Partial Differential Equations of Fluid Dynamics
A Preliminary Step for Pipe Flow Simulations

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Outline

Introduction

Modeling Transport Phenomena Using PDE’s

Discretization of Derivatives

Numerical Solution of PDE’s
Role of CFD in Modern Engine Computations 1
Turbulent Intake, Exhaust and Incylinder Flow Using LES (Courtesy of Sandia)
Role of CFD in Modern Engine Computations 2
Fuel Injection and Turbulence Using LES (Courtesy of Sandia)
Role of CFD in Modern Engine Computations 3
Cross-Section of Turbulence in Exhaust Manifold Using LES
Diffusion, convection and radiation are basic transport mechanisms of mass, momentum and energy.

Example 1: heat conduction (diffusion) via walls of a hot engine cylinder.
Example 2: transport of concentration of a radioactive cloud in given wind conditions.
Example 3: convection of hot exhaust gases out of an engine.

The phenomena above can all be modeled with partial differential equations.

This lecture gives an overview of linear PDE’s and the next lecture on the (non-linear) Navier-Stokes equations.
Partial Differential Equations
Can Be Used to Model and Simulate 1D, 2D and 3D Flows

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Numerical Solution of PDE’s
The General Form of Any Transport Phenomenon
Also the Navier-Stokes Equation is of This Form

The Convection-Diffusion Equation for the Quantity $\phi$

$$\frac{\partial \rho \phi}{\partial t} + \nabla \cdot (u \rho \phi) - \nabla \cdot (\rho \nu \nabla \phi) = S_\phi(\phi)$$

- $\phi$ convects and diffuses in a **fluid** (e.g. air, water...).
- $\phi$ could represent e.g. concentration of soot particles in cigarette smoke or water temperature in ocean currents etc.
- $\rho$ is the density of the fluid and $u = u(x,y,z,t)$ the velocity field, and $\nu$ the diffusivity (e.g. heat diffusivity) of $\phi$. 

In 1D the Convection-Diffusion Equation for Temperature $T$ Can Be Written as Follows

1D Form

\[
\frac{\partial T}{\partial t} + \frac{\partial}{\partial x} (uT) - \frac{\partial}{\partial x} (\nu \frac{\partial T}{\partial x}) = 0
\]

Assumption

- Fluid is incompressible i.e. $\rho = \text{constant}$ (e.g. water or low velocity <100m/s air).
When \( u = 0 \) One Obtains the Heat Diffusion Equation

1D Heat Equation

The temporal derivative

\[
\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left( \nu \frac{\partial}{\partial x} T \right)
\]
When \( \nu = \text{Constant} \) the Heat Diffusion Equation Further Simplifies

1D Heat Equation

\[
\frac{\partial T}{\partial t} = \nu \frac{\partial}{\partial x} \left( \frac{\partial T}{\partial x} \right)
\]
When $\nu = 0$ One Obtains the Convection Equation

**1D Convection Equation**

\[
\frac{\partial T}{\partial t} + \frac{\partial}{\partial x} (uT) = 0.
\]

**Assumption**

- Fluid is incompressible i.e. $\rho =$ constant (e.g. water or low velocity $<100$ m/s air).
Again, When \( u = \text{Constant} \) the Convection Equation Further Simplifies

### 1D Convection Equation

\[
\frac{\partial T}{\partial t} + u \frac{\partial}{\partial x} (T) = 0.
\]

### Assumption

- Fluid is incompressible i.e. \( \rho = \text{constant} \) (e.g. water or low velocity <100m/s air).
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Numerical Solution of PDE’s
How to Solve/Simulate the Basic PDE’s Using Computers?

- The continuous equations need to be discretized.
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- This means that the derivatives have to be expressed using Taylor series which allows numerical evaluation of the derivative terms.
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- Space is divided into finite size elements by replacing $dx \rightarrow \Delta x$.
- Time is divided into finite size time steps by replacing $dt \rightarrow \Delta t$.
- The basic idea: timesteps are numbered from $0, 1, 2, ..., n - 1, n, n + 1, ..., N$ corresponding to physical times $0, \Delta t, 2\Delta t, ..., N\Delta t$, where $N = \frac{\text{total simulation period(s)}}{\Delta t}$. 
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- The basic idea: timesteps are numbered from $0, 1, 2, ..., n - 1, n, n + 1, ..., N$ corresponding to physical times $0, \Delta t, 2\Delta t, ..., N\Delta t$, where $N = \frac{\text{total simulation period (s)}}{\Delta t}$.

- At $n^{th}$ timestep we want to know the solution at the $(n + 1)^{th}$ timestep using solution $T_n$. 

How to Solve/Simulate the Basic PDE’s Using Computers? (cont.)

Here $T_n = T_n(k \cdot \Delta x) = T^k_n$, where $k = 0, 1, 2, \ldots, L/\Delta x$ i.e. the solution at timestep is defined in discrete space points $0, \Delta x, 2\Delta x, \ldots$. 

Simulation of e.g. heat or convection equation means that for every single discrete point (or ‘cell’) we want to find a general update formula in order to advance the solution from timestep $n$ to $n+1$. 

Matlab and PDE’s 16/27

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A Preliminary Step for Pipe Flow Simulations
Here \( T_n = T_n(k \cdot \Delta x) = T_n^k \), where \( k = 0, 1, 2, \ldots, L/\Delta x \) i.e. the solution at timestep is defined in discrete space points \( 0, \Delta x, 2\Delta x, \ldots \).

