in a fluid; for instance, u may represent the *concentration of a pollutant* in a liquid. In this case, the equation is also referred to as the *transport-diffusion* equation.

In general, the convection-diffusion equation describes the evolution of a *passive scalar* u (passive means that it does not influence the fluid motion, i.e., the velocity field \mathbf{a} does not depend on u).

The Péclet number

The convection-diffusion equation models the simultaneous presence of two physical phenomena: heat convection along the streamlines and heat diffusion due to molecular interaction.

The trade-off between the two phenomena is described by the *Péclet number*

$$\mathbb{P}e = \frac{AL}{2\nu} \geq 0 ,$$

where $A = \max_{\Omega} \|\mathbf{a}\|$ is the maximum modulus of velocity, whereas L is a characteristic length (such as the diameter of Ω).

- If $\mathbb{P}e$ is comparable to 1, convection and diffusion have comparable importance.
- If $\mathbb{P}e \ll 1$, the diffusive effects are prevailing over the convective ones.
(In particular, if $\mathbb{P}e = 0$, i.e., $\mathbf{a} = \mathbf{0}$ identically, one has diffusion alone, i.e., one is back to the heat equation).
- If $\mathbb{P}e \gg 1$ instead, convection outweighs diffusion; the limit case $\mathbb{P}e = +\infty$, namely $\nu = 0$, corresponds to the pure convection equation (also indicated as *transport equation*)

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u = f .$$

- Convection-diffusion equation ($\mathbb{P}e < \infty$) :

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u - \nu \Delta u = f \quad \text{in } \Omega ,$$

boundary conditions on $\Gamma_{\text{in}} \cup \Gamma_{\text{car}} \cup \Gamma_{\text{out}} .$

- Pure-convection, or transport, equation ($\mathbb{P}e = \infty$) :

$$\frac{\partial u}{\partial t} + \mathbf{a} \cdot \nabla u = f \quad \text{in } \Omega ,$$

boundary conditions on $\Gamma_{\text{in}} .$

When $\mathbb{P}e \gg 1$, the solution to the convection-diffusion equation tends to behave, in most of the domain, like the solution of the purely-convective equation; where this does not happen, thermal *boundary layers* or *internal layers* are formed, i.e., sudden variations of the temperature.

An example is when a boundary layer is created next to Γ_{char} or Γ_{out} : the temperature, flowing along the internal streamlines, is all of a sudden forced to satisfy boundary conditions imposed by the nature of the convection-diffusion equation.

Whether or not convection prevails over diffusion affects the efficiency of discretization schemes as well, and consequently their choice.

At the numerical level the role of the Péclet number is played by the *mesh Péclet number*. Precisely, in each element T of the mesh, with diameter h_T , one defines the *local Péclet number*

$$\mathbb{P}e_T = \frac{\|\mathbf{a}_T\| h_T}{2\nu} \quad \left(\text{vs } \mathbb{P}e = \frac{AL}{2\nu} \right) ;$$

this means that the characteristic velocity and length of the domain Ω are replaced by those of the mesh element T .

The mesh Péclet number is then defined as

$$\mathbb{P}e_h = \max_T \mathbb{P}e_T .$$

One says that the convection-diffusion problem is, relatively to the grid adopted,

- *diffusion-dominated*, if $\mathbb{P}e_h \leq 1$,
- *convection-dominated*, if $\mathbb{P}e_h > 1$.

- For a *diffusion-dominated* problem, the finite-difference or finite-element methods used so far for the heat equation may be successfully adopted also for the convection-diffusion equation.
- For a *convection-dominated* problem, the same methods may be *unstable*, i.e., they may spawn spurious (non-physical) oscillations between the nodes.
Therefore they must be replaced by other kinds of discretizations, that take into account the mainly propagative character of the phenomenon modelled.

