Numerical Simulation and Scientific Computing in Fluid Mechanics:

Fundamental aspects and applications

Francesco Zonta

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Before starting

http://www.sss.tuwien.ac.at/sss/mla/

Fluid dynamics: computations we do

(@Institute of Fluid Mechanics and Heat Transfer, Group of Prof. Soldati)

1. Oil transport
2. Turbulent flow in channels and pipelines: effect of stratification
3. Ocean/atmosphere CO_2 exchange: phytoplankton
4. Ocean/atmosphere CO_2 exchange: effect of waves
5. Oil/water emulsions
6. Oil/water emulsions with surfactants
7. Flows in porous media

Oil Transport

Method and apparatus for measuring characteristics of core-annular flow
US PATENT 20050033545 A1
Abstract
An apparatus and method are disclosed […] core-annular flow (CAF) in a pipe […] the CAF may be developed from a lubricating fluid, such as water, and a fluid to be transported, such as oil, where the fluid to be transported forms the core region and the lubricating fluid forms the annular region.

Credit: ALFA Research Group

"There is a strong tendency for two fluids to arrange themselves so that the low-viscosity constituent is in the region of high shear.
This gives rise to a kind of a gift of nature in which the lubricated flows are stable, and it opens up very interesting possibilities for technological applications in which one fluid is used to lubricate another "

D:D: Joseph et al, Core-anular flows, ARFM (1997)

Oil Transport

$$We = \frac{\rho u_\tau^2 h}{\sigma} = 0.5 \qquad Re_\tau = \frac{\rho u_\tau h}{\eta_o} = 300 \qquad \lambda = \frac{\eta_w}{\eta_o} = \frac{\text{Water Viscosity}}{\text{Oil Viscosity}}$$

S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CEF (2016)

Oil Transport

Explanation: a closer look

$$Re_{local} \propto \frac{h}{\mu} \downarrow$$

DR driven by σ

$$Re_{local} \propto \frac{h}{\mu} \uparrow$$

DR driven by λ

Roccon, Zonta, Soldati, *J. Fluid Mech.*, **70**, 040801 (2019)

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Stratification

Relevant for:

Industrial applications (heat transfer devices), environmental/geophysical applications (atmospheric boundary layer, ocean)

Main parameters of the flow:

(Shear) **Reynolds number:** inertial/viscous forces $\dfrac{\rho u^2/L}{\mu u/L^2} = \dfrac{uL}{\nu}$

$$Re_\tau = \frac{u_\tau h}{\nu_0}$$

Prandtl number: momentum diffusivity/thermal diffusivity

$$Pr = \frac{\nu_0}{\kappa_0}$$

Grashof number: buoyancy/viscous forces $\dfrac{g\Delta\rho}{\mu u_\nu/L^2}$

$$Gr = \frac{g\Delta\rho L^3}{\rho_0 \nu_0^2}$$

(Shear) **Richardson number:** buoyancy/inertial forces

$$Ri_\tau = \frac{g\Delta\rho h}{\rho_0 u_\tau^2}$$

Note: $Ri_\tau \to 0$, Forced conv.

$Ri_\tau \uparrow$, Buoyancy controlled/dominated

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Stratification

Visualization of temperature on a cross section

$Ri_\tau = 0$

$Ri_\tau = 200$

Neutrally buoyant

- Higher mixing
- Mixing is driven by turbulence structures

Stably stratified

- Lower mixing
- Internal waves act like barriers

Stratification

The temperature distribution has a remarkable effect on the velocity field

$Ri_\tau = 0$

$Ri_\tau = 200$

- Stratified flow is ''faster'' and less homogeneous
- Flow structures in case of stratification are smaller and are ''pushed'' towards the wall

Very important topic: particles dynamics in stratified turbulence

(this is why we have problems with pollution in winter)

Neutrally-buoyant particles in stratified flow

Pollutants are constraint in the proximity of the boundary (in the atmospheric boundary layer)

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Phytoplankton

Phytoplankton is the photosynthetic part of plankton

- Primary production: organize compounds from CO2
- Important part of the global carbon cycle
- Provides 50% of the earth's oxygen
- Sustain the aquatic food web

Phytoplankton

Phytoplankton

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Waves

Transfer rates (for example of CO_2) across an interface depends strongly on the extension of the interface…

Waves

Gravity ↑

Quasy-sinusoidal wavy interface

Surface roughness

Capillarity ↑

Waves

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Oil/Water emulsions

Swarm of drops in turbulence.

- Drop-drop interaction?
- Drop size distribution?
- Effect on turbulence?
- Drag Enhancement or Reduction?

Oil/Water emulsions

COALESCENCE

Two droplets come close and collide due to turbulence fluctuations. During the collision, a small bridge is initially formed; later, surface tension (which tends to reshape the droplet) comes into the picture and complete the coalescence process.

BREAK-UP

A droplet is subjected to a sufficient shear stress, such that it is deformed and stretched until the emerging thin liquid bridge is broken (due to surface tension that acts minimizing the energy stored at the interface).

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Oil/Water emulsions with surfactants

Surface Tension:

The cohesive forces between liquid molecules are the responsible for the phenomenon known as surface tension.

Addition of a surfactant:

Clean system | Surfactant-laden system

Presence of surfactant decreases the surface tension and as a consequence:

-Droplets become more deformable (less surface tension).

-When non-uniform can give rise to tangential forces (Marangoni).

Oil/Water emulsions with surfactants

Clean droplets (no surfactant):

Surfactant-laden droplets:

Oil/Water emulsions with surfactants

Addition of a surfactant

Effects of the surfactant:

- Dispersed phase morphology?
- Droplet size distribution?
- Surfactant distribution?
- Turbulence modifications?

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Flows in porous media

Geological CO2 sequestration

Flows in porous media

A lot of open questions: *role of rock anisotropy & pore scale dynamics*

Study Assistent 1+2 (for 6 months / 5 months)
At the Institute of Visual Computing and Human-Centered Technology, in the Research Unit of Virtual and Augmented Reality, TU Wien is offering a position as student assistant (Studienassistent_in, all genders) for 20 hours/week. Expected start: July 2023.

