Boundary value problems

- Until now, we studied only initial value problems, namely differential equations in which the boundary conditions are all on one side of the computational domain.
- However, we will see when studying partial differential equations that many times one has to deal also with problems where the **boundary conditions are on different sides of the computational domain**. We refer to such problems as **Boundary Value Problems** (BVP).

Boundary value problems

- Let us suppose to have a **model problem** (we will see when studying partial differential equations that this is quite a common example!) of this type:

$$d(x)\frac{d^2Y(x)}{dx^2} + f(x)\frac{dY(x)}{dx} + g(x)Y(x) = h(x) \quad x \in [a,b]$$

  where $d(x)$, $f(x)$, $g(x)$ and $h(x)$ are **known**.

- To completely solve the problem, we have to give some information about the behavior of the solution (or its derivatives) in a and b!

Boundary value problems

- Generally it is sufficient to know **two different values** (since this is a second order differential equation!), e.g.:
  - the solution on the two boundaries, in which case we talk of Dirichlet boundary conditions (**Dirichlet b.c.**);
  - the first derivatives of the solution on the two boundaries (**Neumann b.c.**);
  - the solution on one boundary and its first derivative on the other boundary (**Robin b.c.**).

Boundary value problems

- More specifically, we can distinguish 4 cases:

Case	Known quantities	Name
1	$Y(a)$ and $Y(b)$	Dirichlet b.c.
2	$Y'(a)$ and $Y'(b)$	Neumann b.c.
3	$Y'(a)$ and $Y(b)$	Robin b.c.
4	$Y(a)$ and $Y'(b)$	Robin b.c.

- To start solving the problem, as usual, we assume that we can make a discretization of the spatial domain by dividing the interval $[a,b]$ into N subintervals of width: $h = \dfrac{b-a}{N}$

Boundary value problems

- In such a way we identify $N+1$ discrete points x_j:

$$x_j = a + jh; \qquad j = 0, \ldots, N$$

so that: $x_0 = a$, $x_N = b$.

- Now, as we did for ODEs, we can write our equation on a generic grid-point x_j:

$$d(x_j) \left. \frac{d^2Y(x)}{dx^2} \right|_{x_j} + f(x_j) \left. \frac{dY(x)}{dx} \right|_{x_j} + g(x_j)Y(x_j) = h(x_j)$$

- Now we have to find a suitable approximation for the first and second derivatives in x_j!

Boundary value problems

- We have already studied **the finite difference approximations for the derivatives** on a generic point x_j. For instance, second order f.d. approximations for the first and second derivatives are given by:

$$\left.\frac{dY(x)}{dx}\right|_{x_j} = \frac{Y_{j+1} - Y_{j-1}}{2h} + O(h^2)$$

$$\left.\frac{d^2Y(x)}{dx^2}\right|_{x_j} = \frac{Y_{j+1} - 2Y_j + Y_{j-1}}{h^2} + O(h^2)$$

where, with Y_j we mean $Y(x_j)$, etc.

Boundary value problems

- Now we can put these approximations into the equation:

$$d_j \frac{Y_{j+1} - 2Y_j + Y_{j-1}}{h^2} + f_j \frac{Y_{j+1} - Y_{j-1}}{2h} + g_j Y_j = h_j$$

- We can now re-arrange the terms as:

$$Y_{j-1} \underbrace{\left[\frac{d_j}{h^2} - \frac{f_j}{2h}\right]}_{\lambda_j} + Y_j \underbrace{\left[-\frac{2d_j}{h^2} + g_j\right]}_{\mu_j} + Y_{j+1} \underbrace{\left[\frac{d_j}{h^2} + \frac{f_j}{2h}\right]}_{\xi_j} = h_j$$

where λ_j, μ_j and ξ_j are known quantities.

Boundary value problems

- Therefore, we have **transformed** our **differential equation** in a relation involving **discrete quantities**, as:

$$\lambda_j Y_{j-1} + \mu_j Y_j + \xi_j Y_{j+1} = h_j, \qquad \text{for } j = 0, \ldots, N$$

  where all quantities are known, except Y_j, that are the unknowns of the problem!

- Of course, such a relation makes sense only for

  $j = 1, \ldots, N\text{-}1$, since **we do not have information about the behavior of the solution at the points x_{-1} and x_{N+1}** which appear in the relation for $j=0$ and $j=N$.

Boundary value problems

- Thus, we have $N\text{-}1$ **relations** for $N+1$ **unknowns** Y_j. Of course the missing information can be obtained by taking into account the **boundary conditions**!
- Let us study separately the four cases outlined above.
- Case 1: we know the values of Y_0 and Y_N.
- This is the simplest case: here we have actually $N\text{-}1$ **relations** for $N\text{-}1$ **unknowns**, that is the problem is **perfectly solvable**!