Discretization by finite differences:

On a equally-spaced grid with nodes $\mathbf{x}_{\ell m} = (x_\ell, y_m)$, the convective term $\mathbf{a} \cdot \nabla u$ is discretized by means of second-order centered incremental quotients, in the two directions x and y . We thus have

$$(\mathbf{a} \cdot \nabla u)(\mathbf{x}_{\ell m}) \simeq a_1(\mathbf{x}_{\ell m}) \frac{u_{\ell+1,m} - u_{\ell-1,m}}{2h} + a_2(\mathbf{x}_{\ell m}) \frac{u_{\ell,m+1} - u_{\ell,m-1}}{2h} .$$

In this manner, setting $a_{1,\ell m} = a_1(\mathbf{x}_{\ell m})$ and $a_{2,\ell m} = a_2(\mathbf{x}_{\ell m})$, we obtain the following spatial semi-discretization scheme for the convection-diffusion equation:

$$\begin{aligned} u'_{\ell m} + \frac{a_{1,\ell m}}{2h} (u_{\ell+1,m} - u_{\ell-1,m}) + \frac{a_{2,\ell m}}{2h} (u_{\ell,m+1} - u_{\ell,m-1}) \\ + \frac{\nu}{h^2} (-u_{\ell,m-1} - u_{\ell-1,m} + 4u_{\ell m} - u_{\ell+1,m} - u_{\ell,m+1}) = f_{\ell m}, \\ 1 \leq \ell, m \leq N, \quad 0 < t \leq T, \end{aligned}$$

which must be supplemented with appropriate conditions at the boundary nodes, as well as with initial conditions.

Discretization by finite elements:

The discrete integral formulation of the convection-diffusion equation (assuming for simplicity vanishing boundary conditions) is

$$\begin{cases} u_h(t) \in V_h \text{ and satisfies} \\ \int_{\Omega} \frac{\partial u_h}{\partial t} v_h d\mathbf{x} + \int_{\Omega} (\mathbf{a} \cdot \nabla u_h) v_h d\mathbf{x} + \int_{\Omega} \nu \nabla u_h \cdot \nabla v_h d\mathbf{x} = \int_{\Omega} f v_h d\mathbf{x} \quad \forall v_h \in V_h . \end{cases}$$

It is translated, as usual, into the system of ordinary differential equations

$$\mathbf{B} \mathbf{u}' + \mathbf{A} \mathbf{u} = \mathbf{f} ,$$

where now the “stiffness matrix” \mathbf{A} may be decomposed as

$$\mathbf{A} = \mathbf{C} + \mathbf{D} ,$$

where $\mathbf{D} = (d_{jk})$ with $d_{jk} = \int_{\Omega} \nu \nabla \varphi_k \cdot \nabla \varphi_j d\mathbf{x}$ indicates the by now familiar symmetric and positive-definite matrix that describes diffusion, whereas

$$\mathbf{C} = (c_{jk}) , \quad \text{with} \quad c_{jk} = \int_{\Omega} (\mathbf{a} \cdot \nabla \varphi_k) \varphi_j d\mathbf{x} ,$$

is the matrix that describes convection.

The matrix \mathbf{C} turns out to be as sparse as \mathbf{D} , but it is not symmetric; note that it may depend upon time via \mathbf{a} , namely in general $\mathbf{C} = \mathbf{C}(t)$.

Let us investigate the structure of the *matrix* $\mathbf{C}^{(T)}$ *relative to an element* $T \in \mathcal{T}$; this elemental matrix collects the contribution of the element T to the global matrix \mathbf{C} . With the usual notation, we have

$$\mathbf{C}^{(T)} = \left(c_{\alpha\beta}^{(T)} \right)_{1 \leq \alpha, \beta \leq 3} \in \mathbb{R}^{3 \times 3}, \quad \text{with} \quad c_{\alpha\beta}^{(T)} = \int_T (\mathbf{a} \cdot \nabla \varphi_\beta) \varphi_\alpha d\mathbf{x}.$$

If \mathbf{a}_T denotes a constant that approximates \mathbf{a} on T , we may properly define the matrix by setting

$$c_{\alpha\beta}^{(T)} = \int_T (\mathbf{a}_T \cdot \nabla \varphi_\beta) \varphi_\alpha d\mathbf{x} = \mathbf{a}_T \cdot \nabla \varphi_\beta \int_T \varphi_\alpha d\mathbf{x},$$

since $\mathbf{a}_T \cdot \nabla \varphi_\beta$ is constant on T ; on the other hand,

$$\int_T \varphi_\alpha d\mathbf{x} = \frac{1}{3}|T|, \quad 1 \leq \alpha \leq 3,$$

(volume of the pyramid with base T and height 1). We conclude that

$$c_{\alpha\beta}^{(T)} = \frac{1}{3}|T| \mathbf{a}_T \cdot \nabla \varphi_\beta, \quad 1 \leq \alpha, \beta \leq 3.$$

Let us observe that

$$c_{\alpha\beta}^{(T)} = \frac{1}{3}|T| \mathbf{a}_T \cdot \nabla \varphi_\beta$$

does not depend upon α ; hence, the three rows of the matrix $\mathbf{C}^{(T)}$ are equal.

