Numerical Simulation and Scientific Computing in Fluid Mechanics:

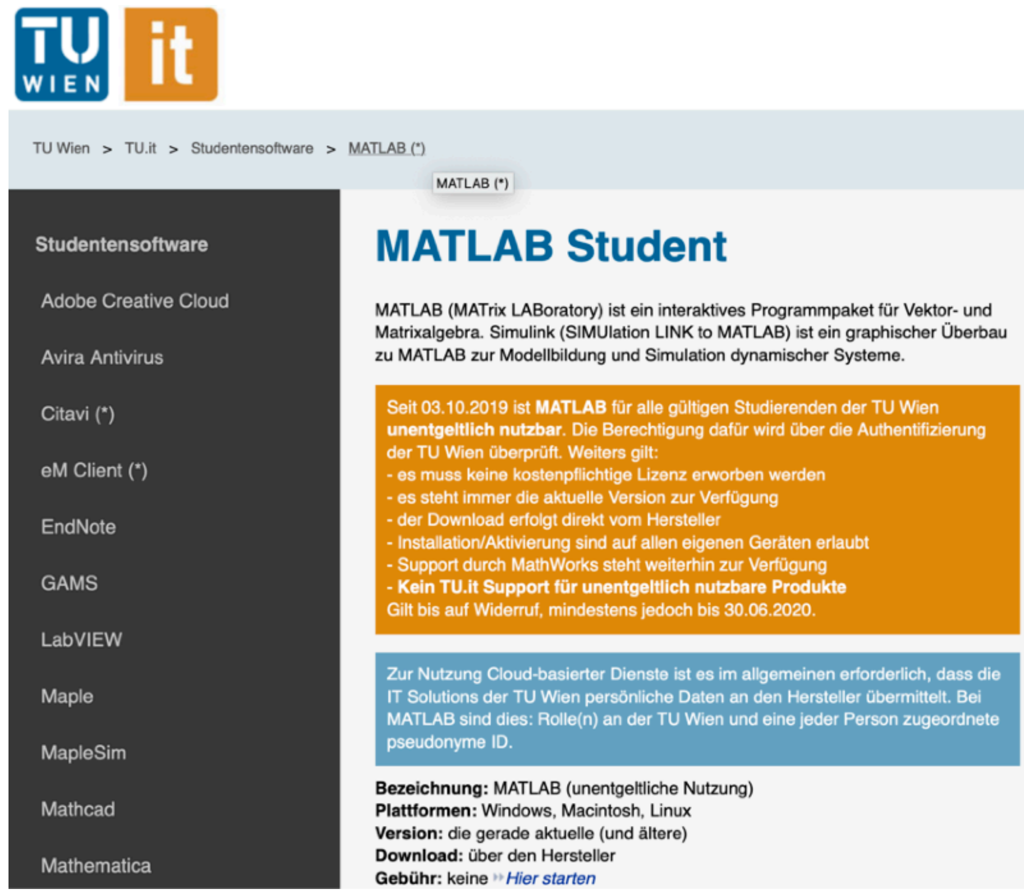
Fundamental aspects and applications

Francesco Zonta

Institute of Fluid Mechanics and Heat Transfer, TU Wien

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
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7. Flows in porous media

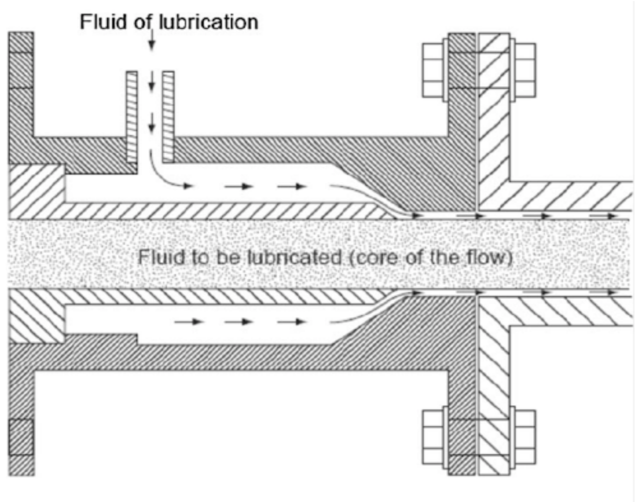
Oil Transport

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.



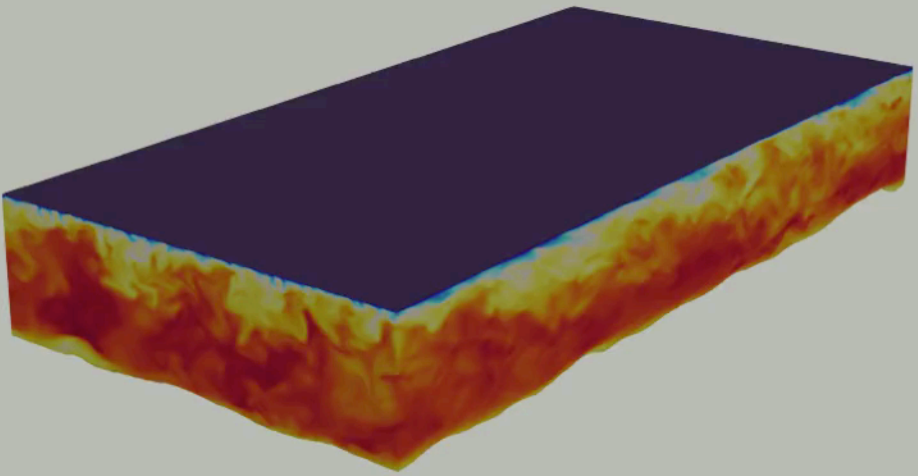
Credit: ALFA Research Group

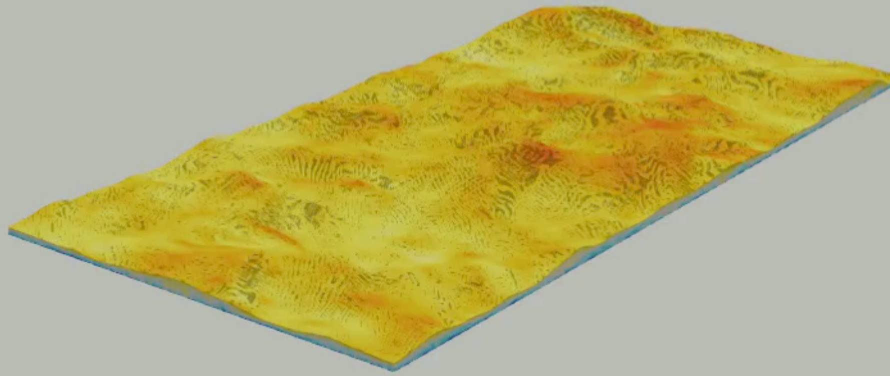
"There is a strong tendency for two fluids to arrange themselves so that the low-viscosity constituent is in the region of high shear.
This gives rise to a kind of a gift of nature in which the lubricated flows are stable, and it opens up very interesting possibilities for technological applications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

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

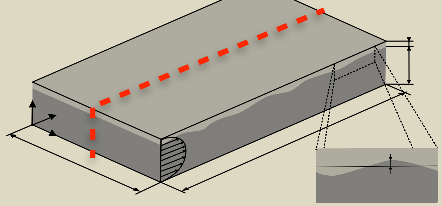
Oil Transport

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

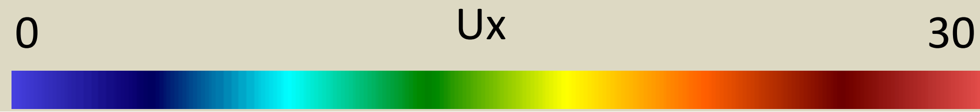


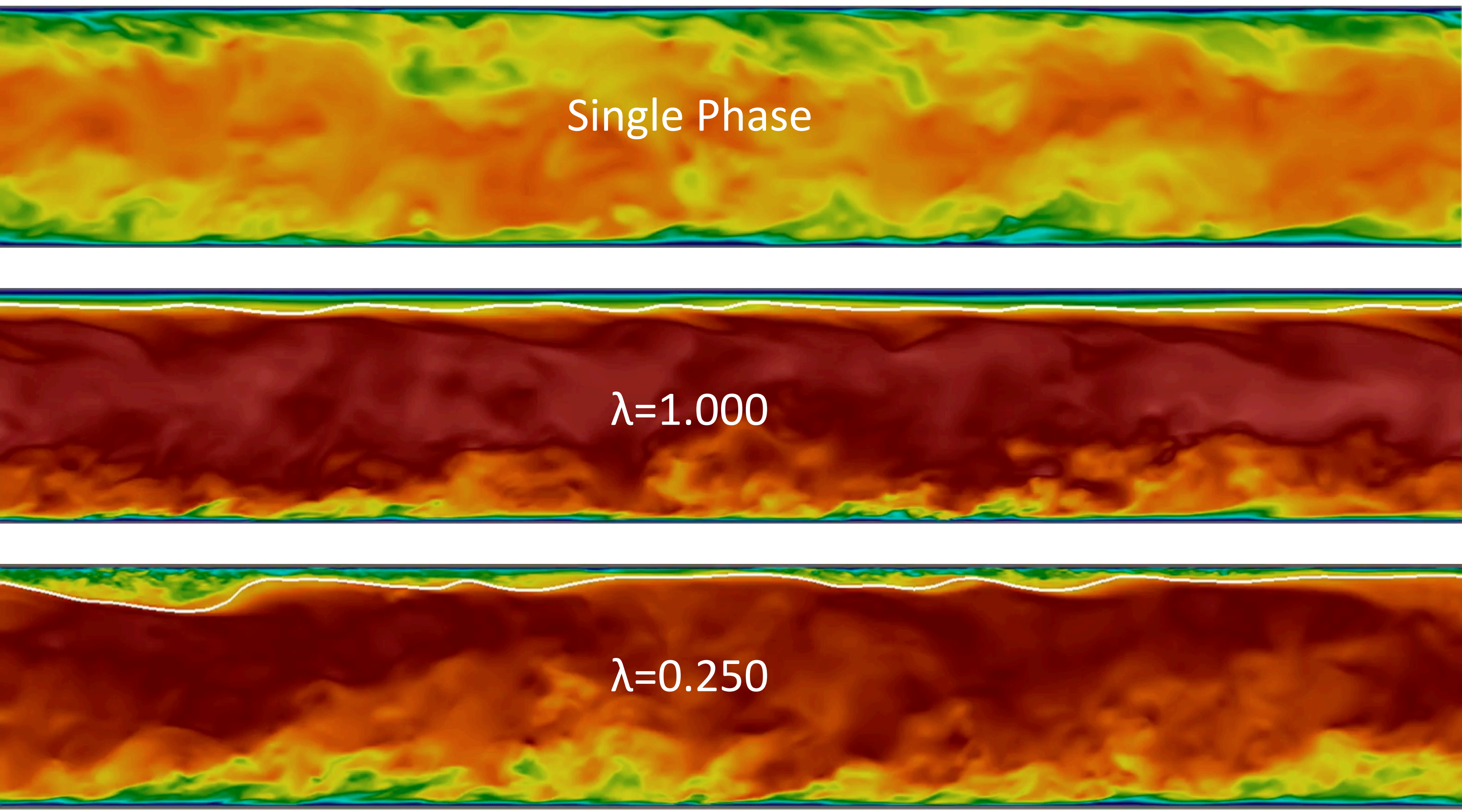


S. Ahmadi et al, Turbulent Drag Reduction by a Near Wall Surface Tension Active Interface, FTAC (2018)
S. Ahmadi et al, Turbulent drag reduction in channel flow with viscosity stratified fluids, CEF (2016)



Oil Transport





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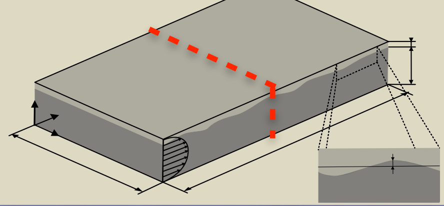
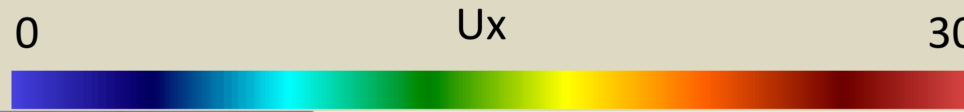
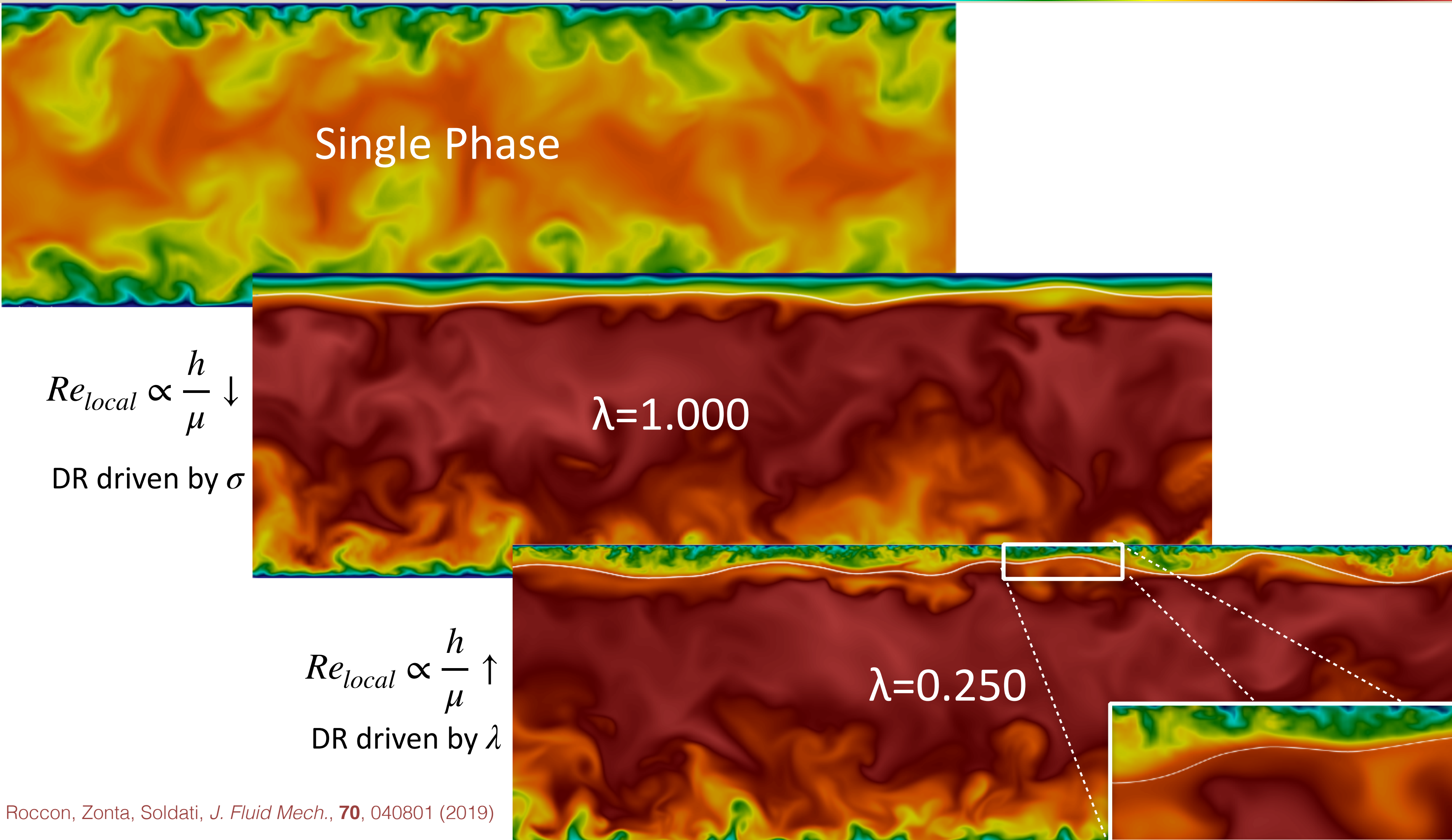


