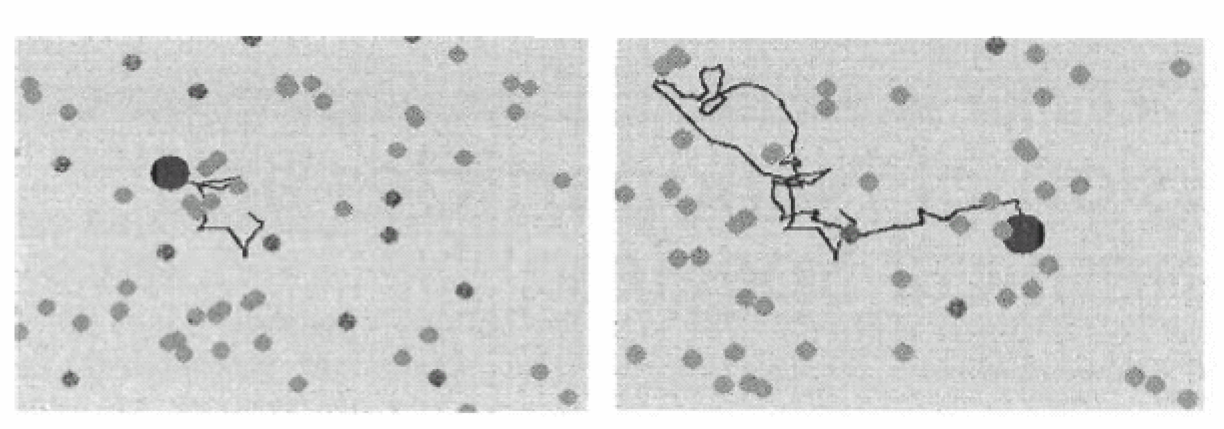
Lecture 8

Flow and Diffusion. Computational flow analysis. Introduction to COMSOL. Multiphysics modelling with COMSOL

Brownian motion

- discovered by R. Brown and J.Ingenhous by observation of pollen grains floating on water



- macroscopic (concentration) and microscopic approach to diffusion

Macroscopic approach to diffusion

- First Fick's law

$$J = -D\nabla c$$

- Second Fick's law

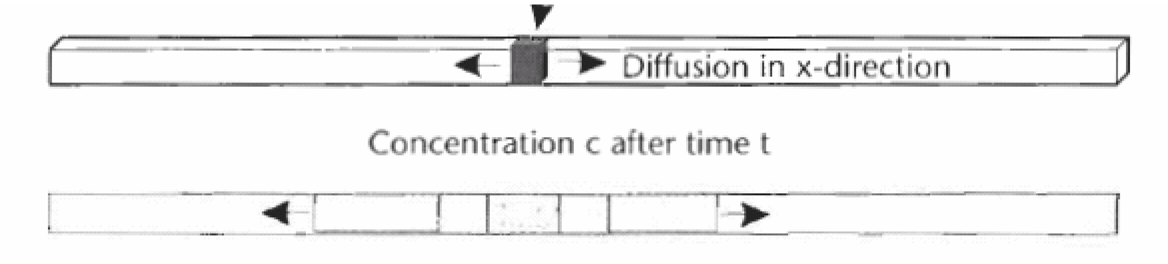
$$\frac{\partial c}{\partial t} = D\Delta c + S$$

source/sink term

- Einstein formula

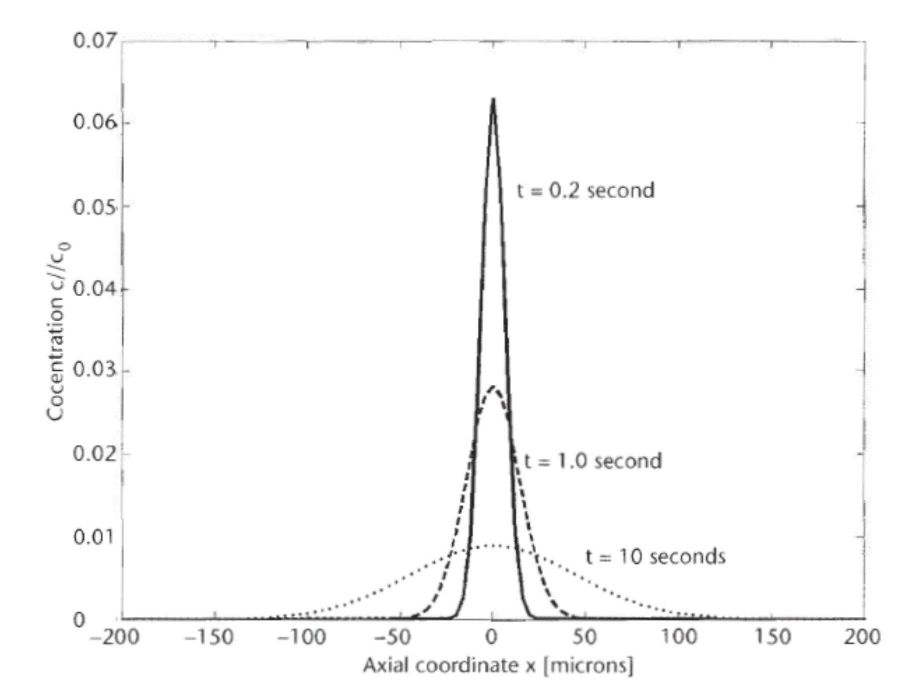
$$D = \frac{kT}{C_D} \qquad D = \frac{kT}{6\pi\eta R}$$

Spreading from a point source in 1D



- solution:

$$c(x,t) = \frac{c_0}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$



Ilkovic's solution

- <u>Problem:</u> consider a half-space with an initial concentration c_0. Concentration on the wall is zero at any time. Find the concentration profile vs time.

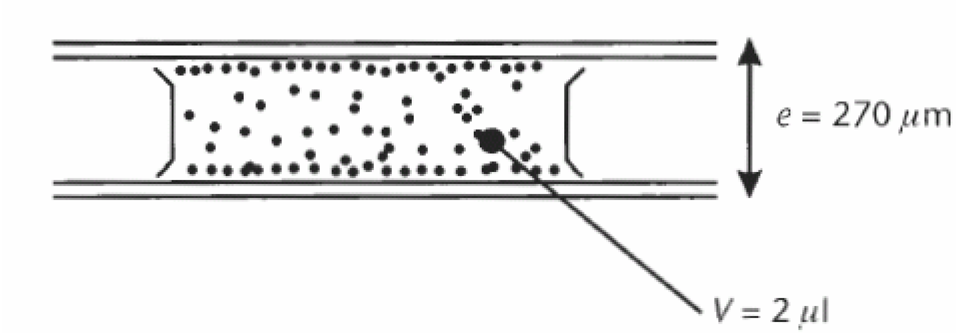
$$c = c_0 erf\left(\frac{x}{\sqrt{4Dt}}\right) \qquad erf(x) = \frac{2}{\sqrt{\pi}}\int_0^\infty e^{-u^2}du$$