Furthermore, the sum of the entries in each row is zero, since

$$\sum_{\beta=1}^3 c_{\alpha\beta}^{(T)} = \frac{1}{3}|T| \mathbf{a}_T \cdot \nabla \left(\sum_{\beta=1}^3 \varphi_\beta \right) = 0 ;$$

this represents a very useful “test” of correctness.

The convection matrix in the one-dimensional case

Let us consider the convection-diffusion equation in an interval $[0, L]$ of the real line, submitted to homogeneous Dirichlet boundary conditions:

$$\begin{cases} \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = f & \text{in } (0, L), \quad 0 < t \leq T, \\ u(0, t) = u(L, t) = 0 & 0 < t \leq T \\ u(x, 0) = u_0(x) & \text{in } (0, L), \end{cases}$$

where $a = a(x, t)$ is a variable coefficient in $[0, L]$, whereas $\nu > 0$ is constant.

Let us discretize the problem by linear finite elements on a subdivision of the interval $[0, L]$ in elements $I_j = [x_{j-1}, x_j]$ of size h_j . With the usual notation, the convection matrix C is given by

$$C = (c_{jk}) , \quad \text{with} \quad c_{jk} = \int_0^L a \frac{d\varphi_k}{dx} \varphi_j dx ;$$

it turns out to be tridiagonal (since $c_{jk} = 0$ if $|j - k| > 1$).

Let us approximate the velocity a in the element I_j by a constant value $a_{j-1/2}$ (for instance, by the value $a((x_{j-1} + x_j)/2, t)$ in the midpoint of the element).

With easy computations, we obtain

$$c_{jk} = \begin{cases} \frac{a_{j-1/2}}{2} - \frac{a_{j+1/2}}{2} & \text{if } k = j, \\ -\frac{a_{j-1/2}}{2} & \text{if } k = j - 1, \\ \frac{a_{j+1/2}}{2} & \text{if } k = j + 1, \\ 0 & \text{otherwise.} \end{cases}$$

Let us observe that if a is constant, then C reduces to the form

$$C = \frac{a}{2} \text{tridiag} [-1 \ 0 \ 1]$$

and is anti-symmetric, i.e., it satisfies $C^T = -C$.

Convection-dominated problems ($\mathbb{P}e_h \gg 1$)

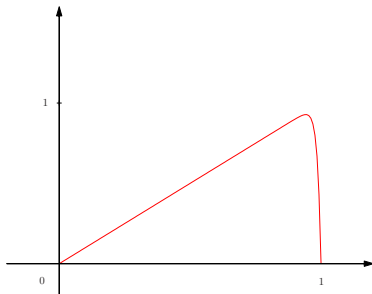
In order to highlight the difficulties arising from the use of standard discretization schemes when $\mathbb{P}e_h \gg 1$, let us consider the *steady* version of the problem

$$\begin{cases} \frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} - \nu \frac{\partial^2 u}{\partial x^2} = f & \text{in } (0, L), \quad 0 < t \leq T, \\ u(0, t) = 0, \quad u(L, t) = 0 & 0 < t \leq T, \\ u(x, 0) = u_0(x) & \text{in } (0, L), \end{cases}$$

namely,

$$\begin{cases} a \frac{du}{dx} - \nu \frac{d^2 u}{dx^2} = f & \text{in } (0, L), \\ u(0) = 0, \quad u(L) = 0, \end{cases}$$

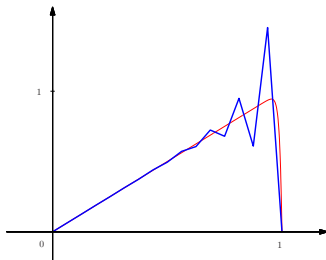
with $a \neq 0$ constant.