Explanation: a closer look





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

DR driven by σ

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

DR driven by λ

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

Fluid dynamics: computations we do

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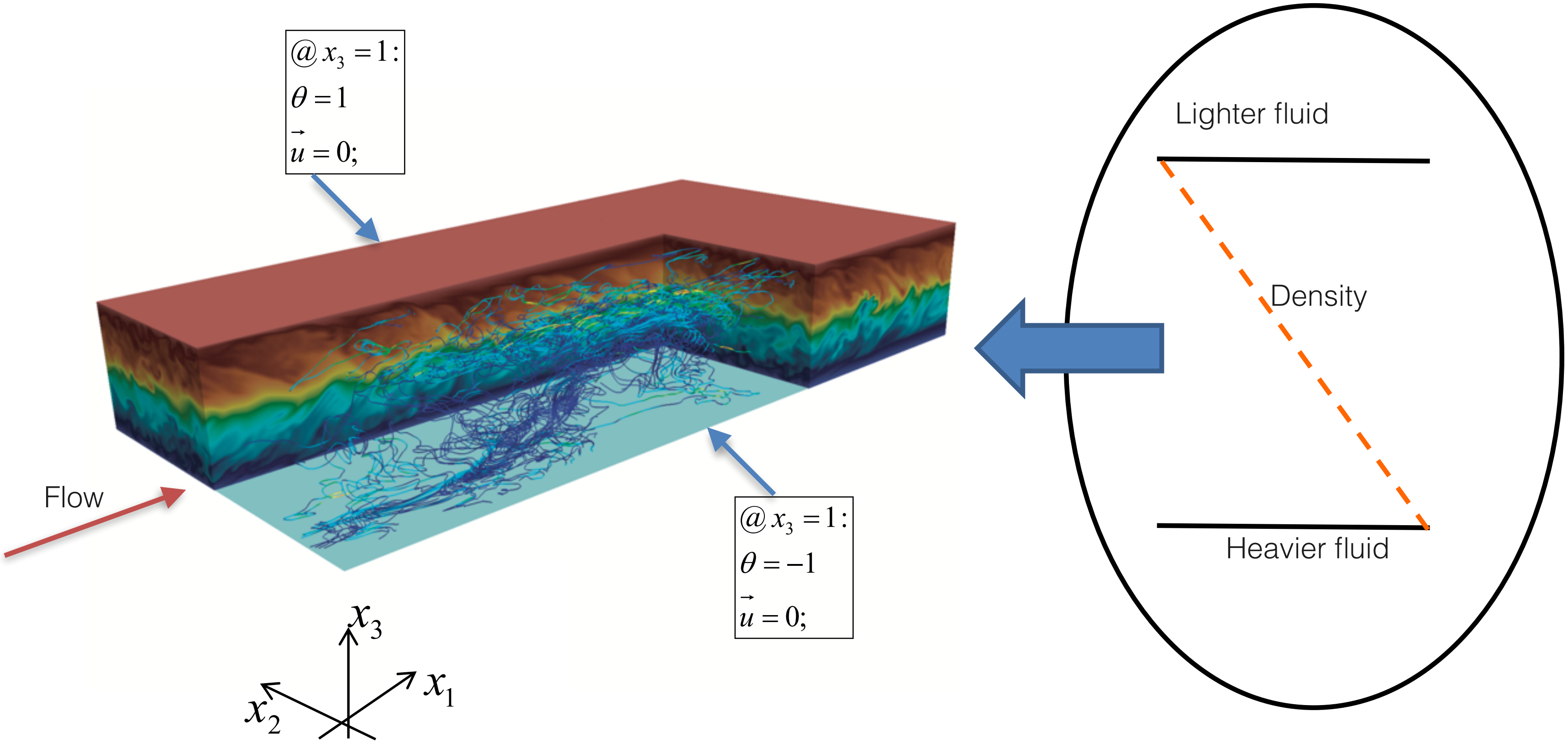
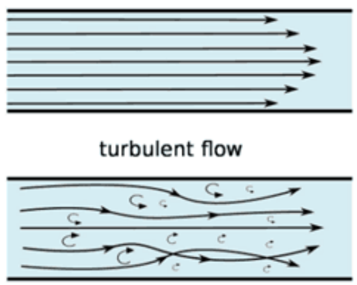
Stratification



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

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

Prandtl number: momentum diffusivity/thermal diffusivity

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

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

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

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

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

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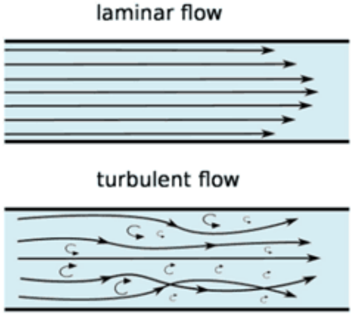

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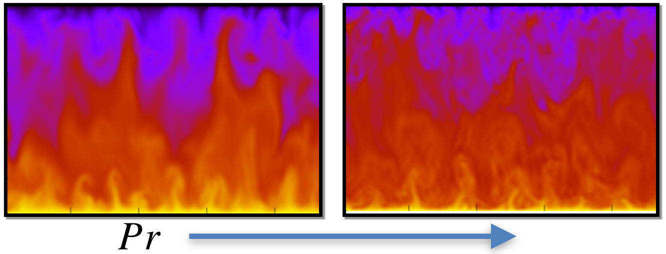

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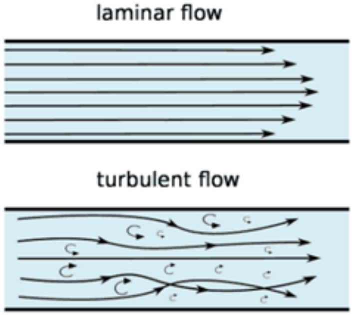

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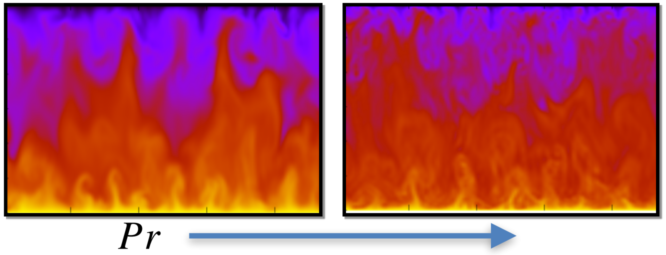

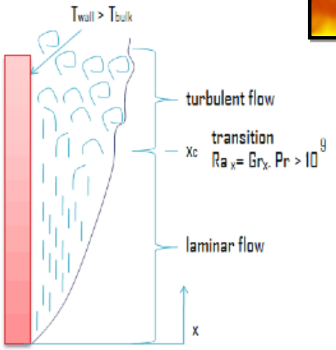

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Flow parameters

Main parameters of the flow:

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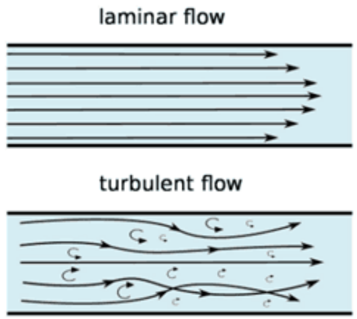

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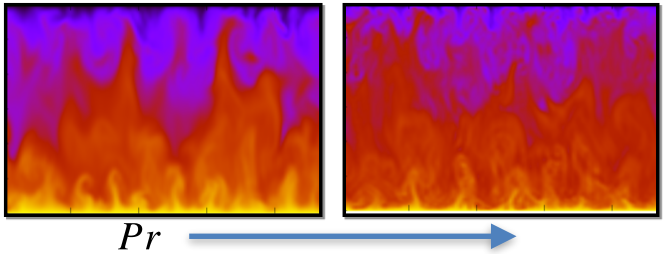

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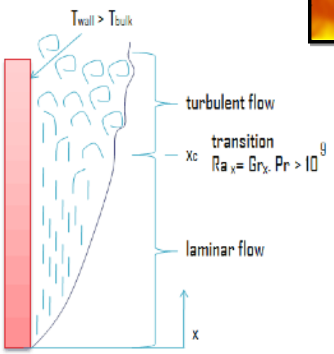

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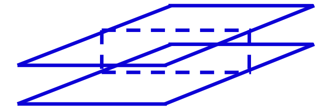
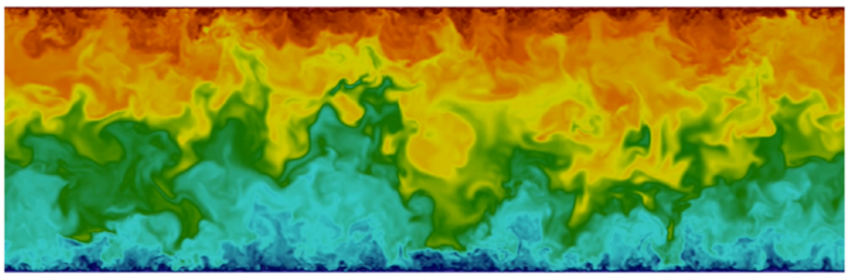
Stratification

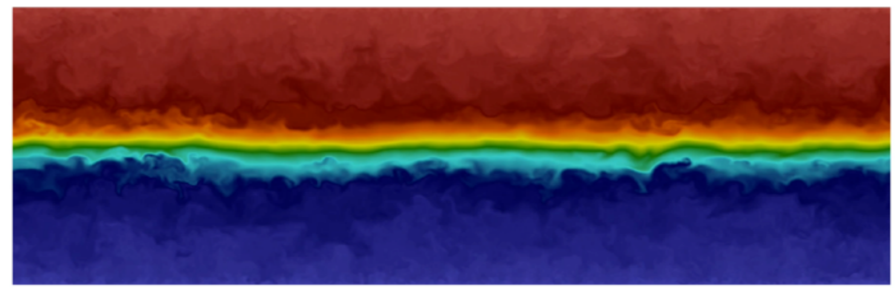
Visualization of temperature on a cross section



$$Ri_\tau = 0$$



$$Ri_\tau = 200$$



Neutrally buoyant

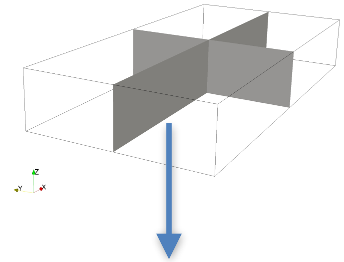
- Higher mixing
- Mixing is driven by turbulence structures

Stably stratified

- Lower mixing
- Internal waves act like barriers

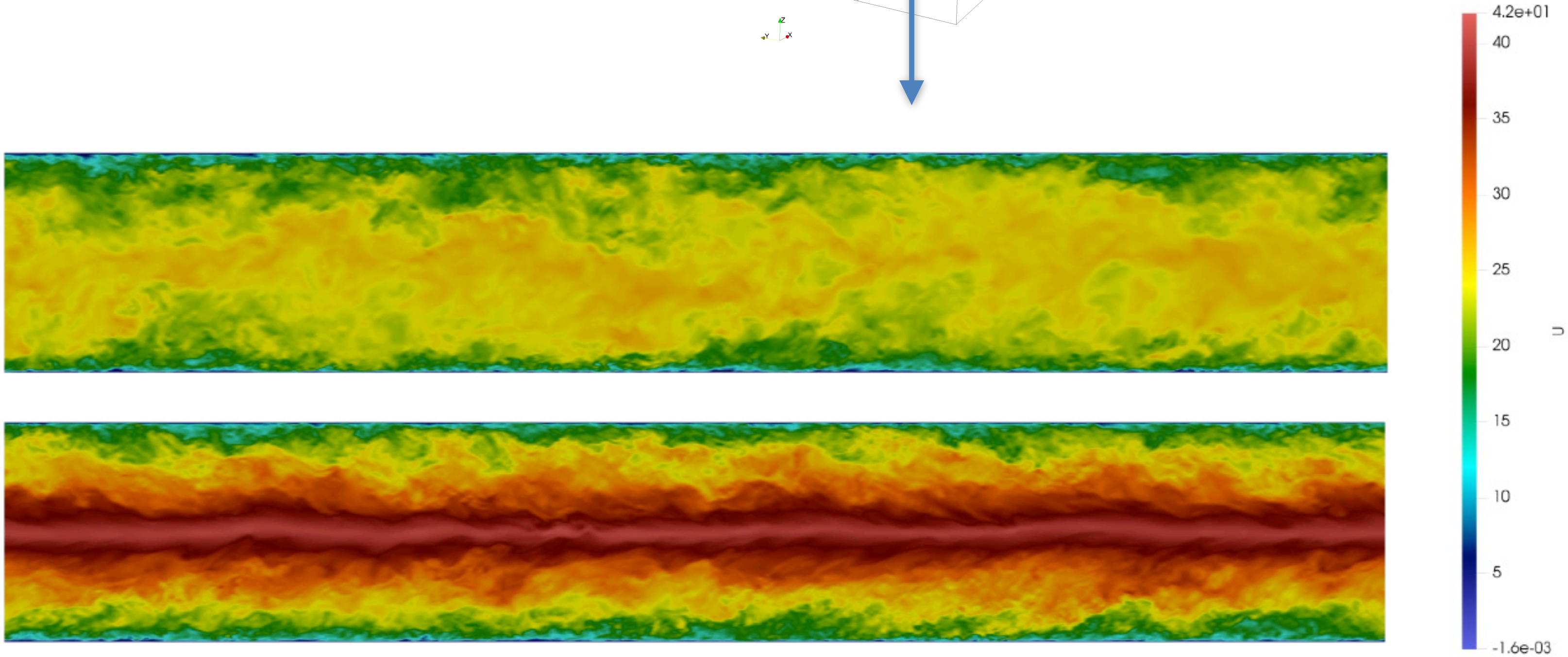
Stratification

The temperature distribution has a remarkable effect on the velocity field



$Ri_\tau = 0$

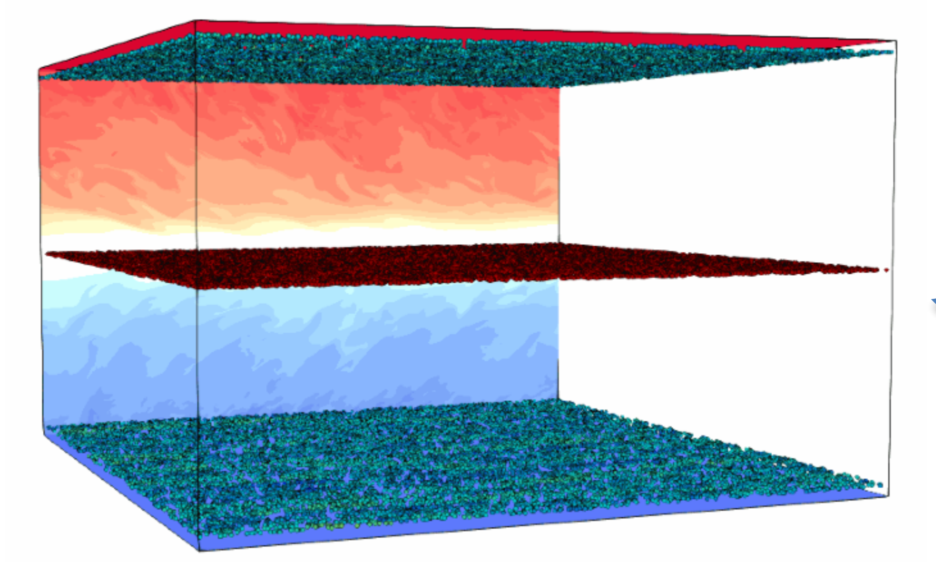
$Ri_\tau = 200$



- 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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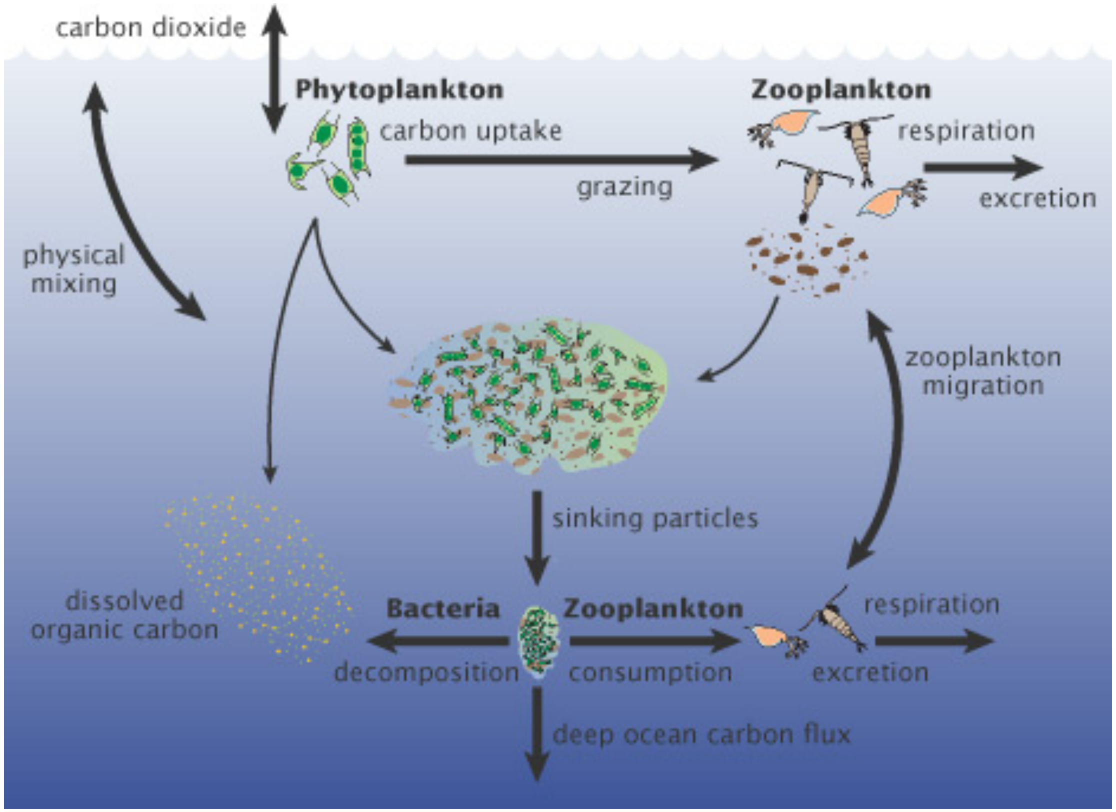
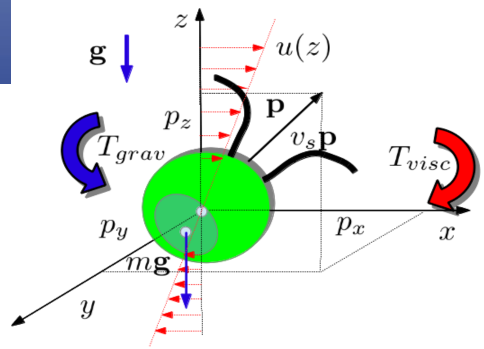
Phytoplankton

