Module 02: Numerical Methods

Unit 04: Ordinary Differential Equation: BVP

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Learning Objectives

- To discretize ordinary differential equation (ODE) along with Boundary Conditions (BC).

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- To discretize ordinary differential equation (ODE) along with Boundary Conditions (BC).
- To derive the algebraic form using discretized ODE and BC(s).

Introduction

- Ordinary Differential Equation with
  - Space discretization: **Boundary Value Problem**
  - Time/ Time-like discretization: Initial Value Problem
- Physical problem in one-dimension can be mathematically conceptualized using ODE along with BC(s).

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- ODE can be solved by using Finite Difference approach.

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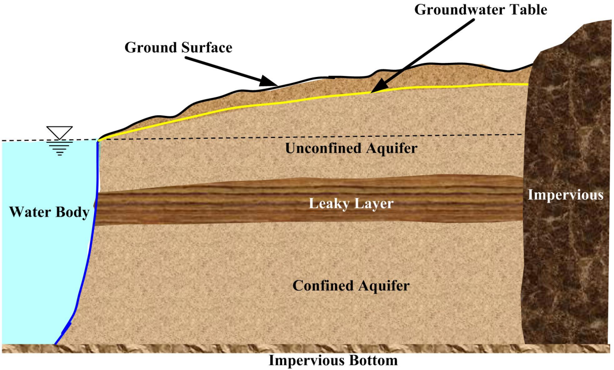
Problem Definition



Mathematical Conceptualization

The differential equation describing the head distribution in the aquifer is given as ,

$$\frac{d^2h}{dx^2} = \frac{C_{\text{conf}}}{T}(h - h_{wt}) \tag{1}$$

where,

$h =$ head,

$T =$ aquifer transmissivity,

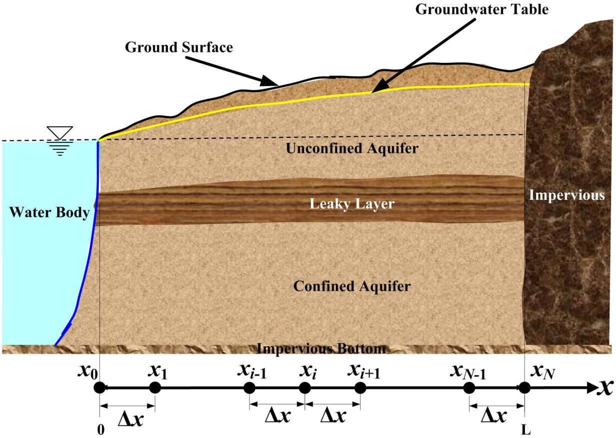
$C_{\text{conf}} =$ hydraulic conductivity/thickness of confining layer,

$h_{wt} =$ overlying water table elevation $(c_0 + c_1 x + c_2 x^2)$.

Boundary Conditions

- Left Boundary is specified head/ Dirichlet boundary: $h(x = 0) = h_s$
- Right Boundary is impervious/ no-flow/ Neumann Boundary: $\left.\frac{dh}{dx}\right|_L = 0$

Domain Discretization



Numerical Discretization
Governing Equation

The governing equation can be discretized as,

$$\frac{h_{i-1} - 2h_i + h_{i+1}}{\Delta x^2} + \mathcal{O}(\Delta x^2) = \frac{C_{\text{conf}}}{T}\left[h_i - h_{wt}(x_i)\right]$$

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The equation can be written as,

$$\frac{1}{\Delta x^2} h_{i-1} - \left(\frac{C_{\text{conf}}}{T} + \frac{2}{\Delta x^2}\right) h_i + \frac{1}{\Delta x^2} h_{i+1} = -\frac{C_{\text{conf}}}{T} h_{wt}(x_i)$$

Only true for interior points: $i = 1,\ 2,\ \cdots,\ N-2,\ N-1.$

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Only true for interior points: $i = 1,\ 2,\ \cdots,\ N-2,\ N-1$.
The equation can be further simplified as,

$$b_i h_{i-1} + d_i h_i + a_i h_{i+1} = r_i$$

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The equation can be further simplified as,

$$b_i h_{i-1} + d_i h_i + a_i h_{i+1} = r_i$$

where the coefficients are given by, $b_i = \frac{1}{\Delta x^2}$, $d_i = -\left(\frac{C_{\text{conf}}}{T} + \frac{2}{\Delta x^2}\right)$, $a_i = \frac{1}{\Delta x^2}$ and $r_i = -\frac{C_{\text{conf}}}{T} h_{wt}(x_i)$

Numerical Discretization

Boundary Conditions

The governing equation is used only for the interior points and the boundary conditions only for the boundary points.