Simulation of e.g. heat or convection equation means that for every single discrete point (or ’cell’) we want to find a general update formula in order to advance the solution from timestep \( n \) to time \( n + 1 \).
Discretization of Time

A Simple First Order Taylor Series Approximation Gives

\[
\frac{\partial T}{\partial t} \approx \frac{T_{n+1} - T_n}{\Delta t} + O(\Delta t).
\]

Above, \( = O(\Delta t) \) is the time discretization error.
Discretization of Time

A Simple First Order Taylor Series Approximation Gives

\[ \frac{\partial T}{\partial t} \approx \frac{T_{n+1} - T_n}{\Delta t} + O(\Delta t). \]

- Above, \( O(\Delta t) \) is the time discretization error.
- \( O(\Delta t) \to 0 \) when \( \Delta t \to 0 \).
Discretization of First Derivative in Space

A Simple Second Order Central Difference Taylor Series Approximation Gives

\[
\frac{\partial T}{\partial x} \approx \frac{T^{k+1} - T^{k-1}}{2\Delta x} + O(\Delta x^2).
\]

Above, \( O(\Delta x^2) \) is the space discretization error.
Discretization of First Derivative in Space

A Simple Second Order Central Difference Taylor Series Approximation Gives

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\frac{\partial T}{\partial x} \approx \frac{T^{k+1} - T^{k-1}}{2\Delta x} + O(\Delta x^2).
\]

Above, \( O(\Delta x^2) \) is the space discretization error.

\( O(\Delta x^2) \to 0 \) when \( \Delta x \to 0 \).
Central Difference Formula for $T''(x)$

\[
\frac{\partial^2 T}{\partial x^2} \approx \frac{T^{k+1} - 2T^k + T^{k-1}}{\Delta x^2} + O(\Delta x^2).
\]

Above, $= O(\Delta x^2)$ is the space discretization error.
Discretization of Second Derivative in Space

Central Difference Formula for $T''(x)$

\[
\frac{\partial^2 T}{\partial x^2} \approx \frac{T^{k+1} - 2T^k + T^{k-1}}{\Delta x^2} + O(\Delta x^2).
\]

- Above, $= O(\Delta x^2)$ is the space discretization error.
- $O(\Delta x^2) \rightarrow 0$ when $\Delta x \rightarrow 0$. 
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Numerical Solution of PDE’s
Explicit Euler Method for the Convection Equation

Update Formula

\[
\frac{T_{n+1}^k - T_n^k}{\Delta t} + u \frac{T_{n+1}^k - T_{n-1}^k}{2\Delta x} = 0.
\]

Or Moving the Known Terms to Right Hand Side

\[
T_{n+1}^k = T_n^k - u \Delta t \frac{T_{n+1}^k - T_{n-1}^k}{2\Delta x} = T_n^k - \frac{u \Delta t}{\Delta x} \frac{\hat{u}}{2} T_{n+1}^k - \frac{u \Delta t}{\Delta x} \frac{T_{n-1}^k - T_{n}^k}{2}
\]

Courant Number
Explicit Euler Method for the Heat (Diffusion) Equation

Update Formula

\[
\frac{T_{n+1}^k - T_n^k}{\Delta t} = \nu \frac{T_{n+1}^k - 2T_n^k + T_{n-1}^k}{\Delta x^2} = 0.
\]

Or Moving the Known Terms to Right Hand Side

\[
T_{n+1}^k = T_n^k + \nu \frac{\Delta t}{\Delta x^2} \left( T_{n+1}^k - 2T_n^k + T_{n-1}^k \right).
\]

Courant-Friedrichs-Lewy Number
Stability Limits

**Courant Number**

- The Courant number $Co = \frac{u \Delta t}{\Delta x}$ describes the propagation distance of information during timestep $\Delta t$. It is necessary that $Co < 1$ for physically meaningful solutions. For explicit Euler methods, $Co < \frac{1}{2}$ sets the limit for the timestep for the algorithm to be numerically stable.
# Stability Limits

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- For explicit Euler method $Co < 1/2$ sets the limit for timestep for the algorithm to be numerically stable.
Stability Limits (cont.)

Courant-Friedrichs-Lewy Number

- The Courant-Friedrichs-Lewy Number $CFL = \frac{\nu \Delta t}{\Delta x^2}$ describes the diffusion distance of information during timestep $\Delta t$. Again, it is necessary that $CFL < 1$ for physically meaningful solution. For explicit Euler method, $CFL < 1/2$ sets the limit for timestep $\Delta t$. A Preliminary Step for Pipe Flow Simulations
Stability Limits (cont.)

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- Again, it is necessary that $CFL < 1$ for physically meaningful solution.
- Again, for explicit Euler method $CFL < 1/2$ sets the limit for timestep for the algorithm to be numerically stable.
Matlab Implementation

- The folder `/demos2012/` shows demo files in which the Explicit Euler method is applied for heat diffusion and convection-diffusion equations.
- `ConvectionDiffusionEquation.m` and `HeatDiffusion.m` demonstrate these examples.
- The files `PlottingFigure.m`, `SurfaceAnimation.m` and `DrawingSurface.m` show how graphs can be drawn, surface motion be animated etc.
Summary

- An introduction to PDE’s and numerical solution using the explicit Euler method was given.
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- It is very easy to extend the present knowledge to e.g. the Runge-Kutta-methods which would provide more robustness and stability.

- In the next lecture we will show that you can already directly apply the learned methods and PDE’s to non-linear the non-linear realistic case of the Navier-Stokes equation for a 1D pipe flow.
The End

Thank you

Questions?