Numerically Solving Partial Differential Equations (Discretization)

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The world of our own is continuous
But the world of computer is discontinuous

https://minecraft.net/static/pages/img/index-hero-og.0757cc783ca4.jpg
Question

How can we mimic the real world (continuous world) with the discrete world?
This procedure is called “Discretization”
Partial differential equation

Partial differential equation (PDE) is the function of the form of:

\[
f \left( x_1, \ldots, x_n, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_n}, \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_1 \partial x_n}, \ldots \right) = 0.\]

https://en.wikipedia.org/wiki/Partial_differential_equation

In a nutshell, equations that contain sort of \( \partial / \partial x \) are the partial differential equations.
But why do we care PDE?

Because a lot of physics phenomena are described with PDEs! Examples are...

Water  https://flic.kr/p/iUFRhK

Fire    https://flic.kr/p/6iBy5G

Cloth   https://flic.kr/p/966FU

And, of course, even more!
Defining the problem

We wish to simulate physics phenomena by mean of computation.

We need to discretize a PDE that corresponds to the target physics phenomenon.
Discretization principle

Integrate over a small domain, and say it satisfies what it should. For example,

\[ f(x) = 0 \]

then it should be also true that:

\[ \int_{\Omega} f(x) \, dx = 0 \]
Discretization principle

Consider an arbitrary scalar function \( \theta(x) \)
Notice that it also holds that:

\[
\int_{\Omega} f(x) \theta(x) \, dx = 0
\]

Indeed, depending on \( \theta(x) \) the name of scheme turns either Finite Volume Method or Finite Element Method. Let’s dig more :)

Wednesday, May 10, 17
Discretization principle

Now, define $F(x)$ such that:

$$f(x) = \frac{\partial}{\partial x} F(x)$$

then the relation below should hold:

$$\frac{\partial}{\partial x} F(x) \theta(x) = F(x) \frac{\partial}{\partial x} \theta(x) + f(x) \theta(x)$$
Discretization principle

Integrating both sides yields:

\[
\frac{\partial}{\partial x} F(x) \theta(x) = F(x) \frac{\partial}{\partial x} \theta(x) + f(x) \theta(x)
\]

\[
\int \frac{\partial}{\partial x} F(x) \theta(x) \, dx = \int F(x) \frac{\partial}{\partial x} \theta(x) \, dx + \int f(x) \theta(x) \, dx
\]
Discretization principle

Finally, re-arranging gives:

\[ \int \frac{\partial}{\partial x} F(x) \theta(x) \, dx = \int F(x) \frac{\partial}{\partial x} \theta(x) \, dx + \int f(x) \theta(x) \, dx \]

Indeed, this is called, "Integration by parts"
Test function

Now, the key component is $\theta(x)$

Actually, the function is called “Test function”

But how should we define it in the first place?
Here’s some examples.

$\theta_A(x)$

$\theta_B(x)$
Test function

Let’s examine some important properties of the test functions. Here they are:

\[ \theta_A(x) \]

\[ \theta_A(x) = 0 \quad \text{on edges.} \]

\[ \frac{\partial}{\partial x} \theta_A(x) = 0 \]
Test function

Let’s see what happens if we plug them into this:

\[
\int f(x)\theta(x)\,dx = \left[ F(x)\theta(x) \right] - \int F(x) \frac{\partial}{\partial x} \theta(x)\,dx
\]

\[
\int f(x)\theta_A(x)\,dx = \left[ F(x)\theta_A(x) \right]
\]

because

\[
\frac{\partial}{\partial x} \theta_A(x) = 0
\]

\[
\int f(x)\theta_B(x)\,dx = - \int F(x) \frac{\partial}{\partial x} \theta_B(x)\,dx
\]

\[
\theta_B(x) = 0
\] on edges.

because
Test function

Yes, and this is when things start to diverge

\[ \int f(x) \theta_A(x) \, dx = \left[ F(x) \theta_A(x) \right] \]