Left Boundary

$$h_0 = h_s \tag{2}$$

Dirichlet boundary is without any truncation error.
In general equation format,
$b_0 = 0$, $d_0 = 1$, $a_0 = 0$ and $r_0 = h_s$

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Right Boundary

First Order Discretization

$$\frac{h_N - h_{N-1}}{\Delta x} + \mathcal{O}(\Delta x) = 0 \tag{3}$$

In general equation format,
$b_N = -\frac{1}{\Delta x}$, $d_N = \frac{1}{\Delta x}$, $a_N = 0$ and $r_N = 0$

Algebraic Form

$$\underbrace{\begin{bmatrix} d_0 & a_0 & & & & & & & \\ b_1 & d_1 & a_1 & & & & & & \\ & b_2 & d_2 & a_2 & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & \ddots & \ddots & \ddots & & \mathbf{0} & \\ & & \mathbf{0} & & \ddots & \ddots & \ddots & & \\ & & & & & \ddots & \ddots & \ddots & \\ & & & & & b_{N-2} & d_{N-2} & a_{N-2} & \\ & & & & & & b_{N-1} & d_{N-1} & a_{N-1} \\ & & & & & & & b_N & d_N \end{bmatrix}}_{\mathbf{A}_{(N+1)\times(N+1)}} \underbrace{\begin{bmatrix} h_0 \\ h_1 \\ h_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ h_{N-1} \\ h_{N-2} \\ h_N \end{bmatrix}}_{\mathbf{h}_{(N+1)\times 1}} = \underbrace{\begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ r_{N-1} \\ r_{N-2} \\ r_N \end{bmatrix}}_{\mathbf{r}_{(N+1)\times 1}}$$

Solution can be obtained as,

$$\mathbf{A}\mathbf{h} = \mathbf{r} \rightarrow \mathbf{h} = \mathbf{A}^{-1}\mathbf{r} \tag{4}$$

Tridiagonal Matrix Form

Tridiagonal Matrix Form

$$\begin{bmatrix} \bullet & \bullet \end{bmatrix}$$

Tridiagonal Matrix Form

$$\begin{bmatrix} \bullet & \bullet & & & & & \\ \color{blue}{\times} & \color{red}{\times} & \color{green}{\times} & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \end{bmatrix}$$

Tridiagonal Matrix Form

$$\left[\begin{matrix} \bullet & \bullet & & \\ {\color{blue}\times} & {\color{red}\times} & {\color{green}\times} & \\ & {\color{blue}\times} & {\color{red}\times} & {\color{green}\times} \\ & & & \\ & & & \\ & & & \\ & & & \end{matrix}\right.$$

Tridiagonal Matrix Form

$$\begin{bmatrix} \bullet & \bullet & & & \\ \times & \times & \times & & \\ & \times & \times & \times & \\ & & \ddots & \ddots & \ddots \\ & & & & \\ & & & & \end{bmatrix}$$

Tridiagonal Matrix Form

$$\left[\begin{array}{cccccc} \bullet & \bullet & & & & \\ \times & \times & \times & & & \\ & \times & \times & \times & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \quad 0 \\ & & & & & \end{array}\right.$$

Tridiagonal Matrix Form

$$\left[\begin{array}{ccccccc} \bullet & \bullet & & & & & \\ \times & \times & \times & & & & \\ & \times & \times & \times & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & \ddots & \ddots & \ddots & 0 \\ & & & & \ddots & \ddots & \ddots \\ & & & & & & \\ & & & & & & \end{array}\right.$$

Tridiagonal Matrix Form

$$\left[\begin{array}{cccccccc}
\bullet & \bullet & & & & & & \\
{\color{blue}\times} & {\color{red}\times} & {\color{green}\times} & & & & & \\
& {\color{blue}\times} & {\color{red}\times} & {\color{green}\times} & & & & \\
& & {\color{blue}\ddots} & {\color{red}\ddots} & {\color{green}\ddots} & & & \\
& & & {\color{blue}\ddots} & {\color{red}\ddots} & {\color{green}\ddots} & & 0 \\
& & & & {\color{blue}\ddots} & {\color{red}\ddots} & {\color{green}\ddots} & \\
& & & 0 & & {\color{blue}\ddots} & {\color{red}\ddots} & {\color{green}\ddots} \\
& & & & & & & \\
\end{array}\right.$$