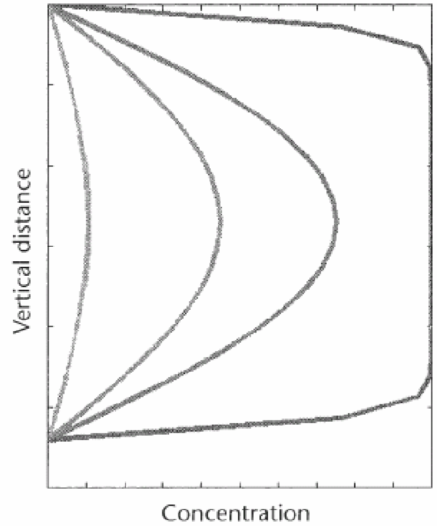
$$\frac{\partial c}{\partial x} = c_0 \frac{2}{\sqrt{\pi}} e^{-\frac{x^2}{4Dt}} \frac{1}{\sqrt{4Dt}}$$

$$J = -D\nabla c_{|wall} = -c_0\sqrt{\frac{D}{\pi t}}$$

Example: diffusion between two plates

- A liquid drop contains nanoparticles that are immobilized upon contact with the walls. Find the concentration dependence vs time

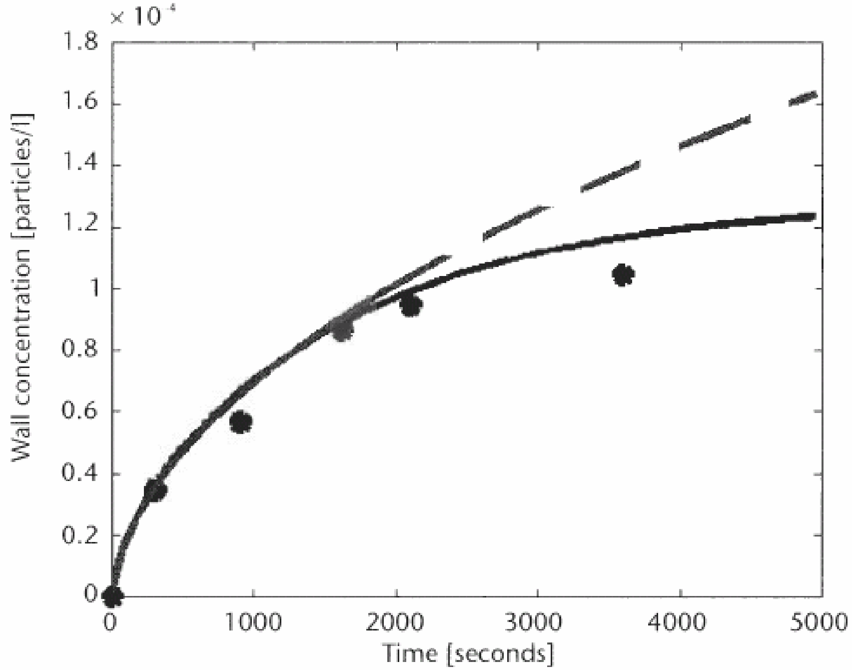




- For times less than $\tau = \dfrac{e/2}{4D}$

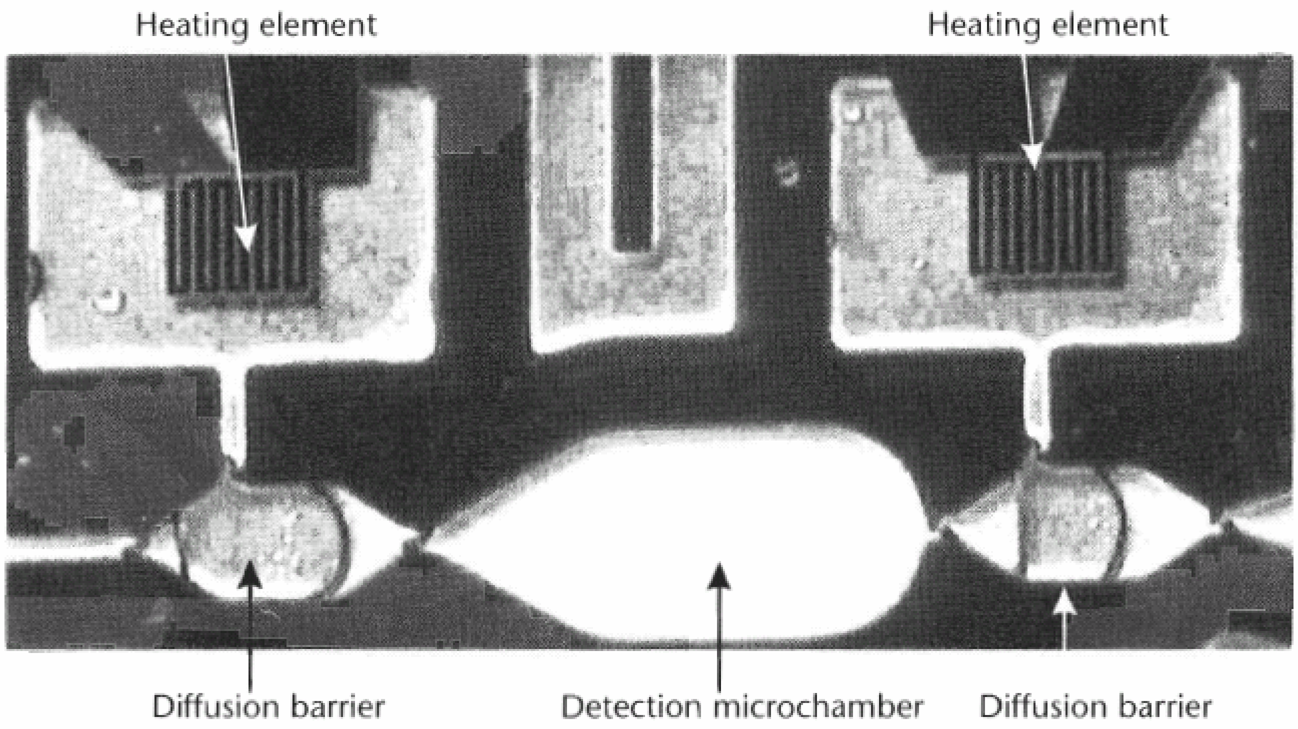
Ilkovic’s solution can be used:

$$J = -2c_0\sqrt{\frac{D}{\pi t}}$$

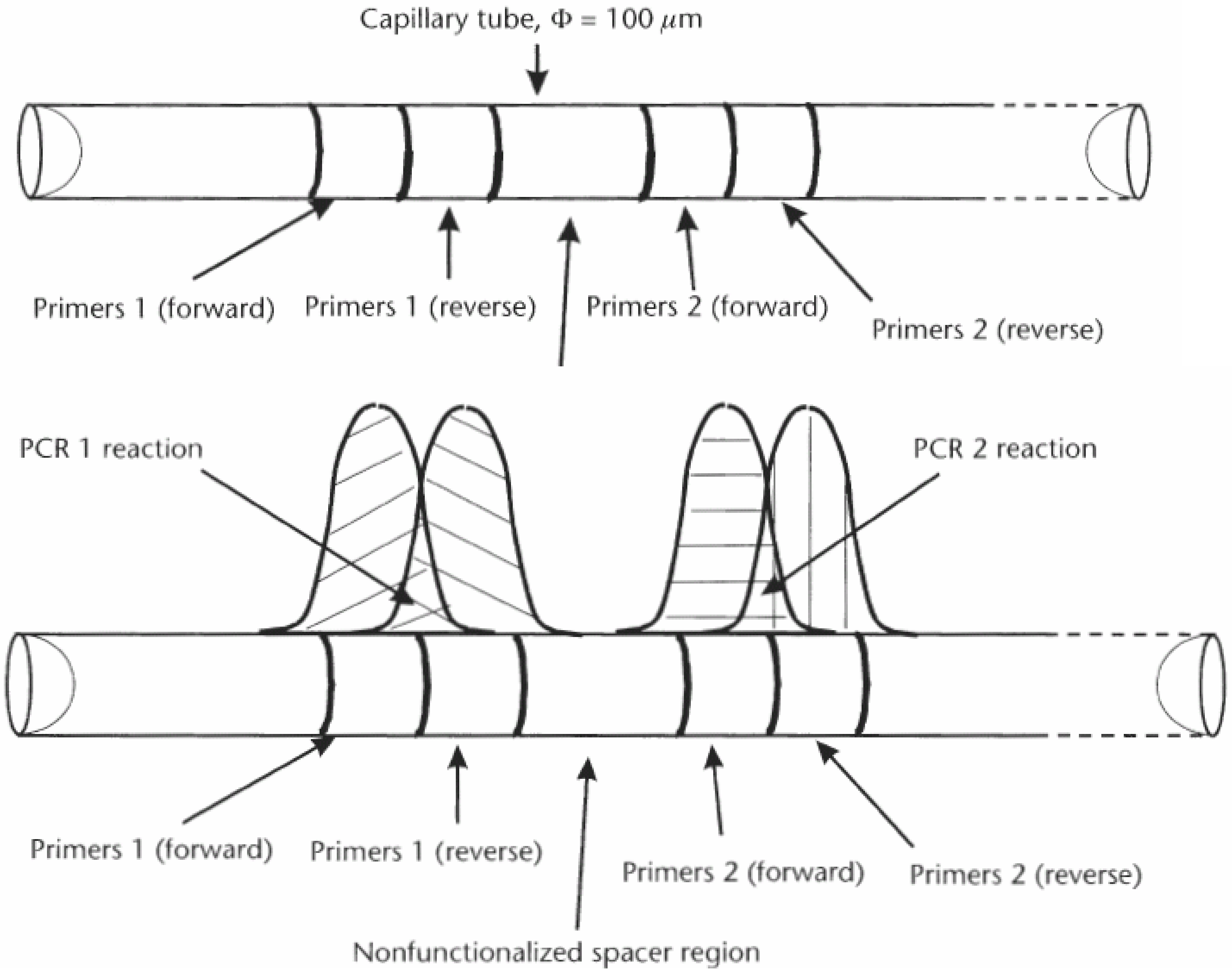


Diffusion inside a microchamber

- Problem: a PCR reaction on chip is designed such that DNA strand are brought inside a microchamber (e.g. with magnetic beads) and let them diffuse to hybridize on labeled surface



Example: Simultaneous PCRs in a capillary



Example: Simultaneous PCRs in a capillary

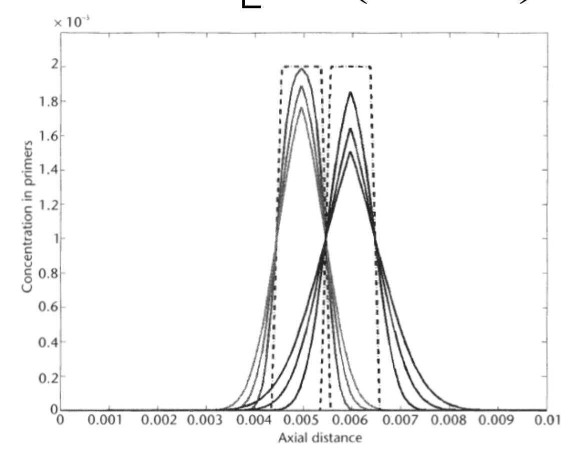
- The system has two characteristic times: diffusion across the capillary and axial diffusion

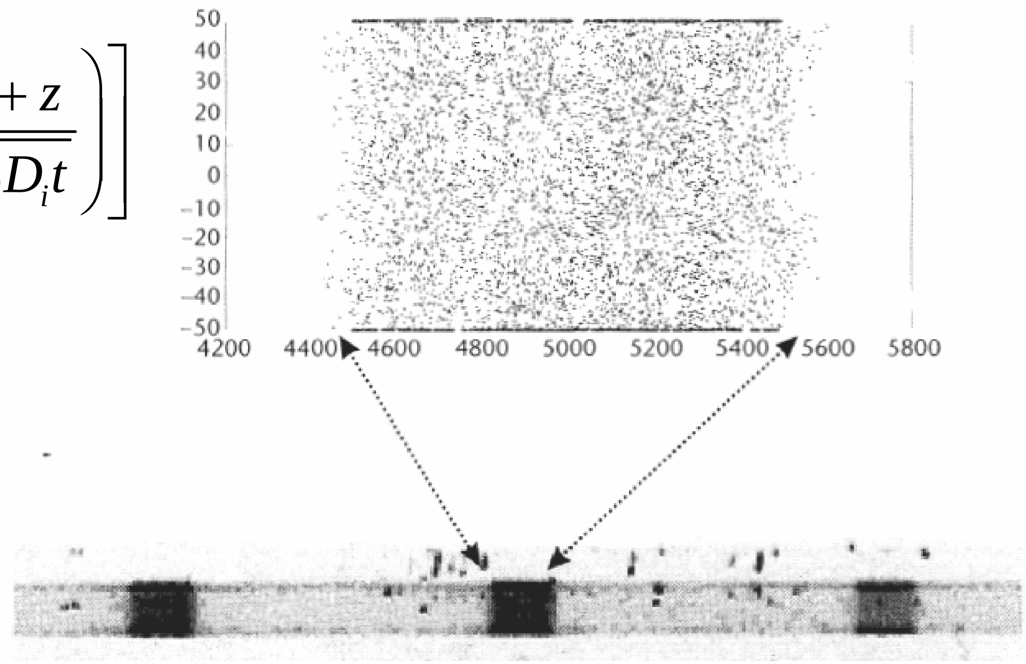
$$\tau \approx \frac{R^2}{4D} \qquad \text{D}=10^{-10}\ \text{m}^2/\text{s, R}=50\ \mu\text{m} \quad \Rightarrow \quad \tau = 6\ \text{s}$$

- After time t uniform concentration across the capillary is achieved.

$$\frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial z^2}$$

$$c_i = \frac{1}{2} c_{0,i} \left[erf\left(\frac{a_i - z}{\sqrt{4D_i t}} \right) + erf\left(\frac{a_i + z}{\sqrt{4D_i t}} \right) \right]$$





Diffusion vs Sedimentation

Does the gravity force affects the diffusion?