Tasks:

- Contributing to a project that brings simulation results from CAE (Computer Aided Engineering) software to stand-alone XR headsets
- Rendering of calculated geometries and physical field quantities
- Implementing XR interactions with objects (e.g. geometric transformations), volumetric data (e.g. defining cutting planes) and simulation (e.g. particles that can be released and followed on their way through the flow)
- Implementation of (network) interfaces for communication between CAE software (e.g. Ansys FLUENT or OpenFOAM), the XR application and auxiliary tools (e.g. file parsers for exported data in cases where CAE software does not provide suitable API)

Your profile:

- Studies in computer science, mechanical engineering, physics, mathematics
- Programming skills in Unity, C#
- Experience with XR interaction
- Knowledge of rendering pipelines and shader programming advantageous
- C++ advantageous
- Experience with Android programming advantageous
- Team spirit

Study Assistent 3: (for 6 months)
At the Institute of Fluid Mechanics and Heat Transfer, TU Wien is offering a position as student assistant (Studienassistent_in, all genders) for 20 hours/week. Expected start: July 2023.

Tasks:

- Contributing to a project that brings simulation results from CAE (Computer Aided Engineering) software to stand alone XR headsets
- Implementation of (network) interfaces for communication between CAE software (e.g. Ansys FLUENT, OpenFOAM or Custom Fortran code), the XR application and auxiliary tools (e.g. file parsers for exported data in cases where CAE software does not provide suitable API).
- Implementation of auxiliary tools (e.g. file parsers for exported data in cases where CAE software does not provide suitable API).
- Implementation of software modules that read, interpolate, resample (if necessary) and write data (geometries and physical field quantities) from the CAE software in datastructures ready for rendering

Your profile:

- Studies in computer science, mechanical engineering, physics, mathematics
- Programming skills in C# or C++
- Knowledge in Fortran advantageous
- Experience in parsing different file formats beneficial
- Knowledge of Unity advantageous
- Experience with Ansys FLUENT or OpenFOAM beneficial
- Team spirit

After this survey on applications, we are now ready to start with an in-depth analysis of transport process and equations…

The main character of the story: The transport process/equation! What is it?

Verona Arena

(a)

(b) (c)

Pettarin et al (2015), *Atmospheric Environment*,**122**, 74-82

We take it as reference!

What do we need to simulate it?

1.**First we need a mathematical model (PDE+BC+IC) of the transport process**: concentration of a chemical species C_i that diffuses and at the same time is advected by the flow. This gives:

$$\boxed{\frac{\partial C_i}{\partial t} + u_j \frac{\partial C_i}{\partial x_j} = D \frac{\partial^2 C_i}{\partial x_j^2}}$$

ADE=Advection Diffusion Equation

Rate of change — Advection — Diffusion

2.**Then we need a discretization strategy** (numerical scheme) to switch from the continuum to the discrete space (Space & Time). The specific method (FD,FE,FV,spectral methods…) is not important here; what matters is the "philosophy"

Before starting: What you will learn

1. You will learn the fundamental concepts on how to solve (numerically) a generic transport equation.

2. I will try to do some “surgery” of the equations, analyzing different aspects one by one (and neglecting other aspects).

3. I will skip some details and technicalities (and I would refer you to specific courses for the purpose).

Maybe at the end of the lecture you will learn how to obtain this:

Distribution of concentration (red= high concentration) in a square cavity filled with air

Introduction: Diffusion and advection

Let's consider our transport equation (1D ADE)

$$\boxed{\frac{\partial C^*}{\partial t^*} + u^* \frac{\partial C^*}{\partial x^*} = D \frac{\partial^2 C^*}{\partial x^{*2}}}$$

We have 1st and 2nd derivatives!

In dimensionless form:

$$\begin{cases} C = \dfrac{C^*}{C_w} \\ x = \dfrac{x^*}{L} \\ u = \dfrac{u^*}{u_{ref}} \\ t = \dfrac{t^* D}{L^2} \end{cases} \rightarrow \frac{D C_w}{L^2} \frac{\partial C}{\partial t} + \frac{u_{ref}\, u\, C_w}{L} \frac{\partial C}{\partial x} = \frac{D C_w}{L^2} \frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} + \frac{u_{ref} \cdot \cancel{C_w}}{\cancel{L}} \frac{L^{\cancel{2}}}{D \cancel{C_w}} u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} + \underbrace{\frac{u_{ref} \cdot L}{D}}_{Pe\ (Peclet)} u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}$$

$$\left[Pe = \frac{\text{diffusion time}}{\text{convection time}} = \frac{L^2/D}{L/u_{ref}} = \frac{L \cdot u_{ref}}{D} \right]$$

$$\boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}}$$

$Pe \ll 1 \Rightarrow$ Diffusion dominates $\rightarrow \boxed{\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}}$

$Pe \gg 1 \Rightarrow$ Advection dominates $\rightarrow \boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = 0}$

Introduction: Diffusion and advection

Question: Diffusion or Advection, which one is more efficient?

Introduction: Diffusion and advection

Question: Diffusion or Advection, which one is more efficient?

$$T_{diff} = \frac{L^2}{D}$$

$$T_{conv} = \frac{L}{U_{ref}}$$

Now we have a physical/mathematical model (ADE); we need a strategy to discretize and solve it!

Introduction: Discretization strategy

How to approximate (discretize) derivatives? The most intuitive way is the following:

(at a given time instant *n*)

Forward approximation

$$\left[\frac{\partial f}{\partial x}\right]_i^n \simeq \frac{f_{i+1}^n - f_i^n}{\Delta x}$$

Backward approximation

$$\left[\frac{\partial f}{\partial x}\right]_i^n \simeq \frac{f_i^n - f_{i-1}^n}{\Delta x}$$

Are they accurate?

Which one is better?

To answer: Taylor series…

Introduction: Discretization strategy

Taylor series

$$f_{i+1}^n = f_i^n + \Delta x \left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + \underbrace{O(\Delta x^3)}_{HOT}$$

$$f_{i-1}^n = f_i^n - \Delta x \left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + HOT$$

It is straightforward to show that

$$\left[\frac{\partial f}{\partial x}\right]_i^n = \frac{f_{i+1}^n - f_i^n}{\Delta x} - \frac{\Delta x}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + HOT$$

$$\left[\frac{\partial f}{\partial x}\right]_i^n = \frac{f_i^n - f_{i-1}^n}{\Delta x} + \frac{\Delta x}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + HOT$$

Our approximation

Error

Forward/Backward discretization=1st order!!

