

# Numerical Simulation and Scientific Computing in Fluid Mechanics: Fundamental aspects and applications

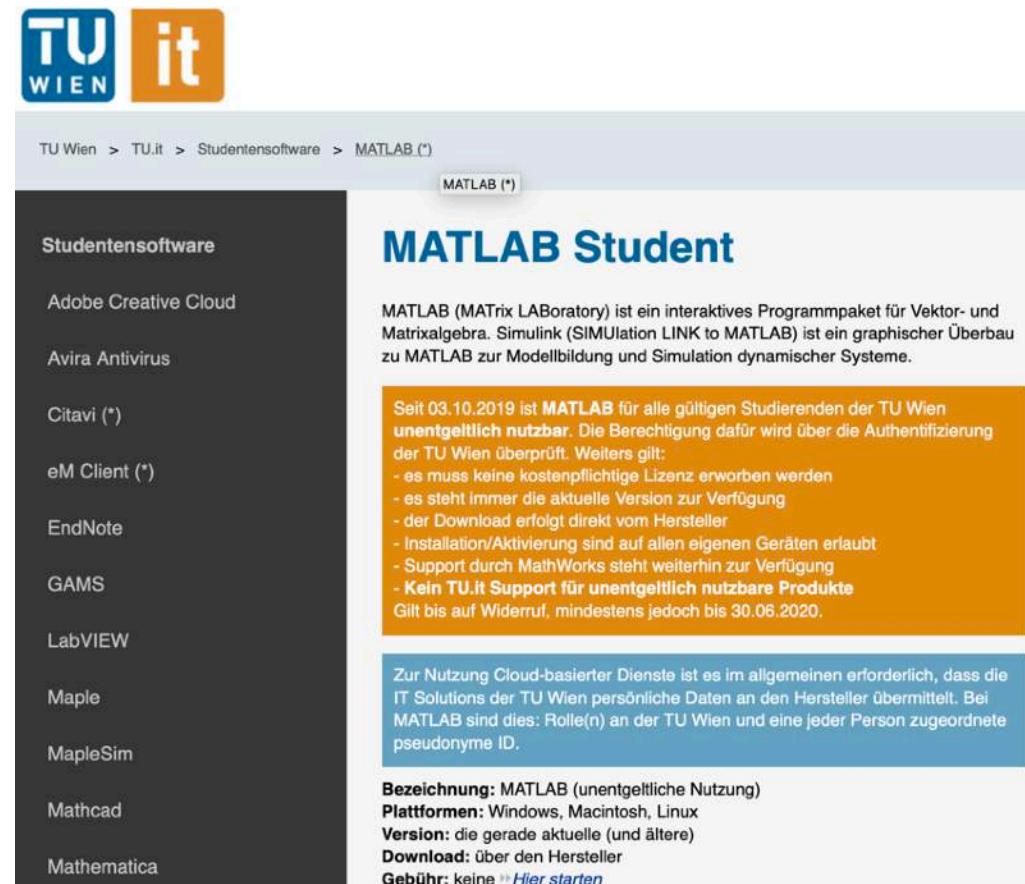
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*Numerical Simulations and Scientific Computing II - Fluid dynamics*

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



The screenshot shows a web page from TU Wien's software distribution portal. At the top, there are two logos: 'TU WIEN' in blue and 'it' in orange. The page title is 'Studentensoftware'. A breadcrumb navigation shows 'TU Wien > TU.it > Studentensoftware > MATLAB (\*)'. A tab labeled 'MATLAB (\*)' is selected. The main content area has a dark grey sidebar on the left containing a list of software titles: Adobe Creative Cloud, Avira Antivirus, Citavi (\*), eM Client (\*), EndNote, GAMS, LabVIEW, Maple, MapleSim, Mathcad, and Mathematica. To the right, the title 'MATLAB Student' is displayed in large blue text. Below it, a text block describes MATLAB as an interactive program package for vector and matrix algebra, mentioning Simulink as a graphical extension. A yellow callout box contains a note about MATLAB being available for all valid students from October 3, 2019, until June 30, 2020. It specifies that no payment is required, the latest version is available, and direct download from the manufacturer is allowed. A blue callout box below provides information about using cloud-based services, mentioning that personal data is sent to the manufacturer. At the bottom, detailed information is provided for MATLAB, including its designation, platforms (Windows, Macintosh, Linux), current version, download source (manufacturer), and a note that no fee is required.

MATLAB Student

MATLAB (MATrix LABoratory) ist ein interaktives Programm paket für Vektor- und Matrixalgebra. Simulink (SIMULATION LINK to MATLAB) ist ein graphischer Überbau zu MATLAB zur Modellbildung und Simulation dynamischer Systeme.

Seit 03.10.2019 ist MATLAB für alle gültigen Studierenden der TU Wien unentgeltlich nutzbar. Die Berechtigung dafür wird über die Authentifizierung der TU Wien überprüft. Weiters gilt:

- es muss keine kostenpflichtige Lizenz erworben werden
- es steht immer die aktuelle Version zur Verfügung
- der Download erfolgt direkt vom Hersteller
- Installation/Aktivierung sind auf allen eigenen Geräten erlaubt
- Support durch MathWorks steht weiterhin zur Verfügung
- Kein TU.it Support für unentgeltlich nutzbare Produkte

Gilt bis auf Widerruf, mindestens jedoch bis 30.06.2020.

Zur Nutzung Cloud-basierter Dienste ist es im allgemeinen erforderlich, dass die IT Solutions der TU Wien persönliche Daten an den Hersteller übermittelt. Bei MATLAB sind dies: Rolle(n) an der TU Wien und eine jeder Person zugeordnete pseudonyme ID.

**Bezeichnung:** MATLAB (unentgeltliche Nutzung)  
**Plattformen:** Windows, Macintosh, Linux  
**Version:** die gerade aktuelle (und ältere)  
**Download:** über den Hersteller  
**Gebühr:** keine [Hier starten](#)

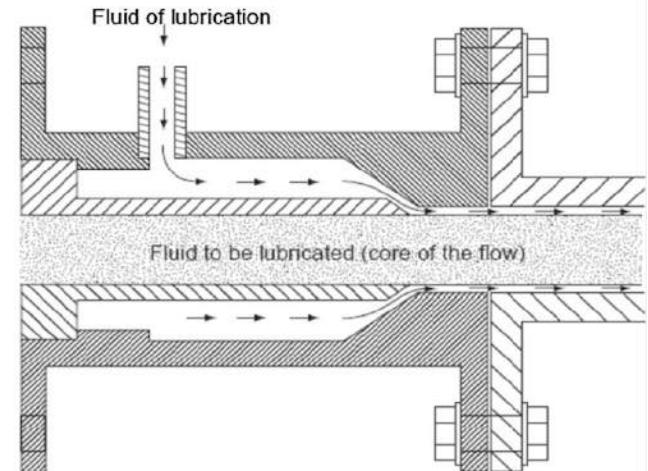
1. Oil transport
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5. Oil/water emulsions
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7. Flows in porous media

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.

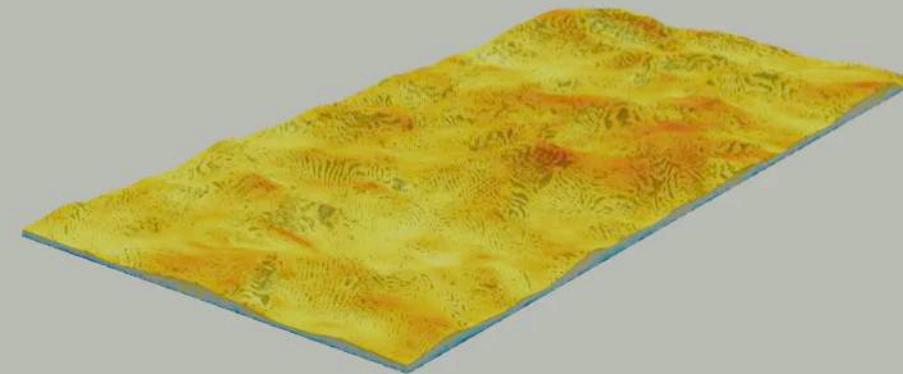
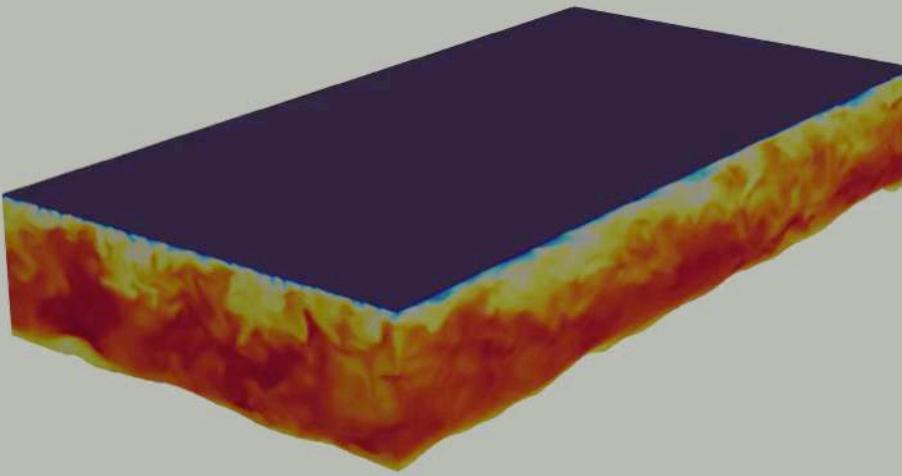


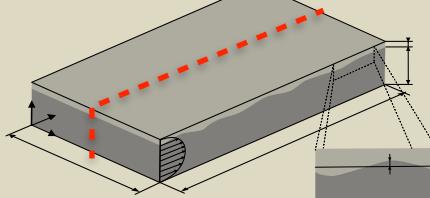
Credit: ALFA Research Group

"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 "

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

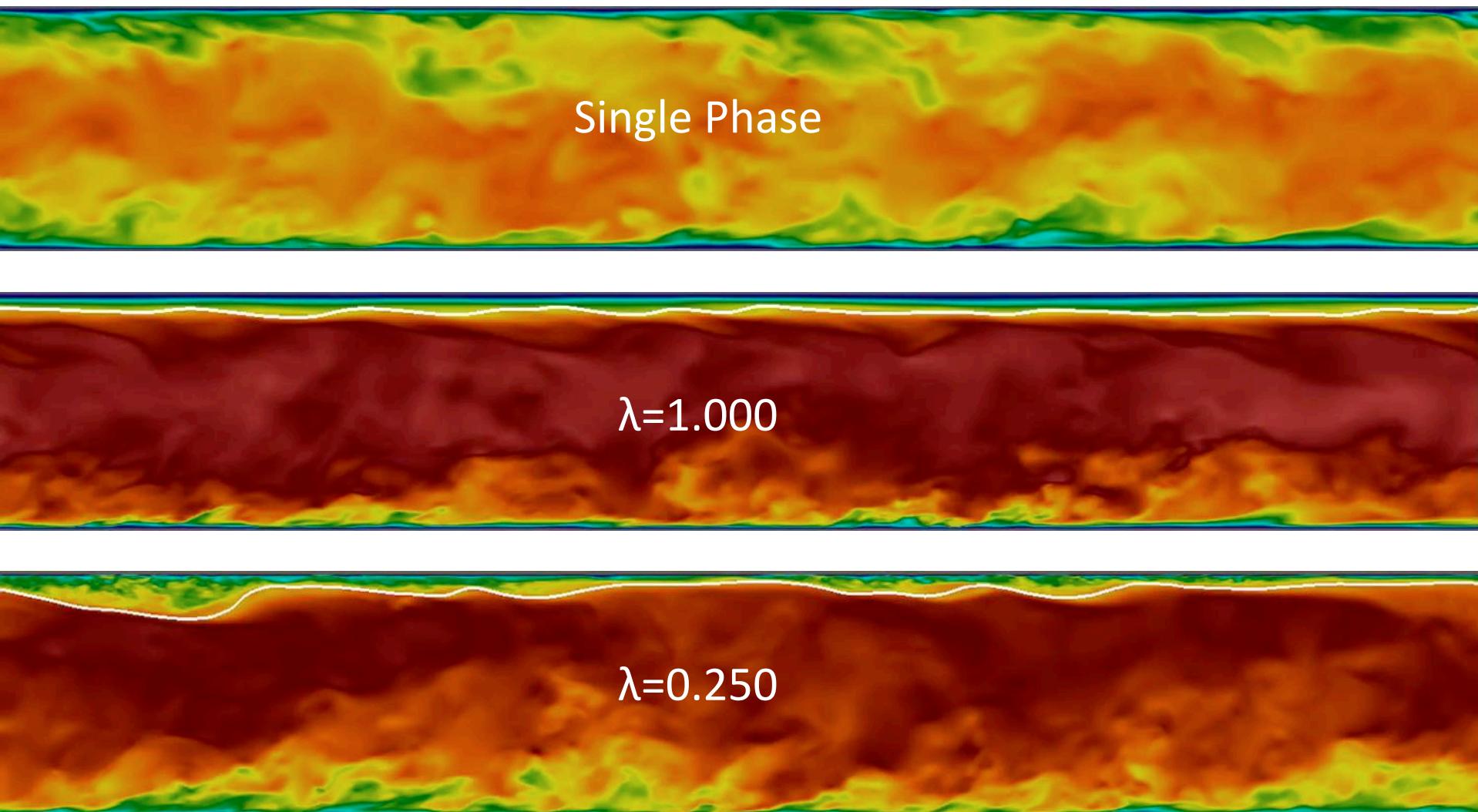




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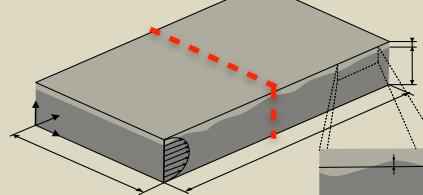
Ux

30

**Oil Transport**

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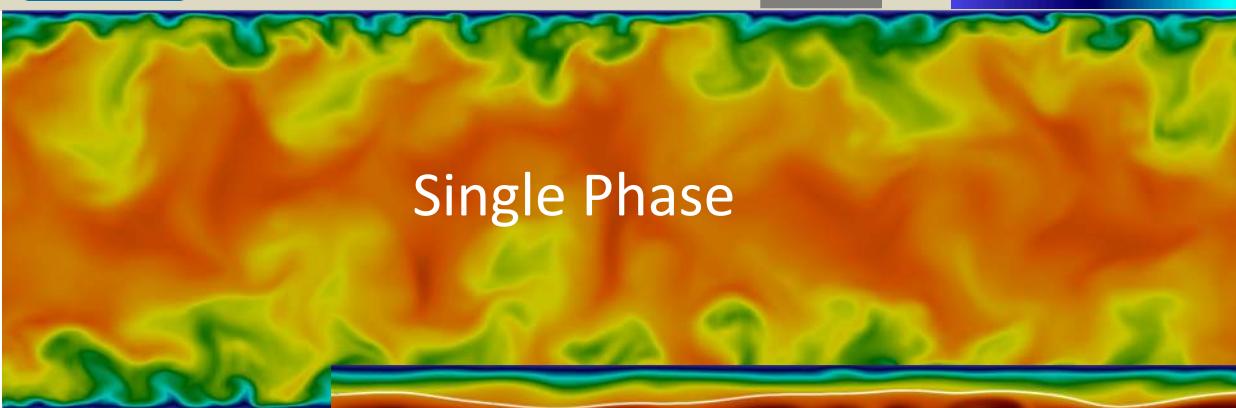
*Numerical Simulations and Scientific Computing II - Fluid dynamics*