- Let's compare diffusion and sedimentation time across a microfluidic chamber
- sedimentation time:

$$C_D V_s = 6\pi\eta R_H V_s = \Delta\rho g \cancel{V}_p$$

$$V_s = \frac{2}{9}\frac{\Delta\rho g R^2}{\eta}$$

$$\tau_1 = d / V_s$$

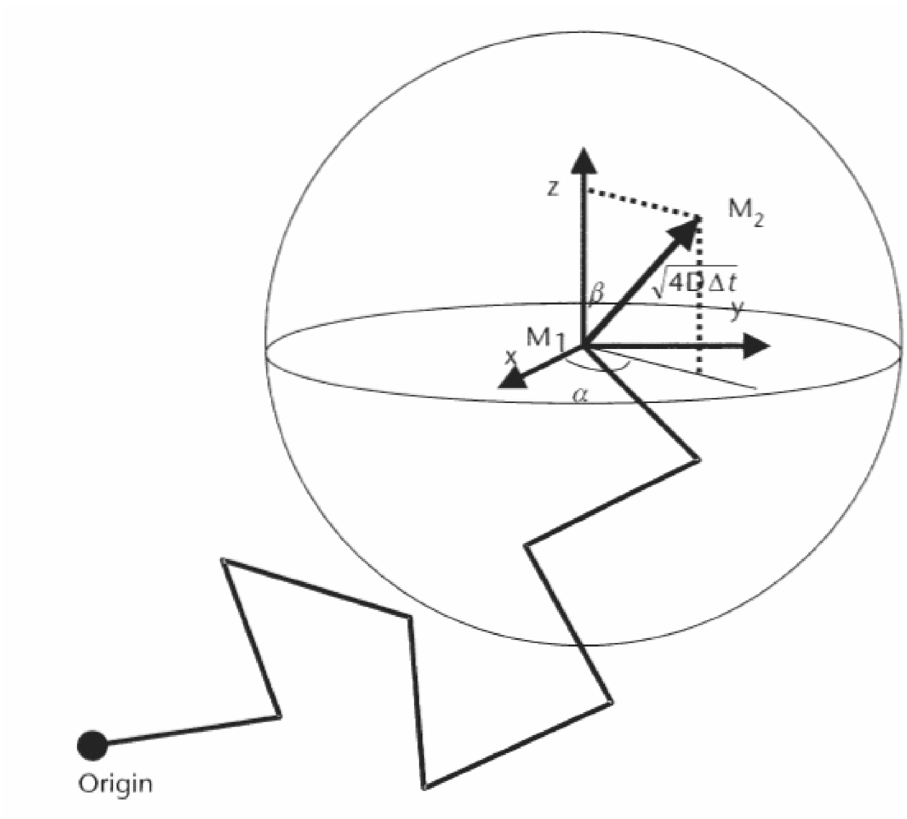
- diffusion time: $\tau_2 = \dfrac{d^2}{4D}$

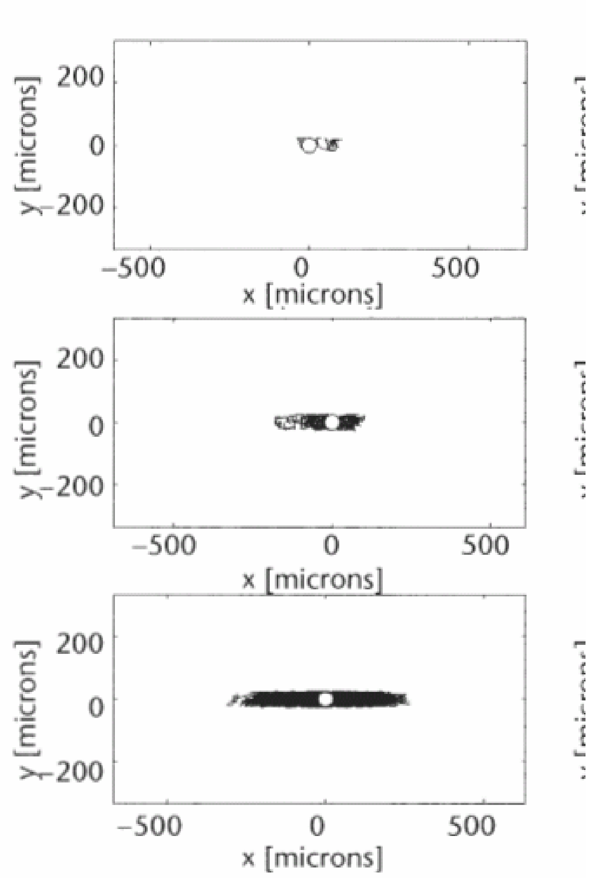
$$\beta = \frac{\tau_1}{\tau_2} = \frac{d}{V_s}\frac{4D}{d^2} = 4\frac{kT}{\Delta mg}\frac{1}{d}$$

- if β<<1 sedimentation dominates

Random walk

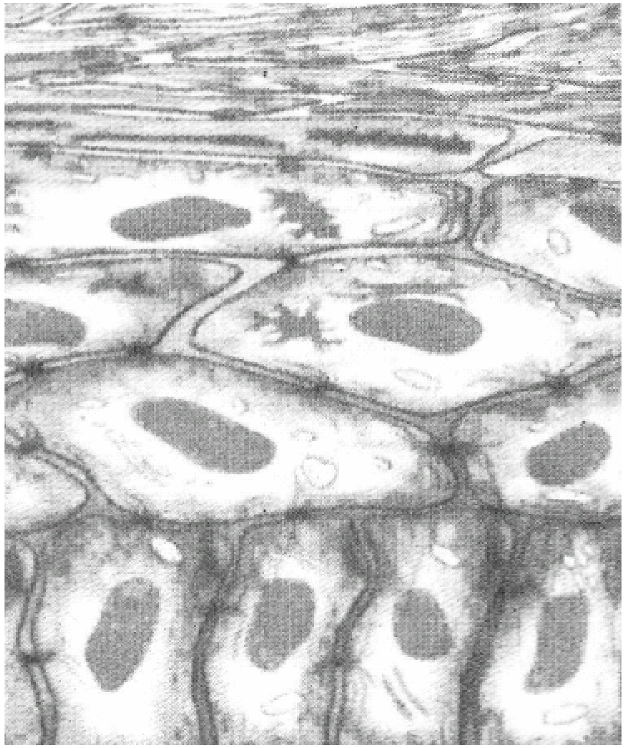
- Diffusion can be modeled as a random walk using Monte-Carlo simulation



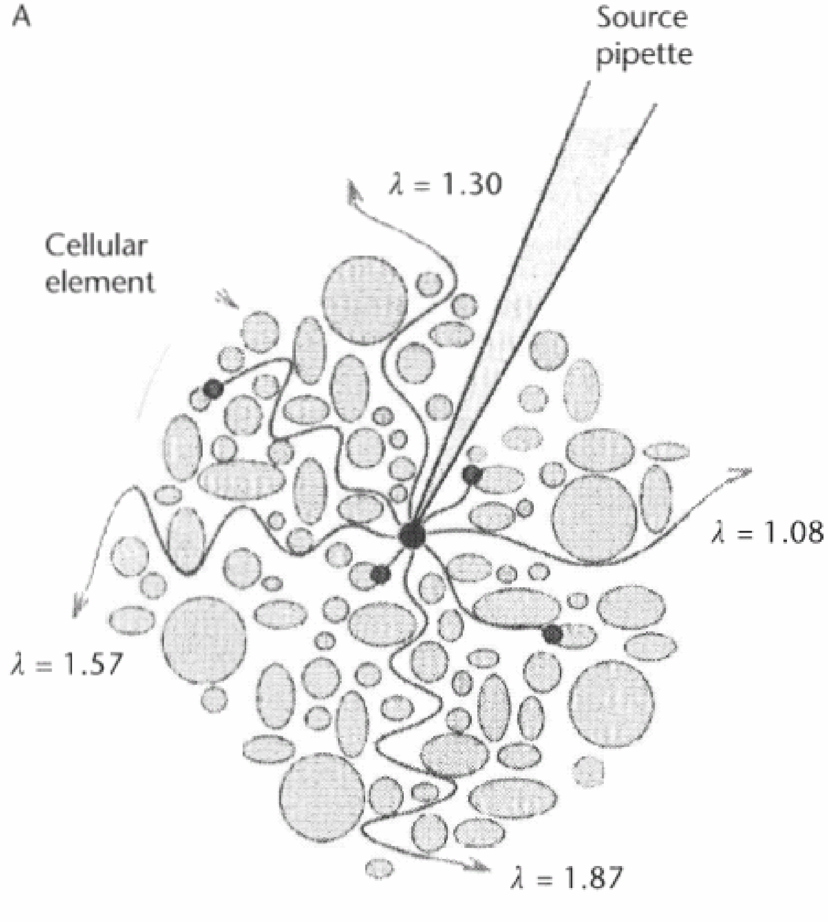


Diffusion in confined volumes

- For example, delivery of drugs relies on a diffusion in ECS of cellular clusters