"Manipulation" of Taylor series. In a more systematic way…

Introduction: Discretization strategy

We wish to approximate the derivatives as follows

$$\boxed{\left[\frac{\partial f}{\partial x}\right]_i^n = a f_{i-1}^n + b f_i^n + c f_{i+1}^n + O(\Delta x^m)}$$

f_{i-1} and f_{i+1} written as Taylor series

$$f_{i-1}^n = f_i^n - \Delta x \left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right] - \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right] + \text{HOT}$$

$$f_{i+1} = f_i^n + \Delta x \left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right] + \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right] + \text{HOT}$$

This finally gives

$$\left[\frac{\partial f}{\partial x}\right]_i^n = a\left[f_i^n - \Delta x\left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right] - \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right] + O(\Delta x^4)\right] + \quad f_{i-1}$$

$$+ b f_i^n \quad f_i$$

$$+ c\left[f_i^n + \Delta x\left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right] + \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right] + O(\Delta x^4)\right] \quad f_{i+1}$$

Introduction: Discretization strategy

After some algebra

$$\left[\frac{\partial f}{\partial x}\right]_i^n = (a+b+c)\, f_i^n + \Delta x (c-a)\left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}(a+c)\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + (c-a)\frac{\Delta x^3}{3}\left[\frac{\partial^3 f}{\partial x^3}\right]_i^n$$

$$\begin{cases} a+b+c=0 \\ (c-a)\Delta x = 1 \\ (a+c)\frac{\Delta x^2}{2} = 0 \end{cases} \rightarrow \quad c = a + \frac{1}{\Delta x}\,; \quad \boxed{a = -\frac{1}{2\Delta x}\,, \quad c = \frac{1}{2\Delta x}\,, \quad b = 0}$$

Therefore

$$\boxed{\left[\frac{\partial f}{\partial x}\right]_i^n = \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} - \overbrace{\frac{\Delta x^2}{6}}^{(c-a)\frac{\Delta x^3}{6}}\left[\frac{\partial^3 f}{\partial x^3}\right]_i^n}$$

Central discretization in space (CS)

2nd order accurate formulation

Introduction: Discretization strategy

Following the same strategy, we can obtain an expression for the second derivative:

$$\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n = a f_{i-1}^n + b f_i^n + c f_{i+1}^n + O(\Delta x^m)$$

And, employing the Taylor series expansion of the function at x_{i-1} and x_{i+1}

$$\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n = a\left(f_i^n - \Delta x\left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n - \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right]_i^n + HOT\right) +$$

$$+ b f_i^n$$

$$+ c\left(f_i^n + \Delta x\left[\frac{\partial f}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + \frac{\Delta x^3}{3!}\left[\frac{\partial^3 f}{\partial x^3}\right]_i^n + HOT\right)$$

$$\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n = \underbrace{(a+b+c)}_{a+b+c=0} f_i^n + \underbrace{\Delta x(c-a)}_{\Delta x(c-a)=0}\left[\frac{\partial f}{\partial x}\right]_i^n + \underbrace{\frac{\Delta x^2}{2}(a+c)}_{(a+c)\frac{\Delta x^2}{2}=1}\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n + \frac{\Delta x^3}{3!}(c-a)\left[\frac{\partial^3 f}{\partial x^3}\right]_i^n + \dots$$

Introduction: Discretization strategy

$$\begin{cases} a+b+c=0 \\ (c-a)\Delta x=0 \\ (a+c)\frac{\Delta x^2}{2}=1 \end{cases} \rightarrow c=a\ ;\ a=\frac{1}{\Delta x^2},\quad c=\frac{1}{\Delta x^2},\quad b=-\frac{2}{\Delta x^2}$$

Therefore, we get

$$\boxed{\left[\frac{\partial^2 f}{\partial x^2}\right]_i^n = \frac{f_{i-1}^n - 2f_i^n + f_{i+1}^n}{\Delta x^2} + \underbrace{\frac{\Delta x^2}{12}}_{(a+c)\frac{\Delta x^4}{4!}}\left[\frac{\partial^4 f}{\partial x^4}\right]}$$

2nd order accurate

To summarize

$$\boxed{\begin{aligned} \left[\frac{\partial f}{\partial x}\right]_i^n &= \frac{f_{i+1}^n - f_{i-1}^n}{2\Delta x} \\ \left[\frac{\partial^2 f}{\partial x^2}\right]_i^n &= \frac{f_{i-1}^n - 2f_i^n + f_{i+1}^n}{\Delta x^2} \end{aligned}}$$

Central discretization in space (CS)

It's all we need for the moment: a model and a discretization strategy!!

Recall: Diffusion and advection

Let's consider our transport equation (1D ADE)

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Diffusion: Explicit method

We focus first on diffusion:

The governing equation is:

$$\boxed{\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2}}$$

Note: An analytical solution exists

$$\boxed{c = 1 - 2\sum_{n=0}^{\infty} \frac{(-1)^n}{(n+\frac{1}{2})\pi} \cos\left[(n+\tfrac{1}{2})\pi x\right] \exp\left[-(n+\tfrac{1}{2})^2\pi^2 t\right]}$$

Now we want to solve the problem numerically

Discretization in space $\Longrightarrow$ $\left[\frac{\partial^2 c}{\partial x^2}\right]_i^n = \frac{c_{i-1}^n - 2c_i^n + c_{i+1}^n}{\Delta x^2}$

Discretization in time $\Longrightarrow$ $\left[\frac{\partial c}{\partial t}\right]_i^n = \frac{c_i^{n+1} - c_i^n}{\Delta t}$

n=known

n+1=unknown

Therefore:

$$\boxed{c_i^{n+1} = c_i^n + \overbrace{\frac{\Delta t}{\Delta x^2}}^{s}\left(c_{i-1}^n - 2c_i^n + c_{i+1}^n\right)}$$

[Explicit method]

Diffusion
Explicit method, Numerical results

$$\Delta x = 4 \cdot 10^{-3}; \Delta t = 8 \cdot 10^{-6}; s = \frac{\Delta t}{\Delta x^2} = 0.5$$

(*Note that: L=1)

Are these results good?

