Introduction to Microfluidics Modeling: Part II - Simulation Techniques

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16.8.2004

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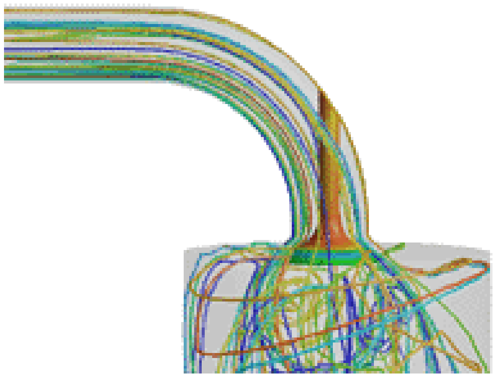
CFD in a Nutshell

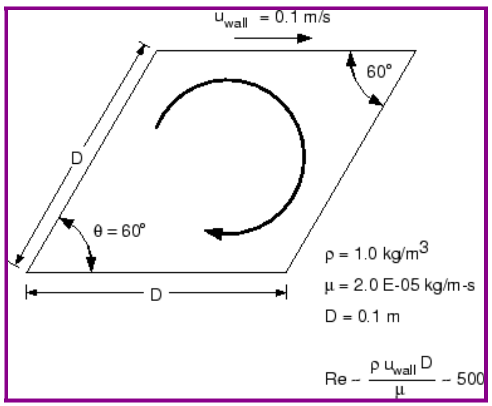
Colorfull? Fluid Dynamics

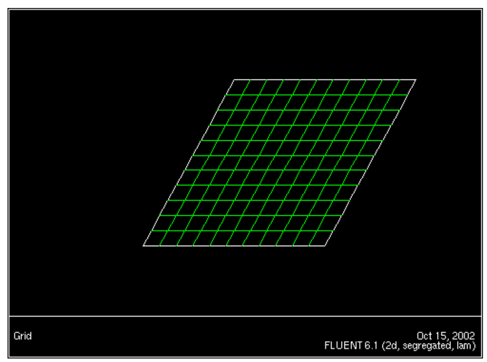
- **C**omputational **F**luid **D**ynamics
- numerical solution of continuum equation for fluidic material
- is not as trivial as it sometimes might appear
- preprocessing ⇒ computation ⇒ postprocessing

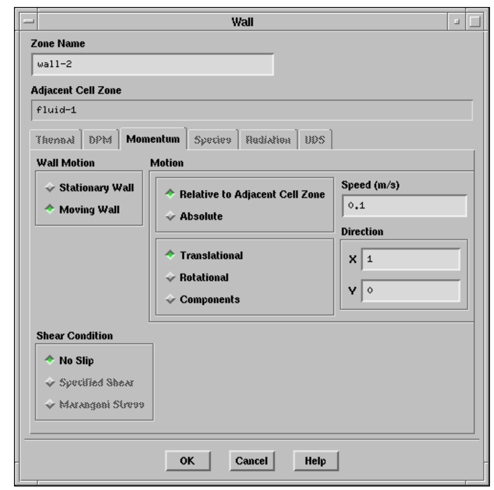


Preprocessing

problem definition ⇒ **geometry and grid generation** ⇒ **physical and numerical settings**