cell arrangement in the human skin

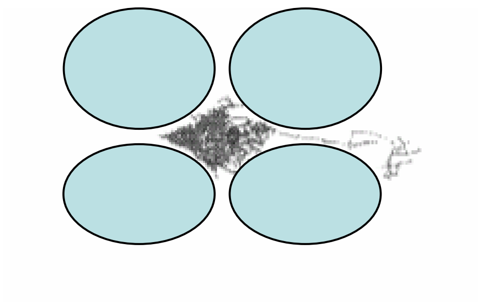


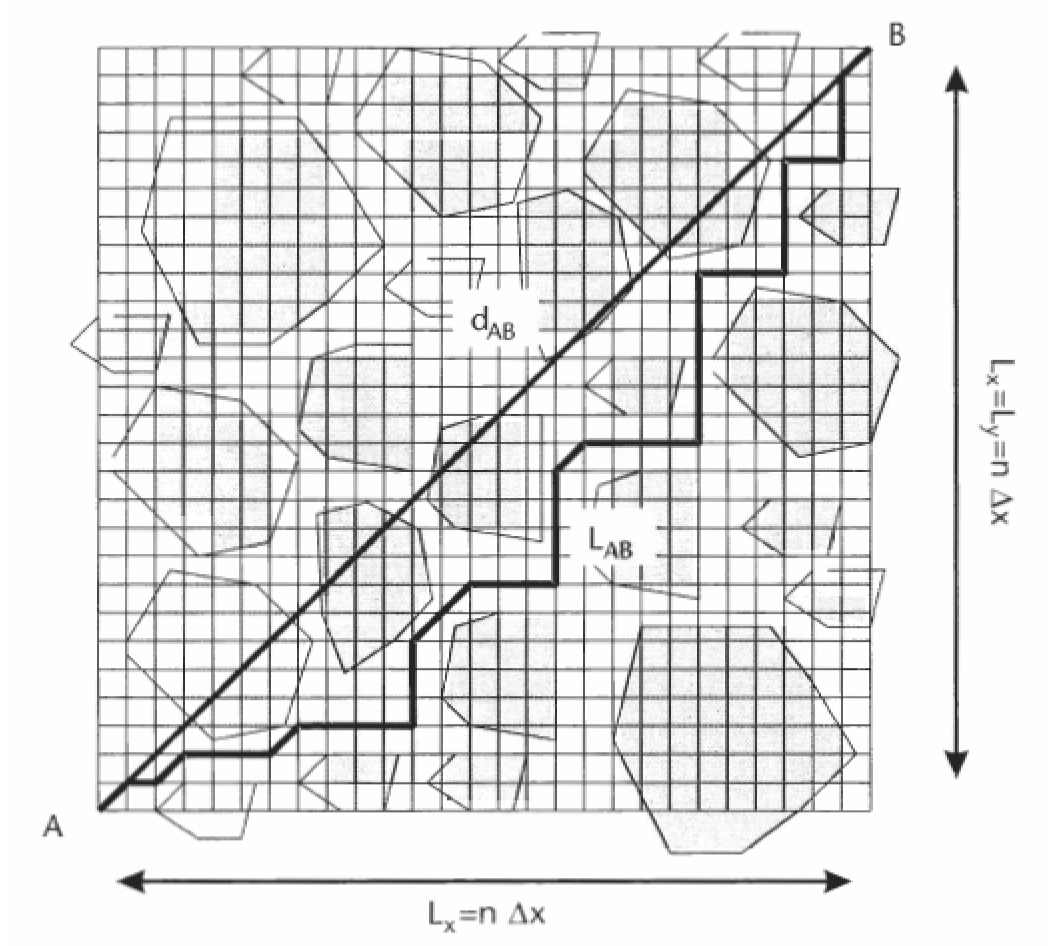
- tortuosity: ration between the distance in liquid and the straight distance between the points

Diffusion in confined volumes

It can be shown that:

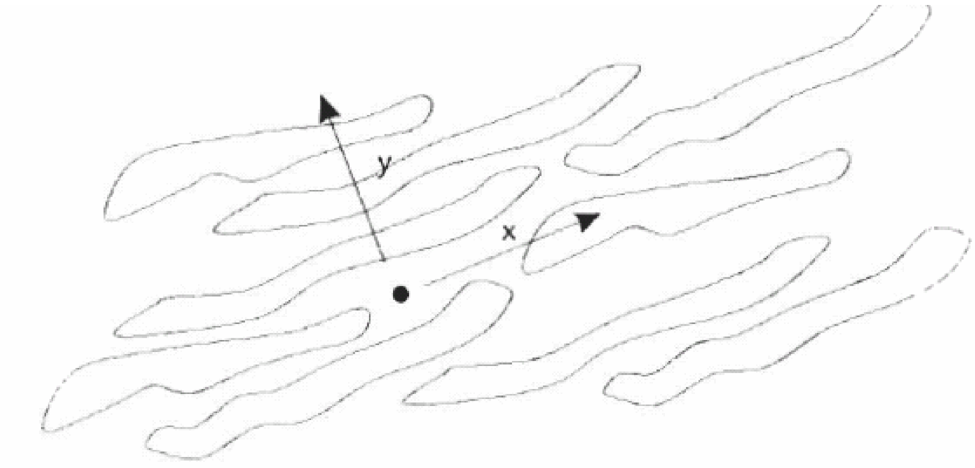
- for any 2D regular isotropic lattice tortuosity is equal to $\tau = \sqrt{2}$
- for 3D: $\tau = \sqrt{3}$
- The situation is more complicated for irregular cells and in the presence of intercleft volumes





How to treat anisotropic media

- to treat a media with a preferential direction we have to introduce a diffusion tensor:



$$[D]=\begin{bmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{bmatrix}$$

$$\begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix} = -[D]\nabla c$$

$$\frac{\partial c}{\partial t} = D_{11}\frac{\partial^2 c}{\partial x^2} + D_{22}\frac{\partial^2 c}{\partial y^2} + D_{33}\frac{\partial^2 C}{\partial z^2} + (D_{23}+D_{32})\frac{\partial c}{\partial y \partial z}$$

$$+(D_{31}+D_{13})\frac{\partial c}{\partial z \partial x} + (D_{12}+D_{21})\frac{\partial c}{\partial x \partial y}$$

- by rotating and scaling the coordinates it's possible to return to a isotropic (scalar) D:

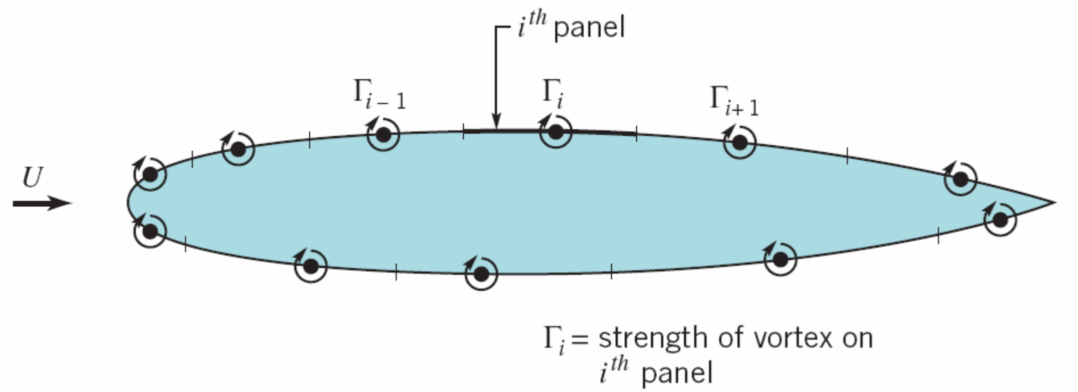
$$\frac{\partial c}{\partial t} = D\left[\frac{\partial^2 c}{\partial \xi^2} + \frac{\partial^2 c}{\partial \eta^2} + \frac{\partial^2 c}{\partial \zeta^2}\right]$$

Computational Fluid Dynamics

- Though the Navier-Stokes equations provide an exact solution for Newtonian fluid, there are only few situation when analytical solution possible
- CFD separates liquid into small volumes where partial differential equations can be approximated with algebraic equations.

Discretization

- **finite element/finite volume method**: flow field is broken into set of elements, conservation equations are (mass, momentum and energy) are written for every element
- **boundary element method** (panel method) : the boundary is broken into discrete elements and singularities like sinks, sources, doublets and vortices are inserted on these elements



- **finite difference method**: flow field is dissected into set of grid points, velocity, pressure etc. fields are approximated by the discrete values at the grid points, derivatives by the differences of values etc.

Discretization: finite difference

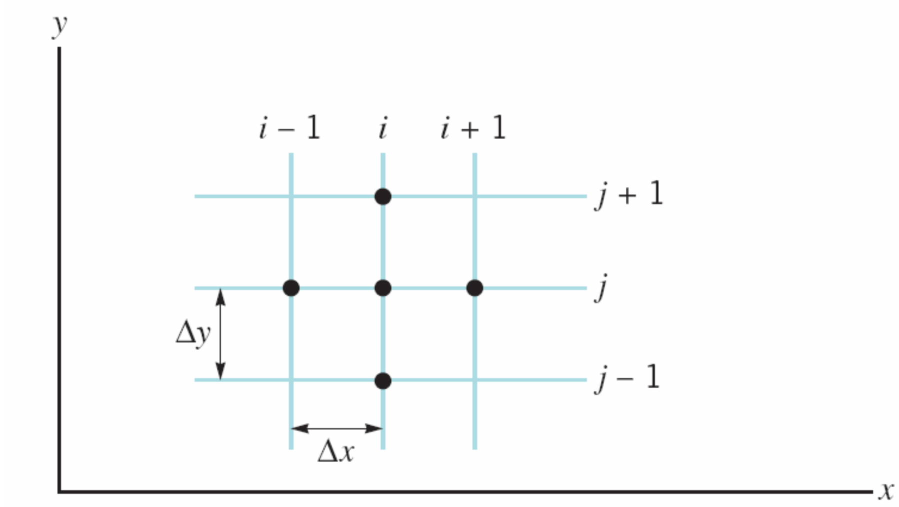
- algebraic approximation for the 1st derivative would be:

$$u_{i+1,j} = u_{i,j} + \left(\frac{\partial u}{\partial x}\right)_{i,j} \frac{\Delta x}{1!} + \left(\frac{\partial^2 u}{\partial x^2}\right)_{i,j} \frac{(\Delta x)^2}{2!} + \left(\frac{\partial^3 u}{\partial x^3}\right)_{i,j} \frac{(\Delta x)^3}{3!} + \dots$$

;

$$\left(\frac{\partial u}{\partial x}\right)_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{\Delta x} + O(\Delta x)$$

truncation of the Taylor series



(5.1.2a)

;

- central difference makes use of the both left and right points as j-1,j and j+1,j and is second order accurate

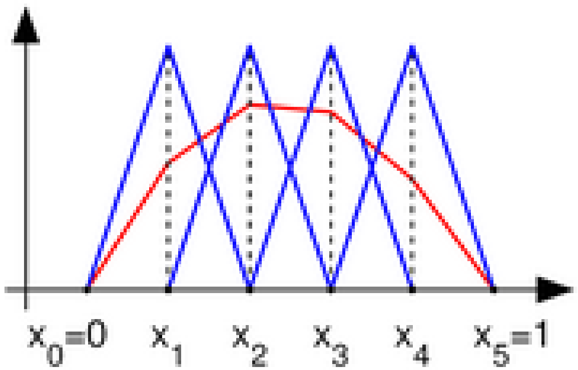
$$\left.\frac{\partial \phi}{\partial \xi}\right|_w = \frac{(\phi_P - \phi_W)}{\Delta \xi} \qquad \left.\frac{\partial \phi}{\partial \eta}\right|_n = \frac{(\phi_N - \phi_P)}{\Delta \eta}$$

$$\left.\frac{\partial \phi}{\partial \xi}\right|_e = \frac{(\phi_E - \phi_P)}{\Delta \xi} \qquad \left.\frac{\partial \phi}{\partial \eta}\right|_s = \frac{(\phi_P - \phi_S)}{\Delta \eta}$$

Finite element method: the idea

- The region is divided into triangular elements
- A basis function Ψ is defined for each node that is equal 1 at the node and drops linearly to zero at all adjacent nodes and is zero anywhere else
- The approximate solution of an equation is than:

$$\overline{\phi} = \sum_{i=!}^{N} \phi_i \Psi_i(x, y)$$



- This solution is searched that satisfy a condition (Galerkin method):

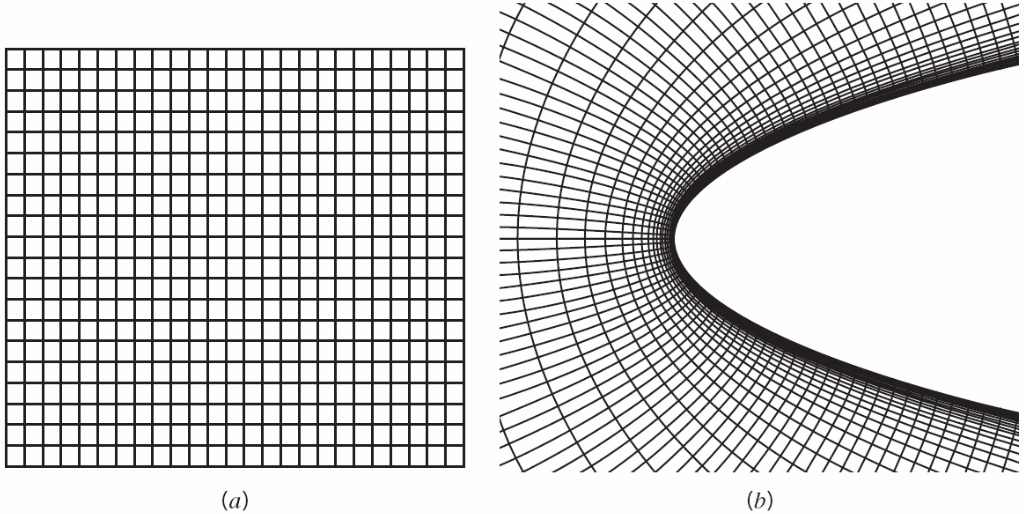
e.g. for diffusion (Poisson equation)