Diffusion
Explicit method: numerical vs analytical results

Symbols: Numerical results

Line: Analytical results (computed up to n=1000)

$$C = 1 - 2\sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1/2)\pi} \cos\left[(n+1/2)\,\pi x\right] \exp\left[-(n+1/2)^2\,\pi^2 t\right]$$

Diffusion
Explicit method: numerical results-2

$$\Delta x = 4 \cdot 10^{-3}; \Delta t = 8.2 \cdot 10^{-6}; s = \frac{\Delta t}{\Delta x^2} = 0.5125$$

Diffusion
Explicit method: numerical vs analytical results-2

Symbols: Numerical results

Line: Analytical results

$$C = 1 - 2\sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1/2)\pi} \cos\left[(n+1/2)\,\pi x\right] \exp\left[-(n+1/2)^2\,\pi^2 t\right]$$

Diffusion
Implicit method

It can be shown that the explicit method is stable only if:

$$\boxed{s = \frac{\Delta t}{\Delta x^2} \leq 0.5}$$

$$\boxed{C_i^{n+1} = C_i^n + \frac{\Delta t}{\Delta x^2}\left(C_{i-1}^n - 2C_i^n + C_{i+1}^n\right)}$$

Otherwise, it is unstable.

→ To overcome this problem, we can use an implicit scheme:

$$\left[\frac{\partial C}{\partial t}\right]_i^n = \frac{C_i^{n+1} - C_i^n}{\Delta t}$$

$$\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n = \frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta x^2}$$

[Evaluated at the new time step "n+1"]

$$\boxed{-sC_{i-1}^{n+1} + (1+2s)C_i^{n+1} - sC_{i+1}^{n+1} = C_i^n}$$

← But now we have a linear system of equations

Unknowns

Diffusion
Implicit method

$$\boxed{-s\,C_{i-1}^{n+1} + (1+2s)\,C_i^{n+1} - s\,C_{i+1}^{n+1} = C_i^n}$$

$$\underbrace{\begin{pmatrix} 1+2s & -s & & \\ -s & 1+2s & -s & \\ & \ddots & \ddots & \ddots \\ & & -s & 1+2s \end{pmatrix}}_{\text{Tridiagonal Matrix}} \underbrace{\begin{pmatrix} C_1^{n+1} \\ \vdots \\ C_i^{n+1} \\ \vdots \\ C_m^{n+1} \end{pmatrix}}_{\text{unew1}} = \underbrace{\begin{pmatrix} C_1^{n} \\ \vdots \\ C_i^{n} \\ \vdots \\ C_m^{n} \end{pmatrix}}_{\text{D}}$$

$\boxed{\text{[Thomas algorithm]}}^{*}$ → *Code*

```
function [ unew1 ] = tridiag(n,a,b,c,D)

alfa=zeros(n,1);
gamma=zeros(n,1);
v=zeros(n,1);
unew1=zeros(n,1);

%    Tridiagonal solver
    alfa(1)=a(1);
    gamma(1)=c(1)/(a(1));
    v(1)=D(1)/(a(1));

    for i=2:n
      alfa(i)=a(i)-b(i)*gamma(i-1);
      gamma(i)=c(i)/alfa(i);
      v(i)=(D(i)-b(i)*v(i-1))/(alfa(i));
    end

    unew1(n)=v(n);

    for i=n-1:-1:1
        unew1(i)=v(i)-gamma(i)*unew1(i-1);
    end
```

If we now run the simulations...

*Thomas algorithm-details

Thomas algorithm

$$\underbrace{\begin{bmatrix} a_1 & c_1 & 0 & 0 \\ b_2 & a_2 & c_2 & 0 \\ 0 & b_3 & a_3 & c_3 \\ 0 & 0 & b_4 & a_4 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \alpha_1 & 0 & 0 & 0 \\ \beta_2 & \alpha_2 & 0 & 0 \\ 0 & \beta_2 & \alpha_3 & 0 \\ 0 & 0 & \beta_4 & \alpha_4 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & \gamma_1 & 0 & 0 \\ 0 & 1 & \gamma_2 & 0 \\ 0 & 0 & 1 & \gamma_3 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{U}$$

Suppose we want to solve: $\boxed{A \cdot C = R}$ Variable

$$\begin{cases} A \cdot C = R \\ \uparrow \\ A = L \cdot U \end{cases} \Rightarrow L \underbrace{U \cdot C}_{y} = R \xrightarrow{\text{Decomposed}} \begin{cases} L \cdot y = R & \text{Problem A} \\ U \cdot C = y & \text{Problem B} \end{cases}$$

*Thomas algorithm-details

Problem A

$$\underbrace{\begin{pmatrix} \alpha_1 & 0 & 0 & 0 \\ \beta_2 & \alpha_2 & 0 & 0 \\ 0 & \beta_3 & \alpha_3 & 0 \\ 0 & 0 & \beta_4 & \alpha_4 \end{pmatrix}}_{L} \cdot \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_{y} = \underbrace{\begin{bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{bmatrix}}_{R}$$

Note: $\alpha_i, \beta_i, \gamma_i$ from $A = L \cdot U$

$\alpha_1 = a_1$

$\alpha_1 \gamma_1 = c_1 \rightarrow \gamma_1 = \frac{c_1}{\alpha_1}$

$\beta_2 = b_2$

$a_2 = \beta_2 \gamma_1 + \alpha_2 \rightarrow \alpha_2 = a_2 - b_2 \frac{c_1}{a_1}$

$c_2 = \alpha_2 \gamma_2 \rightarrow \gamma_2 = \frac{c_2}{\alpha_2}$

$\Downarrow$

$\alpha_1 y_1 = R_1 \rightarrow y_1 = \frac{R_1}{\alpha_1} = \frac{R_1}{a_1}$

$\beta_2 y_1 + \alpha_2 y_2 = R_2 \rightarrow \begin{cases} y_2 = \frac{R_2 - \beta_2 y_1}{\alpha_2} \\ \alpha_2 = a_2 - b_2 \frac{c_1}{a_1} \end{cases}$

For a generic node i:

loop over i

$$\begin{cases} \alpha_i = a_i - b_i \gamma_{i-1} \\ \beta_i = b_i \\ \gamma_i = c_i / \alpha_i \\ y_i = (R_i - b_i y_{i-1}) / \alpha_i \end{cases}$$