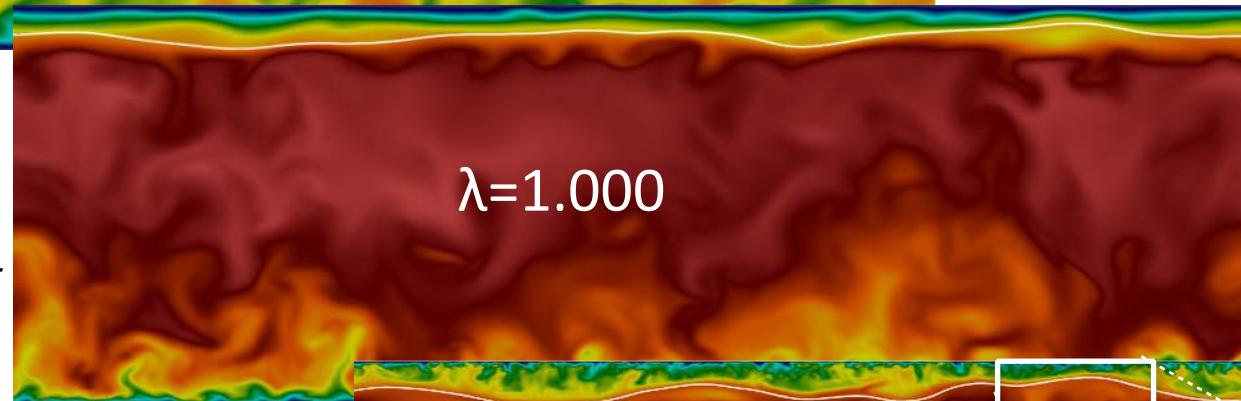
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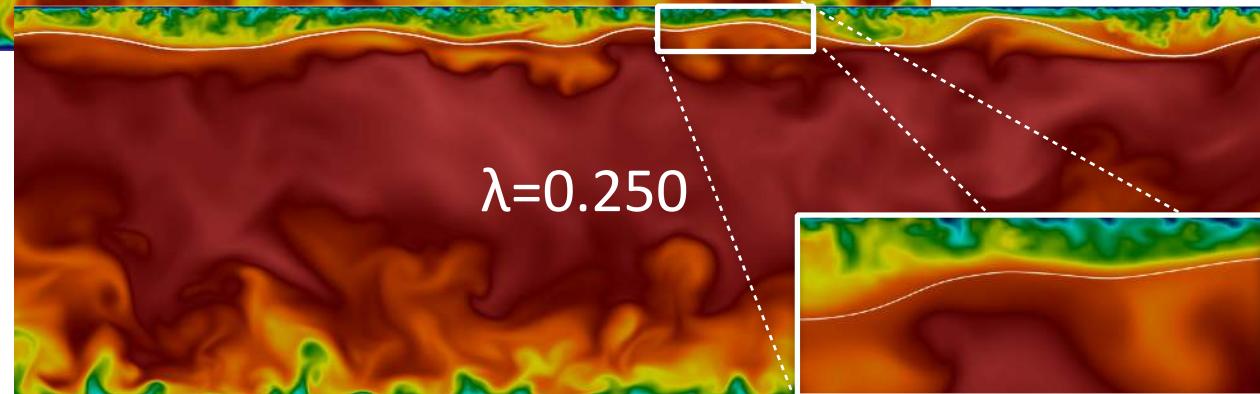
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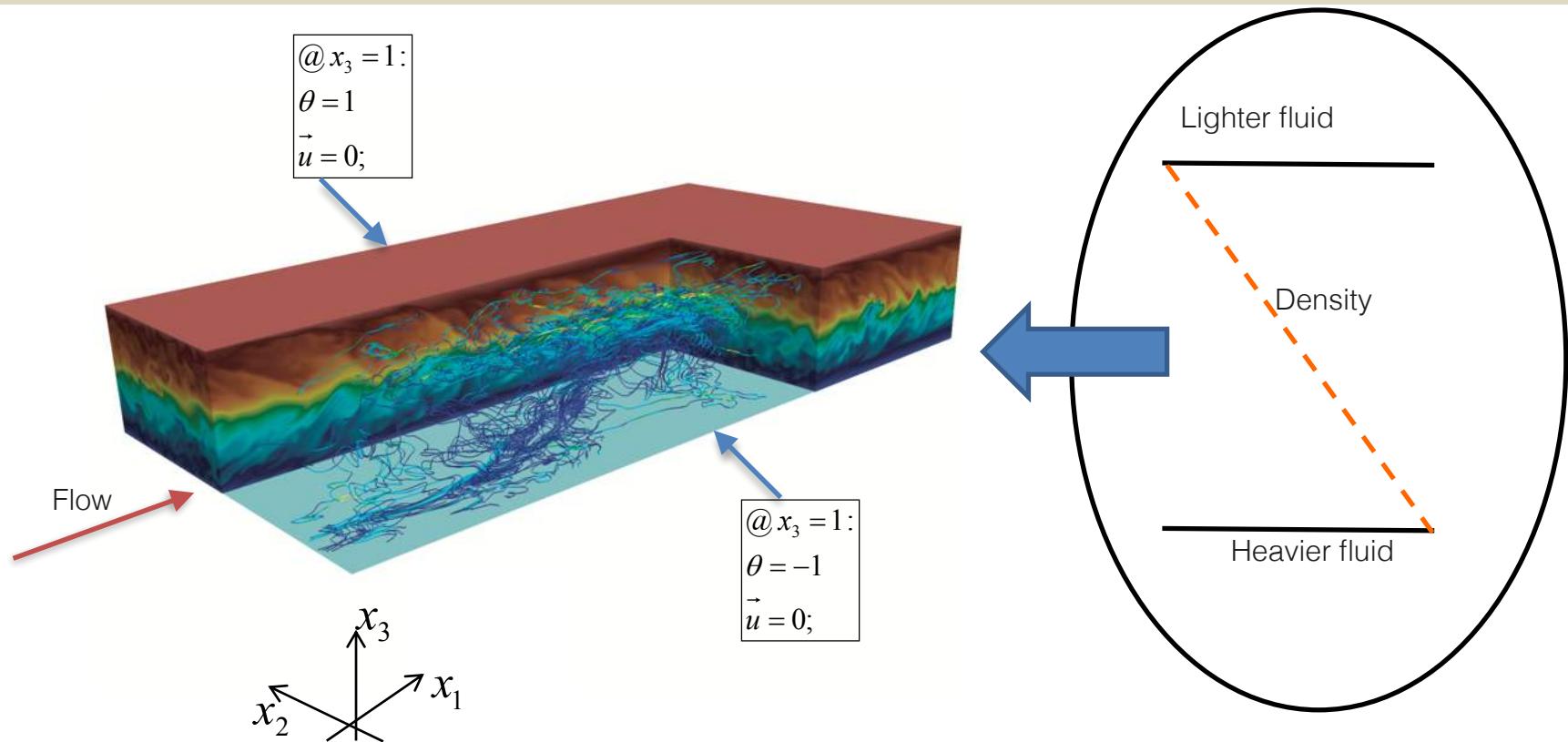
$$Re_{local} \propto \frac{h}{\mu} \downarrow$$

DR driven by  $\sigma$ 

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

DR driven by  $\lambda$ 

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Relevant for:

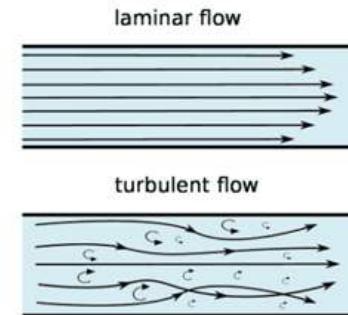
Industrial applications (heat transfer devices), environmental/geophysical applications (atmospheric boundary layer, ocean)

### Main parameters of the flow:

(Shear) **Reynolds number:** inertial/viscous forces

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

$$\frac{\rho u^2 / L}{\mu u / L^2} = \frac{uL}{\nu}$$



**Prandtl number:** momentum diffusivity/thermal diffusivity

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

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

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

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

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

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

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

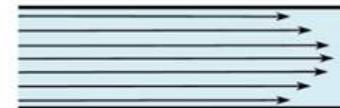
### Main parameters of the flow:

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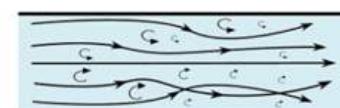
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laminar flow

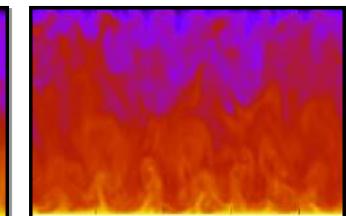
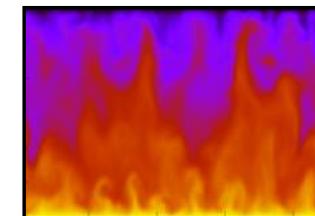


turbulent flow



**Prandtl number:** momentum diffusivity/thermal diffusivity

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



$Pr$  →

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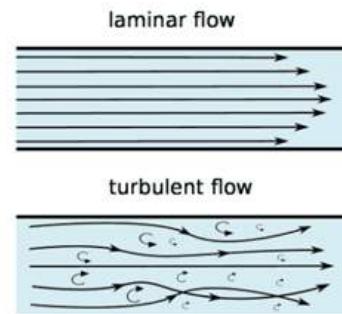
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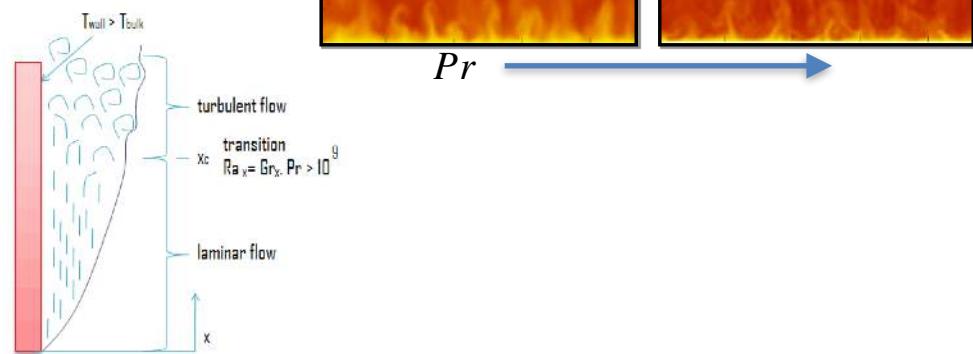
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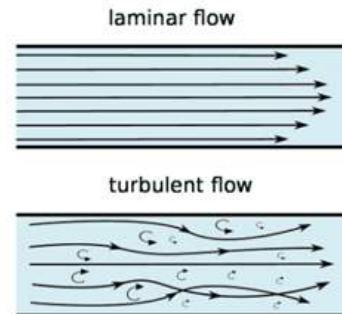


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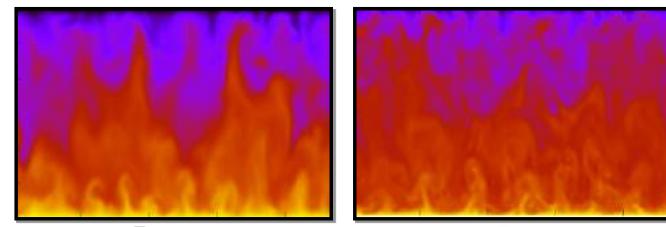
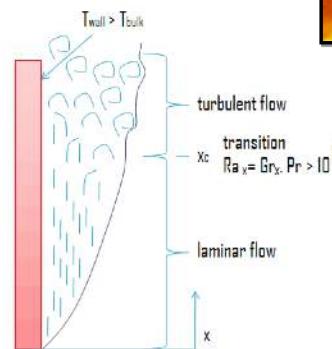
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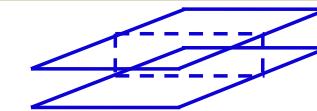
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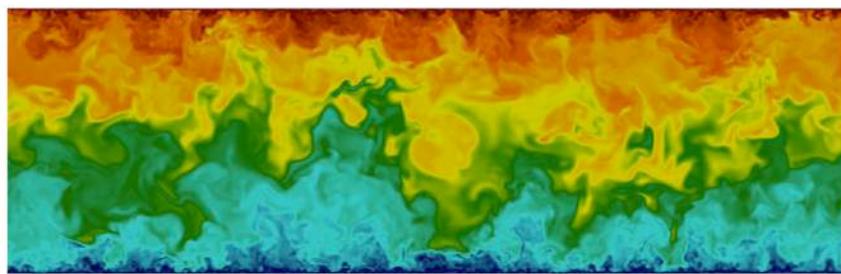
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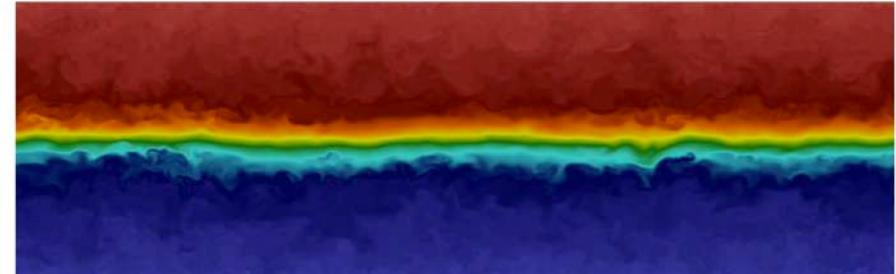
Visualization of temperature on a cross section



$$Ri_\tau = 0$$



$$Ri_\tau = 200$$



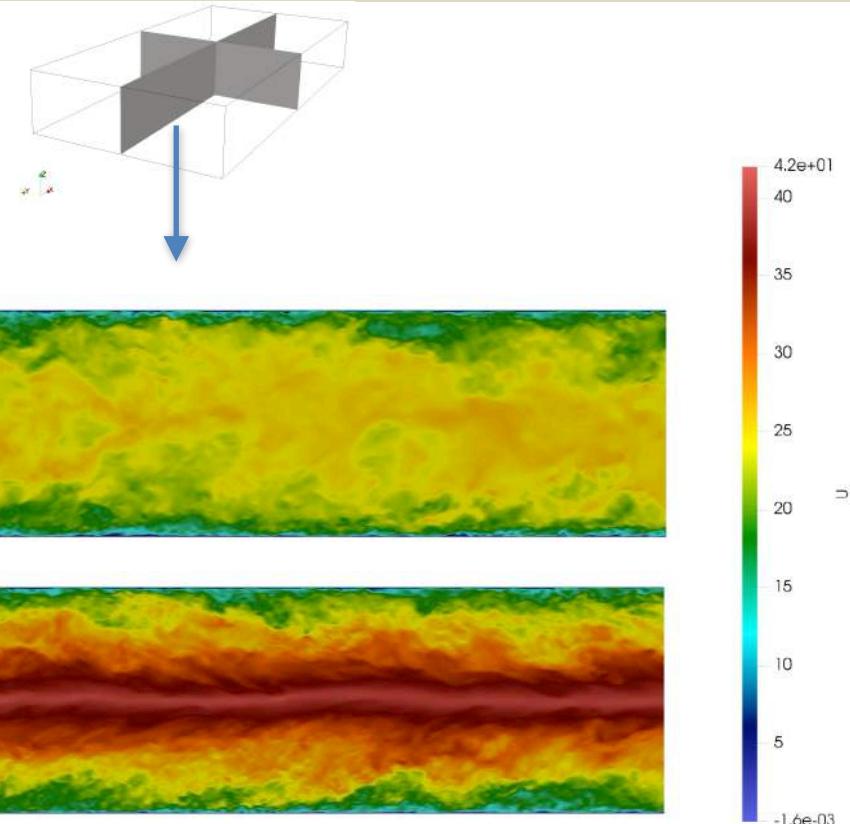
### Neutrally buoyant

- Higher mixing
- Mixing is driven by turbulence structures

### Stably stratified

- Lower mixing
- Internal waves act like barriers

The temperature distribution has a remarkable effect on the velocity field



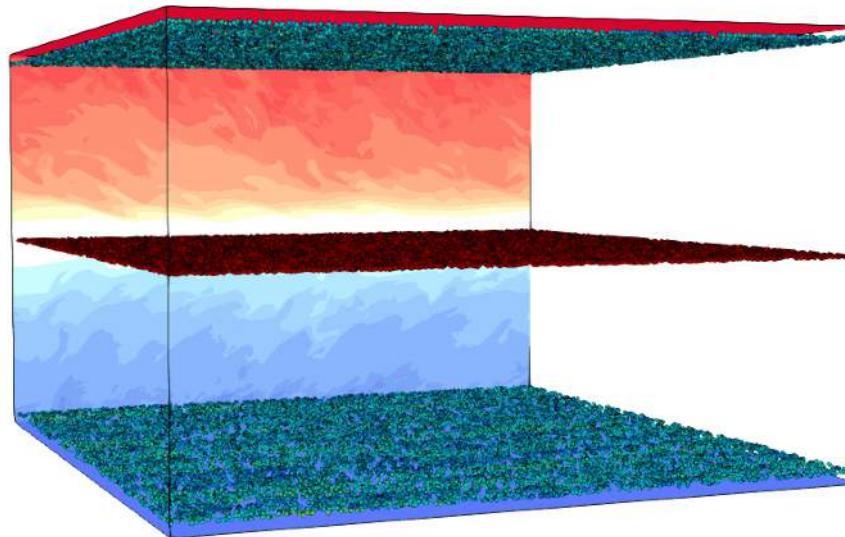
$$Ri_\tau = 0$$

$$Ri_\tau = 200$$

- 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)

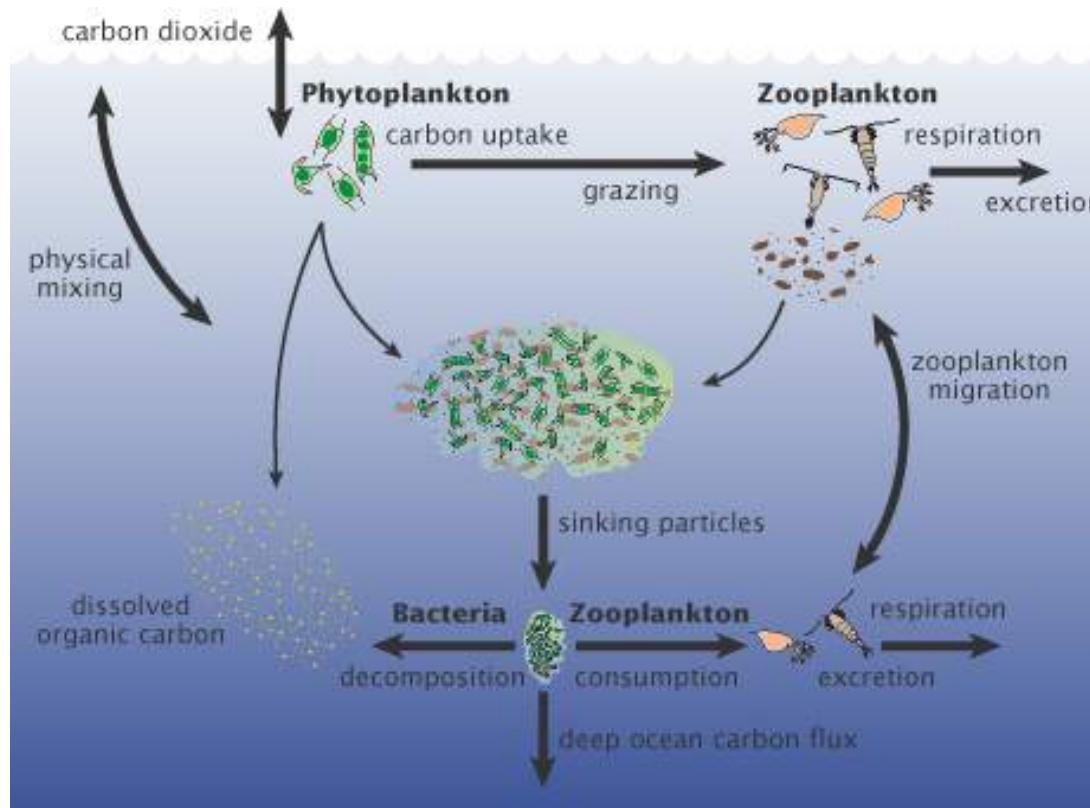


Neutrally-buoyant particles in stratified flow



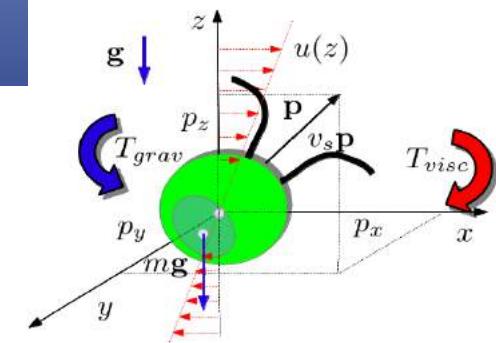
Pollutants are constraint in the proximity of the boundary (in the atmospheric boundary layer)