Finite Volume Method (FVM)

\[ \int f(x) \theta_B(x) \, dx = - \int F(x) \frac{\partial}{\partial x} \theta_B(x) \, dx \]

Finite Element Method (FEM)
Pros and cons

Choose whichever easier for you. Especially...

\[ \int f(x) \theta_A(x) \, dx = \left[ F(x) \theta_A(x) \right] \]

Pick this guy if the boundary is easier to evaluate

\[ \int f(x) \theta_B(x) \, dx = - \int F(x) \frac{\partial}{\partial x} \theta_B(x) \, dx \]

Pick this guy if the inner integration is easier for you.
Finally

Find a solution that this holds true everywhere for all the set of test functions like:

FVM style

FEM style
Defining the function

We said that everything is discrete in this virtual world, and so should $f(x)$, but how do we define it? Here for an easy illustration, let’s work on Laplace problem:

$$f(x) = \frac{\partial^2}{\partial x^2} g(x)$$

And define $g(x)$ as:

$g(x)$

Yes, it looks kinda line chart.
Defining the function

Actually, \( g(x) \) can be expressed with the linear combination of test functions (type B) such that:

\[
g(x) = \phi_1 N_1(x) + \phi_2 N_2(x) + \cdots + \phi_n N_n(x)
\]

where

\[
N(x) = \theta_B(x) =
\]

\( N(x) \) is often called "basis function," and \( \phi_n \) is what we actually solve for, often called "the degree of freedom"
Defining the function

Actually, $g(x)$ can be expressed with a linear combination of test functions (type B) such that:

$$g(x) = \sum$$
Finite Volume Method

Recall that
\[ f(x) = \frac{\partial^2}{\partial x^2} g(x) \]
so
\[ F(x) = \frac{\partial}{\partial x} g(x) \]

hence the below holds:
\[
\int_{-1}^{1} f(x) \theta_A(x) \, dx = \left[ F(x) \theta_A(x) \right]_{-1}^{1} = F(1) - F(-1)
\]

Recall that \( \theta_A(x) = 1 \) everywhere except outer domain.
Finite Volume Method

Recall that

\[ g(x) = \phi_1 N_1(x) + \phi_2 N_2(x) + \cdots + \phi_n N_n(x) \]

and thus

\[ \frac{\partial}{\partial x} g(x) = \phi_1 \frac{\partial}{\partial x} N_1(x) + \phi_2 \frac{\partial}{\partial x} N_2(x) + \cdots + \phi_n \frac{\partial}{\partial x} N_n(x) \]

so let’s simplify

\[ \frac{\partial}{\partial x} g(x) = \phi_1 N'_1(x) + \phi_2 N'_2(x) + \cdots + \phi_n N'_n(x) \]
Finite Volume Method

Now, take this equation with you for a while

$$\frac{\partial}{\partial x} g(x) = \phi_1 N_1'(x) + \phi_2 N_2'(x) + \cdots + \phi_n N_n'(x)$$

Note that our $N(x)$ looks like this:

On the other hand, $N'(x)$ looks like this:
Finite Volume Method

Let’s see how the integration turns out:

\[
\int_{-1}^{1} f(x) \theta_A(x) \, dx = F(1) - F(-1)
\]

\[
= \frac{\partial}{\partial x} g(1) - \frac{\partial}{\partial x} g(-1)
\]

\[
= \frac{\partial}{\partial x} \left( g(1) - g(-1) \right)
\]

\[
= \sum_n \phi_n \left( N'_n(1) - N'_n(-1) \right)
\]
Finite Volume Method

Alright, but this is very confusing!
What exactly is this? Let’s work out via illustration:

$$= \sum_n \phi_n (N'_n(1) - N'_n(-1))$$

$N'_1(x) \quad N'_2(x) \quad N'_3(x)$

\(-1\) \hspace{2cm} 1
Finite Volume Method

By looking at this illustration,

\[ N'_1(x) \quad N'_2(x) \quad N'_3(x) \]

you notice that:

\[
\begin{align*}
N'_1(-1) &= -1 \\
N'_1(1) &= 0 \\
N'_2(-1) &= 1 \\
N'_2(1) &= -1 \\
N'_3(-1) &= 0 \\
N'_3(1) &= 1
\end{align*}
\]
Finite Volume Method