*Thomas algorithm-details

Problem B

$$\underbrace{\begin{pmatrix} 1 & \gamma_1 & 0 & 0 \\ 0 & 1 & \gamma_2 & 0 \\ 0 & 0 & 1 & \gamma_3 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{U} \cdot \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

$$U \cdot C = y$$

Starting from the bottom:

$$c_4 = y_4$$

$$c_3 + \gamma_3 c_4 = y_3 \rightarrow c_3 = y_3 - \gamma_3 c_4$$

$$\vdots$$

In general

$$c_n = y_n$$

$$\text{loop}_i \text{ over} \Rightarrow \left[c_i = y_i - \gamma_i y_{i+1} \right.$$

Note on Neumann BC for the implicit method

Neumann BC (assume it is imposed @x=0) means that:

$$\frac{\partial C}{\partial x}\Big|_{x=0} = c \rightarrow \frac{C_2^{n+1} - C_0^{n+1}}{2\Delta x} = c$$

The equation written @x=0 (i.e. i=1):

$$\begin{cases} (1+2s)\,C_1^{n+1} - s\,C_2^{n+1} - s\,C_0^{n+1} = C_1^{n+1} \\ C_2^{n+1} - C_0^{n+1} = 2\Delta x \cdot c \rightarrow C_0^{n+1} = C_2^{n+1} - 2\Delta x \cdot c \end{cases}$$

$$(1+2s)\,C_1^{n+1} - s\,C_2^{n+1} - s\,C_2^{n+1} - 2sc\Delta x = C_1^{n}$$

$$\boxed{(1+2s)\,C_1^{n+1} - s\,C_2^{n+1} - s\,C_2^{n+1} = C_1^{n} + 2sc\Delta x}$$

This means that with Dirichlet/Neumann BC we have $n = n_y - 1$ equations, whereas with Dirichlet/Dirichlet we have $n = n_y - 2$ equations

Diffusion
Implicit method, Numerical results

$$\Delta x = 4 \cdot 10^{-3}; \Delta t = 2 \cdot 10^{-4}; s = \frac{\Delta t}{\Delta x^2} = 12.5$$

A further consideration : Accuracy

Previous schemes are 1st order accurate in time. A 2nd order scheme would be desired in many applications

To do that → Crank-Nicolson scheme

$$\frac{\partial C}{\partial t} = F(c,x) \Rightarrow \left[\frac{\partial C}{\partial t}\right]_i^n = \frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{F^{n+1}(C,x) + F^n(C,x)}{2}$$

For the present case:

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{1}{2}\left[\frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta x^2} + \frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2}\right]$$

Note:

$$s = \frac{1}{2}\frac{\Delta t}{\Delta x^2}$$

This equation can be rearranged as:

$$\boxed{-sC_{i-1}^{n+1} + (1+2s)C_i^{n+1} - sC_{i+1}^{n+1} = sC_{i-1}^n + (1-2s)C_i^n + sC_{i+1}^n}$$

[Thomas algorithm]

Diffusion
Implicit method: 1st vs 2nd order

$$\Delta x = 1 \cdot 10^{-2}; \Delta t = 1 \cdot 10^{-4}; s = \frac{\Delta t}{\Delta x^2} = 1$$

1st Order

2nd Order

(Percentage) Average error $\rightarrow \frac{1}{n_y} \sum |u_{th} - u_n|$

Further considerations: Extension to 2D case (brief discussion)

Now the stencil has five points, not three

With an explicit scheme:

$$\boxed{C^{n+1}_{i,j} - C^{n}_{i,j} = \frac{\Delta t \cdot D}{\Delta x^2}\left[C^{n}_{i-1,j} - 2C^{n}_{i,j} + C^{n}_{i+1,j}\right] + \frac{\Delta t \cdot D}{\Delta y^2}\left[C^{n}_{i,j-1} - 2C^{n}_{i,j} + C^{n}_{i,j+1}\right]}$$

For stability $\rightarrow \left(\frac{D\Delta t}{\Delta x^2} + \frac{D\Delta t}{\Delta y^2}\right) \leq \frac{1}{2}$ [severe condition]

Also, Fully implicit methods would lead to a pentadiagonal system (Time consuming)

↳ Solution 1: Splitting methods

↳ Solution 2: Iterative solvers (Jacobi, Gauss-Seidel, relaxation)

*Diffusion
Further considerations

Implicit formulation

$$\boxed{\frac{\partial c}{\partial t} = F^{n+1}(x, y, t)}$$

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n}}{\Delta t} = D_{ij}\left[\frac{C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}}{\Delta x^2} + \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta y^2}\right]$$

We obtain

$$\boxed{S_x C_{i+1,j}^{n+1} + S_x C_{i-1,j}^{n+1} - (2S_x + 2S_y - 1) C_{i,j}^{n+1} + S_y C_{i,j+1}^{n+1} + S_y C_{i,j-1}^{n+1} = C_{i,j}^{n}}$$

$$S_x = D_{ij}\frac{\Delta t}{\Delta x^2}$$

$$S_y = D_{ij}\frac{\Delta t}{\Delta y^2}$$

(Pentadiagonal system)

*Diffusion
Further considerations

Splitting methods (Alternating Directions Implicit Method, ADI):

Sweep along 1 direction

$$\frac{C_{i,j}^{n+\frac{1}{2}} - C_{i,j}^{n}}{\left(\frac{\Delta t}{2}\right)} = D_{ij}\left[\frac{C_{i+1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{C_{i,j+1}^{n} - 2C_{i,j}^{n} + C_{i,j-1}^{n}}{\Delta y^2}\right]$$

Sweep along the other direction

$$\frac{C_{i,j}^{n+1} - C_{i,j}^{n+\frac{1}{2}}}{\left(\frac{\Delta t}{2}\right)} = D_{i,j}\left[\frac{C_{i+1,j}^{n+\frac{1}{2}} - 2C_{i,j}^{n+\frac{1}{2}} + C_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}}{\Delta x^2}\right]$$

(Two tridiag. systems)

*Diffusion
Further considerations

Iterative methods. Assume a generic 2D diffusion equation (Poisson eq.)