Tridiagonal Matrix Form

$$
\left[
\begin{array}{ccccccccc}
\bullet & \bullet & & & & & & & \\
\times & \times & \times & & & & & & \\
 & \times & \times & \times & & & & & \\
 & & \ddots & \ddots & \ddots & & & & \\
 & & & \ddots & \ddots & \ddots & & 0 & \\
 & & & & \ddots & \ddots & \ddots & & \\
 & & & 0 & & \ddots & \ddots & \ddots & \\
 & & & & & & \times & \times & \times \\
 & & & & & & & &
\end{array}
\right.
$$

Tridiagonal Matrix Form

$$\begin{bmatrix} \bullet & \bullet & & & & & & & \\ \times & \times & \times & & & & & & \\ & \times & \times & \times & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & \ddots & \ddots & \ddots & & 0 & \\ & & & & \ddots & \ddots & \ddots & & \\ & & 0 & & & \ddots & \ddots & \ddots & \\ & & & & & & \times & \times & \times \\ & & & & & & & \times & \times & \times \end{bmatrix}$$

Tridiagonal Matrix Form

$$\begin{bmatrix}
\bullet & \bullet & & & & & & & \\
\times & \times & \times & & & & & & \\
 & \times & \times & \times & & & & & \\
 & & \ddots & \ddots & \ddots & & & & \\
 & & & \ddots & \ddots & \ddots & & 0 & \\
 & & & & \ddots & \ddots & \ddots & & \\
 & & 0 & & & \ddots & \ddots & \ddots & \\
 & & & & & & \times & \times & \times \\
 & & & & & & & \bullet & \bullet
\end{bmatrix}$$

- Sparse matrix structure
- Minimum storage requirement: $\mathbf{a}_{N+1}$, $\mathbf{b}_{N+1}$, $\mathbf{d}_{N+1}$

Accuracy of Boundary Condition

Right Boundary

Second Order Discretization

$$\frac{3h_N - 4h_{N-1} + h_{N-2}}{2\Delta x} + \mathcal{O}(\Delta x^2) = 0 \tag{5}$$

In general equation format,
$b_N = -\frac{4}{2\Delta x}$, $d_N = -\frac{3}{2\Delta x}$, $a_N = 0$ and $r_N = 0$
$e_N = \frac{1}{2\Delta x}$

Algebraic Form

$$
\underbrace{\begin{bmatrix}
d_0 & a_0 & & & & & & & \\
b_1 & d_1 & a_1 & & & & & & \\
 & b_2 & d_2 & a_2 & & & & & \\
 & & \ddots & \ddots & \ddots & & & & \\
 & & & \ddots & \ddots & \ddots & & \mathbf{0} & \\
 & & \mathbf{0} & & \ddots & \ddots & \ddots & & \\
 & & & & & \ddots & \ddots & \ddots & \\
 & & & & & b_{N-2} & d_{N-2} & a_{N-2} & \\
 & & & & & & b_{N-1} & d_{N-1} & a_{N-1} \\
 & & & & & & e_N & b_N & d_N
\end{bmatrix}}_{\mathbf{A}_{(N+1)\times(N+1)}}
\underbrace{\begin{bmatrix}
h_0 \\ h_1 \\ h_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ h_{N-1} \\ h_{N-2} \\ h_N
\end{bmatrix}}_{\mathbf{h}_{(N+1)\times 1}}
=
\underbrace{\begin{bmatrix}
r_0 \\ r_1 \\ r_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ r_{N-1} \\ r_{N-2} \\ r_N
\end{bmatrix}}_{\mathbf{r}_{(N+1)\times 1}}
$$

Solution can be obtained as,

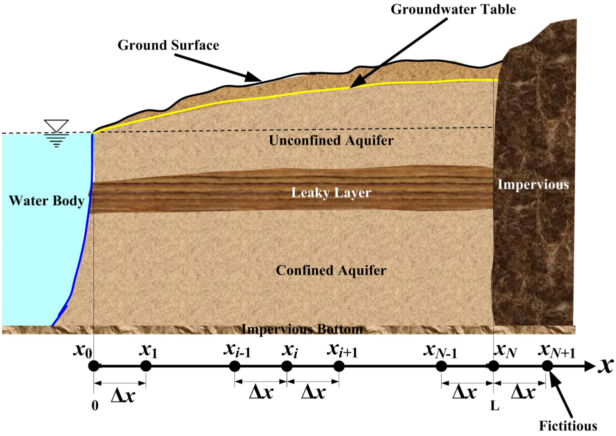
$$\mathbf{A}\mathbf{h} = \mathbf{r} \rightarrow \mathbf{h} = \mathbf{A}^{-1}\mathbf{r} \qquad (6)$$