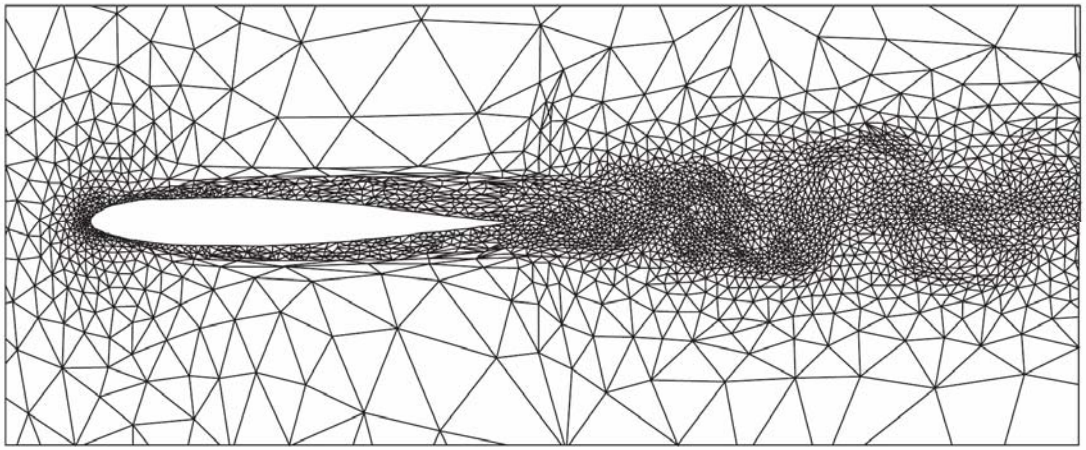
$$D\Delta\phi + S(x, y) = 0$$

$$\int_{\Omega} \Psi_j \left[\nabla \cdot \kappa \nabla \overline{\phi} + S(x, y) \right] d\Omega = 0$$

Grids

- arrangement of the discrete points in finite difference method is called **grid** or **mesh**;
- grid must have sufficient resolution to catch details of flow
- grids could be structured (regular pattern) or unstructured. Other types could be hybrid (several structured elements), moving (time dependent)

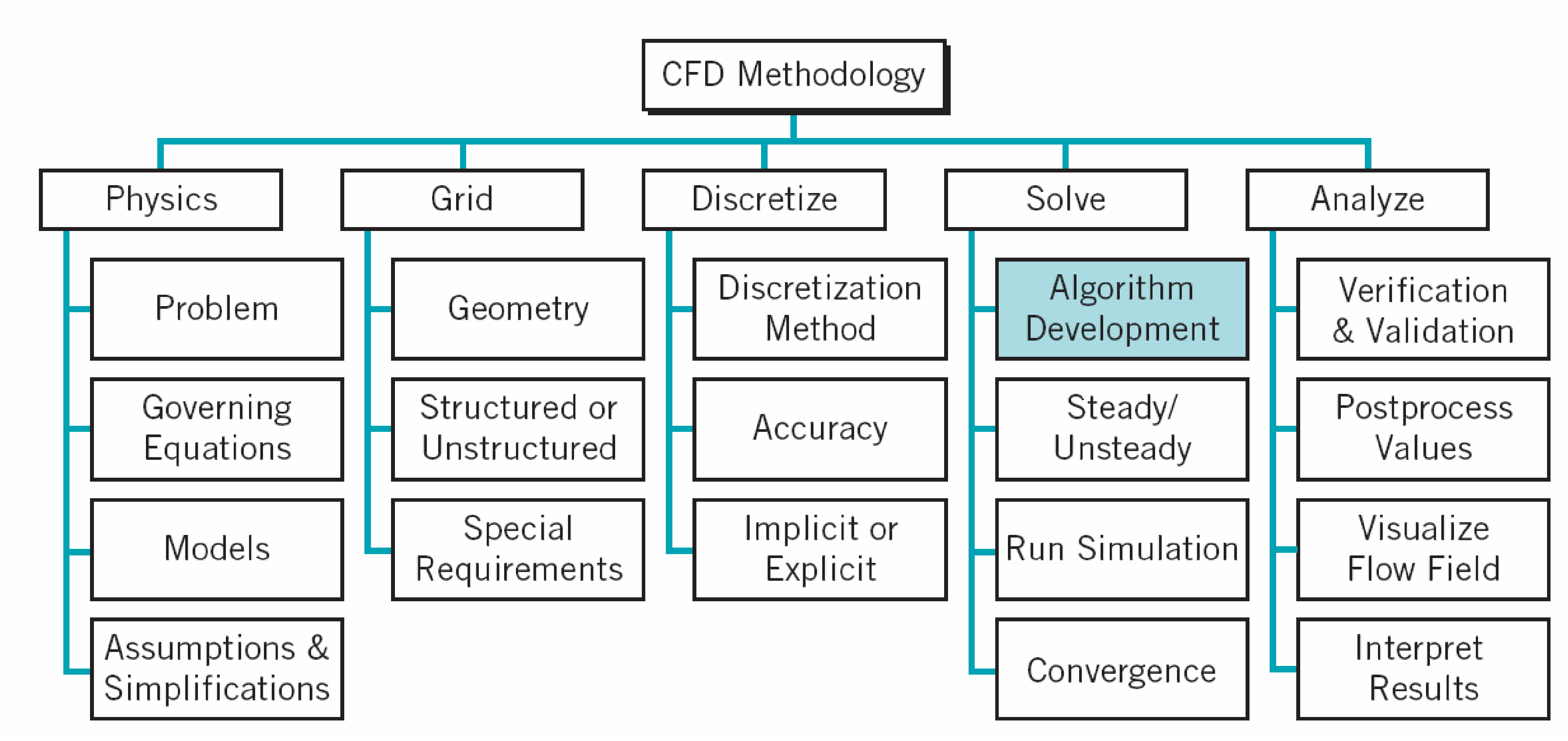




Boundary conditions

- Boundary conditions are essential part of the problem as they characterize the geometry of the problem
- proper definition of the boundary condition are important for accurate representation of the physical problem.

Methodology of CFD



Process flow in CFD

1. Defining governing **equations**. Formulating the problem.
2. Defining **geometry**.
3. Setting **boundary conditions**.
4. Defining the **mesh** (grid): flow field is broken into set of elements
5. **Solving:** conservation equations are (mass, momentum and energy) are written for every element and solved.
6. **Postprocessing:** solution is visualized and hopefully understood