Dirichelet boundary conditions

- Let us write the relations for a simple case $N=5$.
- In this case, the grid-points are: $x_0, x_1, x_2, x_3, x_4, x_5$ and the unknowns are: Y_1, Y_2, Y_3, Y_4.
- The discrete form of the equation becomes:

$$
\begin{array}{llllllllll}
j=1 & \mu_1 Y_1 & + & \xi_1 Y_2 & & & & & = & h_1 - \lambda_1 Y_0 \\
j=2 & \lambda_2 Y_1 & + & \mu_2 Y_2 & + & \xi_2 Y_3 & & & = & h_2 \\
j=3 & & & \lambda_3 Y_2 & + & \mu_3 Y_3 & + & \xi_3 Y_4 & = & h_3 \\
j=4 & & & & & \lambda_4 Y_3 & + & \mu_4 Y_4 & = & h_4 - \xi_4 Y_5
\end{array}
$$

that is a **tridiagonal system** of algebraic equations!

Dirichelet boundary conditions

- In the general case, we get a tridiagonal system of *N-1* equations in *N-1* unknowns $Y_1, \ldots, Y_{N-1}$:

$$
\begin{array}{lrcl}
j=1 & \mu_1 Y_1 + \xi_1 Y_2 & = & h_1 - \lambda_1 Y_0 \\
j=2,\ldots,N-2 & \lambda_j Y_{j-1} + \mu_j Y_j + \xi_j Y_{j+1} & = & h_j \\
j=N-1 & \lambda_{N-1} Y_{N-2} + \mu_{N-1} Y_{N-1} & = & h_{N-1} - \xi_{N-1} Y_N
\end{array}
$$

- This can be solved, for instance, with the **LU factorization algorithm**!
- Case 2: we know the values of Y'_0 and Y'_N.

Neumann boundary conditions

- In this case, we consider **the whole set of $N+1$ equations** in which appear the quantities Y_{-1} and Y_{N+1}, but we can **use the boundary conditions** to get information about the latter.
- In fact, by writing the FD approximation for the first derivative for $j=0$ and $j=N$, we have:

$$Y'_0 = \frac{Y_1 - Y_{-1}}{2h} \quad \Rightarrow \quad Y_{-1} = Y_1 - 2hY'_0$$

$$Y'_N = \frac{Y_{N+1} - Y_{N-1}}{2h} \quad \Rightarrow \quad Y_{N+1} = Y_{N-1} + 2hY'_N$$

Neumann boundary conditions

- First, let us consider the particular case $N=5$ as an example. Now $x_j=x_0, x_1, x_2, x_3, x_4, x_5$ and the unknowns are: $Y_j = Y_0, Y_1, Y_2, Y_3, Y_4, Y_5$.
- The values of Y_{-1} and $Y_{N+1}=Y_6$ are:

$$Y_{-1} = Y_1 + 2hY'_0 \qquad Y_6 = Y_4 + 2hY'_5$$

and the discrete equations for $j=0$ and $j=5$ reads:

$$\lambda_0 Y_{-1} + \mu_0 Y_0 + \xi_0 Y_1 = h_0 \quad \Rightarrow \mu_0 Y_0 + (\xi_0 + \lambda_0) Y_1 = h_0 - 2h\lambda_0 Y'_0$$
$$\lambda_5 Y_4 + \mu_5 Y_5 + \xi_5 Y_6 = h_5 \quad \Rightarrow (\xi_5 + \lambda_5) Y_4 + \mu_5 Y_5 = h_5 - 2h\xi_5 Y'_5$$

Neumann boundary conditions

- We then get the tridiagonal system:

$$\begin{array}{llllllllllll}
\mu_0 Y_0 & + & (\xi_0+\lambda_0)Y_1 & & & & & & & & & = h_0 - 2h\lambda_0 Y_0' \\
\lambda_1 Y_0 & + & \mu_1 Y_1 & + & \xi_1 Y_2 & & & & & & & = h_1 \\
 & & \lambda_2 Y_1 & + & \mu_2 Y_2 & + & \xi_2 Y_3 & & & & & = h_2 \\
 & & & & \lambda_3 Y_2 & + & \mu_3 Y_3 & + & \xi_3 Y_4 & & & = h_3 \\
 & & & & & & \lambda_4 Y_3 & + & \mu_4 Y_4 & + & \xi_4 Y_5 & = h_4 \\
 & & & & & & & & (\xi_5+\lambda_5)Y_4 & + & \mu_5 Y_5 & = h_5 - 2h\xi_5 Y_5'
\end{array}$$

of six equations for the six unknowns $Y_0, \ldots, Y_5$.