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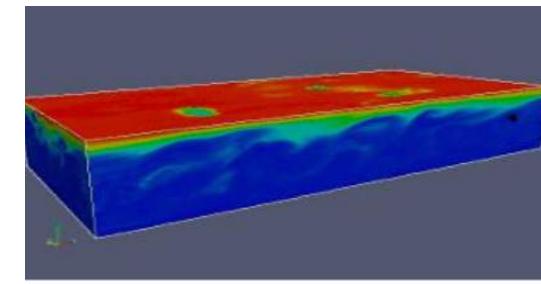
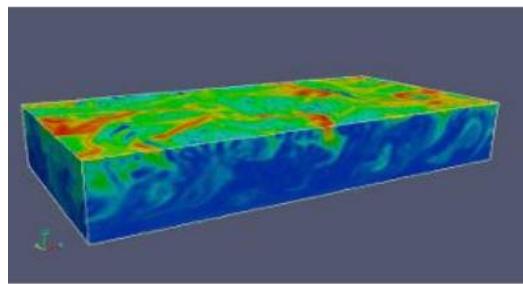
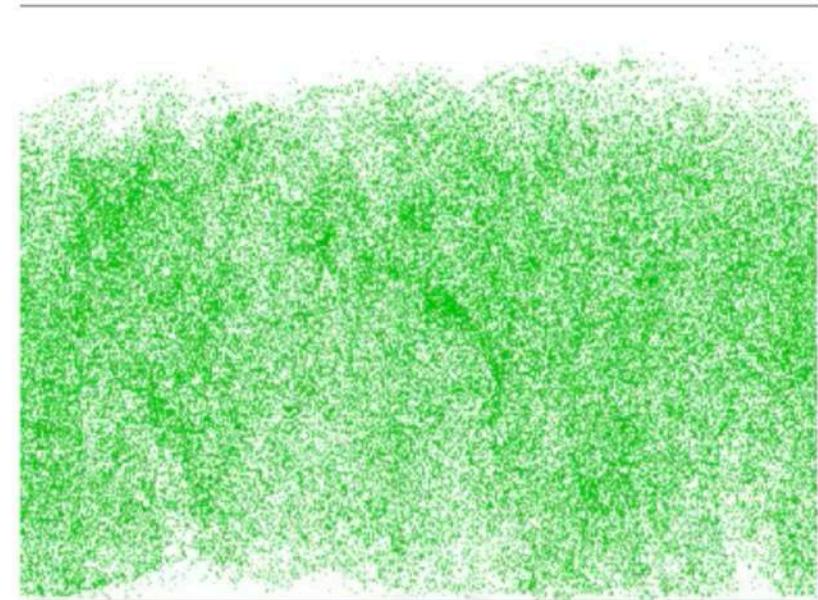
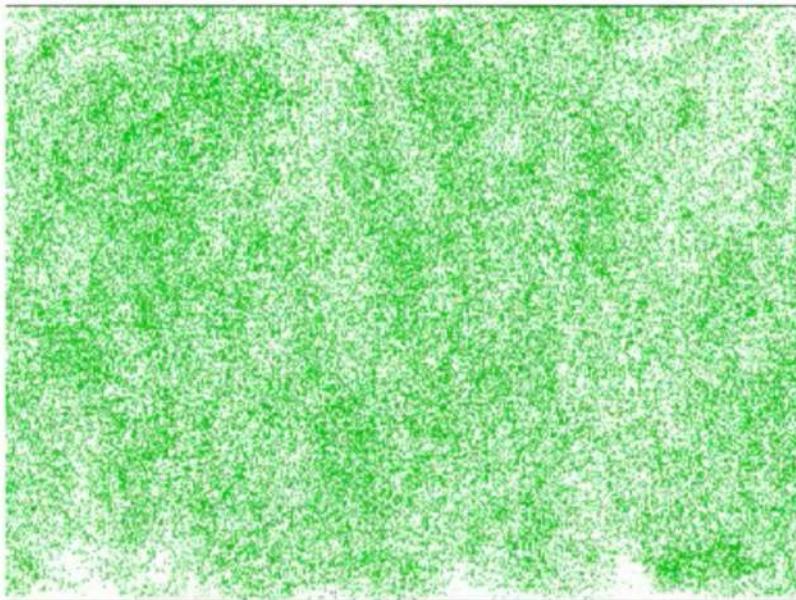


**Phytoplankton** is the photosynthetic part of plankton

- Primary production: organize compounds from CO<sub>2</sub>
- Important part of the global carbon cycle
- Provides 50% of the earth's oxygen
- Sustain the aquatic food web

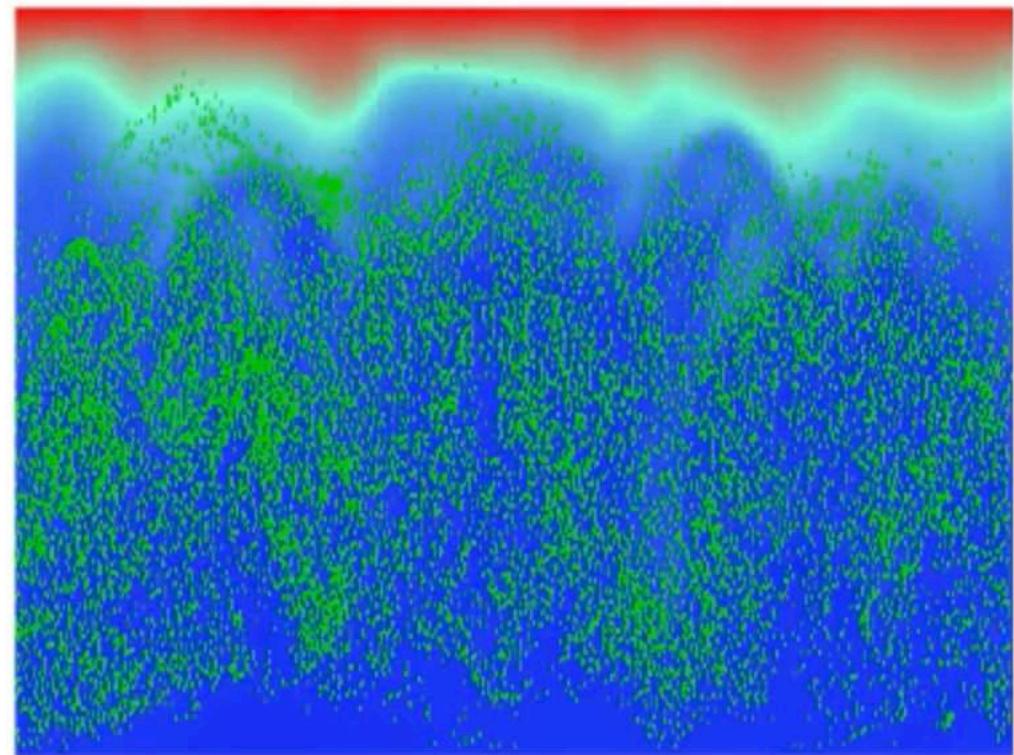
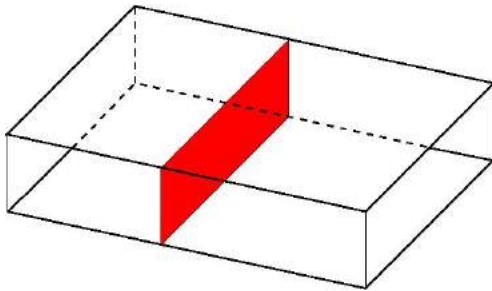


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*Numerical Simulations and Scientific Computing II - Fluid dynamics*



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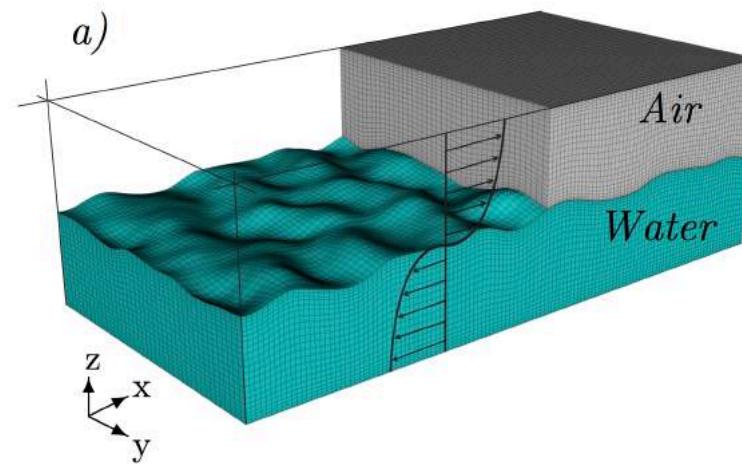
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Transfer rates (for example of CO<sub>2</sub>) across an interface depends strongly on the extension of the interface...

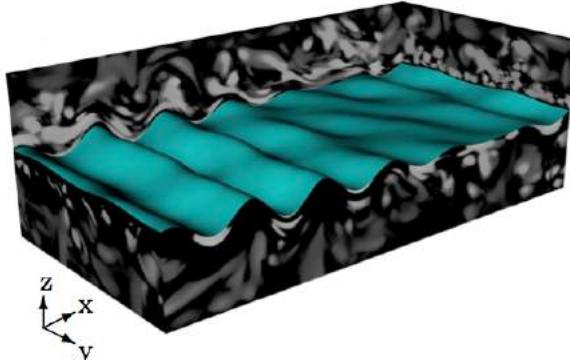


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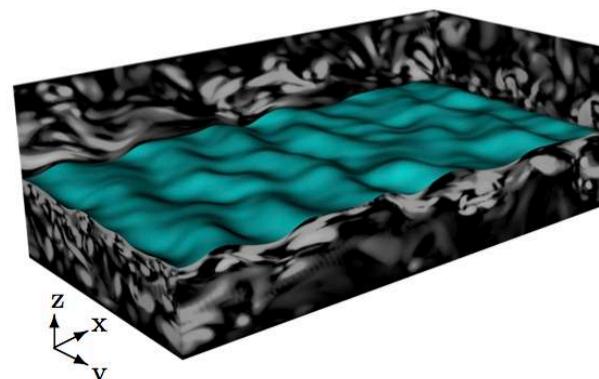


Gravity ↑

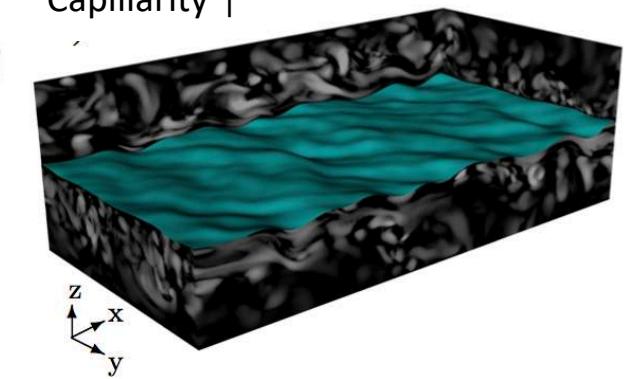


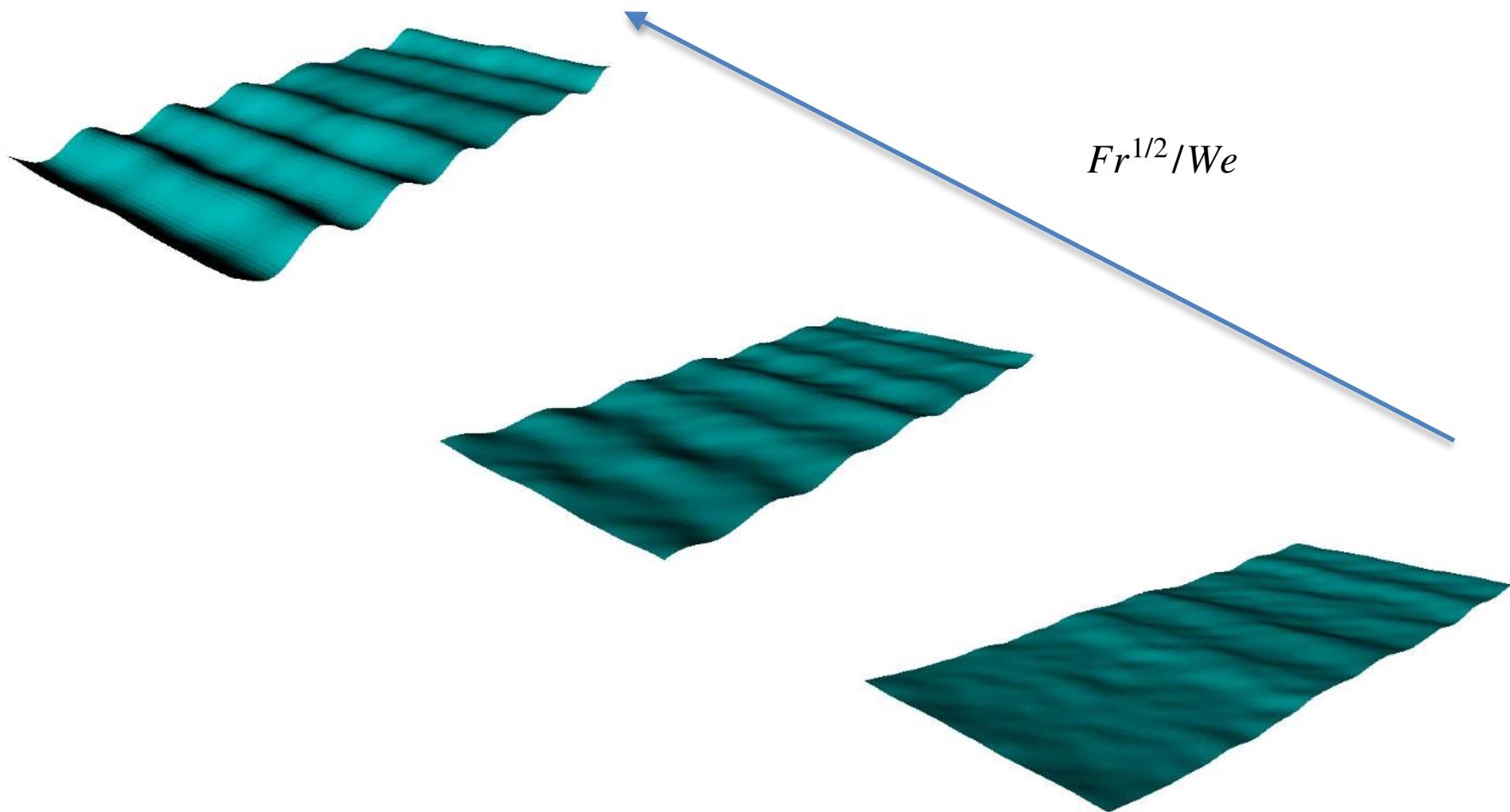
Quasy-sinusoidal wavy interface

Capillarity ↑

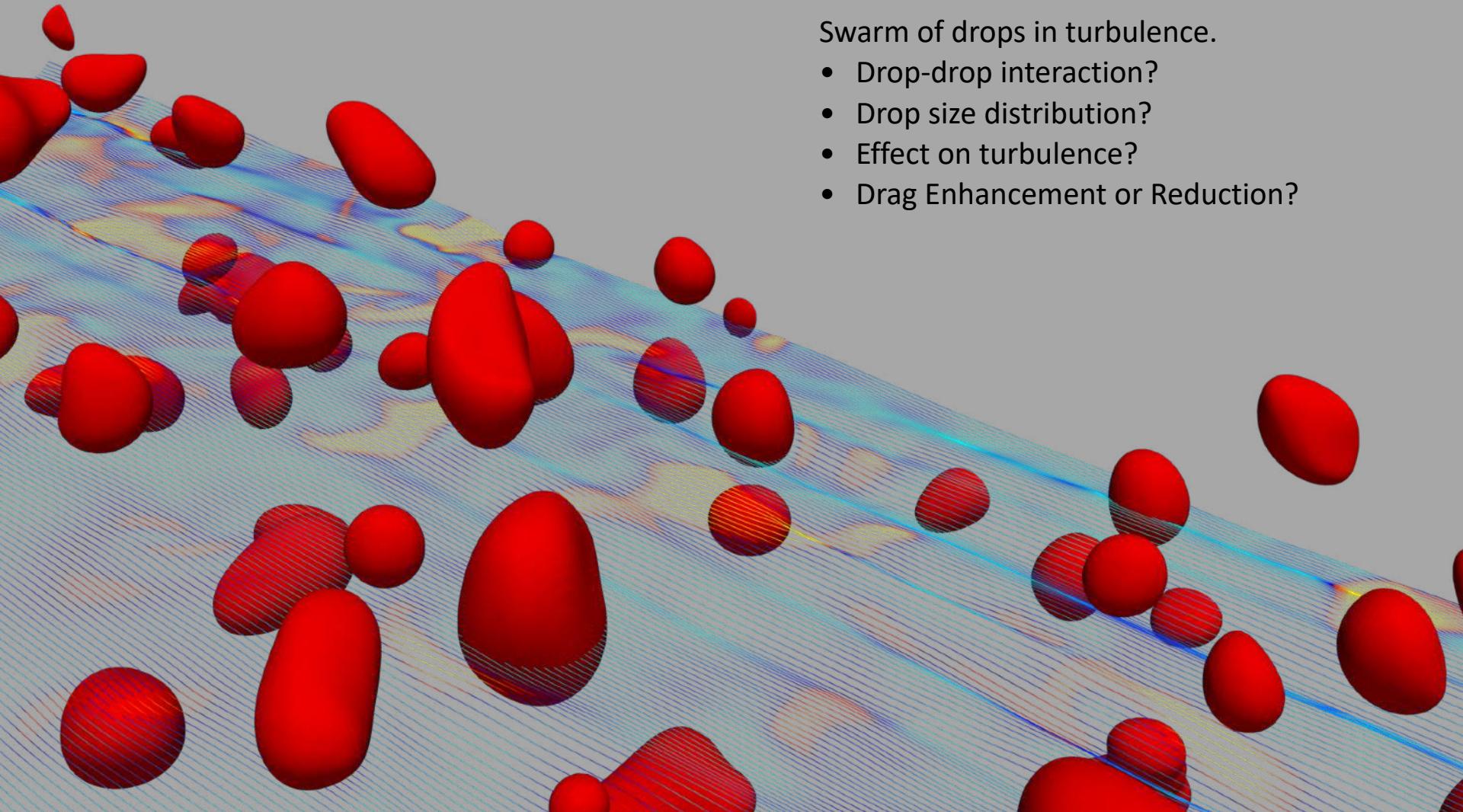


Surface roughness





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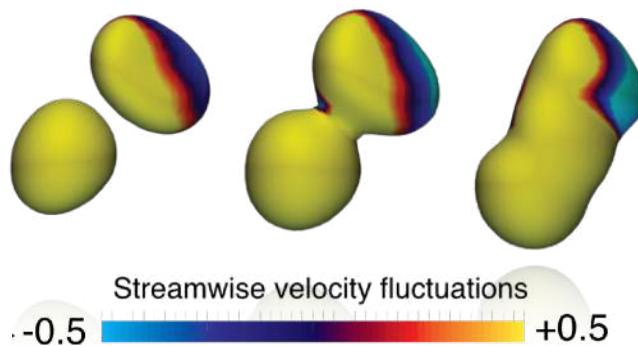


Swarm of drops in turbulence.