$$\boxed{\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = f(x,y)}$$

After discretization:

$$C_{i+1,j} - 2C_{i,j} + 2C_{i-1,j} + \underbrace{\left(\frac{\Delta x^2}{\Delta y^2}\right)}_{\beta^2}\left[C_{i,j-1} - 2C_{i,j} + C_{i,j+1}\right] = f$$

$$\underbrace{\begin{bmatrix} 2 & 1 & 0 & 0 & \beta^2 & 0 \\ 1 & \ddots & \ddots & & & \ddots \\ 0 & \ddots & \ddots & \ddots & & 0 \\ 0 & & \ddots & \ddots & \ddots & \\ \beta^2 & & 0 & \ddots & \ddots & \\ 0 & \ddots & & & & \end{bmatrix}}_{\text{Pentadiagonal}} \begin{bmatrix} \\ C \\ \\ \end{bmatrix} = \begin{bmatrix} \\ D \\ \\ \end{bmatrix}$$

*Diffusion
Further considerations

Iterative solvers

- JACOBI

$$-2C_{i,j} - 2\beta^2 C_{i,j} = -C_{i+1,j} - C_{i-1,j} - \beta^2 C_{i,j-1} - \beta^2 C_{i,j+1}$$

$$\boxed{C_{i,j}^{k+1} = \frac{C_{i+1,j}^{k} + C_{i-1,j}^{k} + \beta^2 C_{i,j-1}^{k} + \beta^2 C_{i,j-1}^{k}}{2(1+\beta^2)}}$$

- POINT GAUSS SEIDEL

[Assume that the algorithms loops along i and then along j

$$\boxed{C_{i,j}^{k+1} = \frac{1}{2(1+\beta^2)}\left[C_{i+1,j}^{k} + C_{i-1,j}^{k+1} + \beta^2\left(C_{i,j+1}^{k} + C_{i,j-1}^{k+1}\right)\right]}$$

*Diffusion
Further considerations

• **LINE GAUSS-SEIDEL**

Instead of focusing on a single point, we focus on a line:

Therefore, we can write a tridiagonal system

$$\boxed{C^{K+1}_{i-1,j} - 2(1+\beta^2)C^{K+1}_{i,j} + C^{K+1}_{i+1,j} = -\beta^2 C^{K}_{i,j+1} - \beta C^{K+1}_{i,j-1}}$$

*Diffusion
Further considerations

• POINT SUCCESSIVE OVER RELAXATION METHODS (PSOR)
(Extrapolation to accelerate convergence)

↳ Assume you apply a GAUSS-SEIDEL

$$C^{calc}_{i,j} = \frac{1}{2(1+\beta^2)}\left[C^{k}_{i+1,j} + C^{k+1}_{i-1,j} + \beta^2\left(C^{k}_{i,j+1} + C^{k+1}_{i,j-1}\right)\right]$$

↳ Relaxation:

$$\boxed{C^{k+1}_{i,j} = C^{calc}_{i,j}\cdot\omega + (1-\omega)\,C^{k}_{i,j}}$$

Recall: Diffusion and advection

Let's consider our transport equation (1D ADE)

$$\boxed{\frac{\partial C^*}{\partial t^*} + u^* \frac{\partial C^*}{\partial x^*} = D \frac{\partial^2 C^*}{\partial x^{*2}}}$$

In dimensionless form:

$$\begin{cases} C = \dfrac{C^*}{C_w} \\ x = \dfrac{x^*}{L} \\ u = \dfrac{u^*}{u_{ref}} \\ t = \dfrac{t^* D}{L^2} \end{cases} \rightarrow \frac{D C_w}{L^2} \frac{\partial C}{\partial t} + \frac{u_{ref}\, u\, C_w}{L} \frac{\partial C}{\partial x} = \frac{D C_w}{L^2} \frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} + \frac{u_{ref} \cdot \cancel{C_w}}{\cancel{L}} \frac{L^{\cancel{2}}}{D \cancel{C_w}} u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}$$

$$\frac{\partial C}{\partial t} + \underbrace{\frac{u_{ref} \cdot L}{D}}_{Pe\ (\text{Peclet})} u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}$$

$$\left[Pe = \frac{\text{diffusion time}}{\text{convection time}} = \frac{L^2/D}{L/u_{ref}} = \frac{L \cdot u_{ref}}{D} \right]$$

$$\boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}}$$

$Pe \ll 1 \Rightarrow$ Diffusion dominates $\rightarrow \boxed{\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}}$

$Pe \gg 1 \Rightarrow$ Advection dominates $\rightarrow \boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = 0}$

Advection: Introduction

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = 0$$

Analytical solution exists

$$\begin{cases} C(x,t) = C_0(x - Ut) \\ C(x,0) = C_0(x) \end{cases}$$

Advection: Discretization strategy

In this case we do not use the usual "central" approximation:

$$\left[\frac{\partial C}{\partial x}\right]_i^n = \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}$$

It can be proven that this scheme is unstable

We use what is usually called an "upwind" approximation:

$[U>0]$

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + U\,\frac{C_i^n - C_{i-1}^n}{\Delta x} = 0$$

$[U = Pe \cdot u]$

This gives:

$$C_i^{n+1} = C_i^n - \underbrace{\frac{U\Delta t}{\Delta x}}_{C_0\ (\text{Courant})}\left(C_i^n - C_{i-1}^n\right) \rightarrow \boxed{C_i^{n+1} = C_i^n(1-C_0) + C_0 \cdot C_{i-1}^n}$$

Stability: It can be shown that (Von-Neumann*)

$$G = 1 - C_0(1-\cos\theta) - i\,C_0\sin\theta \rightarrow |G| = 1 + \overbrace{(1-\cos\theta)}^{\geq 0}(C_0 - 1)\overbrace{2C_0}^{\geq 0} \rightarrow \boxed{C_0 \leq 1} \quad \left(\begin{matrix}\text{small}\\ \Delta t\end{matrix}\right)$$

Advection: Accuracy

What about the accuracy (Truncation error)

(Taylor series)

$$\begin{cases} C_i^{n+1} = C_i^n + \Delta t \left[\frac{\partial C}{\partial t}\right]_i^n + \frac{\Delta t^2}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n + HOT & \text{Time} \\ C_{i-1}^n = C_i^n - \Delta x \left[\frac{\partial C}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n + HOT & \text{Space} \end{cases}$$

Therefore:

$$\boxed{C_i^{n+1} = (1-C_0)C_i^n + C_0 C_{i-1}^n}$$

$$C_i^n + \Delta t \left[\frac{\partial C}{\partial t}\right]_i^n + \frac{\Delta t^2}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n = (1-C_0)C_i^n + C_0\left[C_i^n - \Delta x\left[\frac{\partial C}{\partial x}\right]_i^n + \frac{\Delta x^2}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n\right]$$