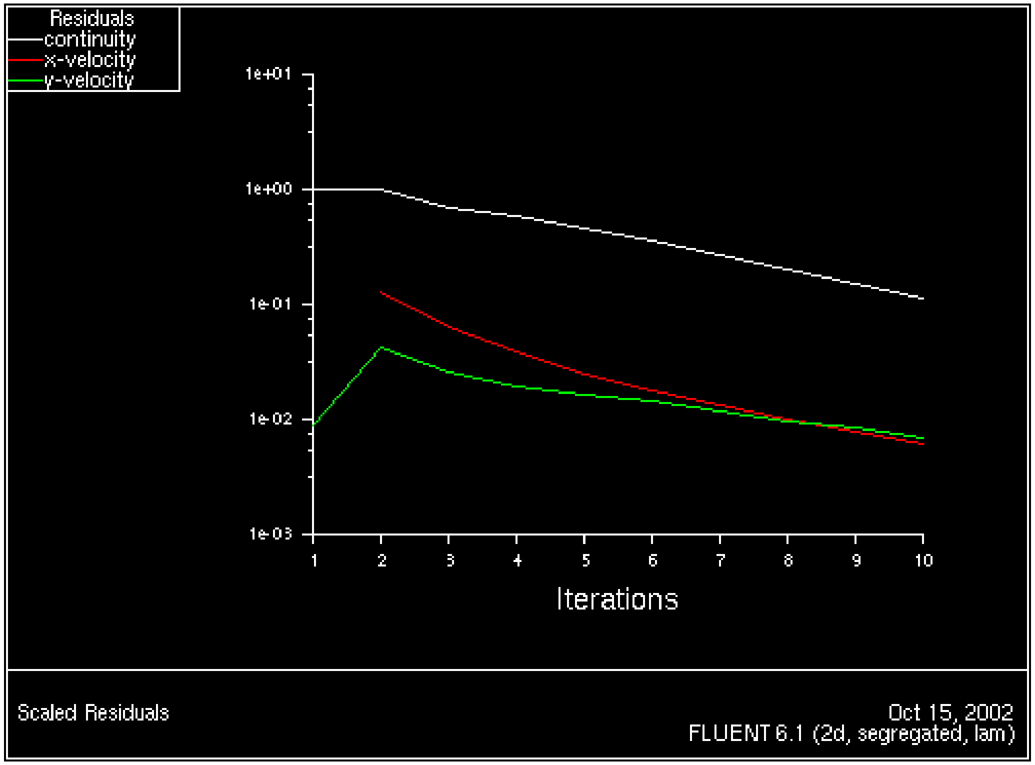




Pictures taken from Fluent.Inc Fluent 6 User Guide

Number Crunching

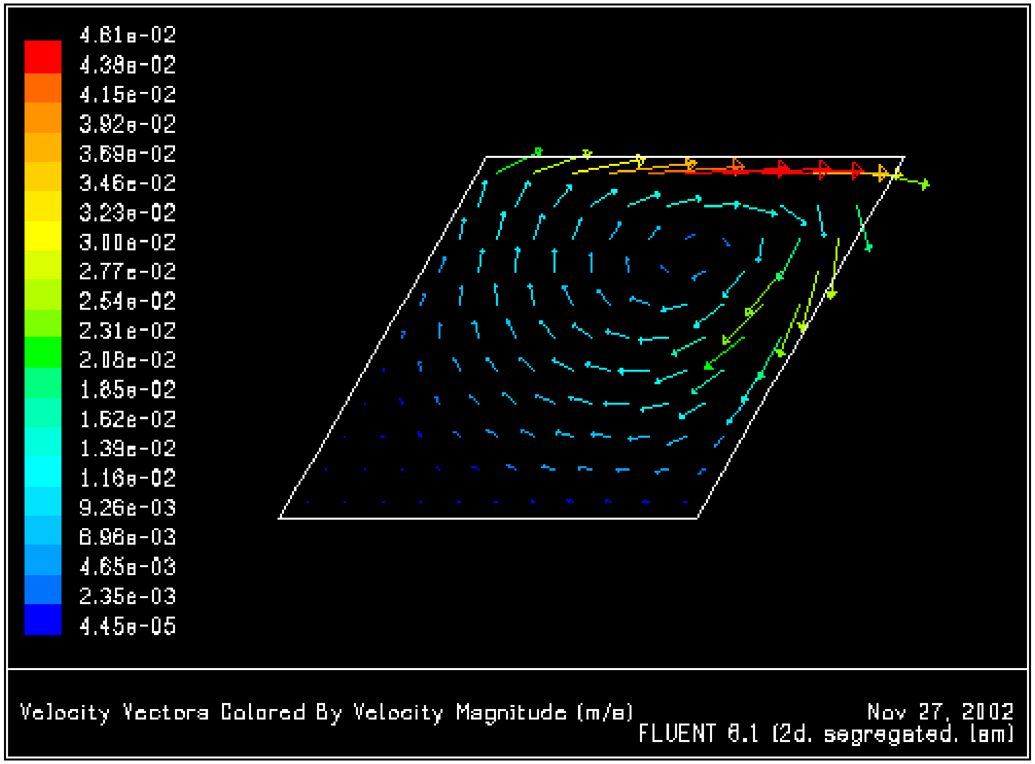
- numerical solution of discretized equations
- different types of methods and techniques
- guidelines for correct choice
- parallel processing
- convergence



Picture taken from Fluent.Inc Fluent 6 User Guide

Post Processing

- Colorfull Fluid Dynamics
- three dimensional post-processing difficult
- transient postprocessing even more difficult
- large datasets from parallel processing
- what do I want to visualize?



Picture taken from Fluent.Inc Fluent 6 User Guide

CFD Strategy

preprocessing ⇒ numerical solution ⇒ postprocessing

THINK! ⇒ PRAY! ⇒ GET EXITED!

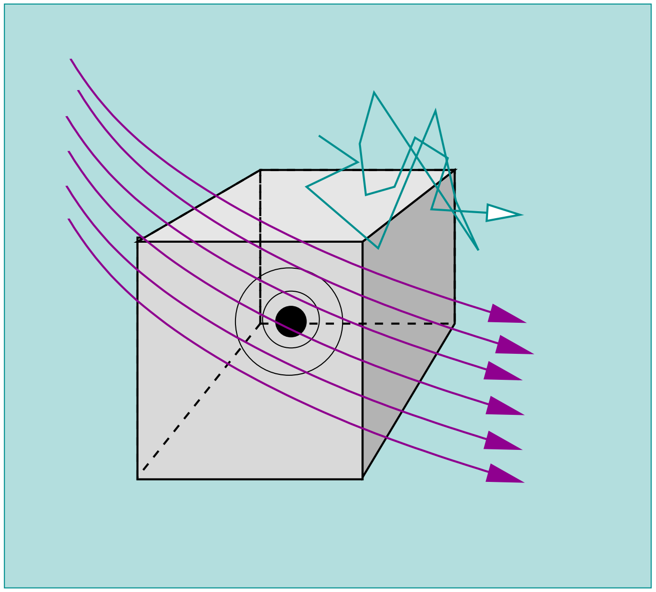
or GET A CLUE!