So let’s calculate!

\[ \sum_{n} \phi_n (N_n' (1) - N_n' (-1)) = \phi_1 (N_1' (1) - N_1' (-1)) + \phi_2 (N_2' (1) - N_2' (-1)) + \phi_3 (N_3' (1) - N_3' (-1)) \]

Plug this relation here

- \( N_1' (-1) = -1 \), \( N_1' (1) = 0 \)
- \( N_2' (-1) = 1 \), \( N_2' (1) = -1 \)
- \( N_3' (-1) = 0 \), \( N_3' (1) = 1 \)

Finally, we get:

\[ = \phi_1 (0 - (-1)) + \phi_2 (-1 - (1)) + \phi_3 (1 - (0)) = \phi_1 - 2\phi_2 + \phi_3 \]
Finite Volume Method

Each test function yields one line of equation

\[ N_1(x) \quad N_2(x) \quad N_3(x) \quad N_4(x) \quad N_5(x) \]

\[ \theta_1(x) \quad \theta_2(x) \quad \theta_3(x) \quad \theta_4(x) \quad \theta_5(x) \]

For example, as you have seen,

\[ \int f(x) \theta_3(x) \, dx = \phi_2 - 2\phi_3 + \phi_4 \]
Finite Volume Method

So let’s do this for all the sets!

\[ \int f(x)\theta_1(x)dx = \phi_2 - \phi_1 \rightarrow 0 \]
\[ \int f(x)\theta_2(x)dx = \phi_1 - 2\phi_2 + \phi_3 \rightarrow 0 \]
\[ \int f(x)\theta_3(x)dx = \phi_2 - 2\phi_3 + \phi_4 \rightarrow 0 \]
\[ \int f(x)\theta_4(x)dx = \phi_3 - 2\phi_4 + \phi_5 \rightarrow 0 \]
\[ \int f(x)\theta_5(x)dx = \phi_4 - \phi_5 \rightarrow 0 \]
Finite Volume Method

Conveniently, you can simplify with a matrix form:

\[
\begin{bmatrix}
-1 & 1 \\
1 & -2 & 1 \\
1 & -2 & 1 \\
1 & -1 \\
\end{bmatrix}
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4 \\
\phi_5 \\
\end{bmatrix}
= 
\begin{bmatrix}
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]
Finite Volume Method

In practice, you want to specify the boundary values like:

<table>
<thead>
<tr>
<th></th>
<th>-1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>-2</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
</tbody>
</table>

\[ \phi_2 \] \hspace{1cm} \phi_3 \hspace{1cm} \phi_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}

Fix the value
Finite Volume Method

Then the linear system can be more simplified:

\[
\begin{array}{c}
-2 & 1 & \ \ & \ \ & \ \ & \ \ \\
1 & -2 & 1 & \ \ & \ \ & \ \ \\
1 & 1 & -2 & \ \ & \ \ & \ \ \\
\end{array}
\begin{array}{c}
\phi_2 \\
\phi_3 \\
\phi_4 \\
\end{array}
= \begin{array}{c}
0 \\
0 \\
-4 \\
\end{array}
\]

You can solve this by matrix inversion to get the actual numbers for \( \phi_n \).
Finite Volume Method

Once you get the numbers, you can now plot your solution!
Summary (FVM)

- Partial differential equation describes the behaviors of many physics phenomena.
- Discretization starts with integrating a PDE within a small domain.
- Test function turns the method either Finite Volume Method or Finite Element Method.
- Basis function serves to define the shape of a function.
- Finally, discretization is a powerful tool to bridge between discrete and continuous world!