Matrix Form

$$
\begin{bmatrix}
\bullet & \bullet & & & & & & & & \\
\times & \times & \times & & & & & & & \\
& \times & \times & \times & & & & & & \\
& & \ddots & \ddots & \ddots & & & & & \\
& & & \ddots & \ddots & \ddots & & 0 & & \\
& & 0 & & \ddots & \ddots & \ddots & & & \\
& & & & & \ddots & \ddots & \ddots & & \\
& & & & & & \times & \times & \times & \\
& & & & & & & \times & \times & \times \\
& & & & & & & \bullet & \bullet & \bullet
\end{bmatrix}
$$

- Tridiagonal Structure is broken.
- Completely second order scheme.
- Need to preserve the matrix structure.

Impermeable Boundary Treatment



Zero Neumann condition can be written as,

$$\frac{h_{N+1} - h_{N-1}}{2\Delta x} + \mathcal{O}(\Delta x^2) = 0 \Rightarrow h_{N+1} = h_{N-1}$$

Fictitious Point Method

Writing the discretized governing equation at $i = N$:

$$b_N h_{N-1} + d_N h_N + a_N h_{N+1} = r_N$$

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Using the boundary condition, this can be written as,

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$$b_N h_{N-1} + d_N h_N + a_N h_{N-1} = r_N$$

This can be simplified as,

$$(b_N + a_N) h_{N-1} + d_N h_N = r_N$$

where the coefficients are given by, $b_N = \frac{1}{\Delta x^2}$,
$d_N = -\left(\frac{C_{\text{conf}}}{T} + \frac{2}{\Delta x^2}\right)$, $a_N = \frac{1}{\Delta x^2}$ and $r_N = -\frac{C_{\text{conf}}}{T} h_{wt}(x_N)$

Algebraic Form

$$\underbrace{\begin{bmatrix} d_0 & a_0 & & & & & & \\ b_1 & d_1 & a_1 & & & & & \\ & b_2 & d_2 & a_2 & & & & \\ & & \ddots & \ddots & \ddots & & & \\ & & & \ddots & \ddots & \ddots & \mathbf{0} & \\ & \mathbf{0} & & & \ddots & \ddots & \ddots & \\ & & & & & \ddots & \ddots & \ddots \\ & & & & & b_{N-2} & d_{N-2} & a_{N-2} & \\ & & & & & & b_{N-1} & d_{N-1} & a_{N-1} \\ & & & & & & & b_N + a_N & d_N \end{bmatrix}}_{\mathbf{A}_{(N+1)\times(N+1)}} \underbrace{\begin{bmatrix} h_0 \\ h_1 \\ h_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ h_{N-1} \\ h_{N-2} \\ h_N \end{bmatrix}}_{\mathbf{h}_{(N+1)\times 1}} = \underbrace{\begin{bmatrix} r_0 \\ r_1 \\ r_2 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ r_{N-1} \\ r_{N-2} \\ r_N \end{bmatrix}}_{\mathbf{r}_{(N+1)\times 1}}$$

Solution can be obtained as,

$$\mathbf{Ah} = \mathbf{r} \rightarrow \mathbf{h} = \mathbf{A}^{-1}\mathbf{r} \tag{7}$$

Matrix Form

$$
\begin{bmatrix}
\bullet & \bullet & & & & & & & \\
\times & \times & \times & & & & & & \\
 & \times & \times & \times & & & & & \\
 & & \ddots & \ddots & \ddots & & & & \\
 & & & \ddots & \ddots & \ddots & & 0 & \\
 & & 0 & & \ddots & \ddots & \ddots & & \\
 & & & & & \ddots & \ddots & \ddots & \\
 & & & & & \times & \times & \times & \\
 & & & & & & \times & \times & \times \\
 & & & & & & & \bullet & \bullet
\end{bmatrix}
$$

- Tridiagonal Structure is preserved.
- Completely second order scheme.

Thank You