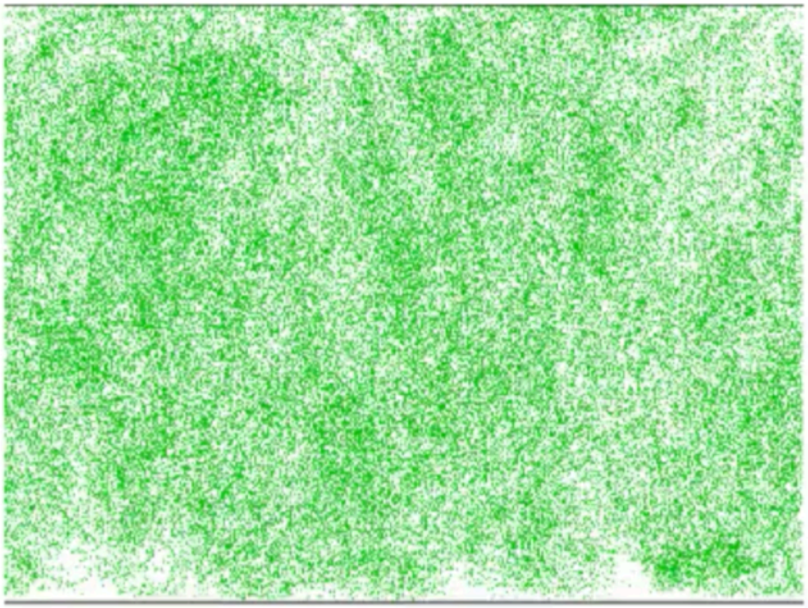


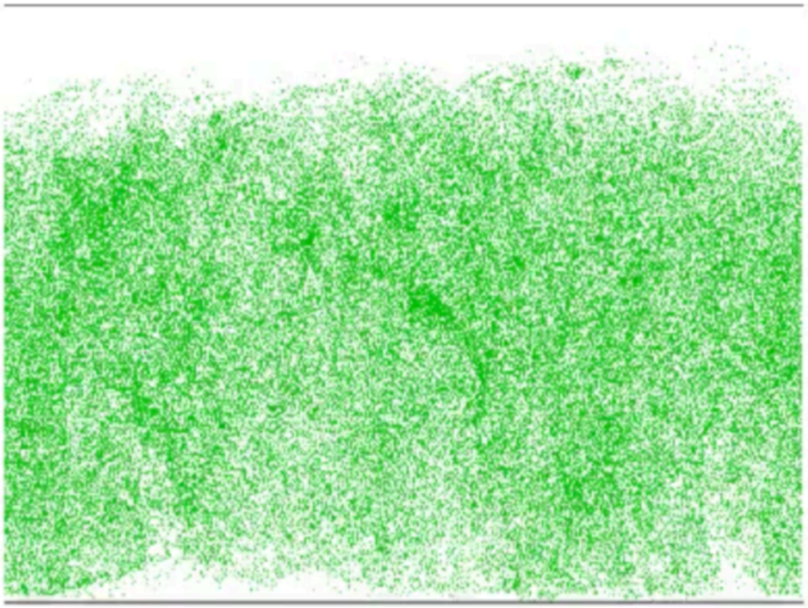
Phytoplankton is the photosynthetic part of plankton

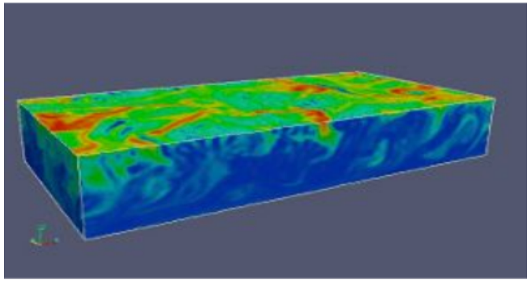
- Primary production: organize compounds from CO2
- Important part of the global carbon cycle
- Provides 50% of the earth's oxygen
- Sustain the aquatic food web

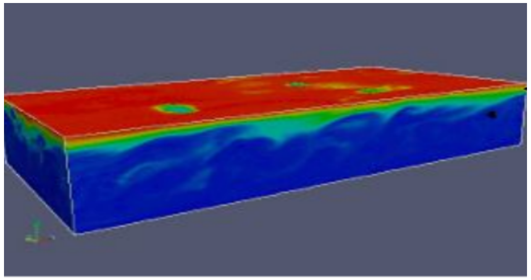


Phytoplankton

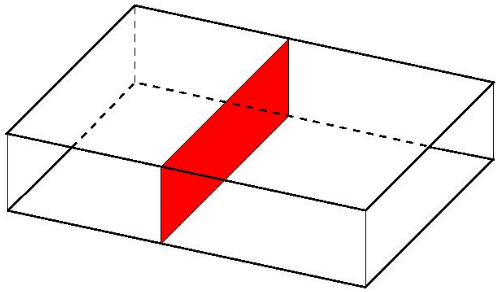


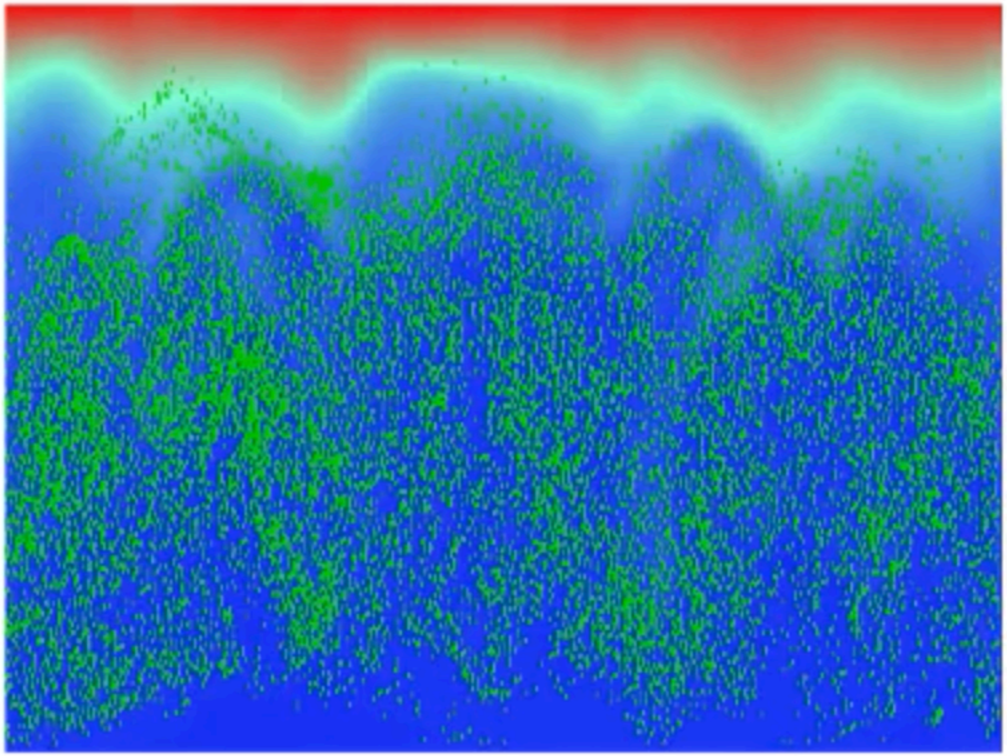






Phytoplankton





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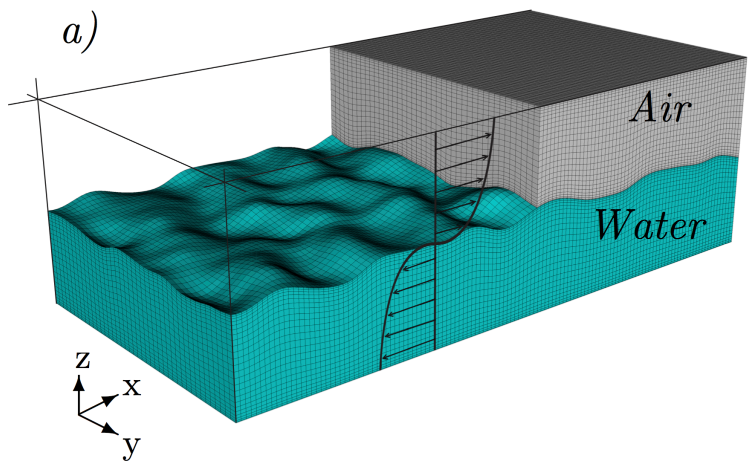
Waves

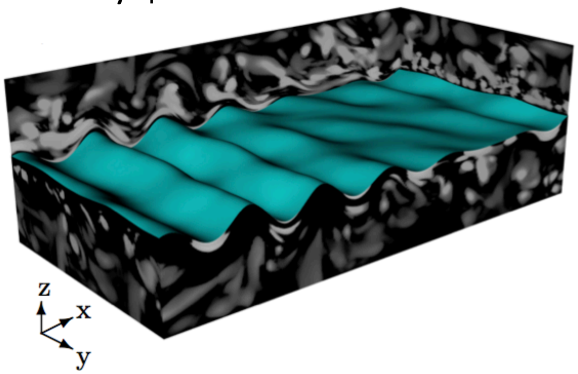
Transfer rates (for example of CO_2) across an interface depends strongly on the extension of the interface…

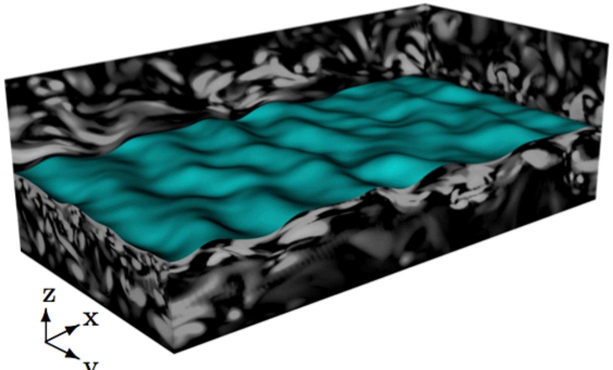
Waves

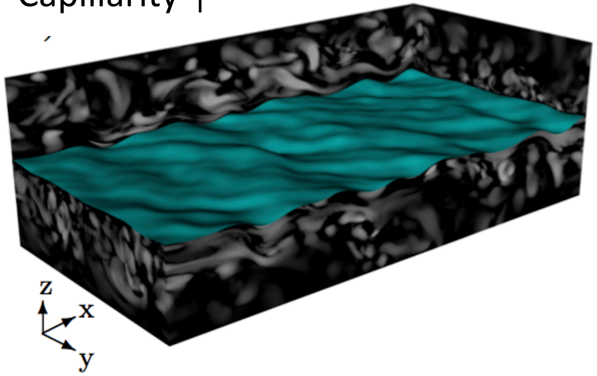


Gravity ↑

Capillarity ↑

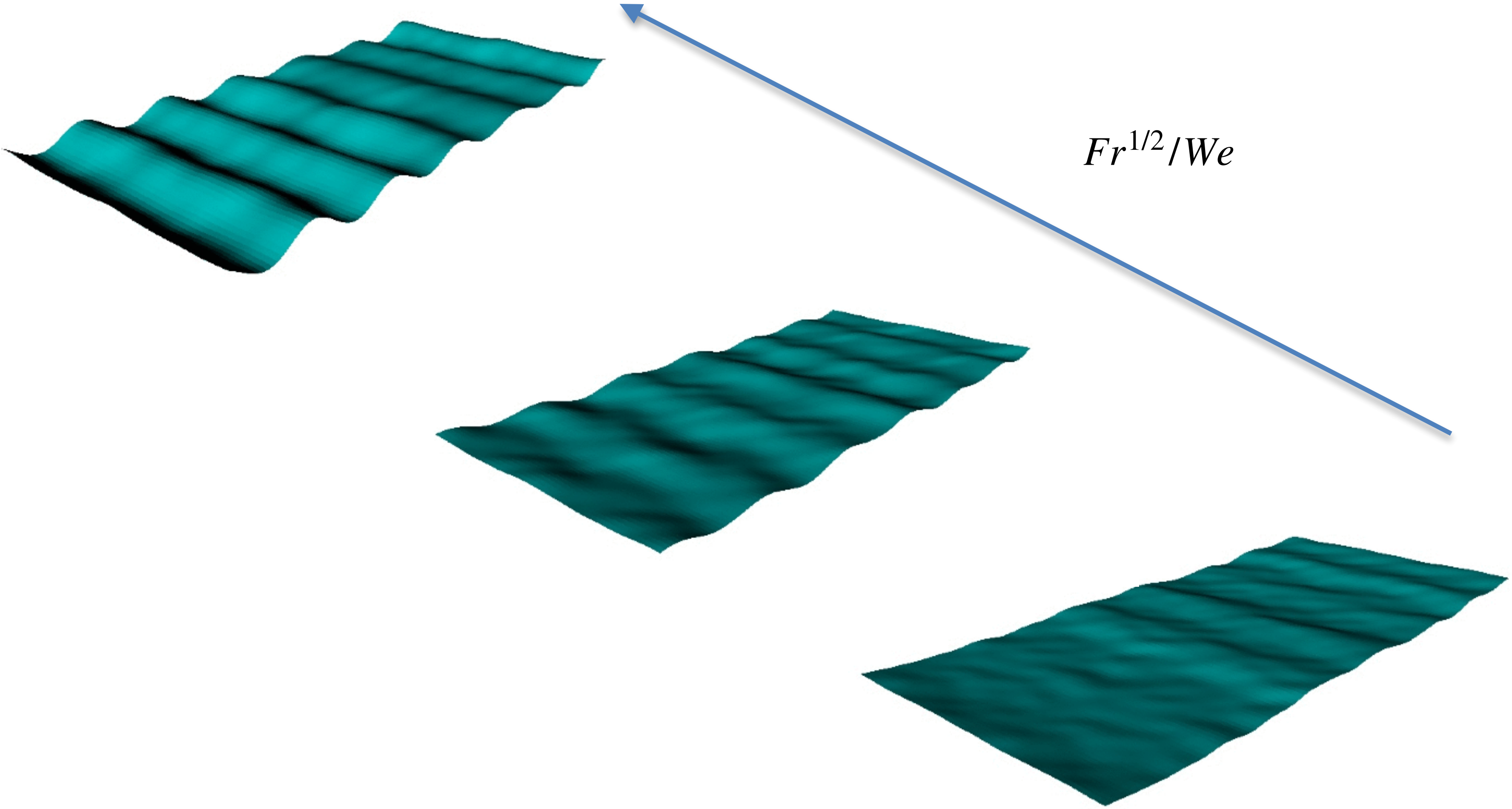






Quasy-sinusoidal wavy interface

Surface roughness


$Fr^{1/2}/We$

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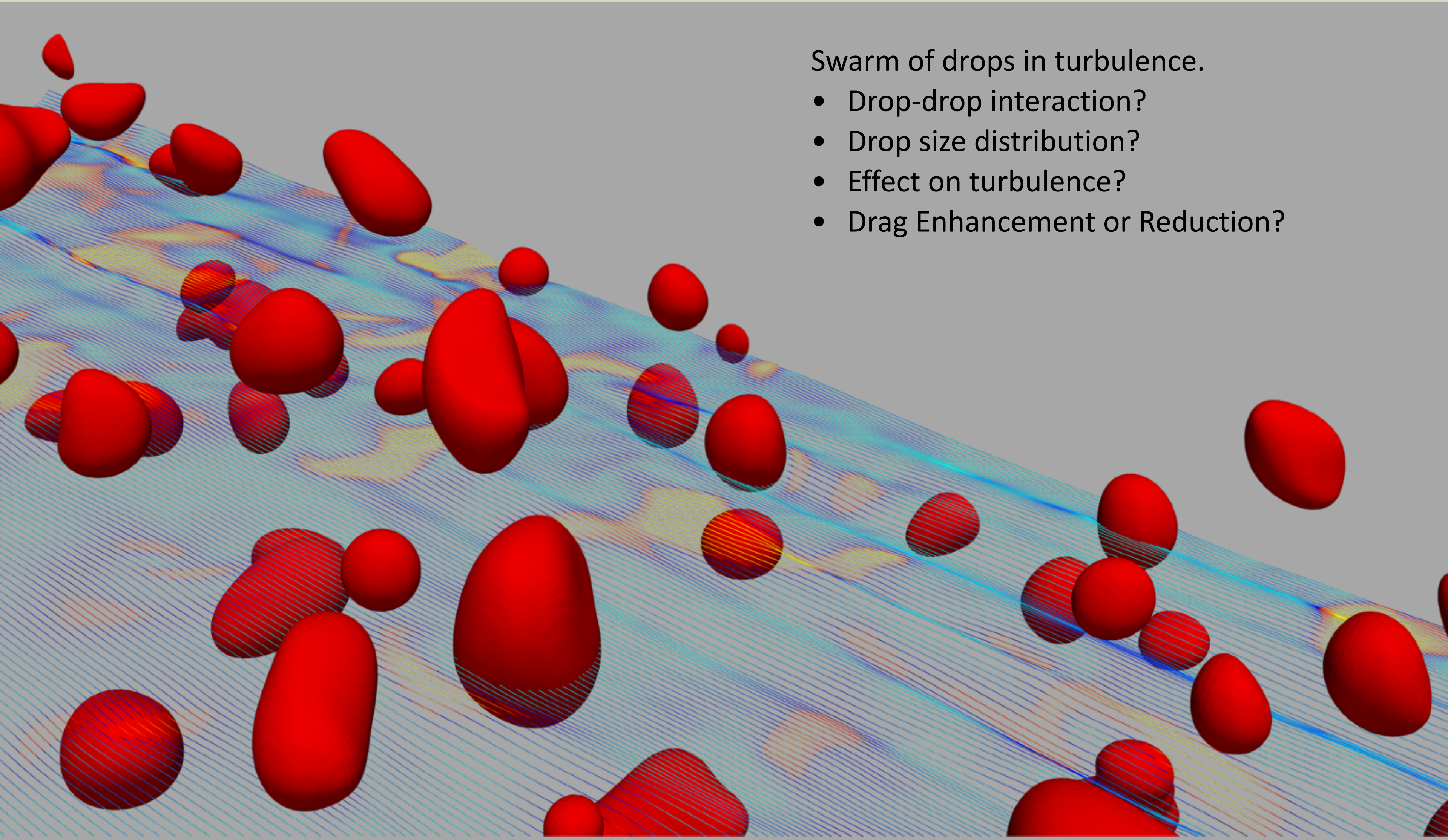
Oil/Water emulsions



Swarm of drops in turbulence.