Let us choose $f = 1$, $a = 1$ and $\nu = 10^{-2}$. In most of the interval, the exact solution is close to the solution $\tilde{u}(x) = x$ of the pure convection problem

$$\begin{cases} a \frac{d\tilde{u}}{dx} = f & \text{in } (0, L) , \\ \tilde{u}(0) = 0 ; \end{cases}$$

only in a neighborhood of size $\mathcal{O}(\nu)$ of the outflow point $x = 1$, u deviates from \tilde{u} in order to adapt itself to the boundary condition enforced therein. Thus, a *boundary layer* appears.



Let us discretize the problem by means of *centered finite differences* on a equally-spaced grid of stepsize h ; we obtain

$$\frac{a}{2h}(u_{j+1} - u_{j-1}) + \frac{\nu}{h^2}(-u_{j-1} + 2u_j - u_{j+1}) = f_j, \quad 1 \leq j \leq N-1,$$

With the same values of f , a and ν given above, the choice $h = 1/16$ yields

$$\mathbb{P}e_h = ah/2\nu = 100/32 > 1.$$

The *spurious inter-node oscillations* are typical **instabilities** created by the use of a centered scheme: this is not appropriate for the convection-dominated regime, characterized by a precise direction of propagation (here from left to right, since $a > 0$).

A similar behavior occurs if we adopt a discretization based on standard linear finite elements, without any specific trick.

- Reduce the meshsize h , i.e., refine the computational grid, to the extent that the corresponding mesh Péclet number is brought to values ≤ 1 .
(Often prohibitive, in dimension 2 and, especially, 3.)
- Use the same grid but change the way the convective term is discretized.
The most natural and simple strategy consists of replacing, in the discretization scheme, the centered incremental quotient

$$a \frac{du}{dx}(x_j) \simeq a \frac{u_{j+1} - u_{j-1}}{2h} ,$$

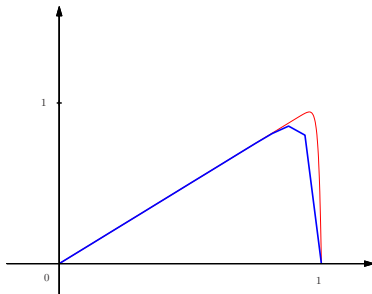
by the *backward incremental quotient*

$$a \frac{du}{dx}(x_j) \simeq a \frac{u_j - u_{j-1}}{h} \quad \text{if } a > 0 ,$$

or by the *forward incremental quotient*

$$a \frac{du}{dx}(x_j) \simeq a \frac{u_{j+1} - u_j}{h} \quad \text{if } a < 0 .$$

In this way, one adopts the philosophy of *upwind schemes*.



Here is what we get in our example by using the backward incremental quotient.

One can show that such a scheme is indeed equivalent to a centered scheme applied to another convection-diffusion equation, namely the one in which ν is replaced by

$$\tilde{\nu} = \nu + \frac{|a|}{2}h$$

(i.e., an *artificial diffusion*, or *numerical diffusion*, proportional to h , has been added), in such a way that the new mesh Péclet number satisfies

$$\tilde{\mathbb{P}}e_h = \frac{|a|h}{2\tilde{\nu}} = \frac{|a|h}{2\nu + |a|h} < 1 .$$

The standard finite element discretization can be modified as well according to the *upwind* philosophy, to account for the presence of a dominant convective term.

For instance, in the popular *SUPG* (*Streamline Upwind Petrov-Galerkin*) method, one adds to the discrete variational formulation a specific stabilization term. In this manner, an artificial diffusion effect is generated, which prevents the onset of spurious oscillations.

A simple form of stabilization is as follows:

$$\int_{\Omega} \frac{\partial u_h}{\partial t} v_h d\mathbf{x} + \int_{\Omega} (\mathbf{a} \cdot \nabla u_h) v_h d\mathbf{x} + S_h(u_h, v_h) + \int_{\Omega} \nu \nabla u_h \cdot \nabla v_h d\mathbf{x} \\ = \int_{\Omega} f v_h d\mathbf{x} \quad \forall v_h \in V_h ,$$

where

$$S_h(u_h, v_h) = \sum_{T \in \mathcal{T}} \tau_T \int_T (\mathbf{a}_T \cdot \nabla u_h) (\mathbf{a}_T \cdot \nabla v_h) d\mathbf{x}$$

with

$$\tau_T = \begin{cases} \frac{h_T}{\|\mathbf{a}_T\|} & \text{if } \mathbb{P}e_T > 1, \\ 0 & \text{otherwise.} \end{cases}$$