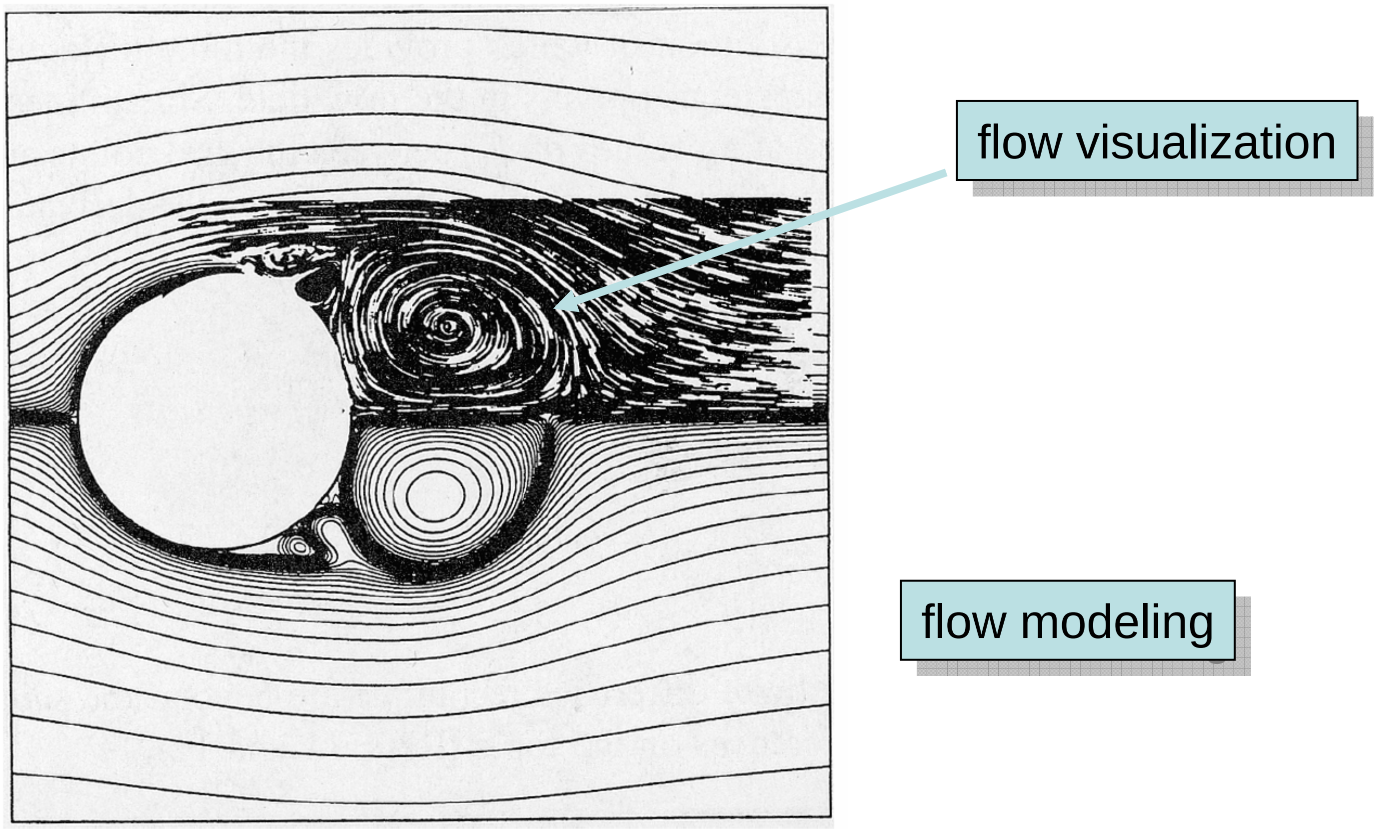
Application of CFD

- Computational fluid dynamics applications:
  - Aerodynamics of aircraft and vehicles
  - Hydrodynamics of ships
  - Microfluidics and biosensors
  - Chemical process engineering
  - Combustion engines and turbines
  - Construction: External and internal environment
  - Electric and electronic engineering: heating and cooling of circuits

Advantages of CFD

- Advantages of CFD
  - Reduction of time and costs
  - Ability to do controlled experiment under difficult and hazardous condition
  - Unlimited level of detail
  - simulate real flow conditions
  - conduct large parametric tests on new designs
  - enhance visualization of complex phenomena
- Difficulties in CFD:
  - dealing with non-linear terms in Navier-Stokes
  - difficulties modeling turbulent flow
  - convergence issues
  - difficulties obtaining quality grid

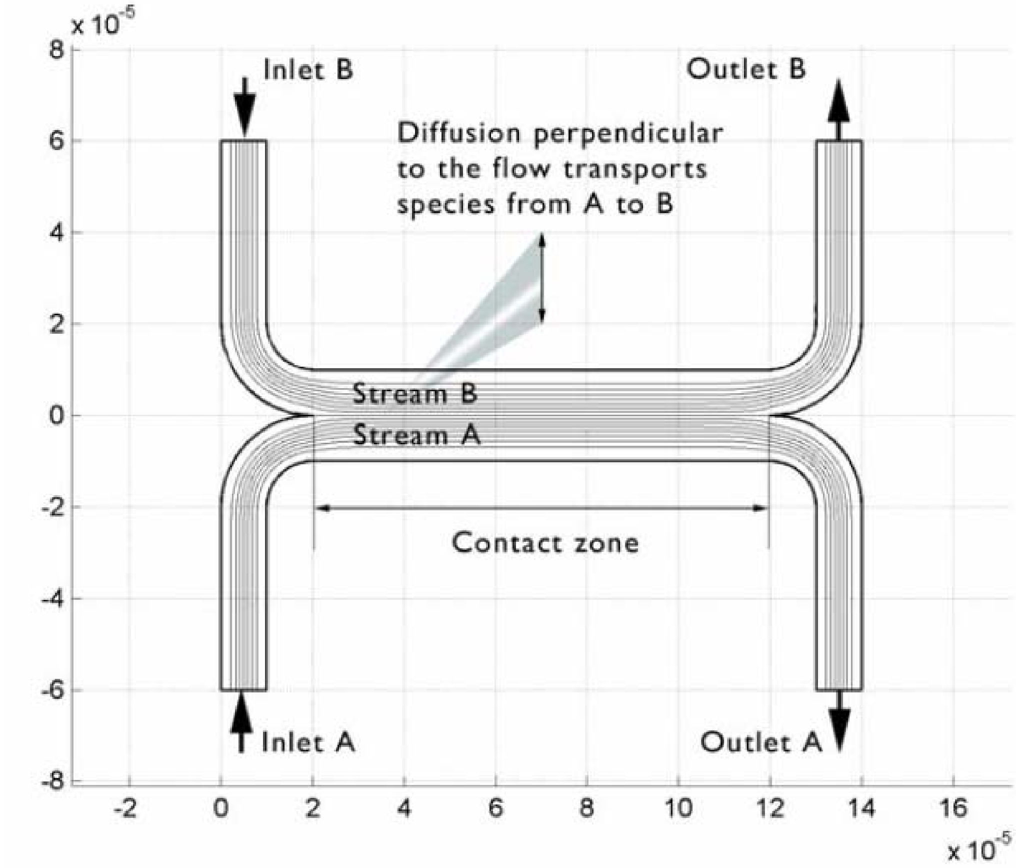
Verification and Validation



- grid convergence testing
- comparison with existing data (e,g, limiting cases)

H-cell model

- H-cell perform separation via diffusion during controlled time
- Small species from A can diffuse into B
- Modelling parameters:
  - P0=2 Pa; D=1e-11



Problem: 2D Viscous flow between the plates

Water is injected between two infinite parallel plates. Solve analytically (in the case of fully developed laminar flow) and numerically (general case) and compare the results. Plot velocity profile across the channel and pressure drop along the channel.

Parameters

flow velocity V=0.001m/s;

height of the channel h=0.4m; length of the channel L=2m

dynamic viscosity (water) $\mu=10^{-3}$ Pa*s; density (water) $\rho=10^{3}$ kg/m^{3}

Questions:

- What is the Reynolds number?
- What is the calculated pressure drop in the channel? What is the entrance pressure drop?
- Is laminar flow fully developed in the channel?