We get:

$$\cancel{C_i^n} + \Delta t \left[\frac{\partial C}{\partial t}\right]_i^n + \frac{\Delta t^2}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n = \cancel{C_i^n} - \cancel{C_0 C_i^n} + \cancel{C_0 C_i^n} - C_0 \Delta x \left[\frac{\partial C}{\partial x}\right]_i^n + C_0 \frac{\Delta x^2}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n$$

$$\left[\frac{\partial C}{\partial t}\right]_i^n + \frac{\Delta t}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n = -\frac{C_0 \Delta x}{\Delta t}\left[\frac{\partial C}{\partial x}\right]_i^n + C_0 \frac{\Delta x^2}{2\Delta t}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n$$

Advection: Accuracy

Finally

$$\underbrace{\left[\frac{\partial C}{\partial t}\right]_i^n + \overbrace{\frac{C_0 \Delta x}{\Delta t}}^{U} \left[\frac{\partial C}{\partial x}\right]_i^n}_{\text{Original equation}} = \underbrace{-\frac{\Delta t}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n + C_0 \frac{\Delta x^2}{2\Delta t}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n}_{\boxed{\text{Error } (\varepsilon)}}$$

We focus now on the error:

$$\varepsilon = -\frac{\Delta t}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n + \frac{U \Delta x}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n$$

$$\hookrightarrow \boxed{\frac{\partial C}{\partial t} = -U\frac{\partial C}{\partial x} \Rightarrow \frac{\partial}{\partial t}\left(\frac{\partial C}{\partial t}\right) = -U\frac{\partial}{\partial x}\left(-U\frac{\partial C}{\partial x}\right) \Rightarrow \boxed{\left[\frac{\partial^2 C}{\partial t^2} = U^2 \frac{\partial^2 C}{\partial x^2}\right]}}$$

$$\varepsilon = -\frac{\Delta t}{2}\left[\frac{\partial^2 C}{\partial t^2}\right]_i^n + \frac{U\Delta x}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n$$

$$= -\frac{\Delta t}{2}\left(U^2\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n\right) + \frac{U\Delta x}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n = \frac{U\Delta x}{2}\left\{\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n - \frac{U\Delta t}{\Delta x}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n\right\}$$

$$= \frac{U\Delta x}{2}\left[\frac{\partial^2 C}{\partial x^2}\right]_i^n (1 - C_0)$$

Advection: Accuracy, numerical diffusion

We have obtained the following expression

$$\boxed{\varepsilon = \underbrace{\frac{U\Delta x}{2}(1-C_0)}_{\alpha' = \text{Numerical viscosity or diffusivity}} \left[\frac{\partial^2 C}{\partial x^2}\right]_i^n}$$

→ We have already seen that $\left[\frac{\partial^2 C}{\partial x^2}\right]$ characterizes diffusion processes

There fore, the equation we are going to solve is:

$$\boxed{\left[\frac{\partial C}{\partial t}\right]_i^n + U\left[\frac{\partial C}{\partial x}\right]_i^n = \alpha' \left[\frac{\partial^2 C}{\partial x^2}\right]_i^n}$$

With the additional constraint that $C_0 \leq 1$, obtained from stability considerations (but also expected...)

Advection
Numerical Results

Discretized equation

$$C_i^{n+1} = (1 - Co)\, C_i^n + Co C_{i-1}^n$$

We first see what happens when $Co = 1.1$

As expected...

Advection
Numerical Results

Now we reduce the Courant number

$Co = 0.5$

$Co = 0.1$

Advection
Numerical Results

A heavier simulation does not necessarily mean a better simulation…

Looking at the truncation error: $$\epsilon = \frac{U\Delta x}{2}(1 - Co)\left[\frac{\partial^2 C}{\partial x^2}\right]$$

$Co = 1$

Now we have seen the fundamental concepts about diffusion & advection, and how to discretize them. It's now time to combine them and to turn into a more complex problem….

The full problem: Physics

Governing equations

$$\begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0 \\ \dfrac{\partial u_i}{\partial t} + u_j \dfrac{\partial u_i}{\partial x_j} = -\dfrac{\partial p}{\partial x_i} + \dfrac{1}{Re}\dfrac{\partial^2 u_i}{\partial x_j^2} \\ \dfrac{\partial C}{\partial t} + u_j \dfrac{\partial C}{\partial x_j} = \dfrac{1}{RePr}\dfrac{\partial^2 C}{\partial x_j^2} \end{cases}$$

$$\boxed{\frac{1}{Pe}}$$

The full problem: Physics

$$u(t) = U \sin(\omega t)$$

Note: transport equation for ω (*see later)

Note: BC for ω obtained from Taylor series expansion of ψ (**see later)

Alternative formulation (ψ, ω)

$$\begin{cases} u_x = \dfrac{\partial \psi}{\partial y} & \text{Riemann} \\ u_y = -\dfrac{\partial \psi}{\partial x} & \\ \omega = \dfrac{\partial u_y}{\partial x} - \dfrac{\partial u_x}{\partial y} & \text{Vorticity} \end{cases}$$

$$\begin{cases} \omega = -\left(\dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{\partial^2 \psi}{\partial y^2}\right) \\ \dfrac{\partial \omega}{\partial t} + u_j \dfrac{\partial \omega}{\partial x_j} = +\dfrac{1}{Re}\dfrac{\partial^2 \omega}{\partial x_j^2} & \text{*Curl(NS)} \\ \dfrac{\partial C}{\partial t} + u_j \dfrac{\partial C}{\partial x_j} = \dfrac{1}{RePr}\dfrac{\partial^2 C}{\partial x_j^2} \end{cases}$$

The full problem: *A note on the vorticity transport equation

(Note: in this slide, ***u=velocity along x***; ***v=velocity along y***; ***subscripts indicate partial derivatives***). To obtain the Vorticity transport eq.:

$$u_t + uu_x + vu_y = -P_x + \mu \nabla^2 u \qquad (A)$$

$$v_t + uv_x + vv_y = -P_y + \mu \nabla^2 v \qquad (B)$$

Then, $\partial/\partial y(A)$ and $\partial/\partial x(B)$

$$u_{ty} + u_y u_x + uu_{xy} + v_y u_y + vu_{yy} = -P_{xy} + \mu \nabla^2 u_y \qquad (C)$$

$$v_{tx} + u_x v_x + uv_{xx} + v_x v_y + vv_{yx} = -P_{xy} + \mu \nabla^2 v_x \qquad (D)$$

