Module 2a: *Introduction to Finite Difference Methods : 1-Dimensional FD Expressions*

David J. Willis

January 28, 2013

Table of contents

Announcements

- First homework posted online this week.
- ECHO360 Lecture capture.
- Permission numbers – refresh today, come see me after class.
- Project description – hopefully posted Thursday evening.

References and Acknowledgements

The following materials were used in the preparation of this lecture:

1. Tannehill, Anderson and Pletcher, *Computational fluid Mechanics and Heat Transfer*.
2. 16.920 Notes

The author of these slides wishes to thank these sources for making the current lecture.

Table of contents

How to solve a simple PDE using a computer

- Consider the 1-D Poisson Equation (ODE) between $x = 0$ and $x = 1$:

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} = f = 1 \tag{1}$$

$$u(x = 0) = 0 \tag{2}$$

$$u(x = 1) = 0 \tag{3}$$

- For this problem, we are going to assume that u represents the deflection of a string, and f represents some applied transverse force.
- Discuss with your neighbor(s):
  1. What is the actual/real solution to this problem?
  2. How can you going to represent the solution u, using a computer code?
  3. How can you represent the geometry/domain in the computer code?
  4. How can you represent the governing ODE in the computer?
  5. Does the solution at a given location depend on the neighboring solutions?

The Exact Solution

Solution Representation

- We will see in this course that there are two ways to numerically represent a solution:
  1. Pointwise
  2. Functional

Pointwise

Functional

Geometry Representation

- We will initially use point-wise representation of the solution.
  - Setup the points where the solution is to be determined $\rightarrow$ discretization or mesh.

Solution Representation

- The solution representation and solution method can have a direct impact on geometry representation in the computer.
- Even if the solution is needed at one location (max deflection), we usually need to solve the problem where dependency exists:
  - **Elliptic**
  - Parabolic
  - Hyperbolic

Solution Representation

- This sub-module: Elliptic equations $\rightarrow$ smooth solutions, infinite domain of influence and dependence.

Table of contents

Finite Difference Approximations to Derivatives

- Let's say we wish to approximate a derivative:

$$\frac{du}{dx} \tag{4}$$

- How can we approximate this derivative?

Finite Difference Approximations to Derivatives

- Fundamental definition of the derivative:
  - Take the value for u at two different $x-$ locations, and simply take the difference between the u-value and divide by the spatial distance (difference in the x-locations.

$$\frac{du}{dx} \simeq \frac{u_{i+1} - u_i}{x_{i+1} - x_i} + error \tag{5}$$

  - As the two points get closer together, the error diminishes.
  - In the limit as the two points approach each other, we recover the derivative.
  - How accurate is this approximation? As $(x_{i+1} - x_i) \rightarrow 0$?

Finite Difference Approximations to Derivatives

- The idea is to approximate derivatives using finite not infinitesimal differences in the variables.
- To make this a viable method, we need to:
  - **GOAL # 1:** Come up with a way to represent a diversity of derivatives, eg:
    - $\frac{\partial^2 u}{\partial x^2}$
    - $\frac{\partial^3 u}{\partial x^3}$
  - **GOAL # 2:** Quantify and reduce the error of the approximation $\rightarrow$ better solution.
  - **GOAL # 3:** Develop expressions and solutions to PDEs using these derivatives.

Mathematics: Taylor Series Expansion

- **GOAL #1, Method 1:** Taylor Series Expansion in positive x-direction:

$$\begin{aligned} u(x_0 + \Delta x) &= u(x_0) + \frac{\partial u}{\partial x}|_0 \Delta x + \\ &+ \frac{\partial^2 u}{\partial x^2}|_0 \frac{(\Delta x)^2}{2!} + ... \\ &+ \frac{\partial^n u}{\partial x^n}|_0 \frac{(\Delta x)^n}{n!} + ... \end{aligned}$$

Geometry and Mathematics of the Taylor Series Expansion

Mathematics: Taylor Series Expansion

- Taylor Series Expansions in negative x-direction:

$$\begin{aligned} u(x_0 - \Delta x) &= u(x_0) - \frac{\partial u}{\partial x}|_0 \Delta x + \\ &+ \frac{\partial^2 u}{\partial x^2}|_0 \frac{(\Delta x)^2}{2!} - ... \\ &+ (-1)^n \frac{\partial^n u}{\partial x^n}|_0 \frac{(\Delta x)^n}{n!} + ... \end{aligned}$$

Mathematics: Taylor Series Expansion

Finite Difference Approximations to Derivatives

- If we start with:

$$
\begin{aligned}
u(x_0 + \Delta x) &= u(x_0) + \frac{\partial u}{\partial x}\|_0 \Delta x + \\
&+ \frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!} + \ldots \\
&+ \frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!} + \ldots
\end{aligned}
$$