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

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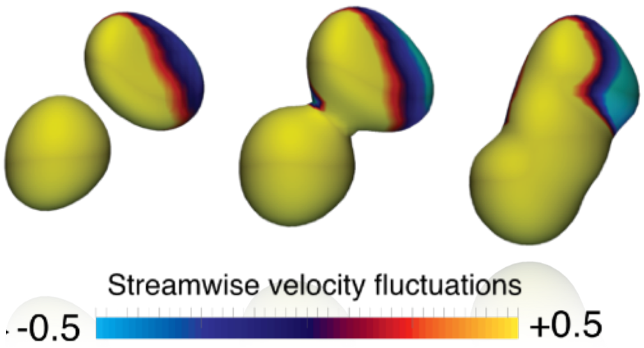
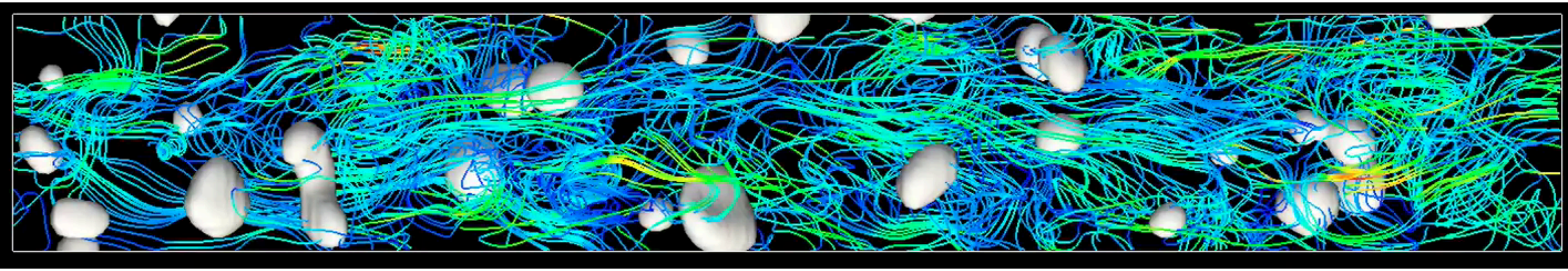
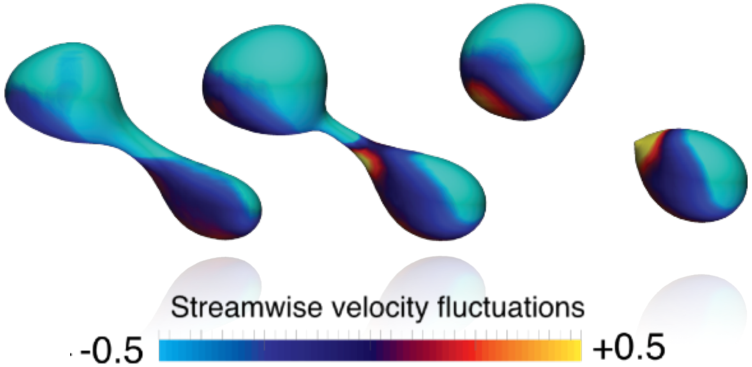
Oil/Water emulsions



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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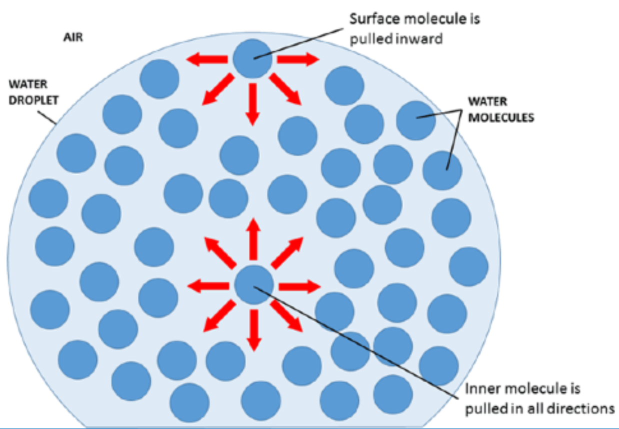
Oil/Water emulsions with surfactants

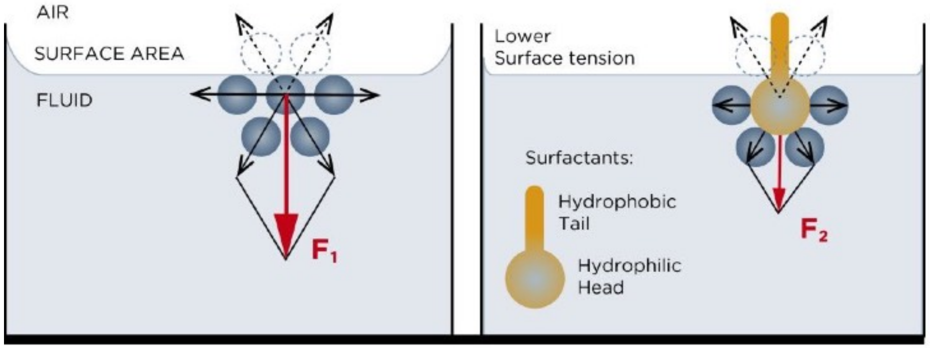
Surface Tension:

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



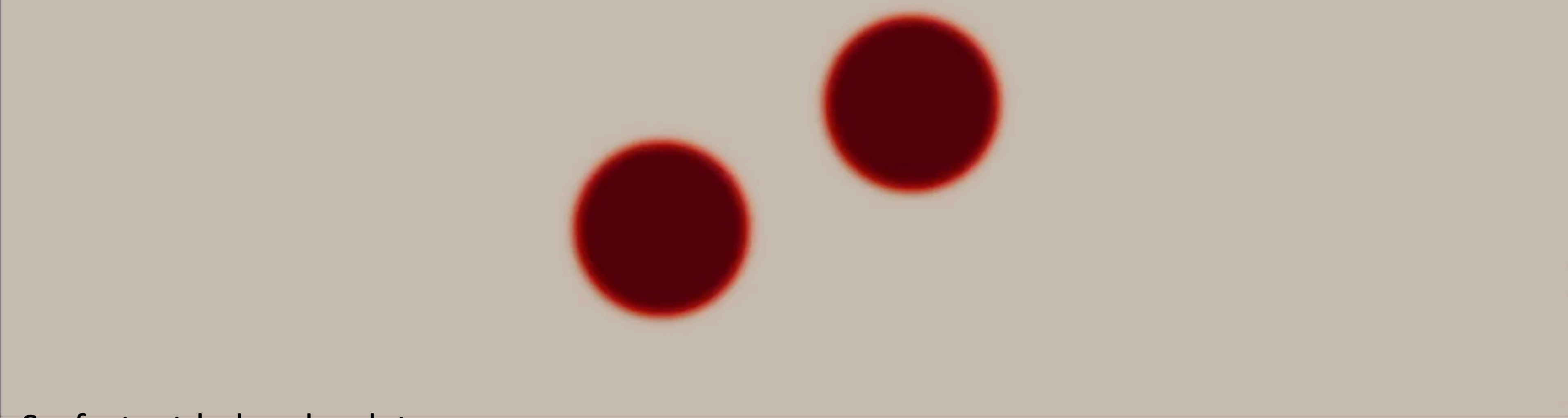
Presence of surfactant decreases the surface tension and as a consequence:

-Droplets become more deformable (less surface tension).

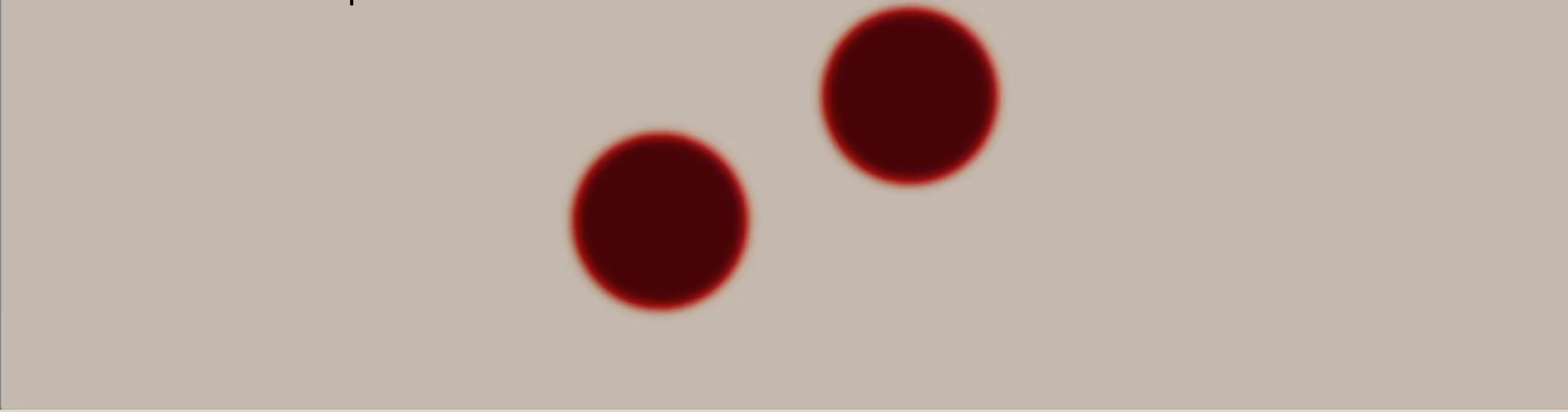
-When non-uniform can give rise to tangential forces (Marangoni).

Oil/Water emulsions with surfactants

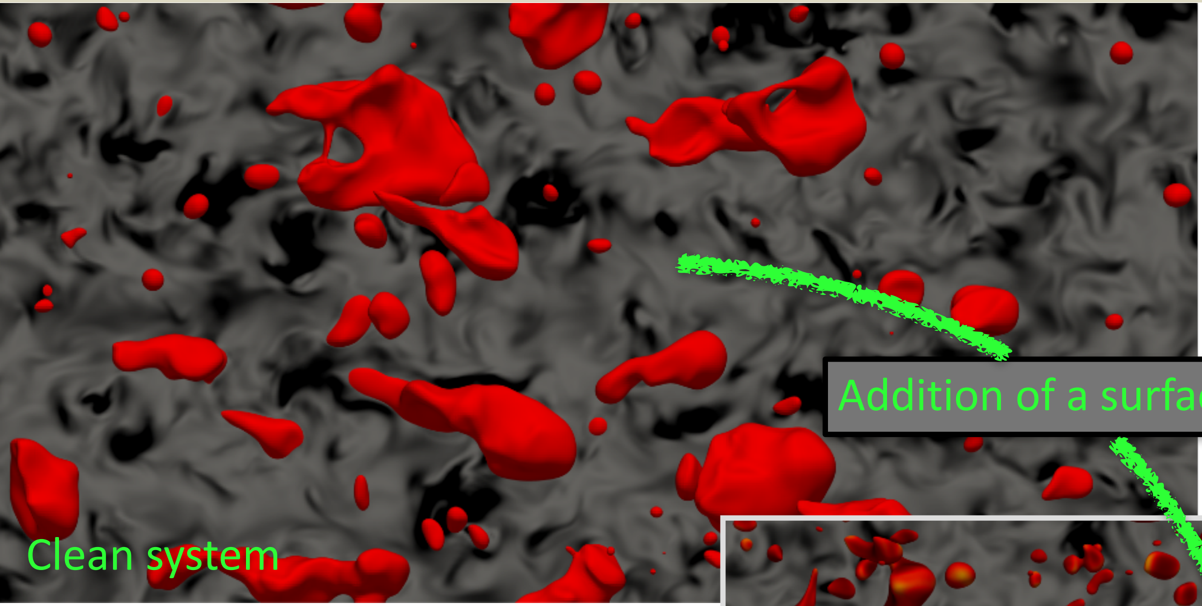
Clean droplets (no surfactant):

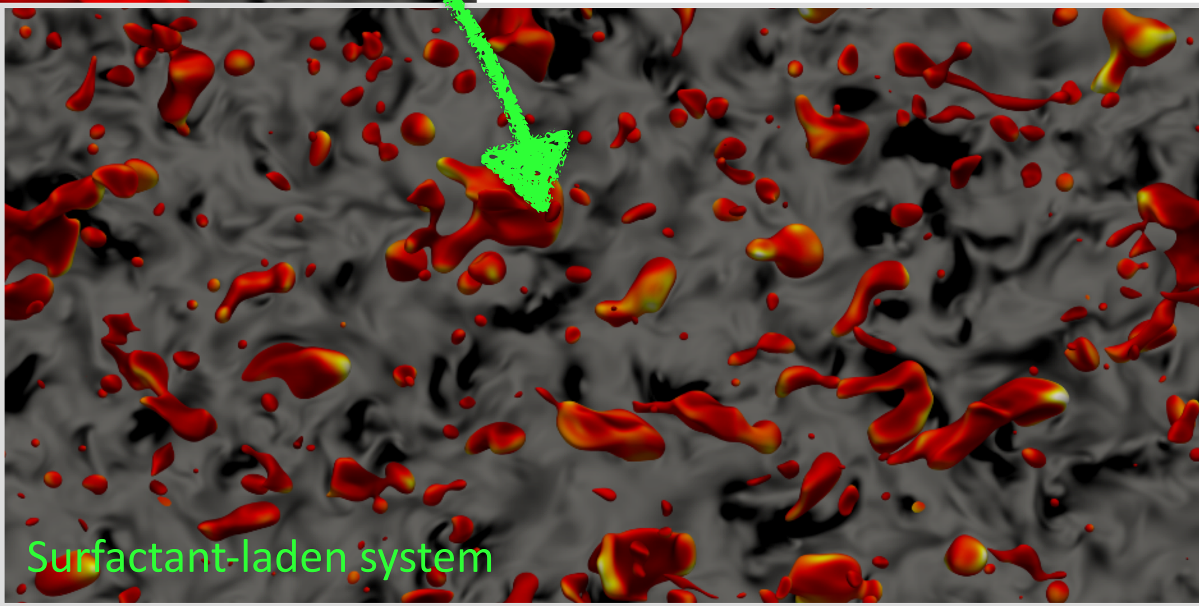


Surfactant-laden droplets:



Oil/Water emulsions with surfactants





Effects of the surfactant:

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

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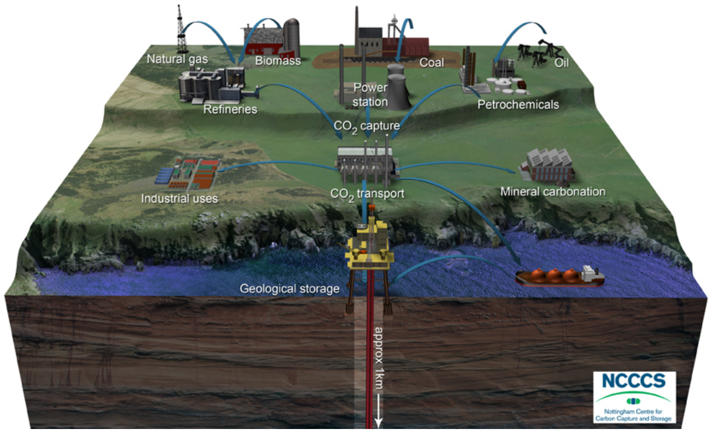
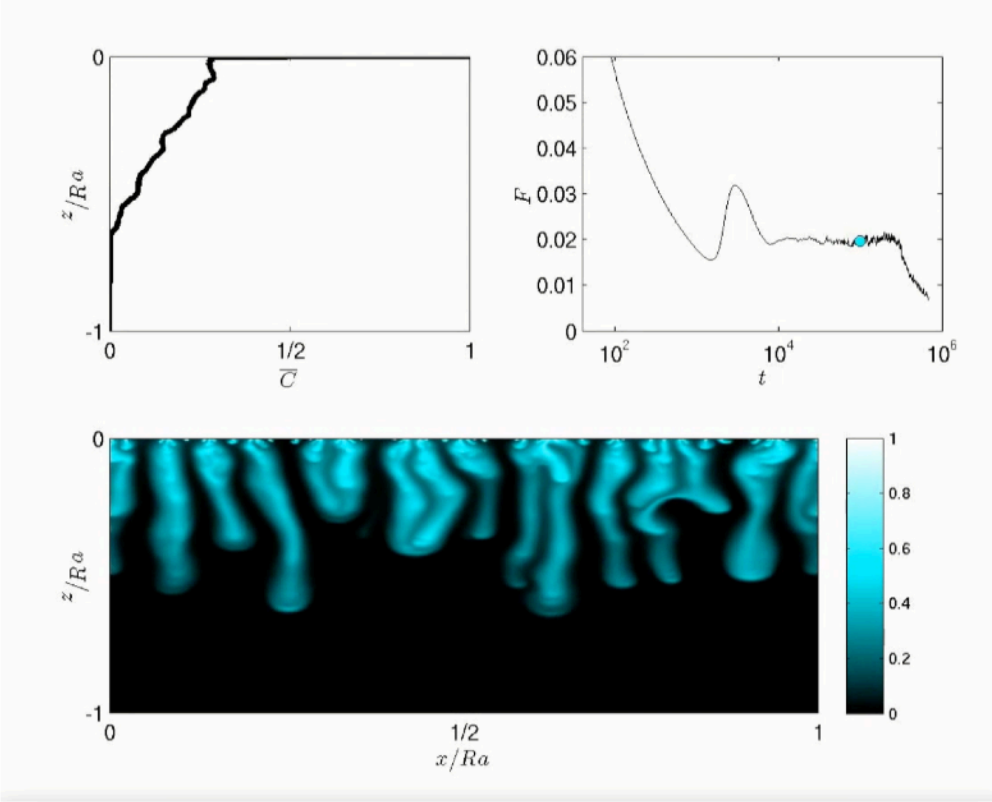
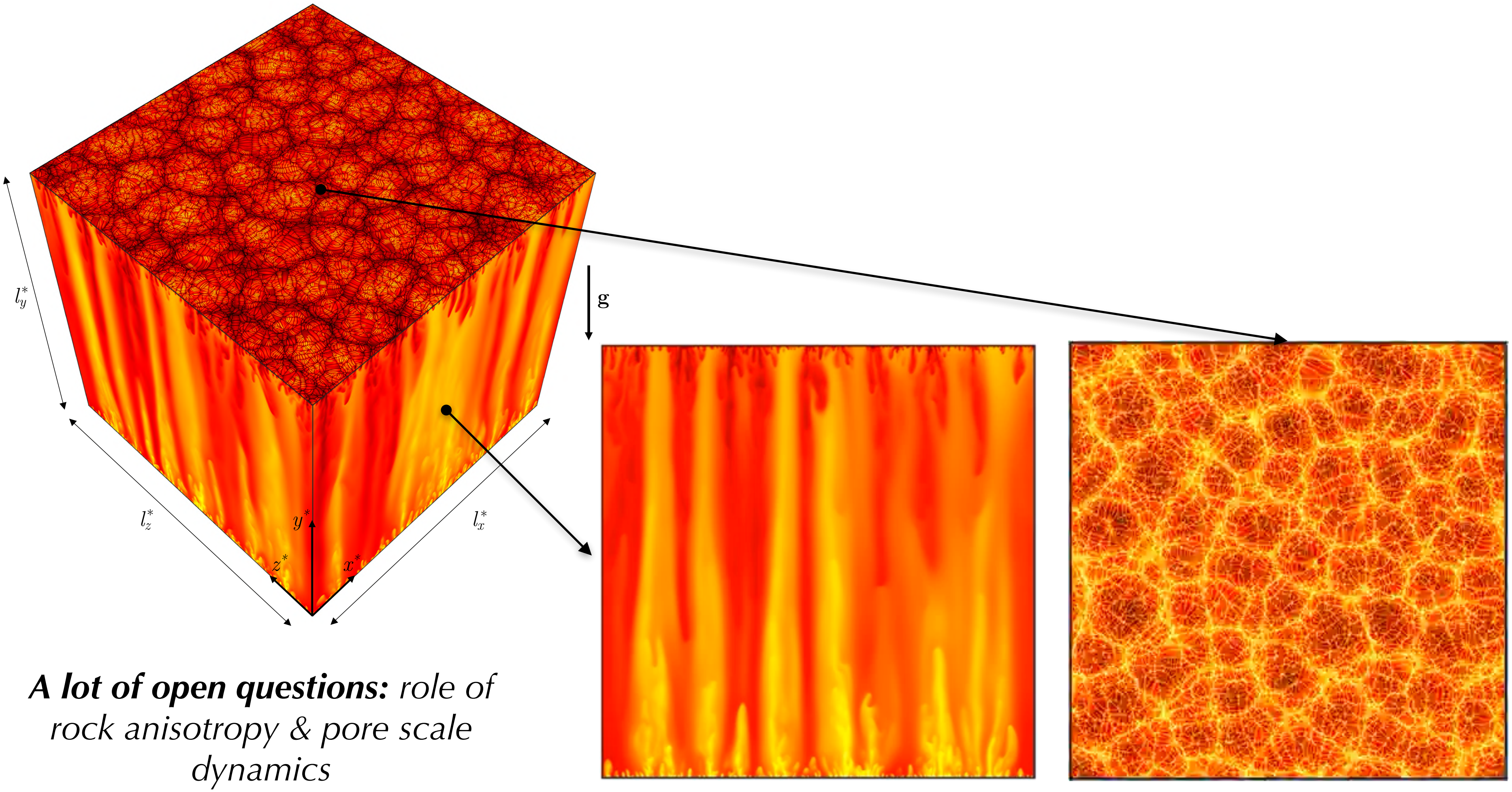


Geological CO2 sequestration



Flows in porous media

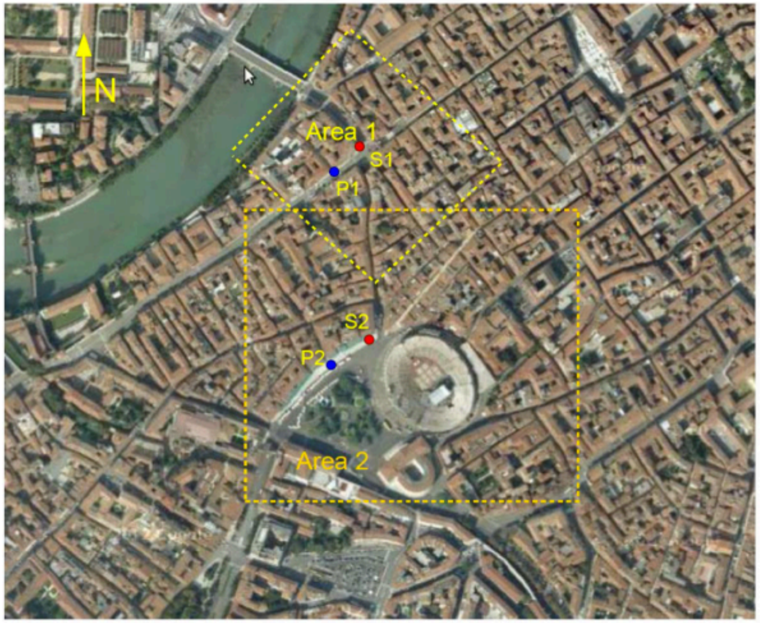


A lot of open questions: *role of rock anisotropy & pore scale dynamics*

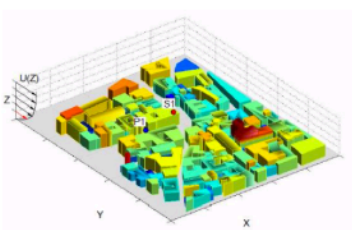
After this survey on applications, we are now ready to start with an in-depth analysis of transport process and equations…

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

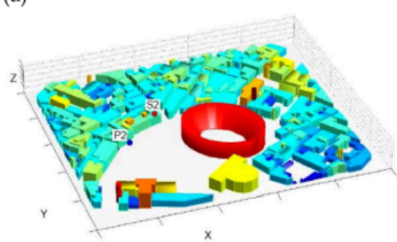
Verona Arena



(a)

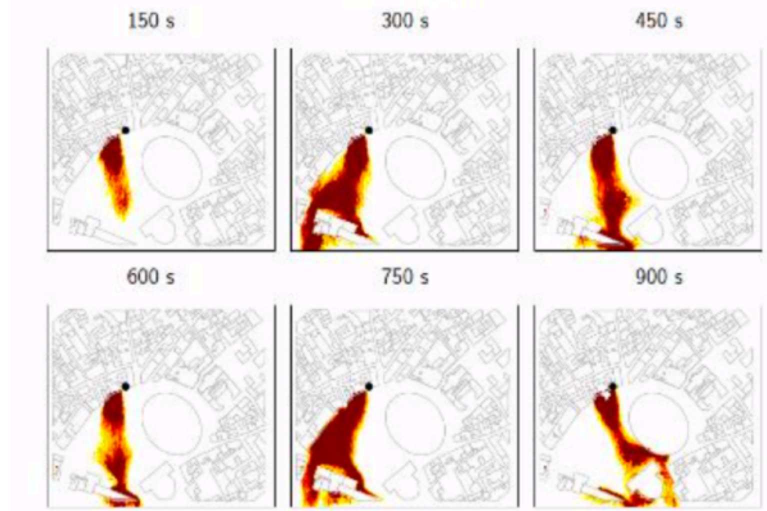


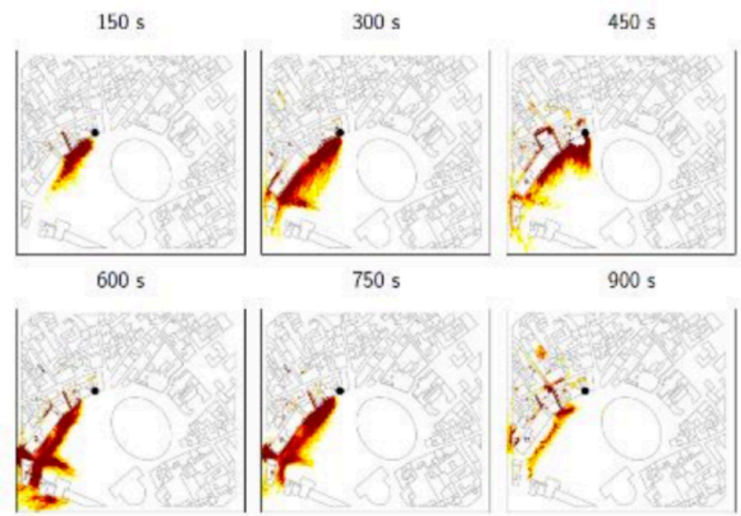
(b)



(c)

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





<u>We take it as reference!</u>

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"

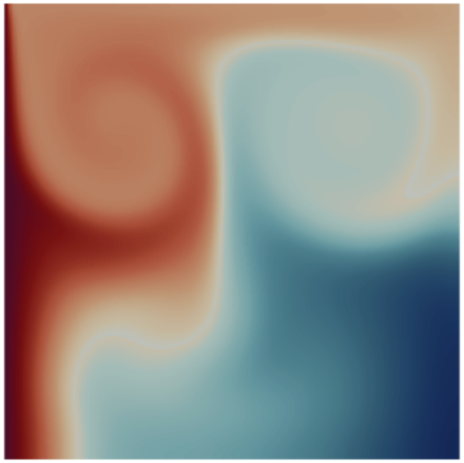
Before starting: What you will learn

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:

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

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

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

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

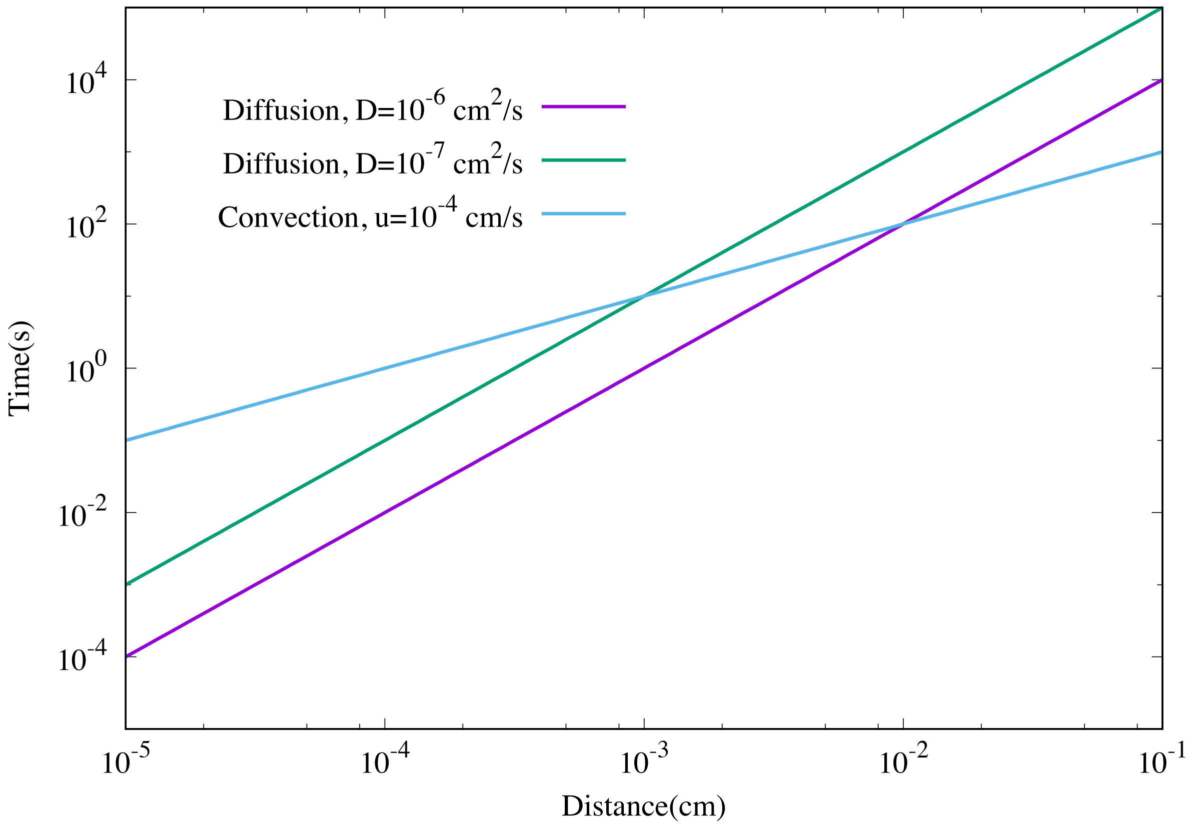
$$\boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}}$$

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

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

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

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



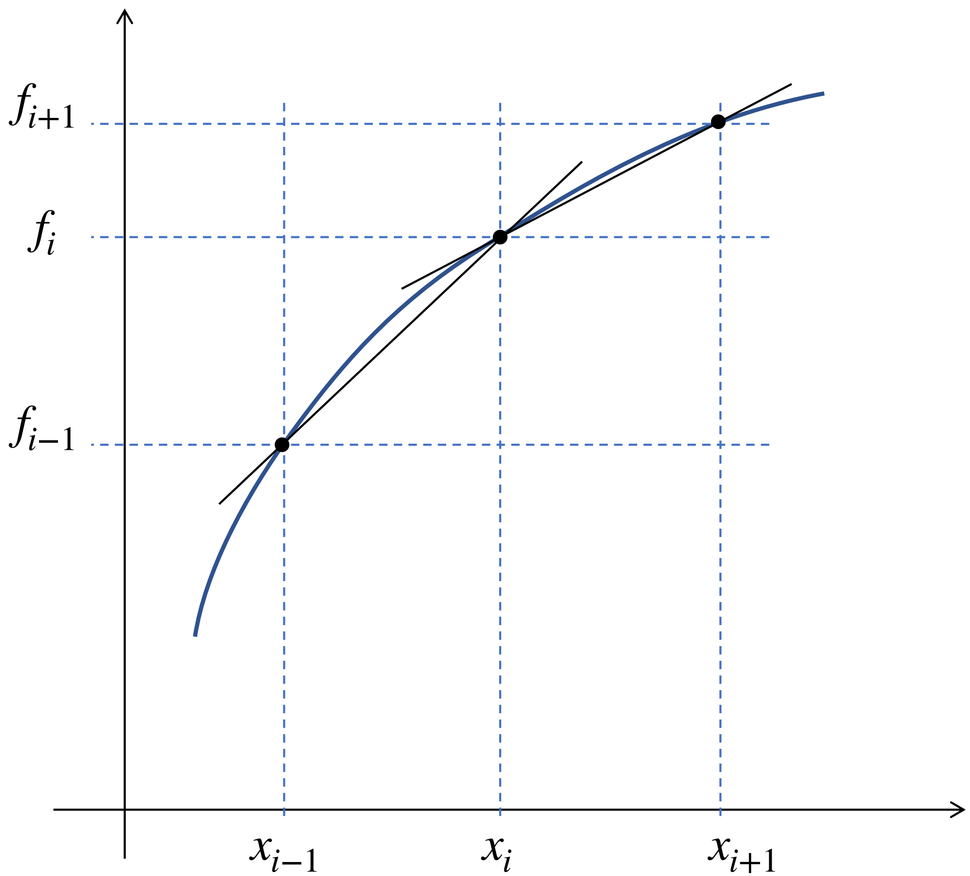
$$T_{diff} = \frac{L^2}{D}$$

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

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?

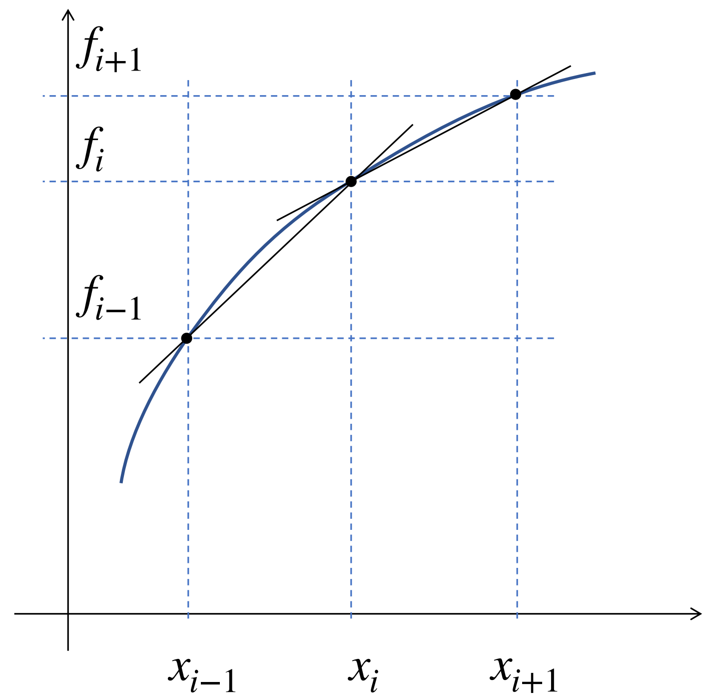
To answer: Taylor series…

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

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

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

Forward/Backward discretization=1st order!!