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

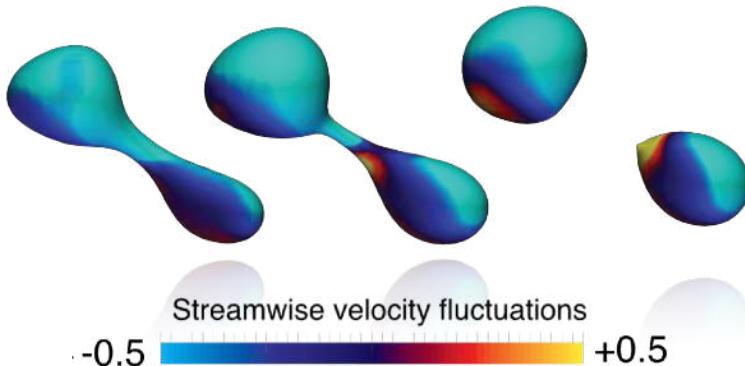
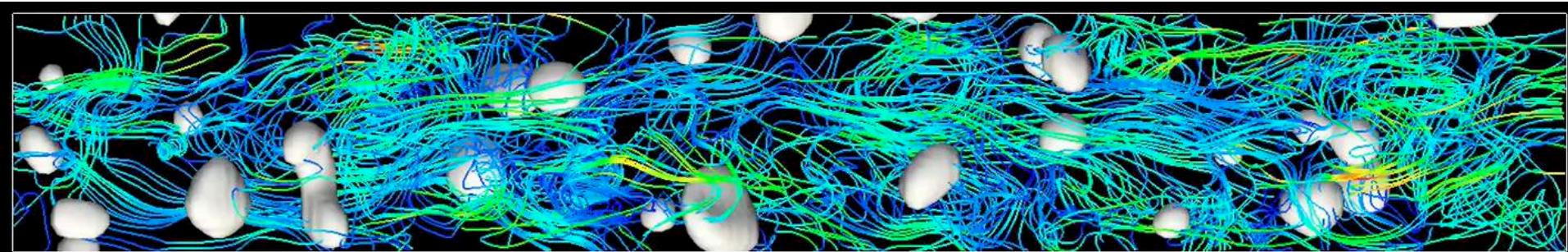
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## COALESCENCE

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.



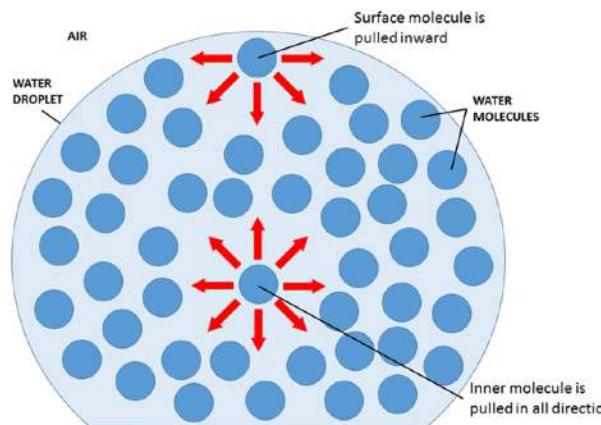
## BREAK-UP

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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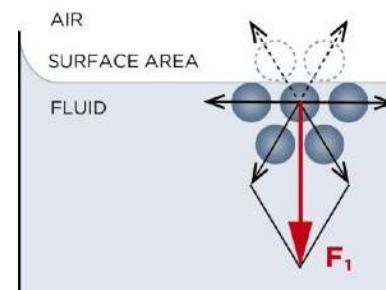
### Surface Tension:

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

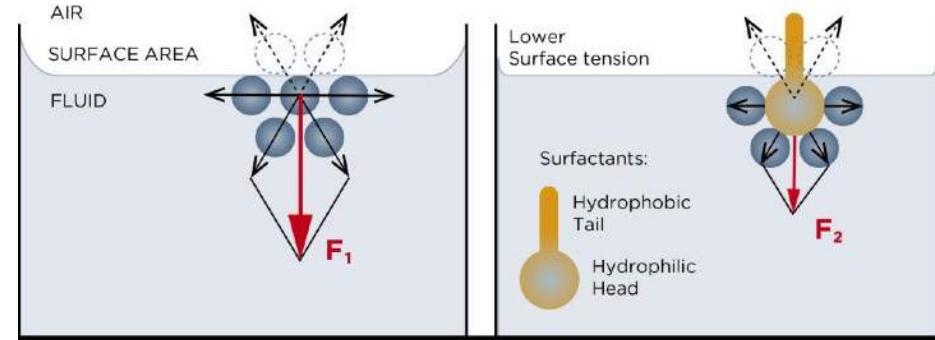


### Addition of a surfactant:

#### Clean system



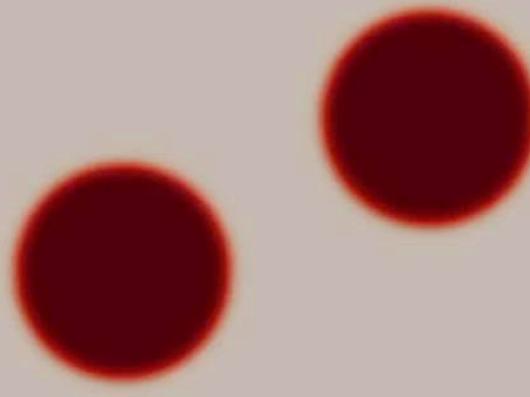
#### Surfactant-laden system



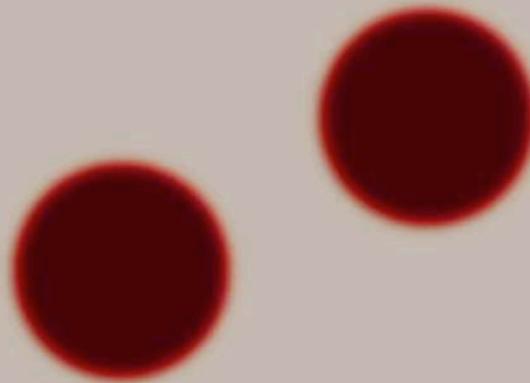
Presence of surfactant decreases the surface tension and as a consequence:

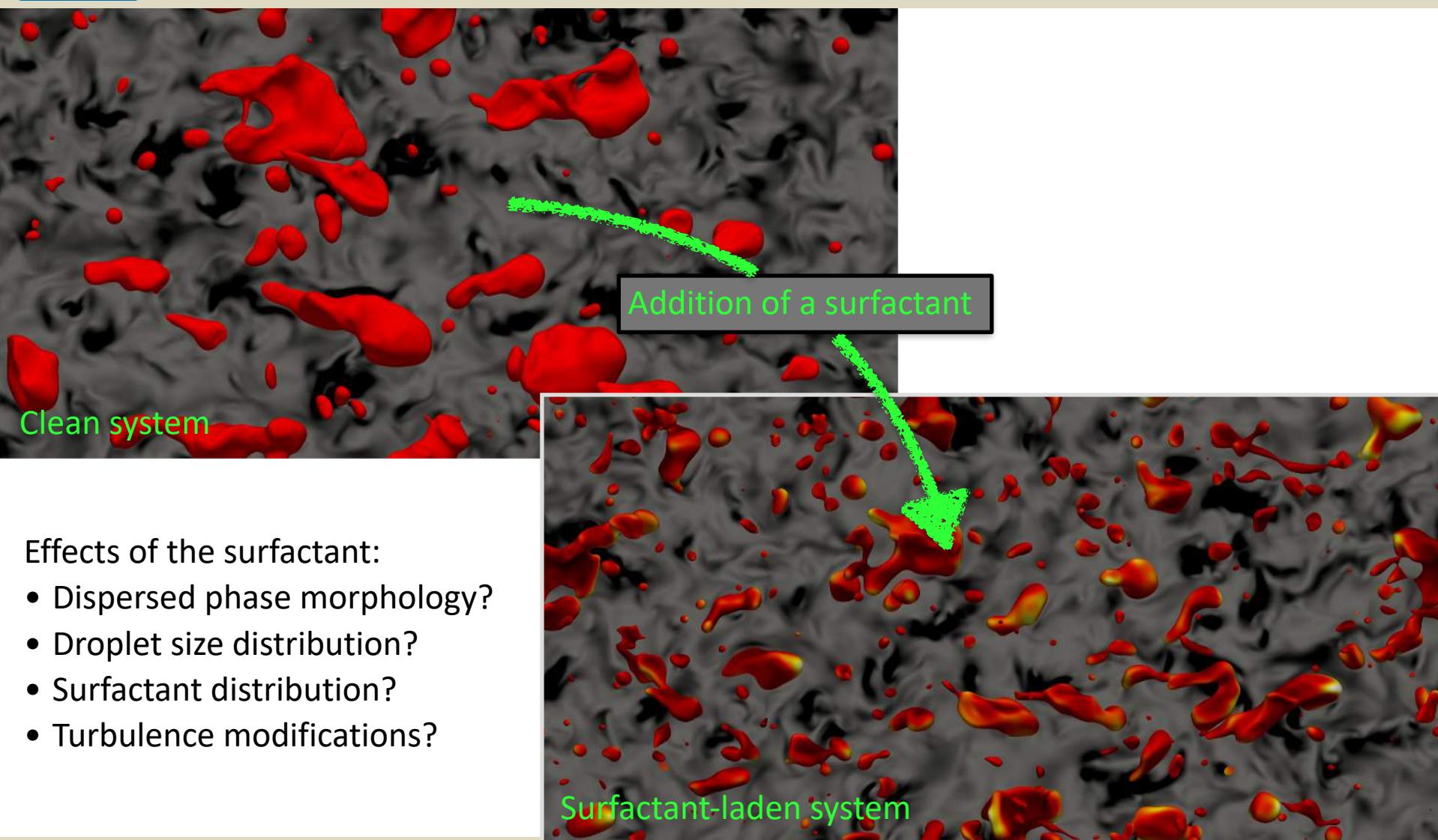
- Droplets become more deformable (less surface tension).
- When non-uniform can give rise to tangential forces (Marangoni).

Clean droplets (no surfactant):



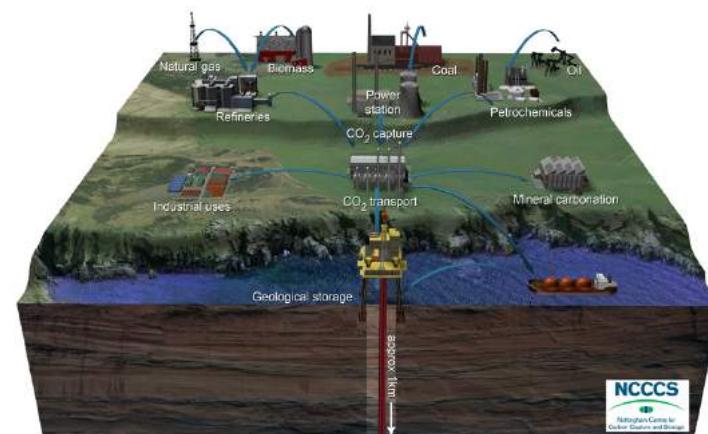
Surfactant-laden droplets:



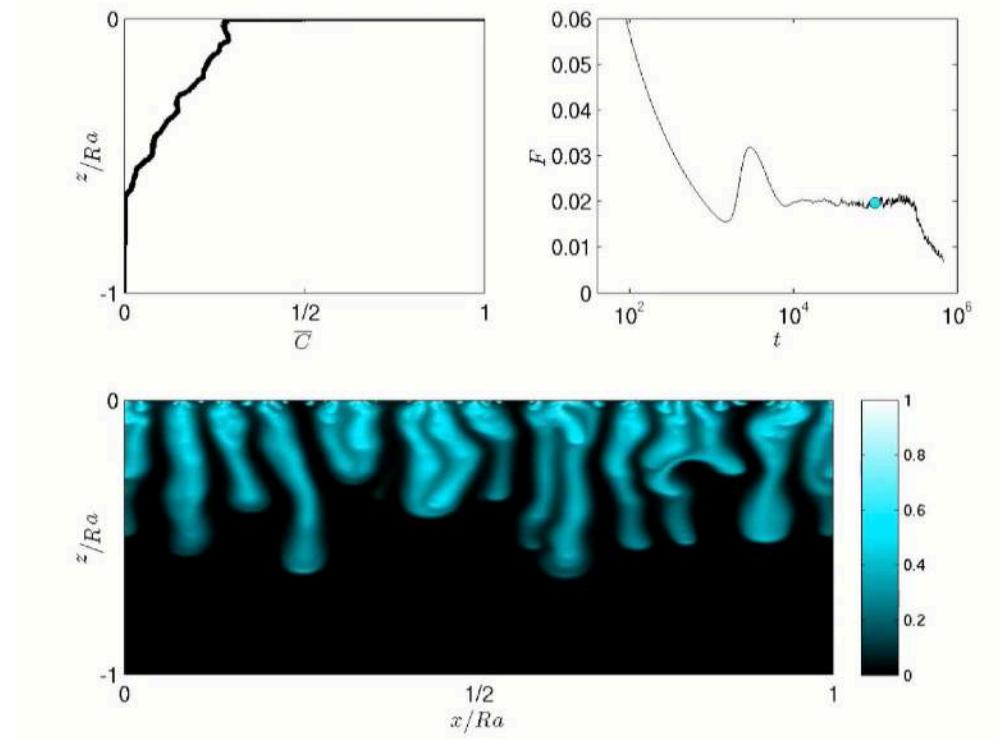


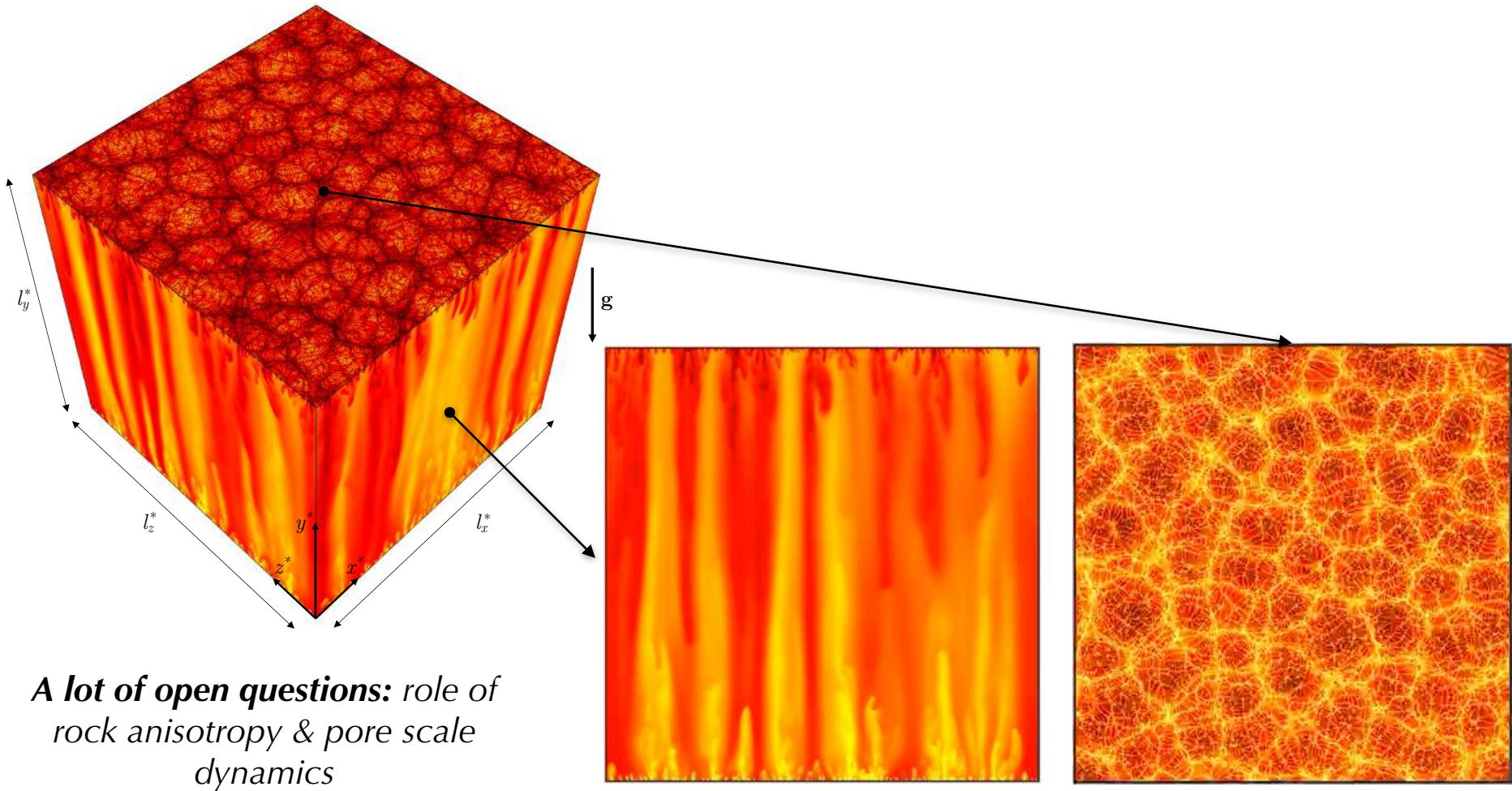
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### *Geological CO<sub>2</sub> sequestration*





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

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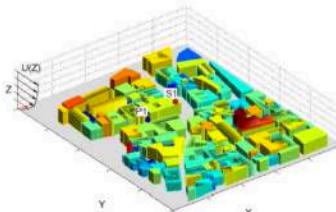
After this survey on applications, we are now ready to start with an in-depth analysis of transport process and equations...