Finite Difference Approximations to Derivatives

- We can re-arrange the equation so that:

$$
\begin{aligned}
\frac{\partial u}{\partial x}\|_0 &= \frac{(u(x_0) - u(x_0 + \Delta x))}{\Delta x} + \\
&+ \frac{\frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!}}{\Delta x} + \ldots \\
&+ \frac{\frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!}}{\Delta x} + \ldots
\end{aligned}
$$

Finite Difference Approximations to Derivatives

- This gives us:

$$\frac{\partial u}{\partial x}\|_0 = \frac{(u(x_0) - u(x_0 + \Delta x))}{\Delta x} + O(\Delta x) \tag{6}$$

- Comment: The error decays proportionally to decreases in Δx

Finite Difference Approximations to Derivatives

- If we start with:

$$
\begin{aligned}
u(x_0 - \Delta x) &= u(x_0) - \frac{\partial u}{\partial x}\|_0 \Delta x + \\
&+ \frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!} - \ldots \\
&+ (-1)^n \frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!} + \ldots
\end{aligned}
$$

- We can re-arrange the equation so that:

$$
\begin{aligned}
\frac{\partial u}{\partial x}\|_0 &= \frac{(u(x_0) - u(x_0 - \Delta x))}{\Delta x} + \\
&+ \frac{\frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!}}{\Delta x} - \ldots \\
&+ (-1)^n \frac{\frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!}}{\Delta x} + \ldots
\end{aligned}
$$

Finite Difference Approximations to Derivatives

- This gives us:

$$\frac{\partial u}{\partial x}\|_0 = \frac{(u(x_0) - u(x_0 - \Delta x))}{\Delta x} + O(\Delta x)$$

- Comment: The error again decays proportionally to decreases in Δx

Finite Difference Approximations to Derivatives

- If we start with:

$$\begin{aligned} u(x_0 - \Delta x) &= u(x_0) - \frac{\partial u}{\partial x}\|_0 \Delta x + \\ &+ \frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!} - \ldots \\ &+ (-1)^n \frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!} + \ldots \end{aligned}$$

- And subtract the expression:

$$\begin{aligned} u(x_0 + \Delta x) &= u(x_0) + \frac{\partial u}{\partial x}\|_0 \Delta x + \\ &+ \frac{\partial^2 u}{\partial x^2}\|_0 \frac{(\Delta x)^2}{2!} \vdots \\ &+ \frac{\partial^n u}{\partial x^n}\|_0 \frac{(\Delta x)^n}{n!} + \ldots \end{aligned}$$

Finite Difference Approximations to Derivatives

$$\frac{\partial u}{\partial x}\|_0 = \frac{u(x_0+\Delta x)-u(x_0-\Delta x)}{2\Delta x} + \\ + \frac{1}{2}\frac{\partial^3 u}{\partial x^3}\|_0 \frac{(\Delta x)^2}{3!} + \ldots$$

- This is a more accurate approximation to the first derivative
- As we reduce the spacing between points by factor of 2, the error in the derivative changes by a factor of 4

Finite Difference Approximations to Derivatives

- Let's define a system that uses i (and j) indices to indicate our position on a grid.
- The spatial difference between i-points is Δx.

Finite Difference Approximations to Derivatives

- Let's look at a couple of common first derivative finite difference approximations:

$$\frac{du}{dx} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x) \tag{7}$$

$$\frac{du}{dx} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x) \tag{8}$$

$$\frac{du}{dx} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2) \tag{9}$$

$$\frac{du}{dx} = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + O(\Delta x^2) \tag{10}$$

$$\frac{du}{dx} = \frac{-3u_i + 4u_{i+1} - u_{i+2}}{2\Delta x} + O(\Delta x^2) \tag{11}$$

$$\frac{du}{dx} = \frac{u_{i+1} - u_i}{\Delta x} + O(\Delta x)$$

$\frac{du}{dx} = \frac{u_i - u_{i-1}}{\Delta x} + O(\Delta x)$

$\frac{du}{dx} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + O(\Delta x^2)$

$$\frac{du}{dx} = \frac{3u_i - 4u_{i-1} + u_{i-2}}{2\Delta x} + O(\Delta x^2)$$

Table of contents

Thought Experiment

- The deflection of a 1-D string.

Thought Experiment

- Now that we have a governing equation, let's determine how to solve it using Finite Differences:

$$\frac{\partial^2 u}{\partial x^2} = f(x) \tag{12}$$

- With boundary conditions on both ends of:

$$u_L = u_R = 0 \tag{13}$$

- How do we solve this?