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

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

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

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

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

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

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

Therefore

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

$\downarrow$ 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}

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

$$+ b f_i^n$$

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

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

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

Introduction: Discretization strategy

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

Therefore, we get

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

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)

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

In dimensionless form:

$$\left\{ \begin{array}{l} C = \dfrac{C^*}{C_w} \\[2ex] x = \dfrac{x^*}{L} \\[2ex] u = \dfrac{u^*}{u_{ref}} \\[2ex] t = \dfrac{t^* D}{L^2} \end{array} \right.$$

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

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

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

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

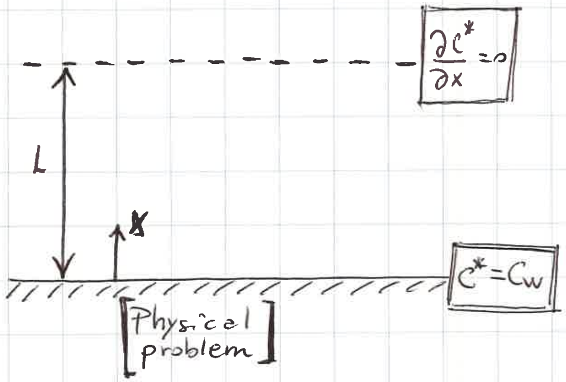
$$\boxed{\frac{\partial C}{\partial t} + Pe \cdot u \frac{\partial C}{\partial x} = \frac{\partial^2 C}{\partial x^2}}$$

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

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

Diffusion: Explicit method

We focus first on diffusion:



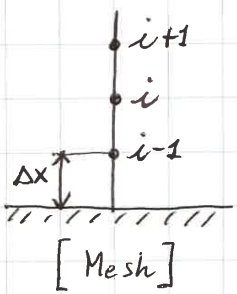
The governing equation is:

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

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

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

n=known

n+1=unknown

Therefore :

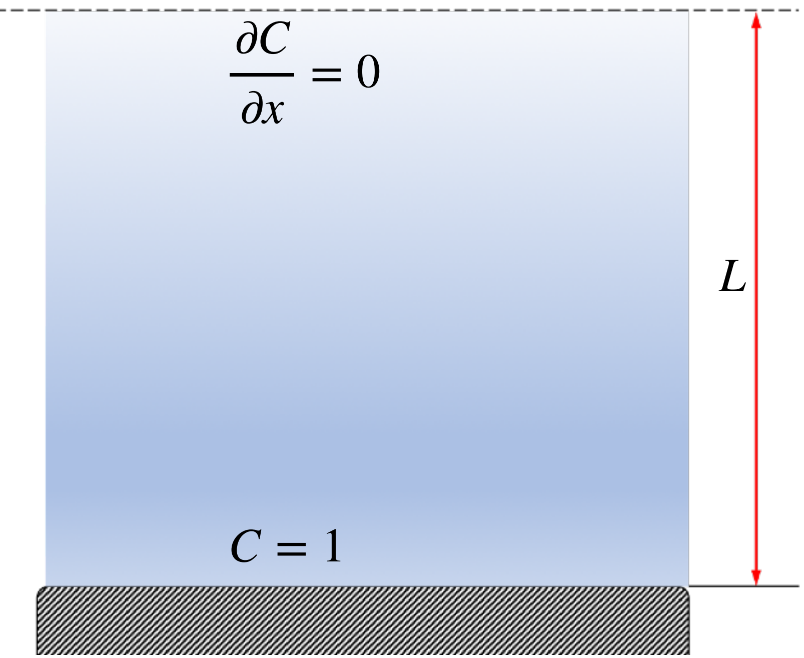
$$\boxed{C_i^{n+1} = C_i^n + \overbrace{\frac{\Delta t}{\Delta x^2}}^{S}\left(C_{i-1}^n - 2C_i^n + C_{i+1}^n\right)}$$

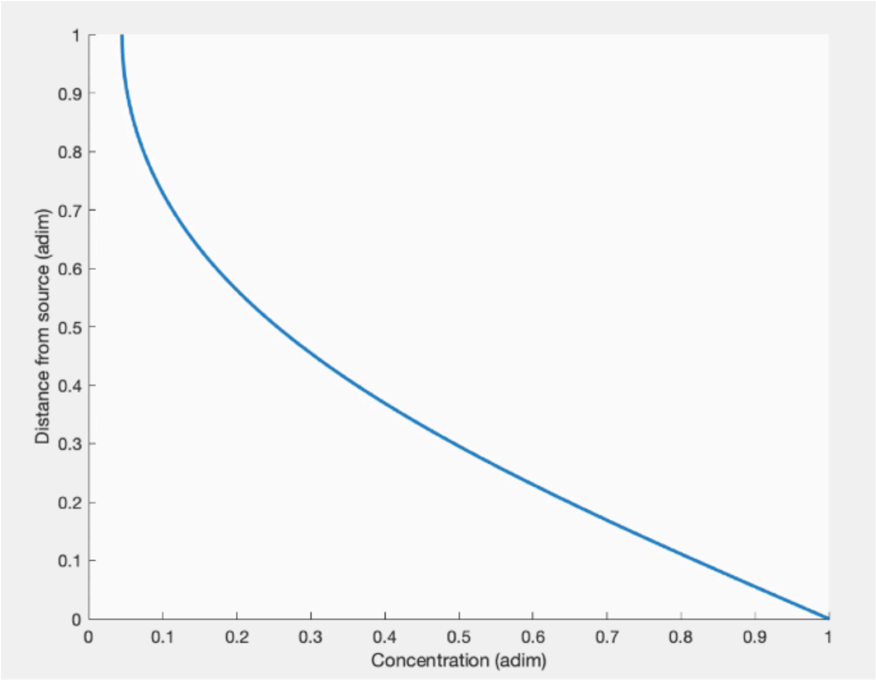
[Explicit method]

Diffusion
Explicit method, Numerical results

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

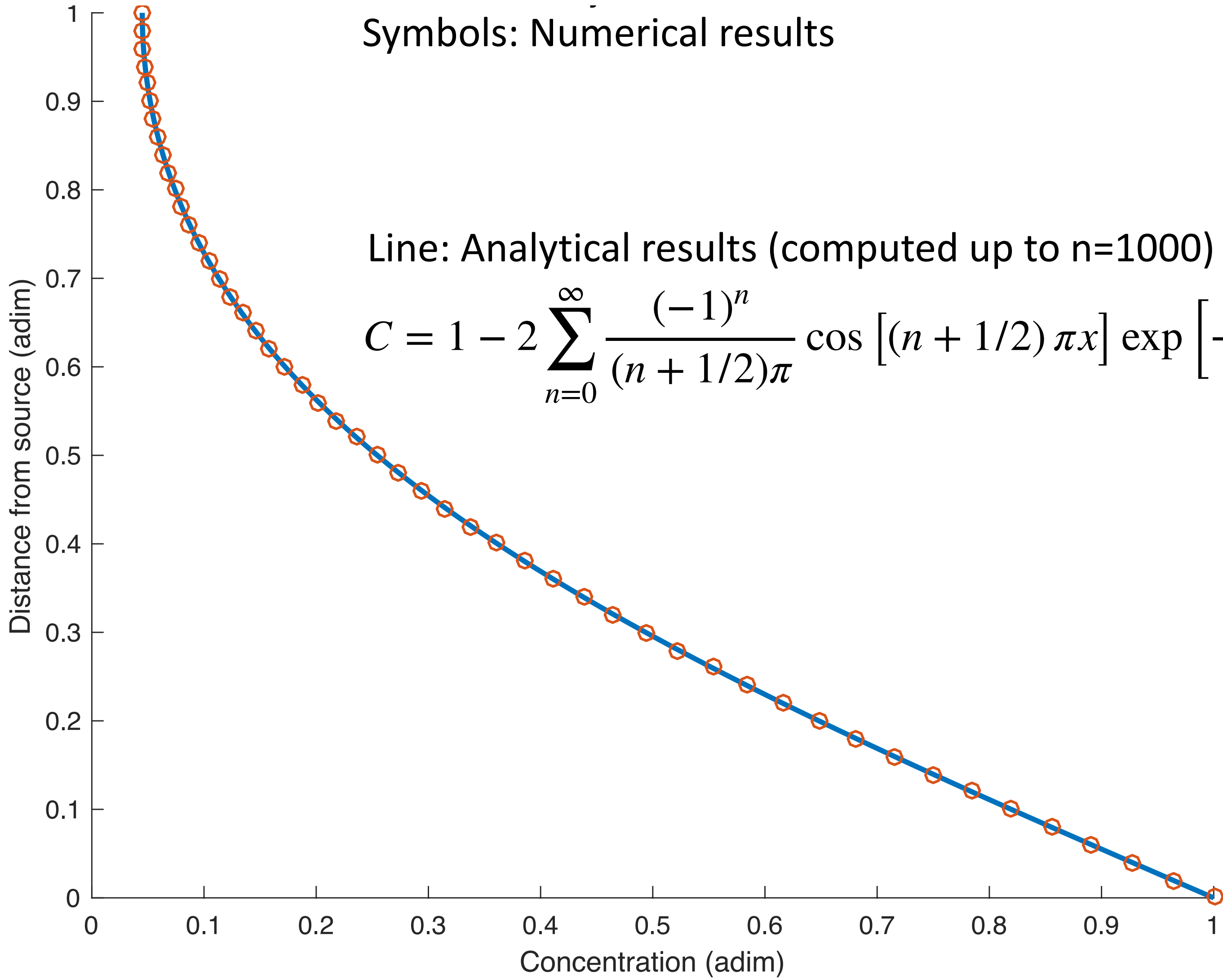
(*Note that: L=1)





Are these results good?

Diffusion
Explicit method: numerical vs analytical results



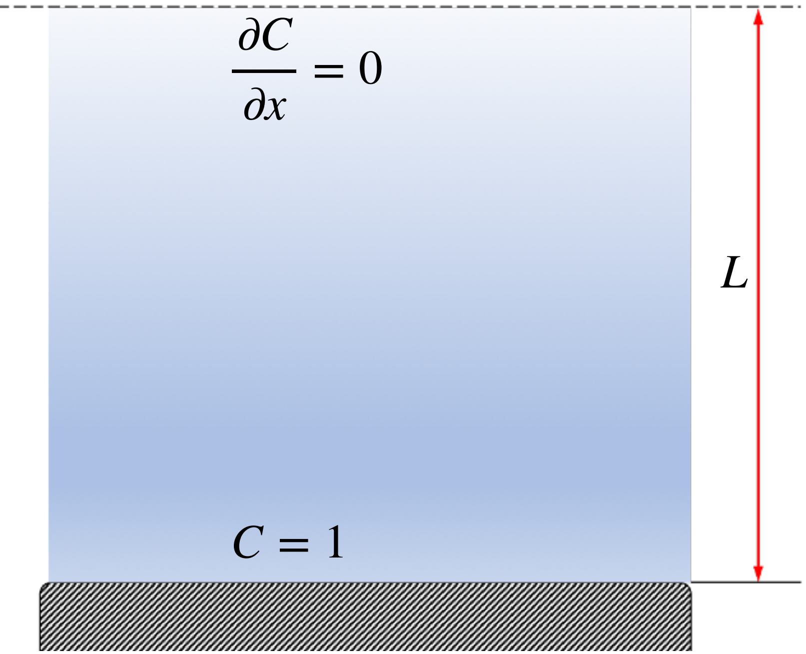
Symbols: Numerical results

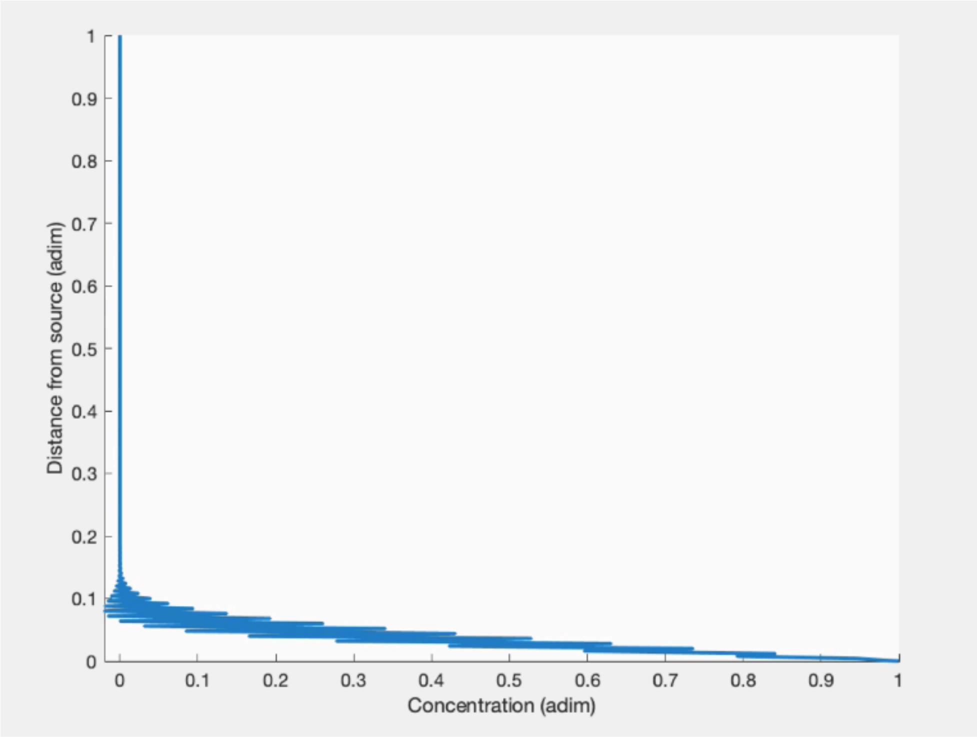
Line: Analytical results (computed up to n=1000)

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

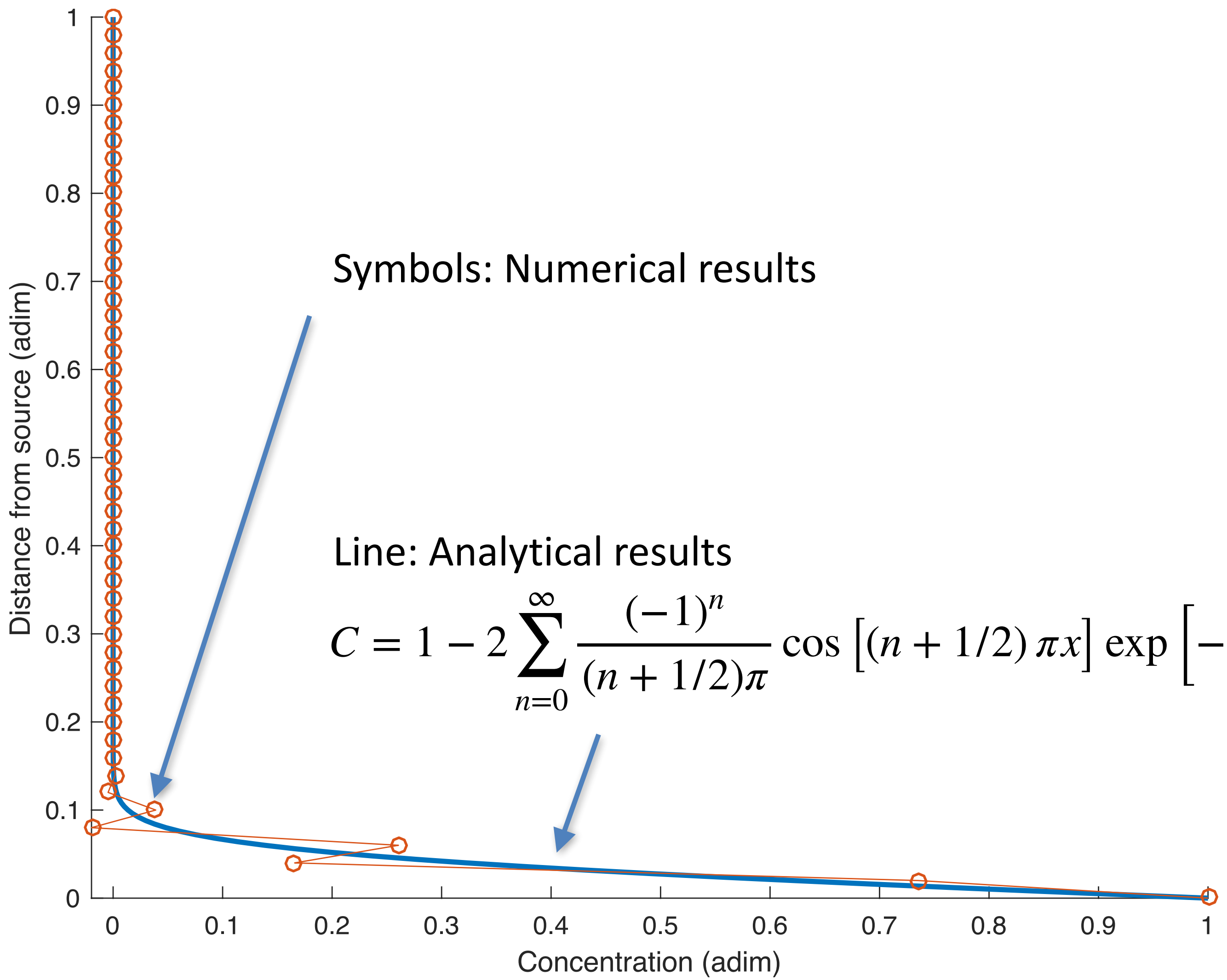
Diffusion
Explicit method: numerical results-2