Making (D)-(C), and taking into account that:

$$\left.\begin{aligned} &\omega = v_y - u_x \\ &u_x + v_y = 0 \quad (continuity) \end{aligned}\right\} \longrightarrow \omega_t + u\omega_x + v\omega_y = Re^{-1}\nabla^2\omega$$

The full problem: Physics

Central approx.

$$\left[\frac{\partial f_{i,j}}{\partial x}\right]^n_{i,j} = \frac{f^n_{i+1,j} - f^n_{i-1,j}}{2\Delta x}$$

$$\left[\frac{\partial^2 f}{\partial x^2}\right]^n_{i,j} = \frac{f^n_{i-1,j} - 2f^n_{i,j} + f^n_{i+1,j}}{\Delta x^2}$$

$$\left[\frac{\partial f_{i,j}}{\partial y}\right]^n_{i,j} = \frac{f^n_{i,j+1} - f^n_{i,j-1}}{2\Delta y}$$

$$\left[\frac{\partial^2 f}{\partial y^2}\right]^n_{i,j} = \frac{f^n_{i,j-1} - 2f^n_{i,j} + f^n_{i,j+1}}{\Delta y^2}$$

Explicit

$$\left[\frac{\partial f}{\partial t}\right]^n_{i,j} = F^n_{i,j}$$

The full problem: **A note on B.C.

Let's focus on B.C. for ψ, ω:

$$u(t) = U \sin(\omega t)$$

- B.C. $\psi = 0$ is used to solve the Poisson equation
- B.C on the derivative of ψ is used to build B.C. for ω.

Using Taylor series expansion for ψ we have:

$$\psi_{i,j-1} = \psi_{i,j} - \Delta y \left[\frac{\partial \psi}{\partial y}\right]_{i,j} + \frac{\Delta y^2}{2}\left[\frac{\partial^2 \psi}{\partial y^2}\right]_{i,j} + \dots$$

$$\omega_{i,j} = \left[\frac{\partial^2 \psi}{\partial y^2}\right]_{i,j}$$

$$\psi_{i,j} = 0; \quad \left[\frac{\partial \psi}{\partial y}\right]_{i,j} = g$$

See *Fletcher, C.A.J,* ***Computational techniques for fluid dynamics — 2 volume*** (1991), Springer-Verlag Berlin Heidelberg

The full problem: Numerics

```
c       WRITE(*,*) 'CALL POISSON'
        call poisson(dx,dy,vor2,psi,psin)

      DO I=1,NX
       DO J=1,NY
        PSI(I,J)=PSIN(I,J)
       ENDDO
      ENDDO


c       WRITE(*,*) 'CALL BC'
        call boundary_vor(dx,dy,psi,uwall,vor2)

      DO I=1,NX
       DO J=1,NY
        VOR(I,J)=VOR2(I,J)
       ENDDO
      ENDDO


c       WRITE(*,*) 'CALL VELOCITY'
        call velocity(dx,dy,psi,u,v)

c       WRITE(*,*) 'CALL TSCHEME'
        call tscheme(re,dx,dy,dt,u,v,vor,vor2)
```

Find ψ^{n+1} from ω^n $\longrightarrow$ $\omega = -\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}\right)$

Apply BC for ω^{n+1} from the knowledge of ψ^{n+1}

$$\omega_{1,j} = \frac{1}{2\Delta x^2}\left(8\psi_{2,j} - \psi_{3,j}\right)$$

$$\omega_{N,j} = \frac{1}{2\Delta x^2}\left(8\psi_{N-1,j} - \psi_{N-2,j}\right)$$

$$\omega_{i,1} = \frac{1}{2\Delta y^2}\left(8\psi_{i,2} - \psi_{i,3}\right)$$

$$\omega_{i,M} = \frac{1}{2\Delta x^2}\left(8\psi_{i,M-1} - \psi_{i,M-2}\right) + \frac{3u}{\Delta y}$$

Solve the transport of vorticity $\omega^{n+1} = \omega^n + \Delta t\left(F^n_{i,j}\right)$

The full problem: Numerics

$$Re = 2000; \quad L = H = 1; \quad N_x = N_y = 100; \quad \Delta t = 10^{-3}$$

$$u(t) = U \sin\left(\frac{t}{3}\right)$$

$$u(t) = U \sin\left(\frac{t}{2}\right)$$

$$u(t) = U \sin\left(\frac{3t}{4}\right)$$

Conclusions

1. Advection-Diffusion Equation

2. Discretization strategies: Basic concepts (1st, 2nd derivatives, Taylor series)

3. Diffusion equation: Explicit and implicit methods; stability and accuracy

4. Linear advection equation: “numerical diffusion" and stability

5. Transport of a scalar in a time dependent field: the full problem and its implementation

Navier-Stokes Eqs. (primitive variables)

$$\begin{cases} \dfrac{\partial u_i}{\partial x_i} = 0 \\ \dfrac{\partial u_i}{\partial t} + u_j \dfrac{\partial u_i}{\partial x_j} = -\dfrac{\partial p}{\partial x_i} + \dfrac{1}{Re}\dfrac{\partial^2 u_i}{\partial x_j{}^2} \end{cases}$$

$$Re = \frac{U_T L}{\nu}, \quad \nu = \frac{\mu}{\rho}$$

ν kinematic viscosity;

ρ density

μ dynamics. viscosity

L Reference Length

U_T Reference Velocity

Streamfunction-Vorticity formulation (ψ, ω)

$$\begin{cases} u_x = \dfrac{\partial \psi}{\partial y} \\ u_y = -\dfrac{\partial \psi}{\partial x} \\ \omega = \dfrac{\partial u_y}{\partial x} - \dfrac{\partial u_x}{\partial y} \end{cases}$$

Riemann equations

Vorticity definition

$$\begin{cases} \omega = -\left(\dfrac{\partial^2 \psi}{\partial x^2} + \dfrac{\partial^2 \psi}{\partial y^2}\right) \\ \dfrac{\partial \omega}{\partial t} + u_j \dfrac{\partial \omega}{\partial x_j} = +\dfrac{1}{Re}\dfrac{\partial^2 \omega}{\partial x_j{}^2} \end{cases}$$

*Curl(NS)