- In the general case of $N+1$ equations, we have:

Neumann boundary conditions

$$\begin{array}{lrcl} j = 0 & \mu_0 Y_0 + (\xi_0 + \lambda_0) Y_1 & = & h_0 - 2h\lambda_0 Y_0' \\ j = 1, \ldots, N-1 & \lambda_j Y_{j-1} + \mu_j Y_j + \xi_j Y_{j+1} & = & h_j \\ j = N & (\xi_N + \lambda_N) Y_{N-1} + \mu_N Y_N & = & h_N - 2h\xi_N Y_N' \end{array}$$

- Finally, for the case of Robin b.c. we have a mixed situation:
  - If we know Y'_0 and Y_N, the system of equations becomes a system of N equations in the N unknowns: Y_0, Y_1, …, Y_{N-1}:

Robin boundary conditions

$$\begin{array}{lrcl}
j=0 & \mu_0 Y_0 + (\xi_0+\lambda_0)Y_1 & = & h_0 - 2h\lambda_0 Y_0' \\
j=1,\ldots,N-2 & \lambda_j Y_{j-1} + \mu_j Y_j + \xi_j Y_{j+1} & = & h_j \\
j=N-1 & \lambda_{N-1} Y_{N-2} + \mu_{N-1} Y_{N-1} & = & h_{N-1} - \xi_{N-1} Y_N
\end{array}$$

- If we know Y_0 and Y'_N, the system of equations becomes a system of N equations in the N unknowns: Y_1, Y_2, ..., Y_N:

$$\begin{array}{lrcl}
j=1 & \mu_1 Y_1 + \xi_1 Y_2 & = & h_1 - \lambda_1 Y_0 \\
j=2,\ldots,N-1 & \lambda_j Y_{j-1} + \mu_j Y_j + \xi_j Y_{j+1} & = & h_j \\
j=N & (\xi_N+\lambda_N) Y_{N-1} + \mu_N Y_N & = & h_N - 2h\xi_N Y_N'
\end{array}$$

An example: Chebyshev's Polynomials

- As an example of solution for a BVP, let us consider the solution of the equation:

$$(1-x^2)\frac{d^2Y(x)}{dx^2} - x\frac{dY(x)}{dx} + n^2Y(x) = 0$$

- It is "easy" to show that this equation has a **denumerable infinity of solutions** for each integer value of n, given by:

$$Y(x) = T_n(x) = \cos(n\theta) \qquad \text{where: } \theta(x) = \arccos(x)$$

- The functions $T_n(x)$ are called **Chebyshev polynomials**.

An example: Chebyshev's Polynomials

- As an example of solution for a BVP, let us consider the solution of the equation:

$$(1-x^2)\frac{d^2Y(x)}{dx^2} - x\frac{dY(x)}{dx} + n^2Y(x) = 0 \qquad x \in [-1,+1]$$

- It is "easy" to show that this equation has a **denumerable infinity of solutions** for each integer value of n, given by:

$$Y(x) = T_n(x) = \cos(n\theta) \qquad \text{where: } \theta(x) = \arccos(x)$$

- The functions $T_n(x)$ are called **Chebyshev polynomials**.

An example: Chebyshev's Polynomials

- This equation corresponds to our general BVP in the case:

$$d(x) = 1 - x^2; \quad f(x) = -x; \quad g(x) = n^2; \quad h(x) = 0.$$

- Are the solutions really "polynomials"? Yes, indeed:

$$T_0(x) = \cos(0 \cdot \arccos(x)) = 1;$$
$$T_1(x) = \cos(1 \cdot \arccos(x)) = x;$$
$$T_2(x) = \cos(2 \cdot \arccos(x)) = 2\cos^2(\arccos(x)) - 1 = 2x^2 - 1$$
$$\ldots$$

An example: Chebyshev's Polynomials

- We can solve this equation by using several kind of boundary conditions, since we know the analytical form of the solution. In particular, we have:

$$T_n(-1) = \cos[n \arccos(-1)] = (-1)^n$$

$$T_n(+1) = \cos[n \arccos(+1)] = +1$$

$$T_n'(x) = \frac{d}{dx}\cos[n\theta(x)] = \frac{d}{d\theta}\cos(n\theta)\cdot\frac{d\theta}{dx} =$$

$$= -\frac{1}{\sqrt{1-x^2}}[-n\sin(n\theta)] = n\frac{\sin[n \arccos(x)]}{\sqrt{1-x^2}}$$

$$\lim_{x\to-1} T_n'(x) = (-1)^n n^2$$

$$\lim_{x\to+1} T_n'(x) = n^2$$

An example: Chebyshev's Polynomials

- Therefore, we can get the solutions of the problem, given by the $T_n(x)$ for different kind of boundary conditions:

Case	Known quantities	Values
1	$Y(a)$ and $Y(b)$	$Y(-1) = (-1)^n; \quad Y(+1) = 1$
2	$Y'(a)$ and $Y'(b)$	$Y'(-1) = (-1)^n n^2; \quad Y'(+1) = n^2$
3	$Y'(a)$ and $Y(b)$	$Y'(-1) = (-1)^n n^2; \quad Y(+1) = 1$
4	$Y(a)$ and $Y'(b)$	$Y(-1) = (-1)^n; \quad Y'(+1) = n^2$