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





Diffusion
Explicit method: numerical vs analytical results-2



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

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:

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

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

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

← But now we have a linear system of equations

Unknowns

Diffusion
Implicit method

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

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

[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

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

$$A = L \quad U$$

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

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

*Thomas algorithm-details

Problem A

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

$$L \cdot y = R$$

$$\Downarrow$$

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

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

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

$$\alpha_1 = a_1$$

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

$$\beta_2 = b_2$$

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

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

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

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

$$U \cdot C = y$$

Starting from the bottom:

$$C_4 = y_4$$

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

$$\vdots$$

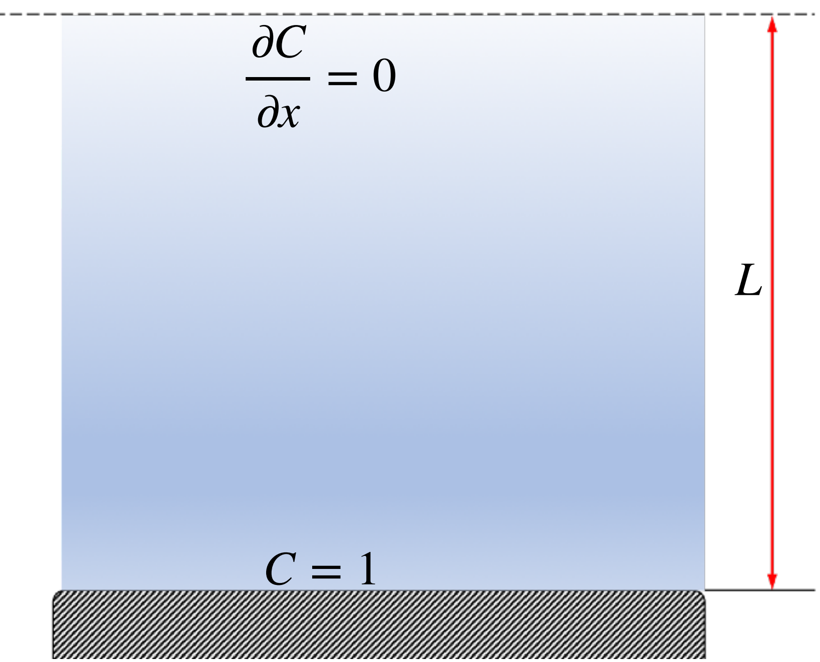
In general

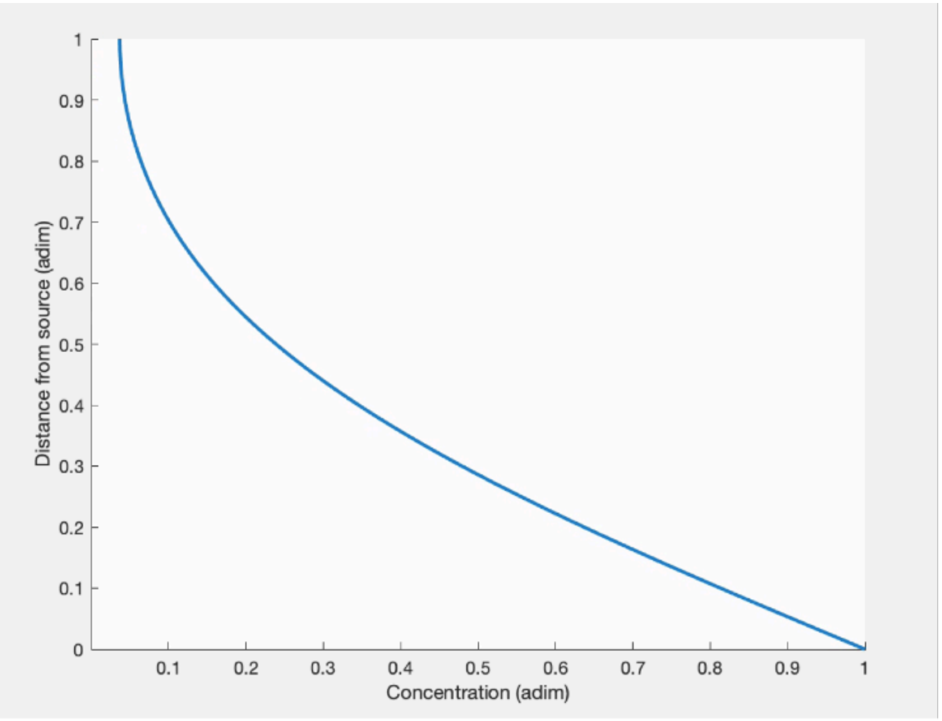
$$C_n = y_n$$

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

Diffusion
Implicit method, Numerical results

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





Diffusion
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

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

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:

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

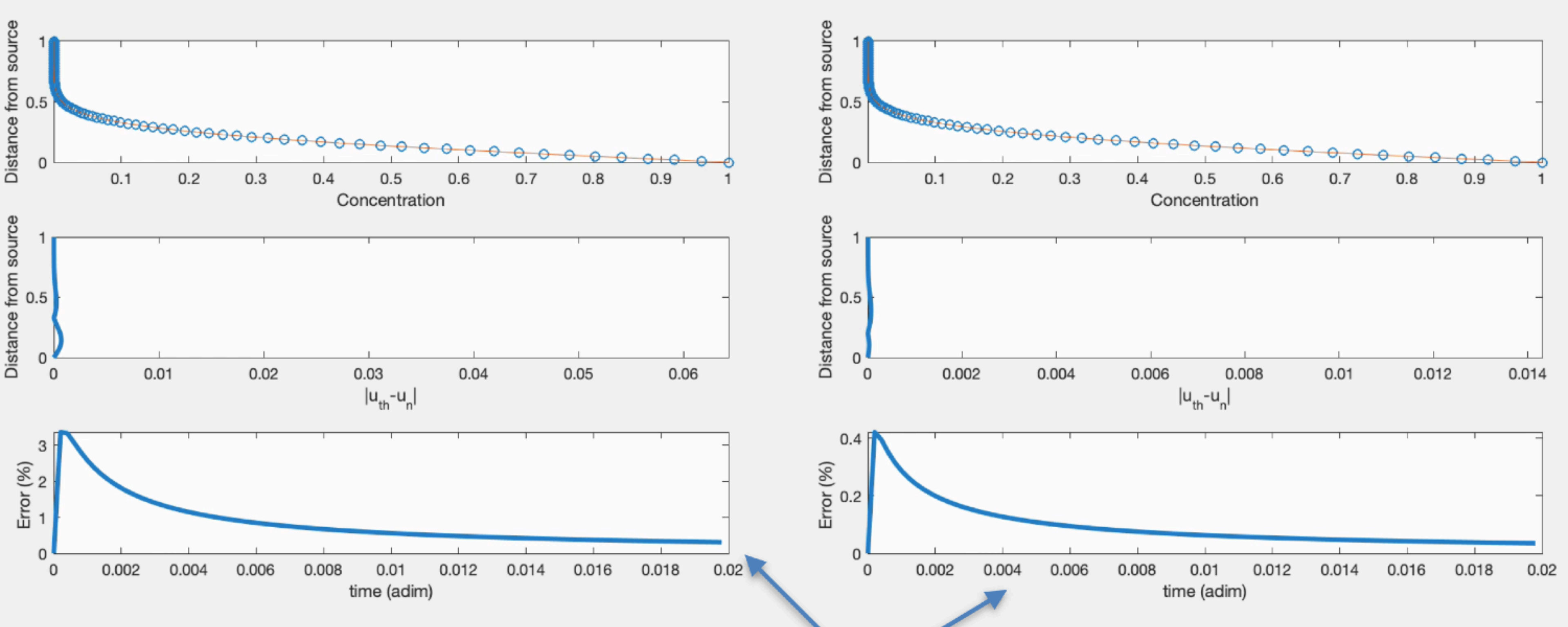
This equation can be rearranged as:

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

[Thomas algorithm]

Diffusion
Implicit method: 1st vs 2nd order

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

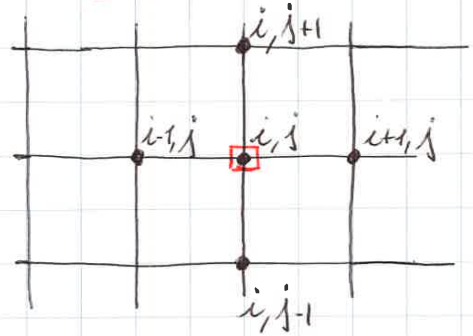


1st Order

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:

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

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)

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:

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

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

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

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

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

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

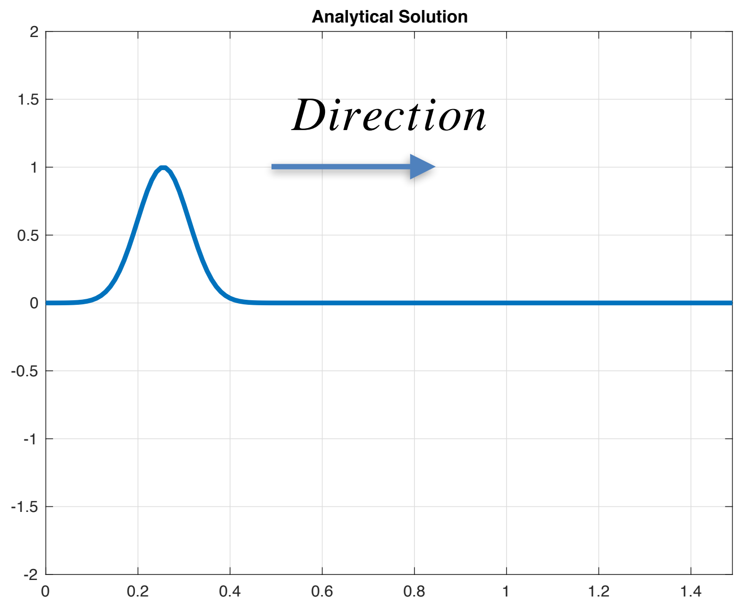
$Pe \gg 1 \Rightarrow$ **Advection dominates** $\rightarrow \boxed{\dfrac{\partial C}{\partial t} + Pe \cdot u \dfrac{\partial C}{\partial x} = 0}$

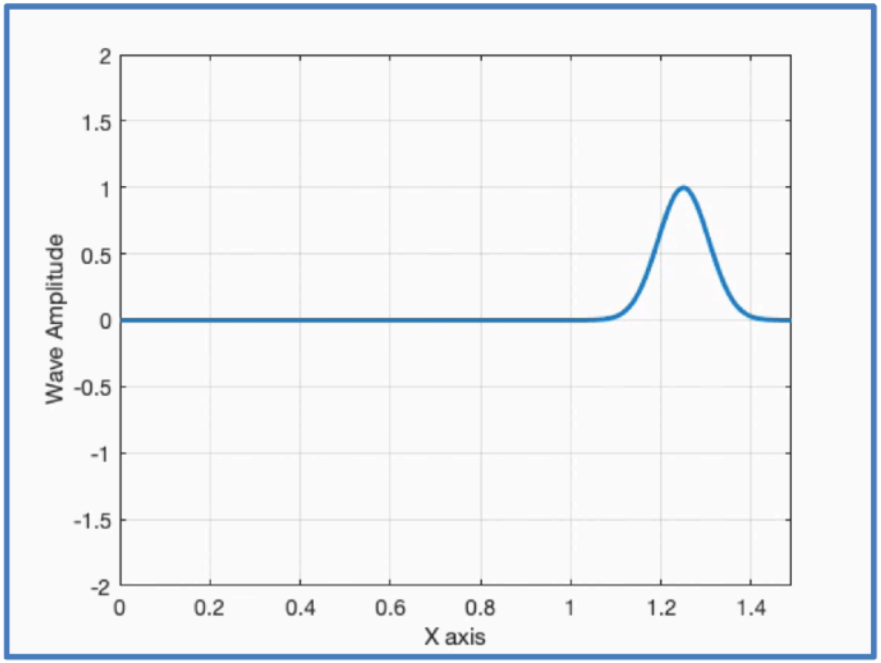
Advection: Introduction

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

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 proved 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:

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

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

$$G = 1 - Co(1-\cos\theta) - i\,Co\sin\theta \rightarrow |G| = 1 + \overbrace{(1-\cos\theta)}^{>0}(Co-1)\overbrace{2Co}^{>0} \;\Big|\rightarrow \boxed{Co \leq 1}$$

(small Δt)

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

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

We get:

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

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

Advection: Accuracy

Finally

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

We focus now on the error:

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

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

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

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

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

We have obtained the following expression

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

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

$$\underbrace{\frac{U\Delta x}{2}(1 - C_0)}_{\alpha' = \text{Numerical viscosity or diffusivity}}$$

Therefore, the equation we are going to solve is:

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

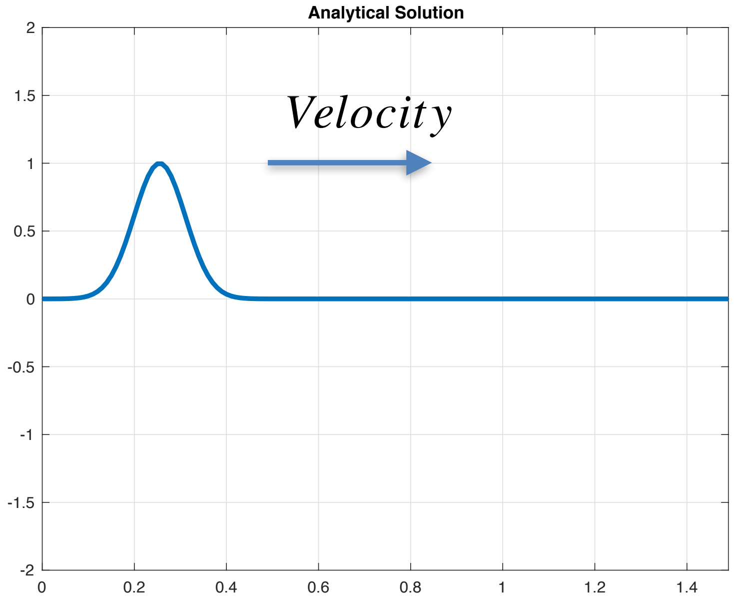
With the additional constraint that $C_0 \leq 1$, obtained from stability considerations (but also expected...)

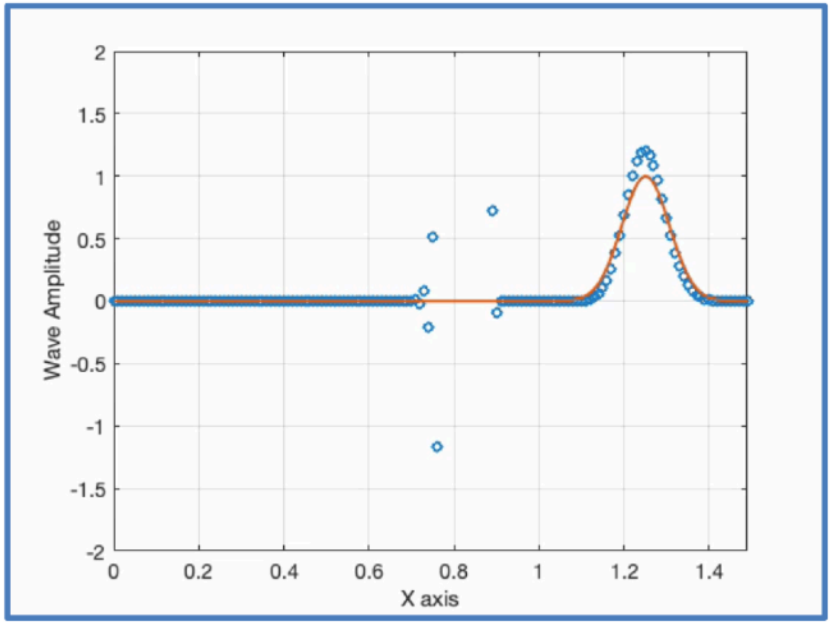
Advection
Numerical Results

Discretized equation

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

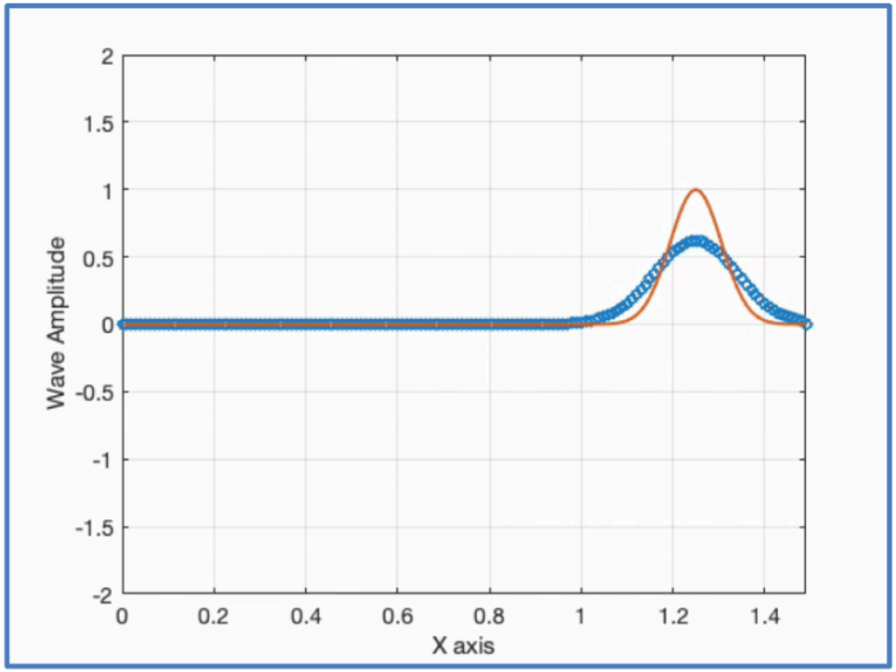
We first see what happens when $Co = 1.1$