Thought Experiment

- Step 1: Discretize the domain into n intervals ($n + 1$ points).
- Step 2: Write finite difference equations for each internal node of the problem
- Step 3: Form a system of linear equations
- Step 4: Enforce the boundary conditions for the end points
- Step 5: Solve the system of equations

Table of contents

Method of Lagrange Interpolation to Find FD Formulae

- **Method 2:** for finding finite difference formula is **Lagrange Interpolation**. This is a more rigorous approach.
- When deriving new finite difference formula, we want to find an approximation of the form:

$$\frac{d^m u}{dx^m} \simeq \sum_{j=-left}^{right} \delta_j^m u_j \tag{14}$$

- We need a way to find the values of the coefficients: δ_j^m

Method of Lagrange Interpolation to Find FD Formulae

- Example of this notation: The first derivative

Method of Lagrange Interpolation to Find FD Formulae

- Start by defining a Lagrange Polynomial:

$$L_j(x) = \frac{(x - x_l)...(x - x_{j-1})(x - x_{j+1})...(x - x_r)}{(x_j - x_l)...(x_j - x_{j-1})(x_j - x_{j+1})...(x_j - x_r)} \tag{15}$$

- The values for the above equation are 1 when $x = x_j$ and 0 when $x_i \neq x_j$.
- Here, x_i is a node other than x_j

Method of Lagrange Interpolation to Find FD Formulae

- We can approximate the solution by adding the appropriate combinations of Lagrange Polynomials together:

$$\hat{u}(x) = \sum_{j=-left}^{right} L_j(x) u_j \tag{16}$$

Method of Lagrange Interpolation to Find FD Formulae

- Rather than the solution $\hat{u}$, we want to represent the derivatives, $\frac{d^m u}{dx^m}$ up to order m.

$$\frac{d^m u}{dx^m} \simeq \frac{d^m \hat{u}}{dx^m}|_{x=x_0} = \sum_{j=-left}^{right} \frac{d^m L_j}{dx^m}|_{x=x_0} u_j \tag{17}$$

- What this means, is that the coefficients δ_j^m that we wish to find are simply (by pattern matching):

$$\delta_j^m = \frac{d^m L_j}{dx^m}|_{x=x_0} \tag{18}$$

Let's Try An Example

- Here we will look for the finite difference equations that are based on a 3-point polynomial.
- Start first by expressing the solution as:

$$
\begin{aligned}
\hat{u}(x) &= \sum_{j=-l}^{r} L_j(x) u_j \\
&= \frac{(x - x_j)(x - x_{j+1})}{(x_{j-1} - x_j)(x_{j-1} - x_{j+1})} u_{j-1} \\
&+ \frac{(x - x_{j-1})(x - x_{j+1})}{(x_j - x_{j-1})(x_j - x_{j+1})} u_j \\
&+ \frac{(x - x_{j-1})(x - x_j)}{(x_{j+1} - x_{j-1})(x_{j+1} - x_j)} u_{j+1}
\end{aligned}
$$

Let's Try An Example

- To find the finite difference equation coefficients (the δ_j^m):
  1. It helps to first expand the polynomial in each numerator
  2. Differentiate the various Lagrangian polynomials with respect to x
  3. Depending upon where the finite difference is centered, insert the appropriate x entry
  4. Simplify the expression to get the value for δ_j^m in terms of Δx

Let's Try An Example

- Start with the term δ^m_{j-1}, where the finite difference is centered at x_{j-1}:

$$
\begin{aligned}
L_{j-1}(x) &= \frac{(x-x_j)(x-x_{j+1})}{(x_{j-1}-x_j)(x_{j-1}-x_{j+1})} \\
L_{j-1}(x) &= \frac{(x^2-xx_j-xx_{j+1}+x_jx_{j+1})}{(x_{j-1}-x_j)(x_{j-1}-x_{j+1})} \\
\frac{dL_{j-1}(x)}{dx} &= \frac{(2x-x_j-x_{j+1})}{(x_{j-1}-x_j)(x_{j-1}-x_{j+1})} \\
\delta^m_{j-1}(x=x_{j-1}) &= \frac{-3\Delta x}{2\Delta x^2} = \frac{-3}{2\Delta x}
\end{aligned}
$$

Let's Try An Example

- Similarly, for Largange polynomials centered at different x points, we can find the following expressions when $x = x_{j-1}$:

$$\delta^m_{j-1} = \frac{-3}{2\Delta x}$$

$$\delta^m_{j} = \frac{2}{\Delta x} = \frac{4}{2\Delta x}$$

$$\delta^m_{j+1} = \frac{-1}{2\Delta x}$$

- See the example sheet for derivations of the other terms and other finite difference expressions.

Let's Try An Example

- The result is:

$$\begin{aligned}\frac{du}{dx} &= \delta^m_{j-1} u_j + \delta^m_j u_{j+1} + \delta^m_{j+1} u_{j+2} \\ &= \frac{-3}{2\Delta x} u_j + \frac{2}{\Delta x} u_{j+1} + \frac{-1}{2\Delta x} u_{j+2} \\ &= \frac{-3u_j + 4u_{j+1} - u_{j+2}}{2\Delta x}\end{aligned}$$

- We have derived the equation for the one sided first derivative.
- Note: We had 3-points, and as such we represented the solution using a polynomial of order 2.
- The error in the first derivative is therefore second order ($O(\Delta x^2)$).

Let's Try An Example

- Applying the same approach, we can find many other finite difference formulas.
- One formula of particular interest is the second derivative, central difference formula:

$$\frac{d^2u}{dx^2} \simeq \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + O(h^2)$$