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

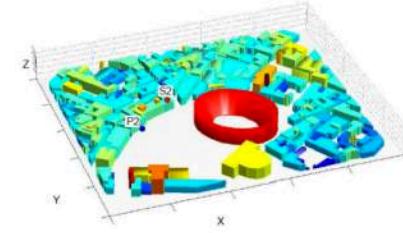
Verona Arena



(a)



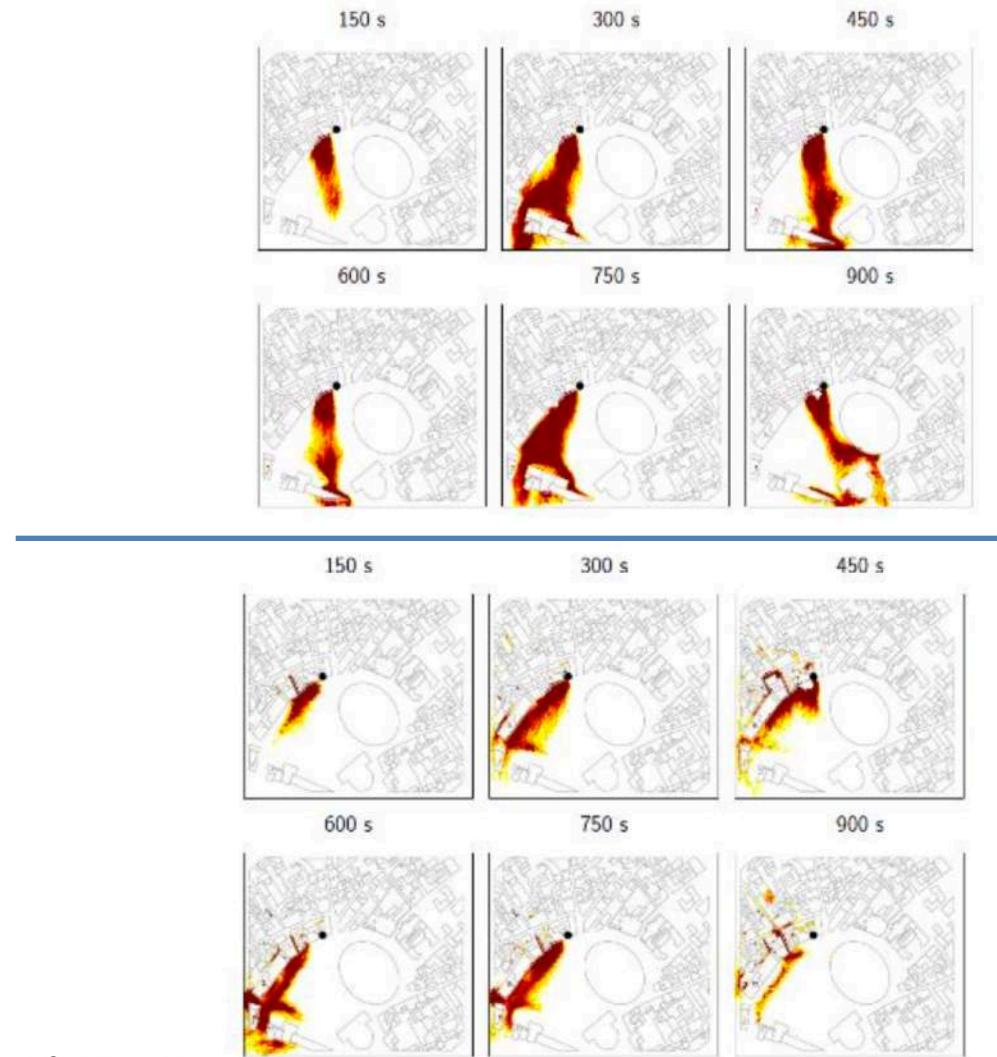
(b)



(c)

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

We take it as reference!



Francesco Zonta

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 adverted by the flow. This gives:

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

ADE=Advection  
Diffusion Equation

Rate of change      Advection      Diffusion

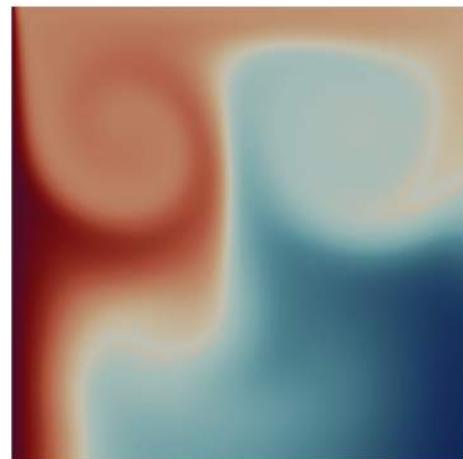
The diagram shows the Advection-Diffusion Equation enclosed in a blue rectangular box. Three blue arrows point from the text labels 'Rate of change', 'Advection', and 'Diffusion' to the corresponding terms in the equation:  $\frac{\partial C_i}{\partial t}$ ,  $u_j \frac{\partial C_i}{\partial x_j}$ , and  $D \frac{\partial^2 C_i}{\partial x_j^2}$  respectively.

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

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

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

We have 1st  
and 2nd derivatives!

In dimensionless form:

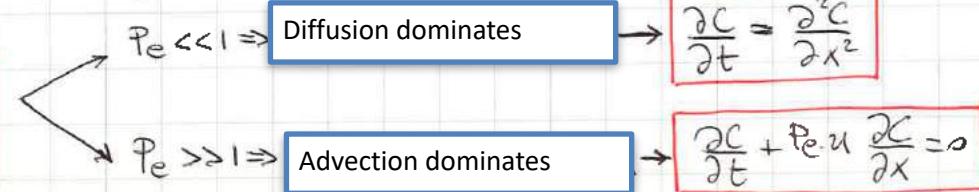
$$\left\{ \begin{array}{l} C = \frac{C^*}{C_w} \\ x = \frac{x^*}{L} \\ u = \frac{u^*}{u_{ref}} \\ t = \frac{t^* D}{L^2} \end{array} \right. \rightarrow \frac{DC_w}{L^2} \frac{\partial C}{\partial t} + \frac{u_{ref} u C_w}{L} \frac{\partial C}{\partial x} = \frac{DC_w}{L^2} \frac{\partial^2 C}{\partial x^2}$$

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

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

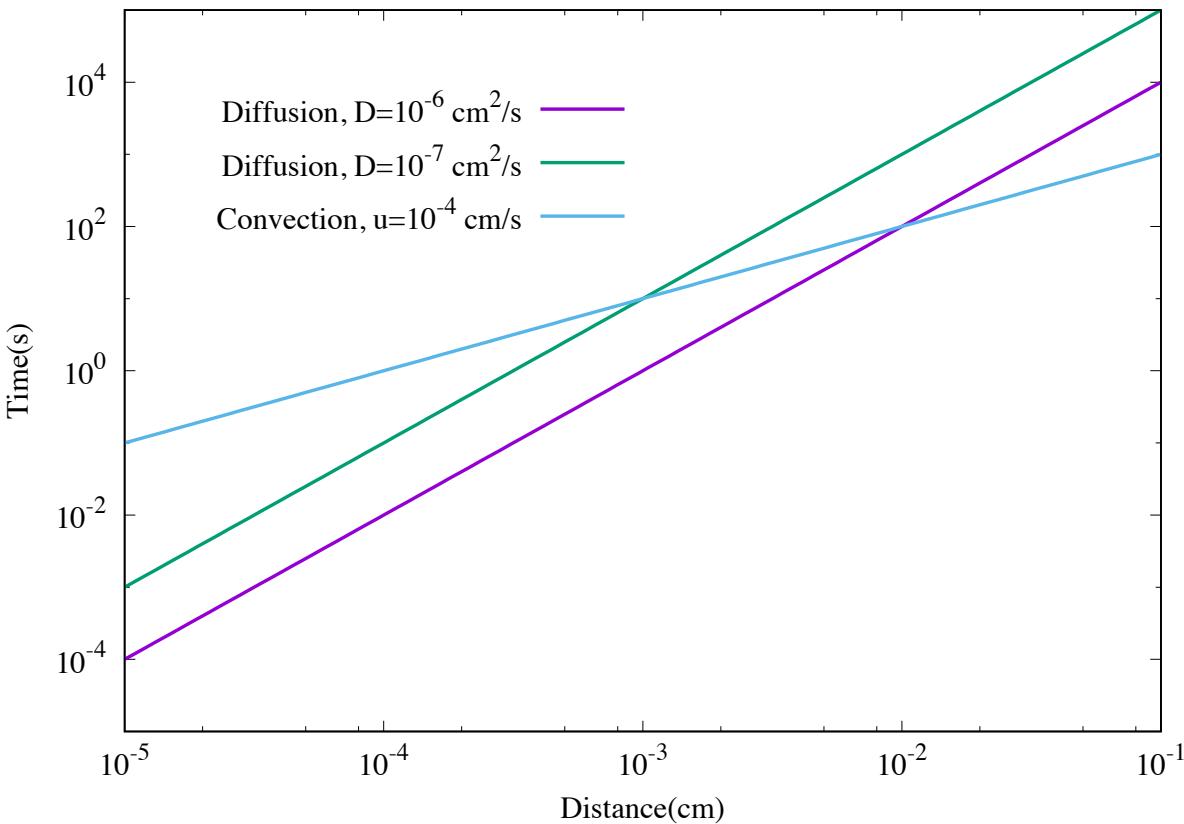
$$Pe = \frac{\text{diffusion time}}{\text{convection time}} = \frac{L^2 / D}{L / u_{ref}} = \frac{L \cdot u_{ref}}{D}$$

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



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

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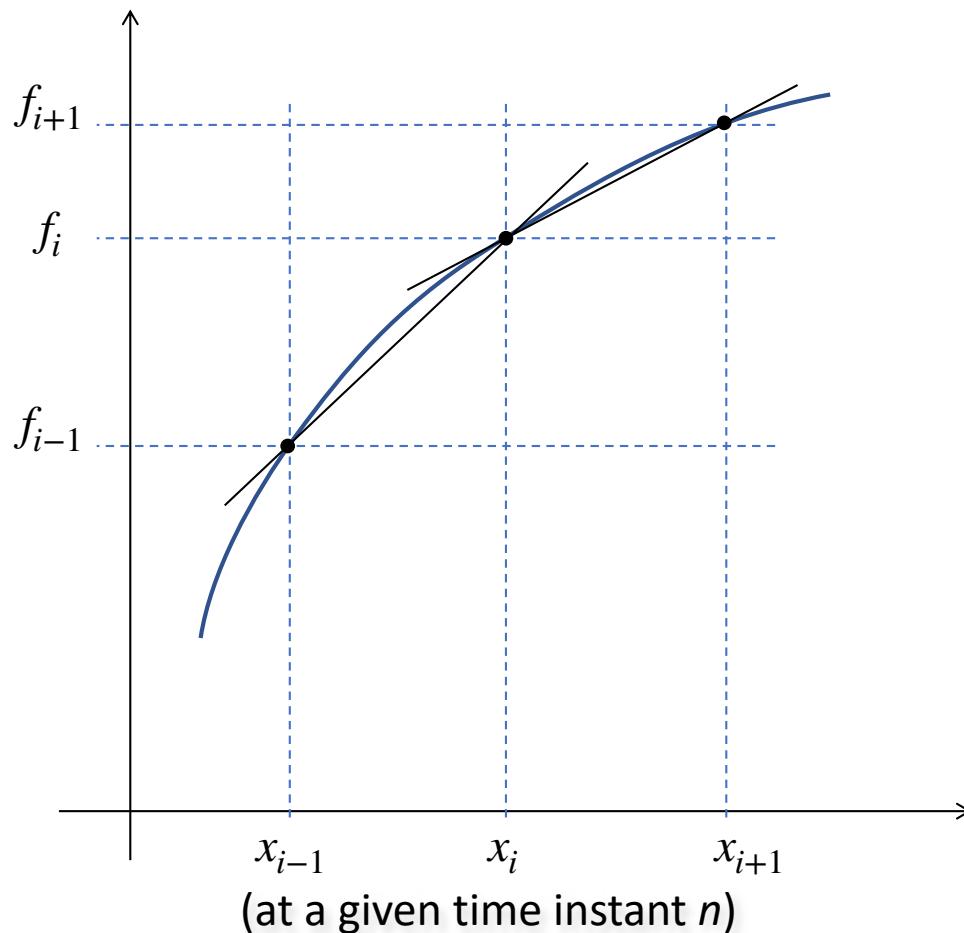


$$T_{diff} = \frac{L^2}{D}$$

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

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

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



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...

## Taylor series

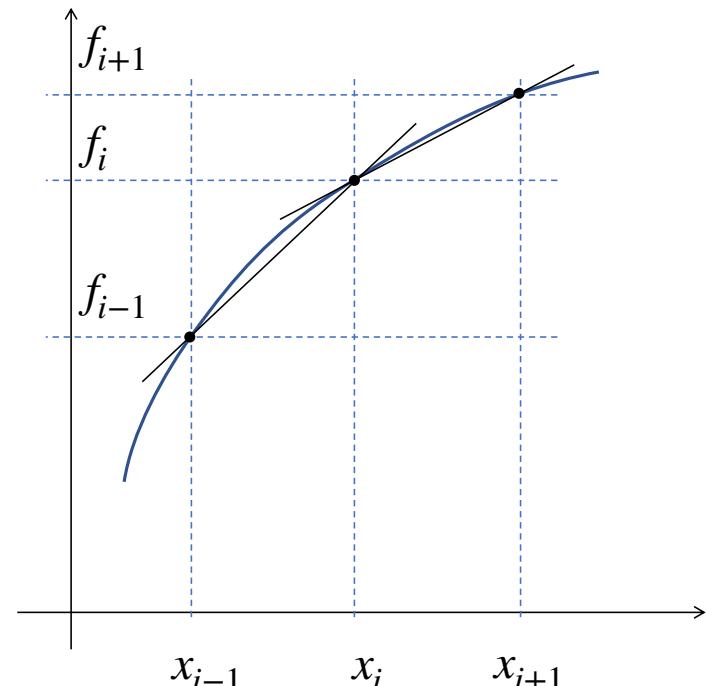
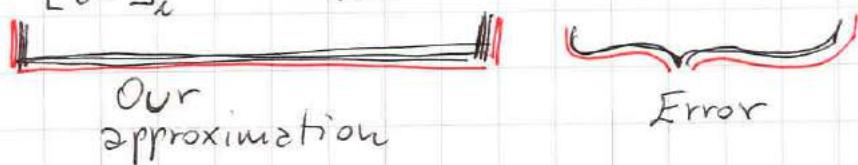
$$f_{i+1}^n = f_i^n + \Delta x \left[ \frac{\partial f}{\partial x} \right]_i^n + \frac{\Delta x^2}{2} \left[ \frac{\partial^2 f}{\partial x^2} \right]_i^n + \underbrace{O(\Delta x^3)}_{\text{HOT}}$$

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

It is straightforward to show that

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

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



**Forward/Backward  
discretization=1st order!!**

“Manipulation” of Taylor series. In a more systematic way...

We wish to approximate the derivatives as follows

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

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

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

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

This finally gives

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

$$+ b f_i^h + c \left[ f_i^h + \Delta x \left[ \frac{\partial f}{\partial x} \right]_i^h + \frac{\Delta x^2}{2} \left[ \frac{\partial^2 f}{\partial x^2} \right]_i^h + \frac{\Delta x^3}{3!} \left[ \frac{\partial^3 f}{\partial x^3} \right]_i^h + O(\Delta x^4) \right] \xrightarrow{f_i}$$

$$\xleftarrow{f_{i+1}}$$

After some algebra

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

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

Therefore

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

↓  
2nd order accurate  
formulation

**Central discretization in  
space (CS)**

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  $x_{i+1}$

$$\begin{aligned} \left[ \frac{\partial^2 f}{\partial x^2} \right]_i^n &= a \left( f_i^n - \Delta x \left[ \frac{\partial f}{\partial x} \right]_i^n + \frac{\Delta x^2}{2} \left[ \frac{\partial^2 f}{\partial x^2} \right]_i^n - \frac{\Delta x^3}{3!} \left[ \frac{\partial^3 f}{\partial x^3} \right]_i^n + \text{HOT} \right) + \\ &\quad + b f_i^n \\ &\quad + c \left( f_i^n + \Delta x \left[ \frac{\partial f}{\partial x} \right]_i^n + \frac{\Delta x^2}{2} \left[ \frac{\partial^2 f}{\partial x^2} \right]_i^n + \frac{\Delta x^3}{3!} \left[ \frac{\partial^3 f}{\partial x^3} \right]_i^n + \text{HOT} \right) \end{aligned}$$

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

$\downarrow$                      $\downarrow$                      $\downarrow$   
 $a+b+c=0$              $\Delta x (c-a)=0$              $(a+c) \frac{\Delta x^2}{2}=1$

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

Therefore, we get

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

↓  
2nd order accurate

To summarize

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

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

## Central discretization in space (CS)

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

## Diffusion and advection

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

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

In dimensionless form:

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

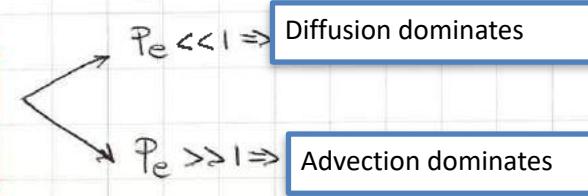
$$\frac{DC_w}{L^2} \frac{\partial C}{\partial t} + \frac{u_{ref} u C_w}{L} \frac{\partial C}{\partial x} = \frac{DC_w}{L^2} \frac{\partial^2 C}{\partial x^2}$$

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

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

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

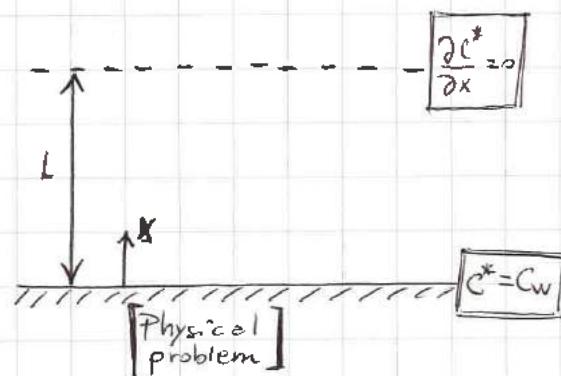
$$\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}$$



$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}$$



We focus first on diffusion:



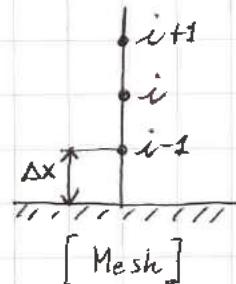
The governing equation is:

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}$$

Note: An analytical solution exists

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

Now we want to solve the problem numerically



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

$$\text{Discretization in time} \Rightarrow \left[ \frac{\partial C}{\partial t} \right]_i^s = \frac{C_i^{n+1} - C_i^n}{\Delta t}$$

$n = \text{known}$

$n+1 = \text{unknown}$

Therefore :

$$C_i^{n+1} = C_i^n + \frac{\Delta t}{\Delta x^2} (C_{i-1}^n - 2C_i^n + C_{i+1}^n) \quad [\text{Explicit method}]$$