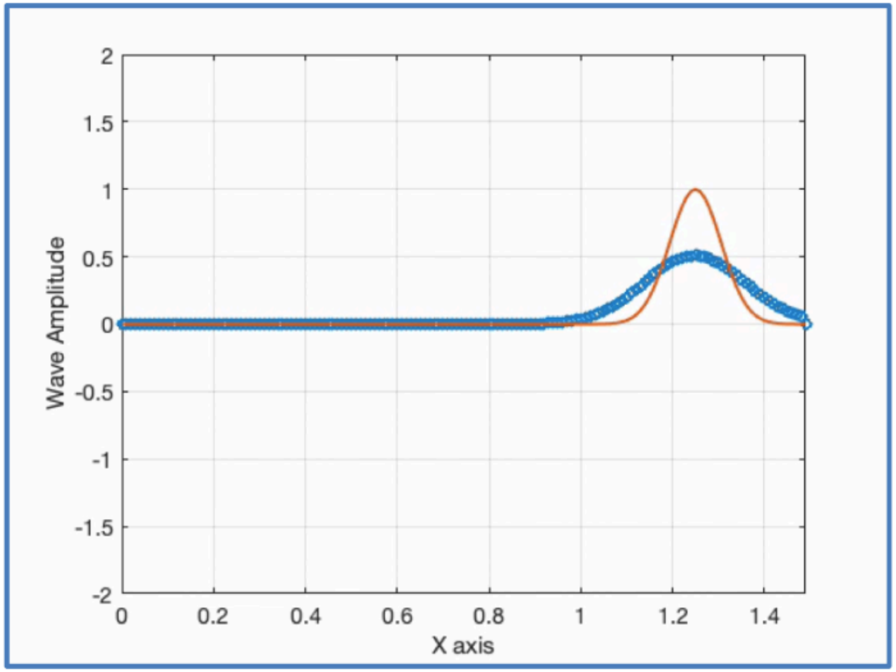




As expected…

Now we reduce the Courant number



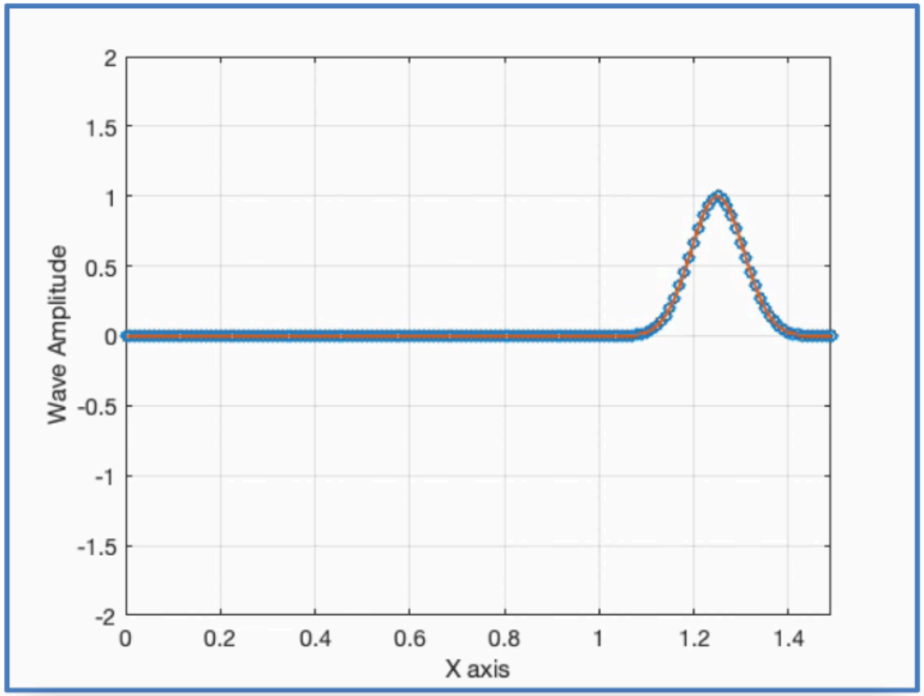


$Co = 0.5$ $\qquad$ $Co = 0.1$

Advection Numerical Results

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

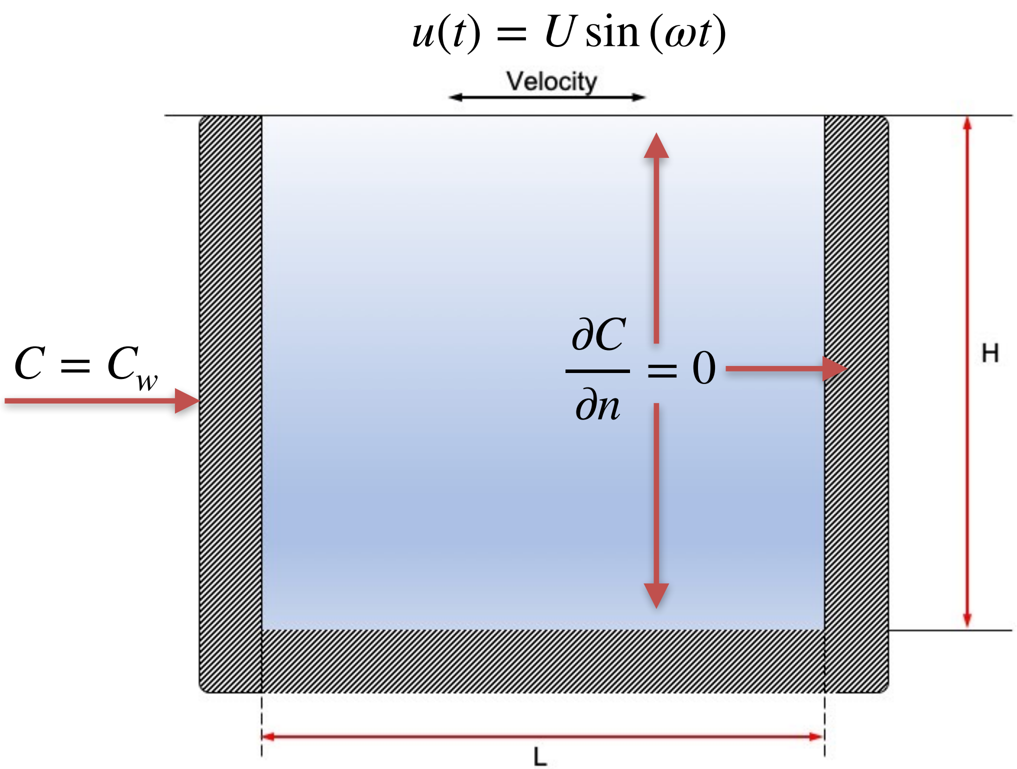
Looking at the truncation error: $$\epsilon = \frac{U\Delta x}{2}(1 - Co)\left[\frac{\partial^2 C}{\partial x^2}\right]$$



$$Co = 1$$

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

The full problem: Physics



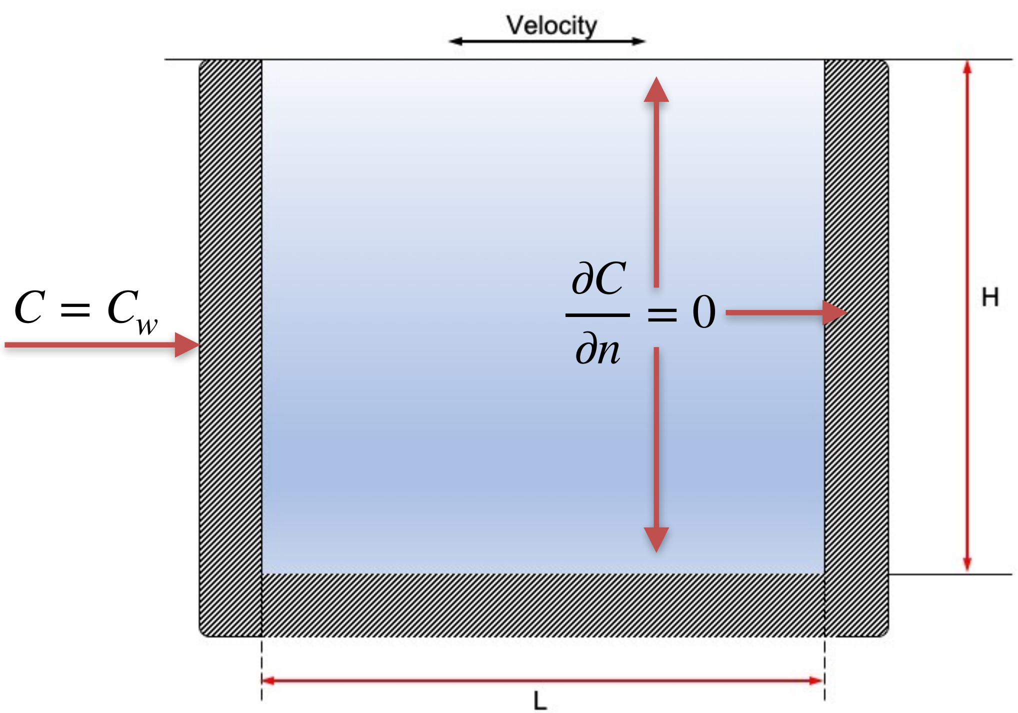
Governing equations

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

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

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)

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

Riemann

Vorticity

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

*Curl(NS)

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 $\partial/\partial x(B)$

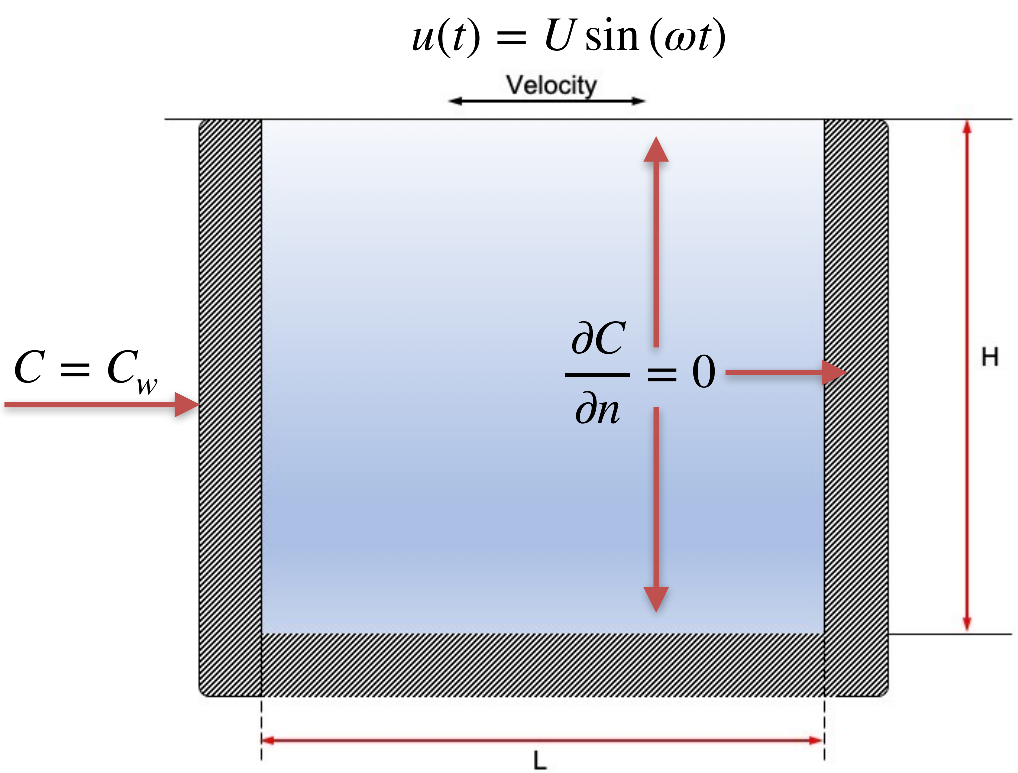
$$u_{ty} + u_y u_x + uu_{xy} + v_y u_y + vu_{yy} = -P_{xy} + \mu\nabla^2 u_y \qquad (C)$$

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

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.

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

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

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

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

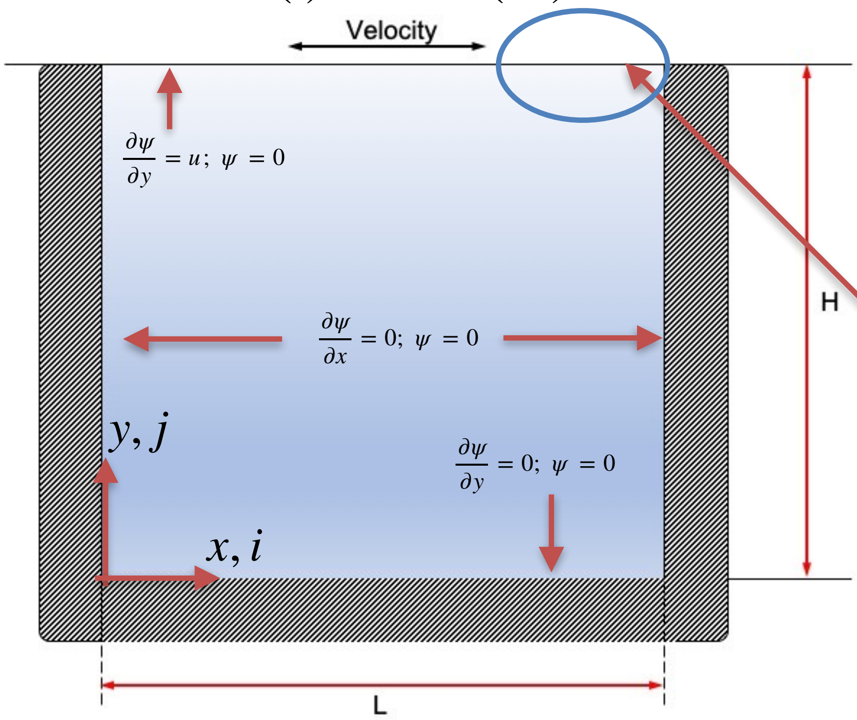
Explicit

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

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 from the knowledge of ψ^{n+1}

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

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

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

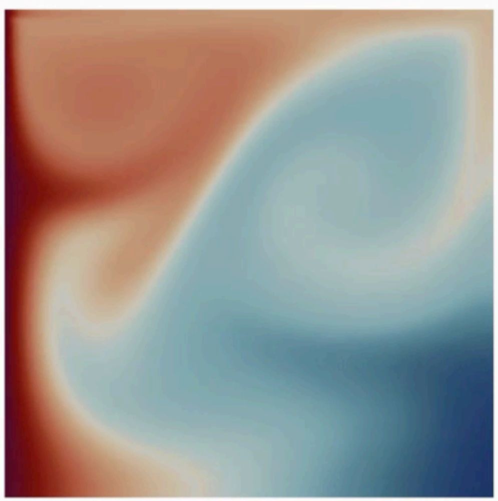
$$\omega_{i,M} = \frac{1}{2\Delta x^2}\left(8\psi_{i,M-1} - \psi_{i,M-2}\right) + \frac{3u}{\Delta y}$$

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

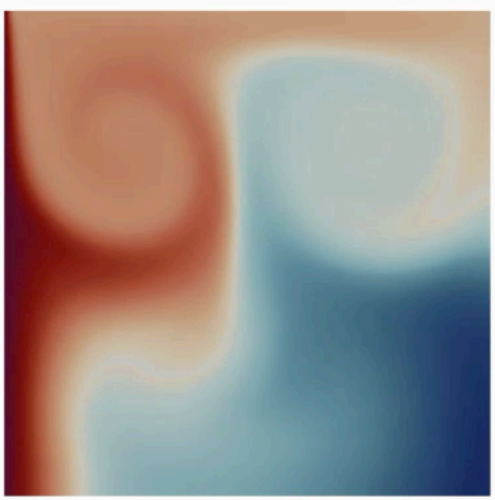
The full problem: Numerics

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

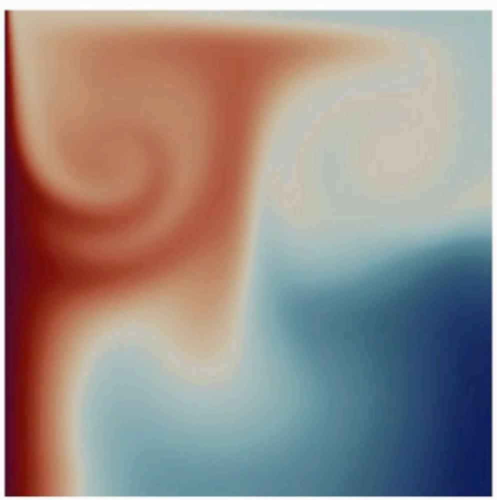
$$u(t) = U \sin\left(\frac{t}{3}\right)$$



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



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



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)