## Explicit method, Numerical results

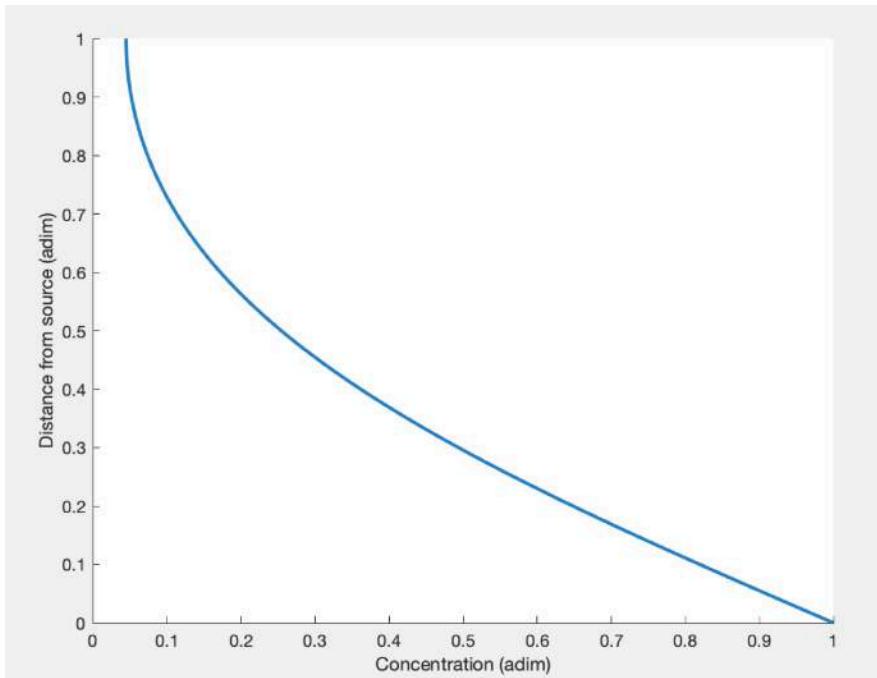
$$\Delta x = 4 \cdot 10^{-3}; \Delta t = 8 \cdot 10^{-6}; s = \frac{\Delta t}{\Delta x^2} = 0.5$$

(\*Note that: L=1)

$$\frac{\partial C}{\partial x} = 0$$



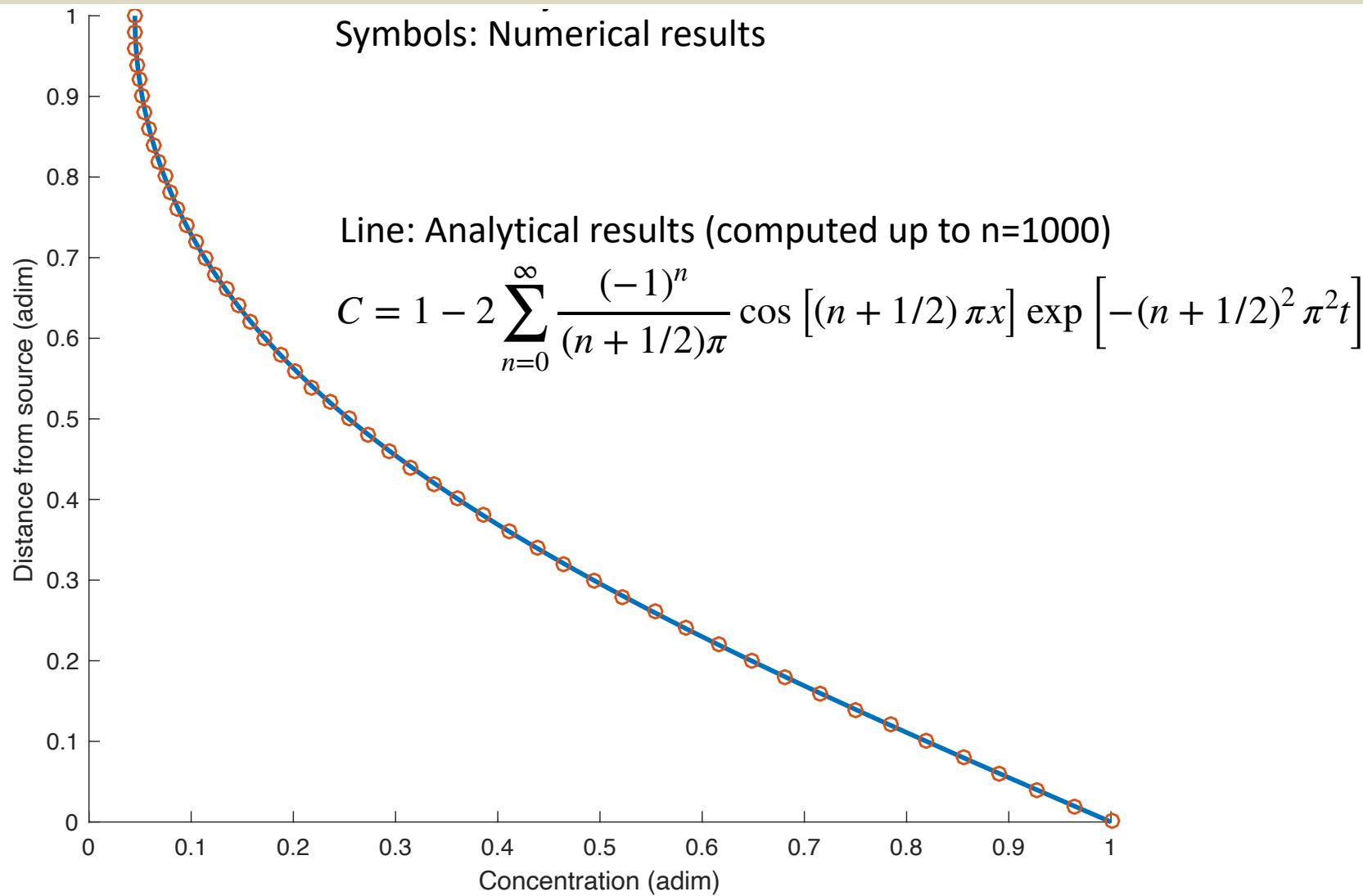
$$C = 1$$



Are these results good?

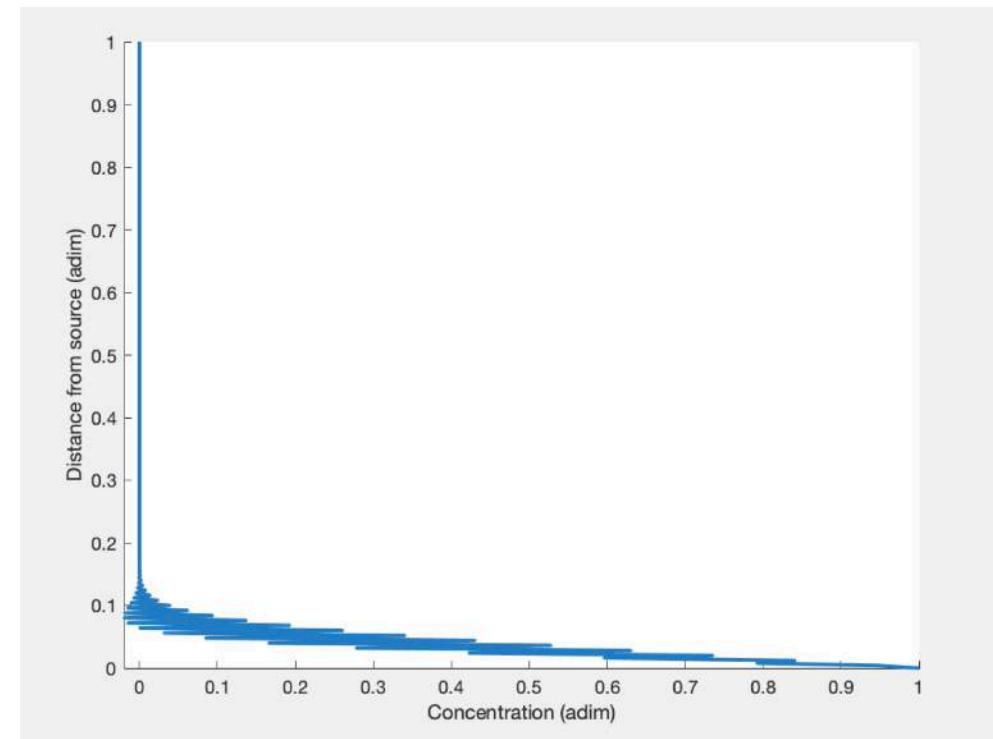
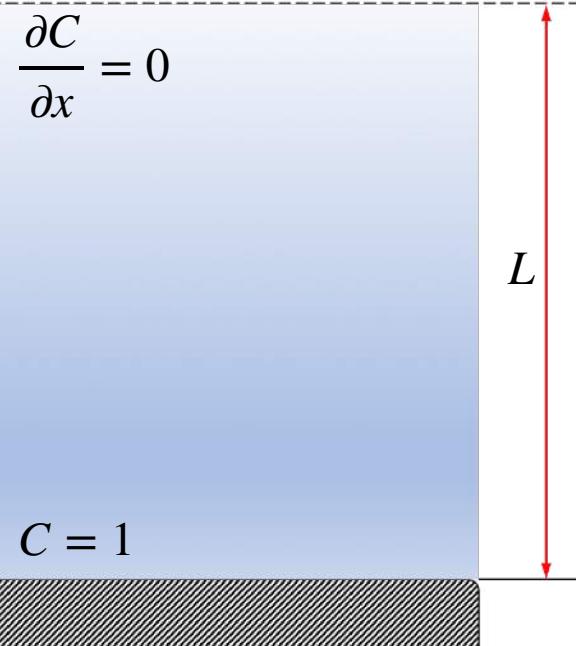
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## Explicit method: numerical vs analytical results

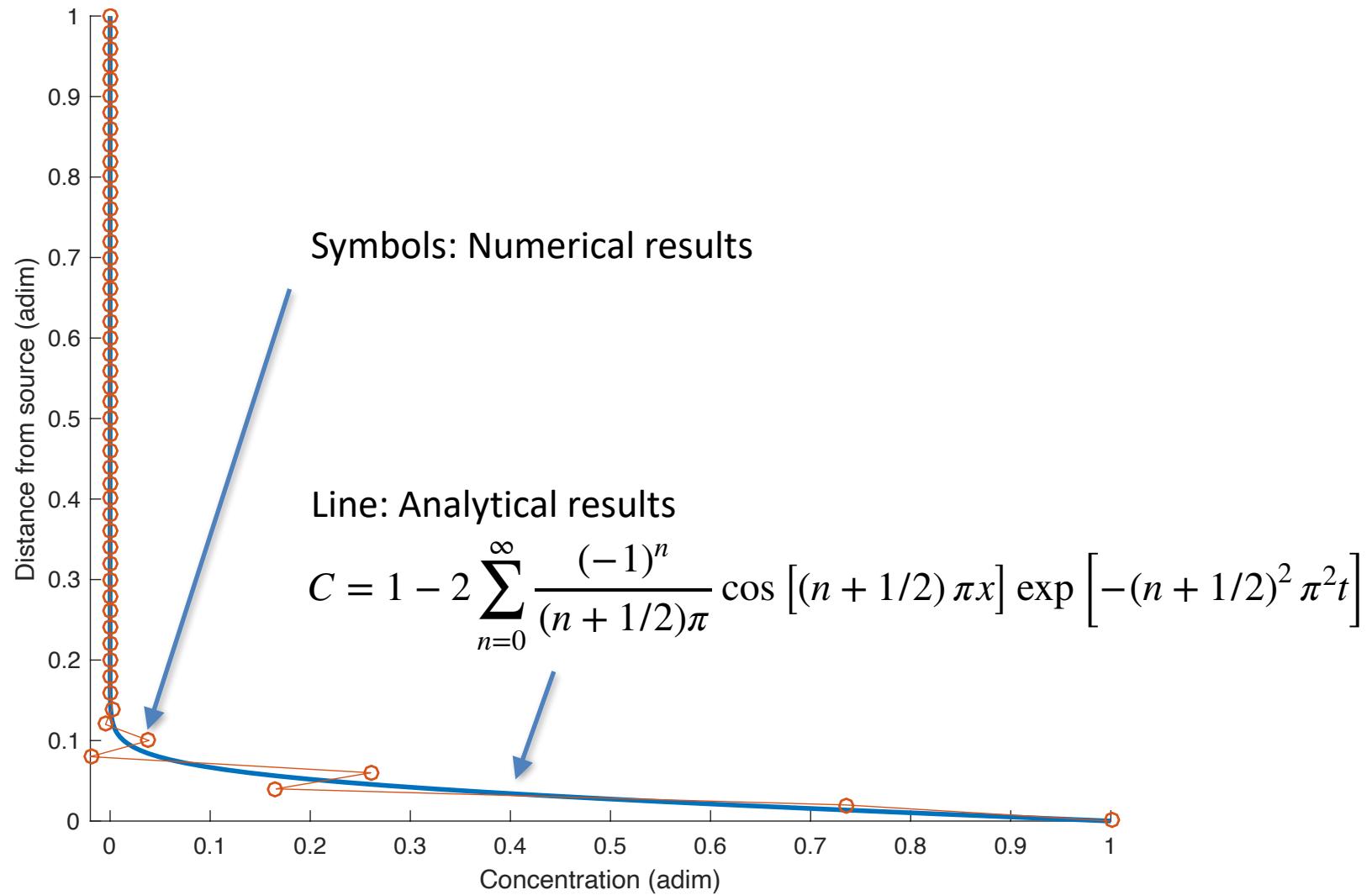


## Explicit method: numerical results-2

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



## Explicit method: numerical vs analytical results-2



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

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

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

Otherwise, it is unstable.

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

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

$$\left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n = \frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1}}{\Delta x^2} \quad [\text{Evaluated at the new time step } "n+1"]$$

$$-SC_{i-1}^{n+1} + (1+2S)C_i^{n+1} - SC_{i+1}^{n+1} = C_i^n$$

But now we have a linear system of equations

Unknowns

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

$$\begin{pmatrix} 1+2\varsigma & -\varsigma & & \\ -\varsigma & 1+2\varsigma & -\varsigma & \\ & -\varsigma & 1+2\varsigma & -\varsigma \\ & & -\varsigma & 1+2\varsigma \end{pmatrix} \begin{pmatrix} C_1^{n+1} \\ C_2^{n+1} \\ \vdots \\ C_m^{n+1} \end{pmatrix} = \begin{pmatrix} C_1^n \\ C_2^n \\ \vdots \\ C_m^n \end{pmatrix}$$

Tridiagonal  
Matrix

Thomas algorithm \*

Code

If we now run the simulations...

```
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
```

Thomas algorithm

$$\begin{bmatrix} \alpha_1 & c_1 & 0 & 0 \\ b_2 & \alpha_2 & c_2 & 0 \\ 0 & b_3 & \alpha_3 & c_3 \\ 0 & 0 & b_4 & \alpha_4 \end{bmatrix} = \begin{bmatrix} \alpha_1 & 0 & 0 & 0 \\ \beta_2 & \alpha_2 & 0 & 0 \\ 0 & \beta_3 & \alpha_3 & 0 \\ 0 & 0 & \beta_4 & \alpha_4 \end{bmatrix} \begin{bmatrix} 1 & r_1 & 0 & 0 \\ 0 & 1 & r_2 & 0 \\ 0 & 0 & 1 & r_3 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$A = L U$$

Suppose we want to solve:  $A \cdot C = R$

$$\begin{array}{c} A \cdot C = R \\ \uparrow \\ A = L \cdot U \end{array} \rightarrow L U \cdot C = R \xrightarrow{\text{Decomposed}} \begin{cases} L \cdot y = R \\ U \cdot C = y \end{cases}$$

Problem A      Problem B

Problem A

$$\begin{pmatrix} \alpha_1 & 0 & 0 & 0 \\ \beta_2 & \alpha_2 & 0 & 0 \\ 0 & \beta_3 & \alpha_3 & 0 \\ 0 & 0 & \beta_4 & \alpha_4 \end{pmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix} = \begin{bmatrix} r_1 \\ r_2 \\ r_3 \\ r_4 \end{bmatrix}$$

$L \cdot y = R$

$$\alpha_1 y_1 = r_1 \rightarrow y_1 = \frac{r_1}{\alpha_1} = \frac{r_1}{\alpha_1}$$

$$\beta_2 y_1 + \alpha_2 y_2 = r_2 \rightarrow \begin{cases} y_2 = \frac{r_2 - \beta_2 y_1}{\alpha_2} \\ \alpha_2 = \alpha_2 - b_2 \frac{c_1}{\alpha_1} \end{cases}$$

For a generic node  $i$ :

loop over  $i$

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

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

$$\alpha_1 = \alpha_1$$

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

$$\beta_2 = b_2$$

$$\alpha_2 = \beta_2 \gamma_1 + \alpha_2 \rightarrow \alpha_2 = \alpha_2 - b_2 \frac{c_1}{\alpha_1}$$

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

Problem B

$$\begin{pmatrix} 1 & \gamma_1 & 0 & 0 \\ 0 & 1 & \gamma_2 & 0 \\ 0 & 0 & 1 & \gamma_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

$\Downarrow \quad \cdot \quad C = y$

Starting from the bottom:

$$C_4 = y_4$$

$$C_3 + \gamma_3 C_4 = y_3 \rightarrow C_3 = y_3 - \gamma_3 C_4$$

 $\vdots$ 

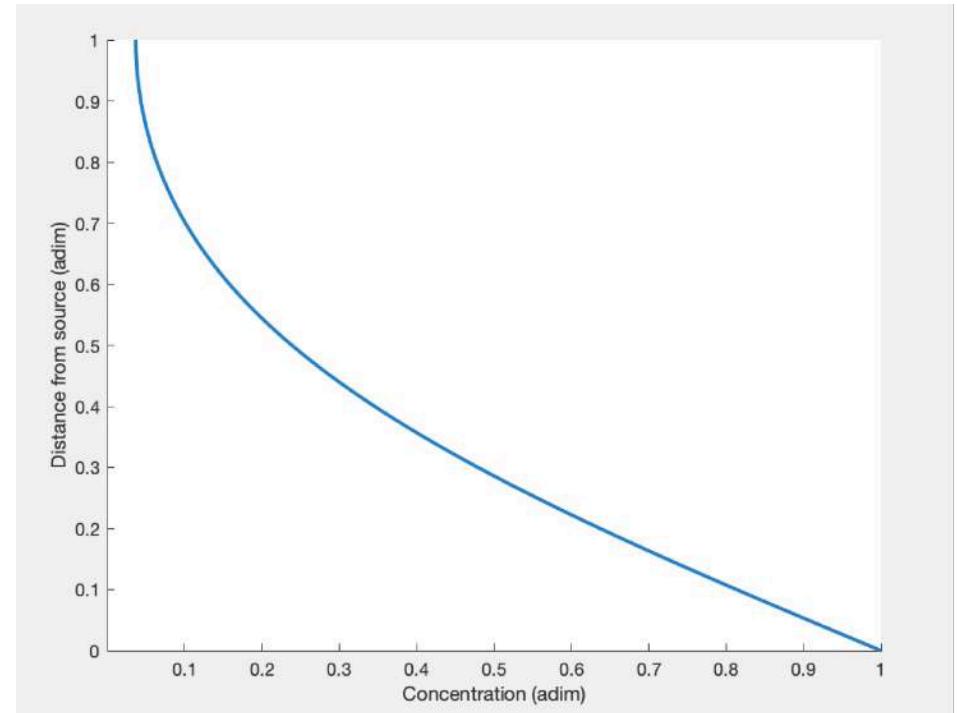
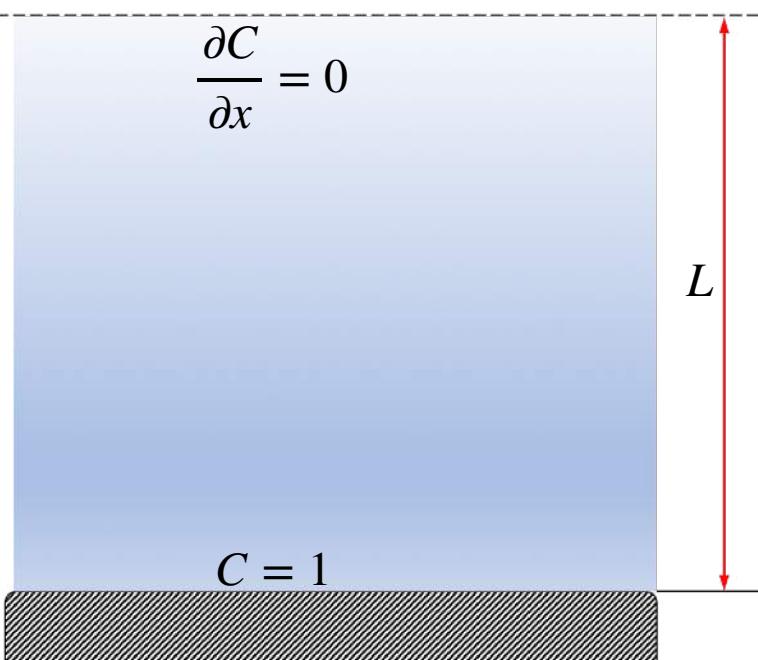
In general

$$C_4 = y_n$$

$$\text{loop } i \text{ over } \Rightarrow [C_i = y_i - \gamma_i y_{i+1}]$$

## 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 note on accuracy

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

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

For the present case:

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

This equation can be rearranged as:

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

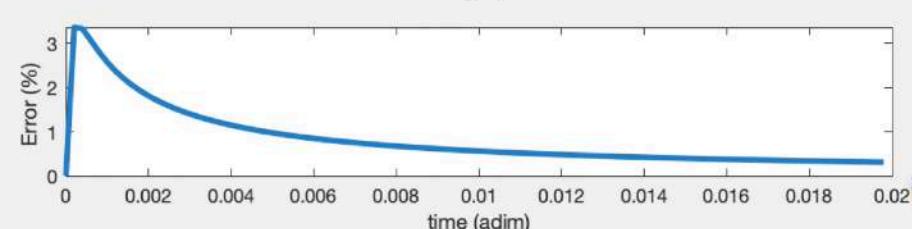
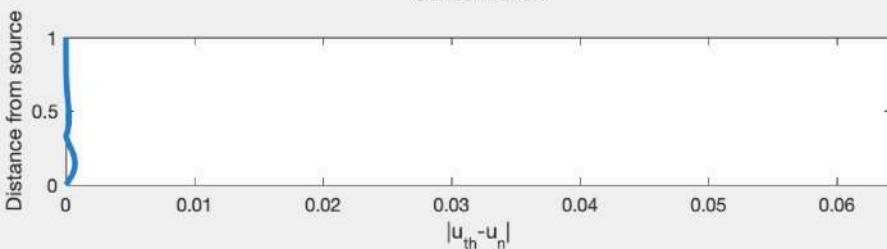
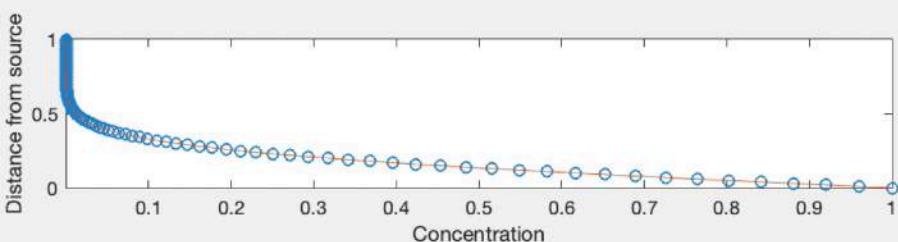
[Thomas algorithm]

Note:

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

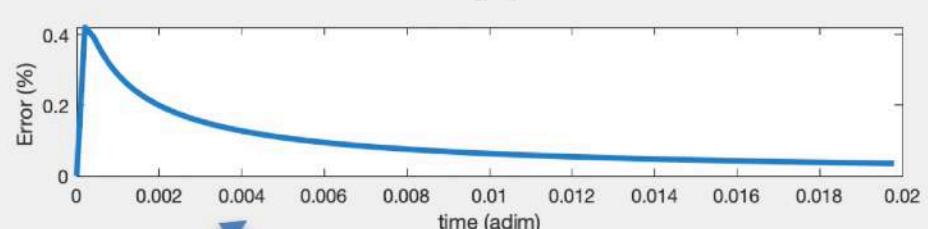
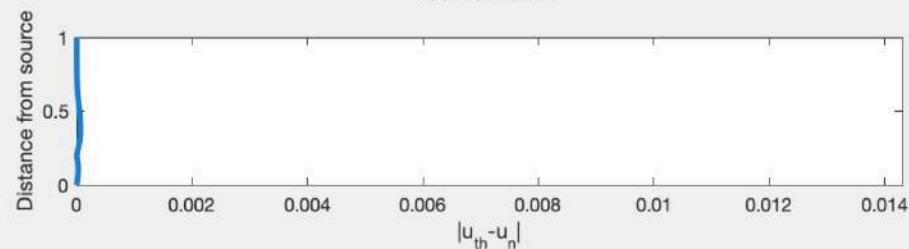
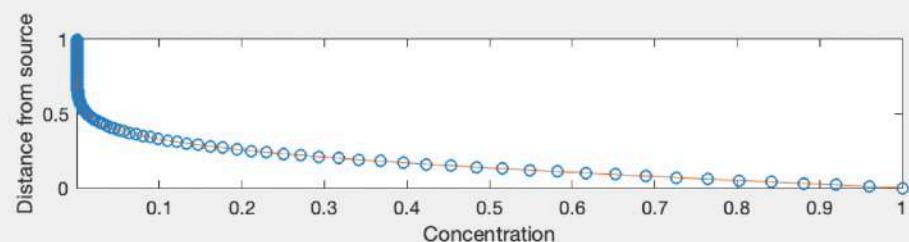
# Implicit method: 1st vs 2nd order

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



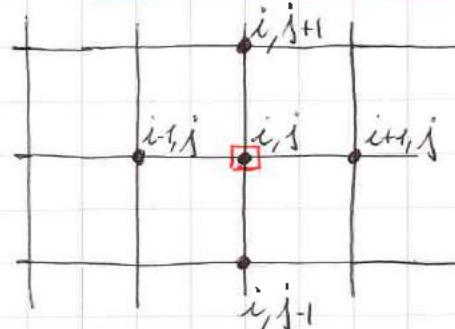
1st Order

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



2nd Order

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



Now the stencil has five points, not three

With an explicit scheme:

$$\begin{aligned} C_{i,j}^{n+1} - C_{i,j}^n &= \frac{\Delta t \cdot D}{\Delta x^2} \left[ C_{i-1,j}^n - 2C_{i,j}^n + C_{i+1,j}^n \right] + \\ &\quad + \frac{\Delta t \cdot D}{\Delta y^2} \left[ C_{i,j-1}^n - 2C_{i,j}^n + C_{i,j+1}^n \right] \end{aligned}$$

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

Also, Fully implicit methods would lead to a penta-diagonal system (Time consuming)

↳ Solution 1: Splitting methods

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

## Diffusion and advection

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

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

In dimensionless form:

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

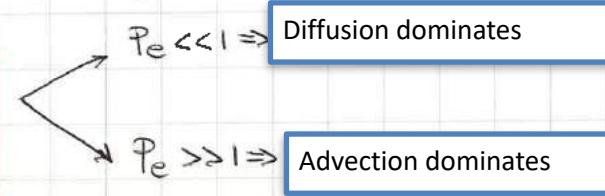
$$\frac{DC_w}{L^2} \frac{\partial C}{\partial t} + \frac{u_{ref} u C_w}{L} \frac{\partial C}{\partial x} = \frac{DC_w}{L^2} \frac{\partial^2 C}{\partial x^2}$$

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

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

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

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



$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2}$$



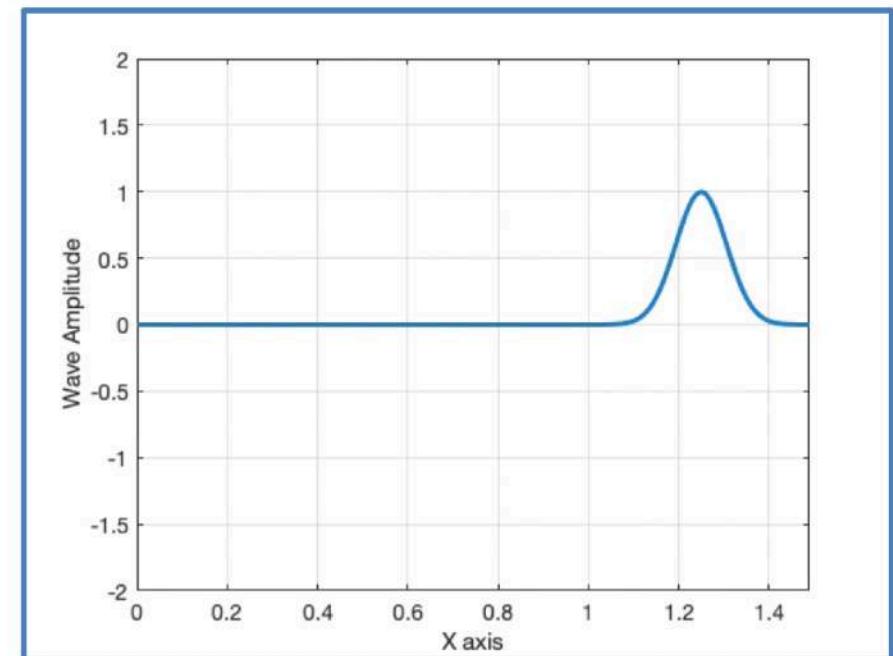
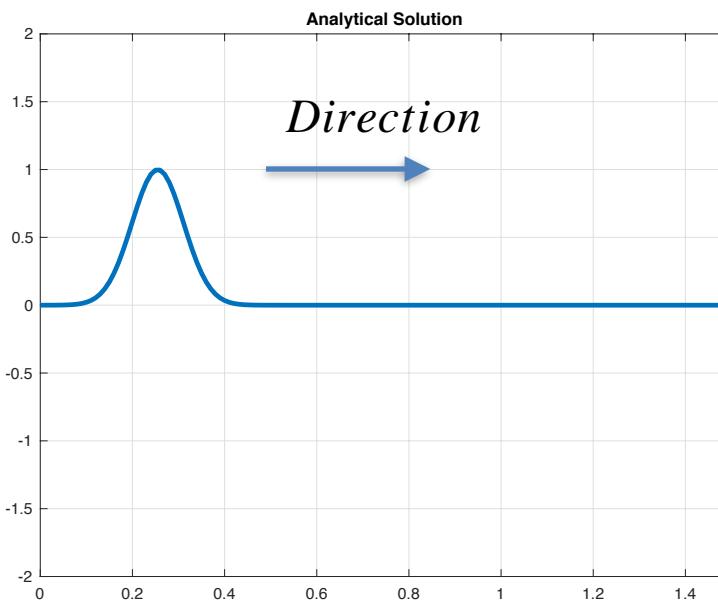
$$\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = 0$$



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

Analytical solution exists

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



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

$$\left[ \frac{\partial C}{\partial x} \right]_i^n = \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} \quad \begin{array}{l} \text{It can be proved that} \\ \text{this scheme is unstable} \end{array}$$

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

$$[U > 0] \quad \frac{C_i^{n+1} - C_i^n}{\Delta t} + U \frac{C_i^n - C_{i-1}^n}{\Delta x} = 0 \quad [U = Pe \cdot u]$$

This gives:

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

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

$$G = 1 - C_0(1 - \cos \theta) - i C_0 \sin \theta \rightarrow |G| = \sqrt{1 + (1 - \cos \theta)^2} (C_0 - 1)^2 C_0 \rightarrow C_0 \leq 1 \quad (\frac{\text{small } \Delta t}{\Delta x})$$

What about the accuracy (Truncation error)

(Taylor series)

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

Therefore:

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

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

We get:

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

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

Finally

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

Error ( $\varepsilon$ )

We focus now on the error:

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

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

$$\begin{aligned} \varepsilon &= -\frac{\Delta t}{2} \left[ \frac{\partial^2 C}{\partial t^2} \right]_i^n + \frac{U \Delta x}{2} \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n \\ &= -\frac{\Delta t}{2} \left( U^2 \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n \right) + \frac{U \Delta x}{2} \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n = \frac{U \Delta x}{2} \left\{ \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n - \frac{U \Delta t}{\Delta x} \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n \right\} \\ &= \frac{U \Delta x}{2} \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^n (1 - C_0) \end{aligned}$$

We have obtained the following expression

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

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

$\zeta'$  = Numerical viscosity  
or diffusivity

Therefore, the equation we are going to solve is:

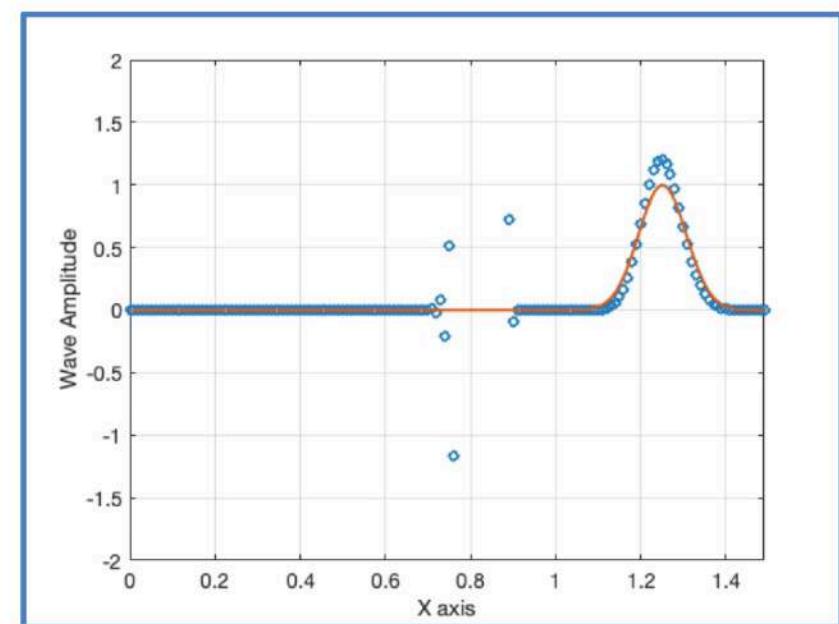
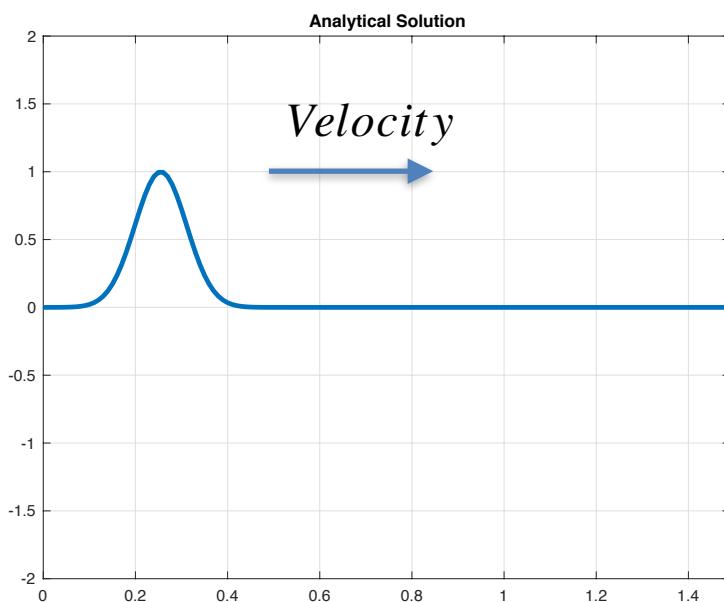
$$\left[ \frac{\partial C}{\partial t} \right]_i^h + U \left[ \frac{\partial C}{\partial x} \right]_i^h = \zeta' \left[ \frac{\partial^2 C}{\partial x^2} \right]_i^h$$

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

Discretized equation

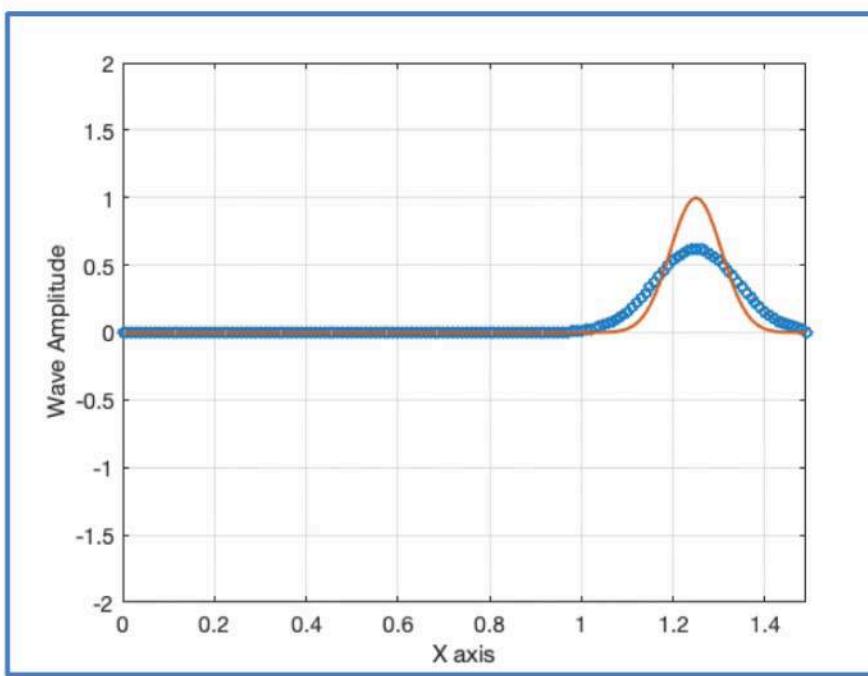
$$C_i^{n+1} = (1 - Co) C_i^n + Co C_{i-1}^n$$

We first see what happens when  $Co = 1.1$

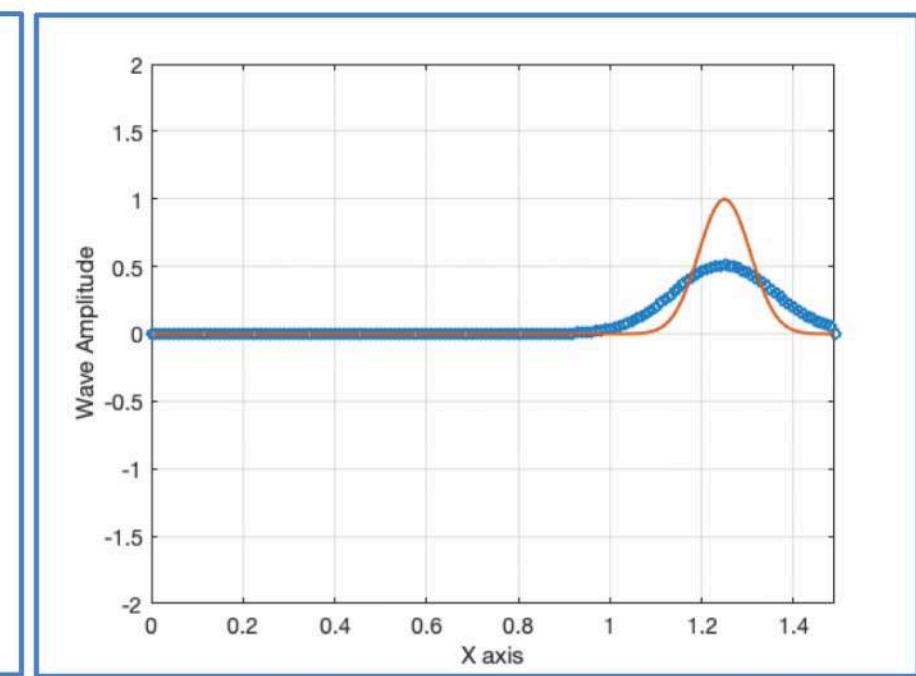


As expected...

Now we reduce the Courant number



$$Co = 0.5$$

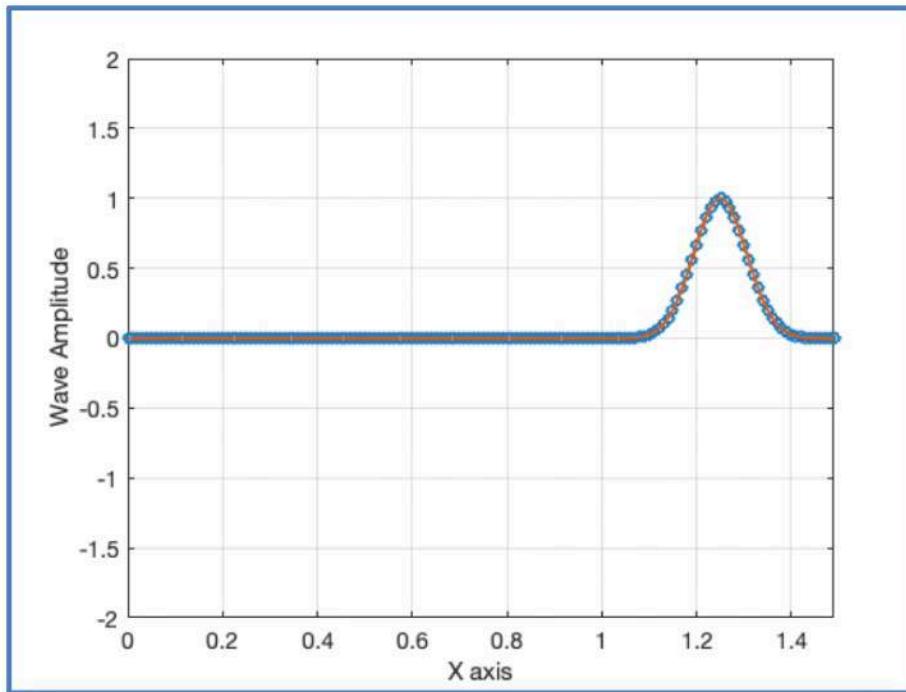


$$Co = 0.1$$

A heavier simulation does not necessarily mean a better simulation...

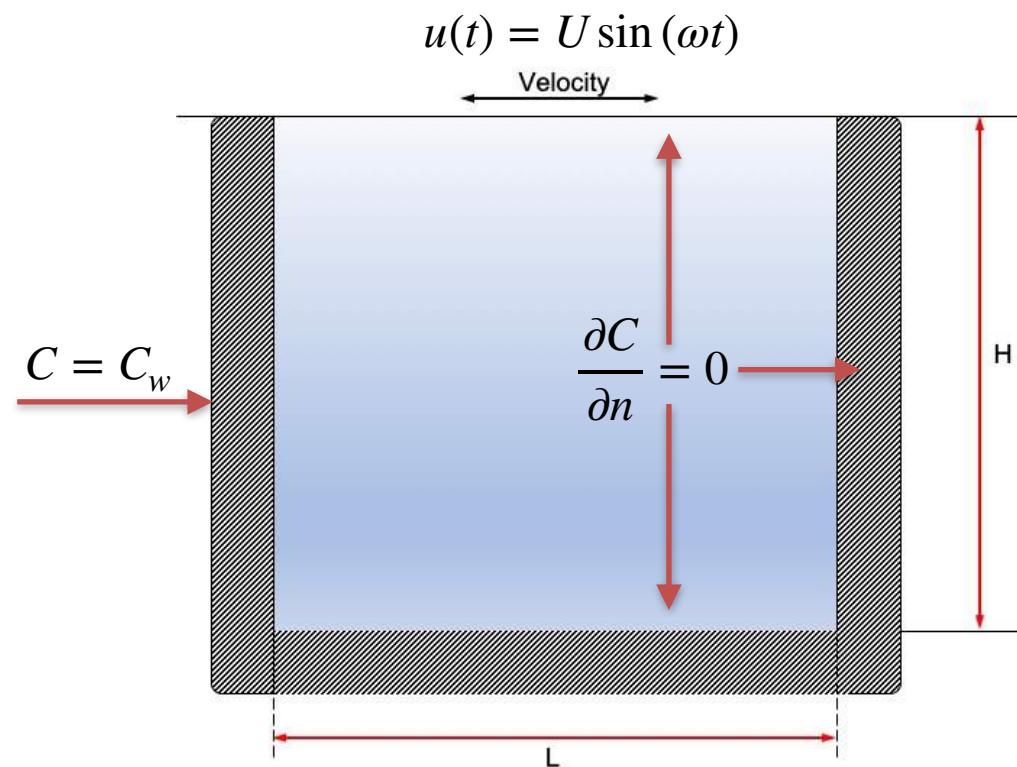
Looking at the truncation error:

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



$$Co = 1$$

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



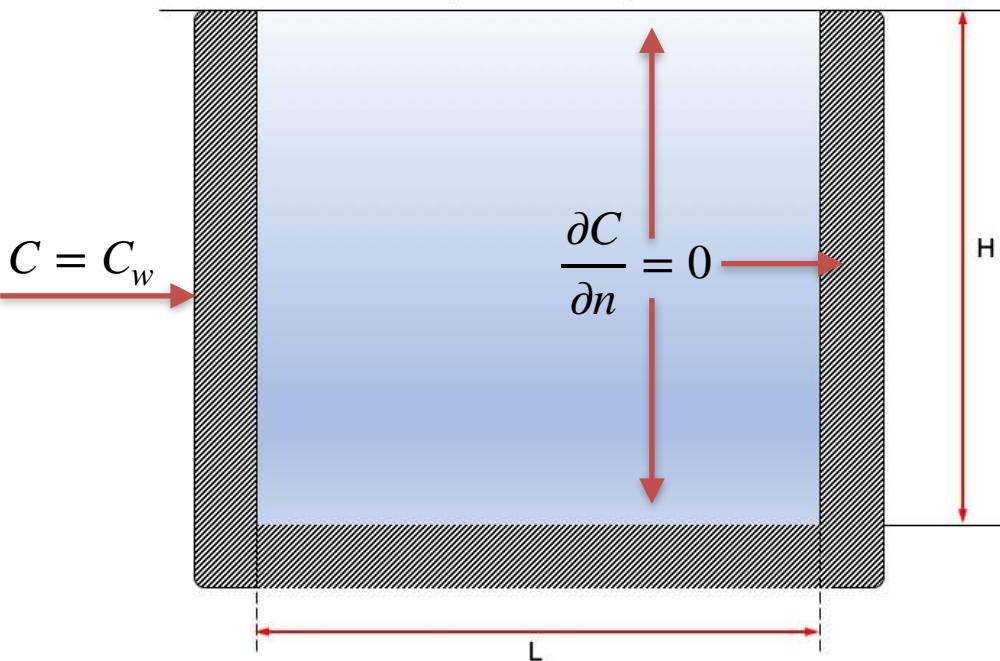
Governing equations

$$\left\{ \begin{array}{l} \frac{\partial u_i}{\partial x_i} = 0 \\ \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j^2} \\ \frac{\partial C}{\partial t} + u_j \frac{\partial C}{\partial x_j} = \frac{1}{RePr} \frac{\partial^2 C}{\partial x_j^2} \end{array} \right.$$

$\frac{1}{Pe}$

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

Velocity



Note: transport equation for  $\omega$  (\*see later)

Note: BC for  $\omega$  obtained from Taylor series expansion of  $\psi$   
(\*\*see later)

Alternative formulation  $(\psi, \omega)$

$$\left\{ \begin{array}{l} u_x = \frac{\partial \psi}{\partial y} \\ u_y = -\frac{\partial \psi}{\partial x} \\ \omega = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \end{array} \right. \begin{array}{l} \text{Riemann} \\ \text{Vorticity} \end{array}$$

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

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

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

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

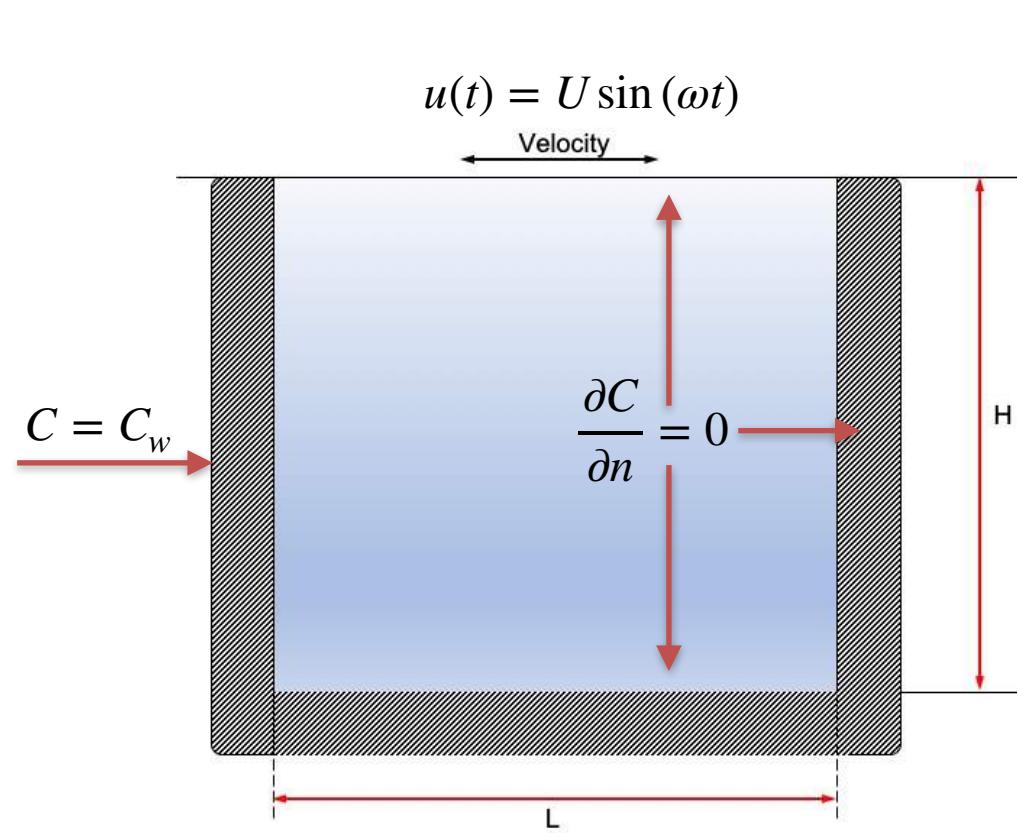
Then,  $\partial/\partial y(A)$  and  $\partial/\partial x(B)$

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

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

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

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



**Central  
approx.**

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

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

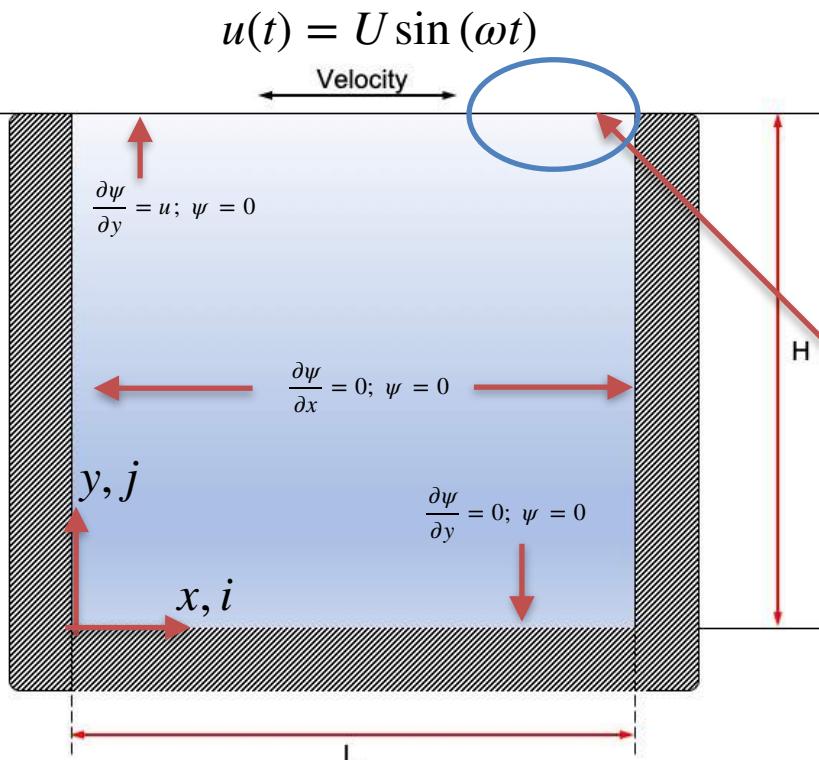
$$\left[ \frac{\partial f_{i,j}}{\partial y} \right]_{i,j}^n = \frac{f_{i,j+1}^n - f_{i,j-1}^n}{2\Delta y}$$

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

**Explicit**

$$\left[ \frac{\partial f}{\partial t} \right]_{i,j}^n = F_{i,j}^n$$

Let's focus on B.C. for  $\psi, \omega$ :



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

Using Taylor series expansion for  $\psi$  we have:

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

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

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

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

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

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

Apply BC for  $\omega^n$  from the knowledge of  $\psi^{n+1}$

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

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

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

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

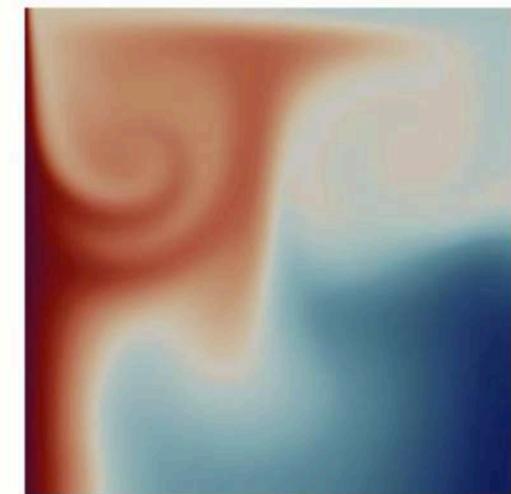
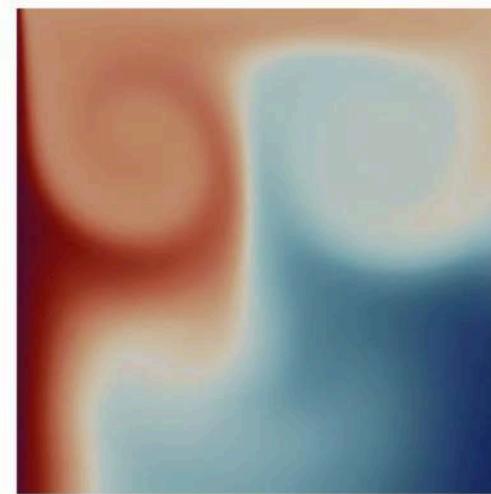
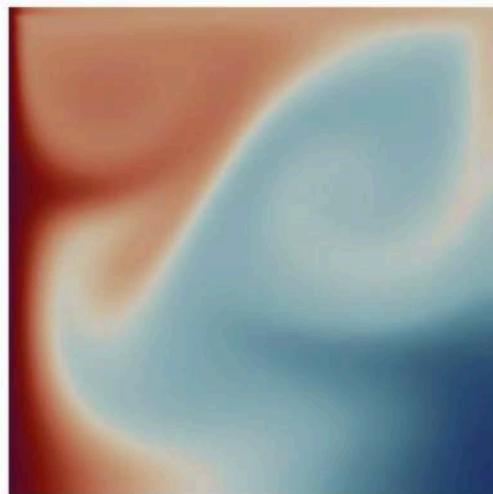
Solve the transport of vorticity  $\omega^{n+1} = \omega^n + \Delta t \left( F_{i,j}^n \right)$

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

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

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

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



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)

$$\left\{ \begin{array}{l} \frac{\partial u_i}{\partial x_i} = 0 \\ \frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = - \frac{\partial p}{\partial x_i} + \frac{1}{Re} \frac{\partial^2 u_i}{\partial x_j^2} \end{array} \right.$$

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

$\nu$  kinematic viscosity;

$\rho$  density

$\mu$  dynamics. viscosity

$L$  Reference Length

$U_T$  Reference Velocity

## Streamfunction-Vorticity formulation ( $\psi, \omega$ )

$$\left\{ \begin{array}{l} u_x = \frac{\partial \psi}{\partial y} \\ u_y = - \frac{\partial \psi}{\partial x} \\ \omega = \frac{\partial u_y}{\partial x} - \frac{\partial u_x}{\partial y} \end{array} \right. \quad \begin{array}{l} \text{Riemann equations} \\ \\ \text{Vorticity definition} \end{array}$$

$$\left\{ \begin{array}{l} \omega = - \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) \\ \frac{\partial \omega}{\partial t} + u_j \frac{\partial \omega}{\partial x_j} = + \frac{1}{Re} \frac{\partial^2 \omega}{\partial x_j^2} \end{array} \right. \quad * \text{Curl(NS)}$$