⇐ ⇐ and GET IT FIXED!

Numerics

Conservation Laws

local change	=	convection
	+	diffusion
	+	production

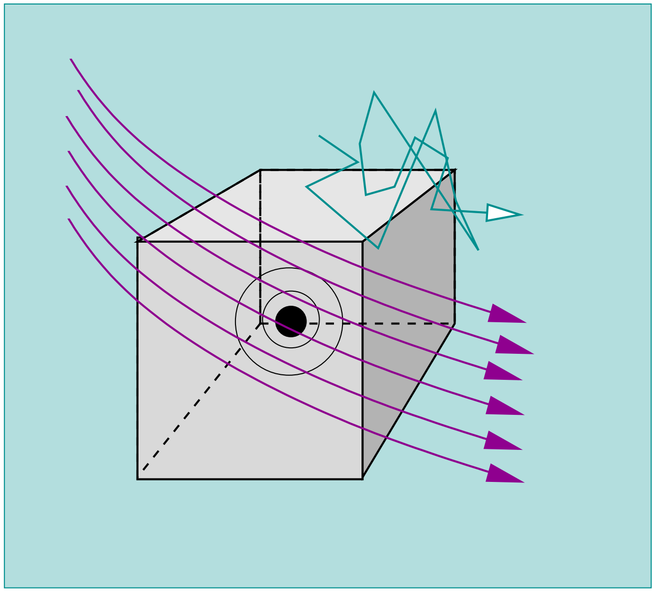


Partial Differential Equations

$$\rho \cdot \frac{\partial \Psi}{\partial t} = -\rho \cdot u \cdot \frac{\partial \Psi}{\partial x}$$

$$+ \quad D \cdot \frac{\partial^2 \Psi}{\partial x^2}$$

$$+ \quad \rho \cdot S$$



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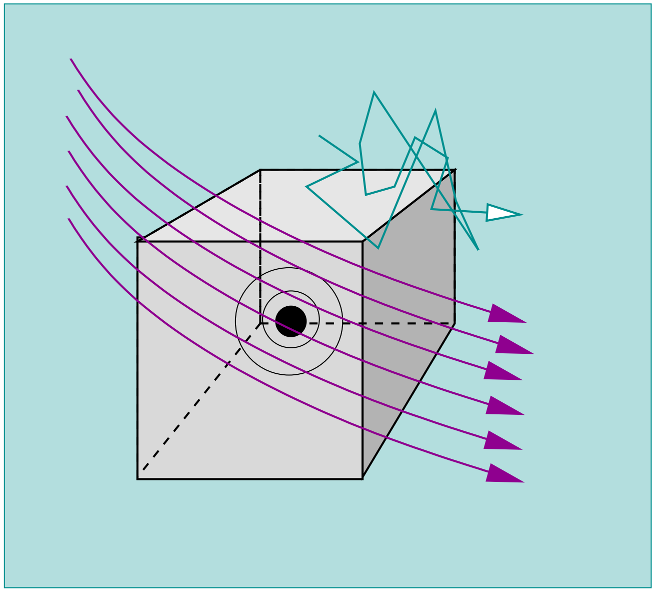
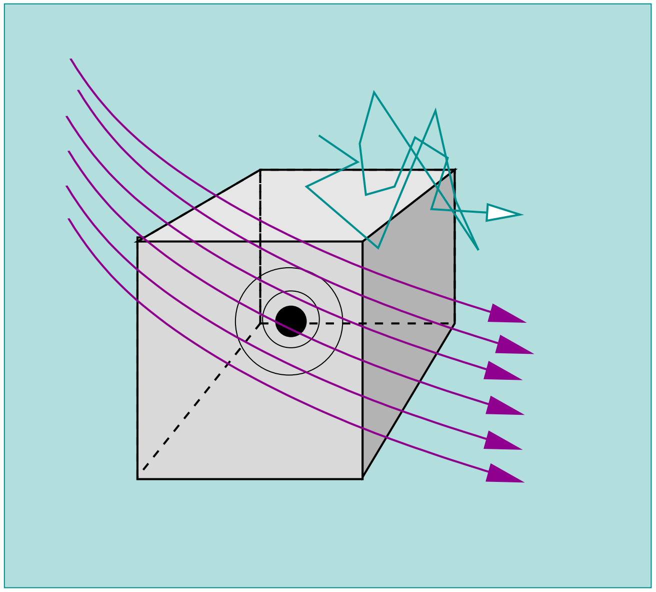


Non-transient Problem (i.e., stationary): $\frac{\partial \Psi}{\partial t} \equiv 0$

Partial Differential Equations

$$\rho \cdot \frac{\partial \Psi}{\partial t} = -\rho \cdot u \cdot \frac{\partial \Psi}{\partial x} + D \cdot \frac{\partial^2 \Psi}{\partial x^2} + \rho \cdot S$$

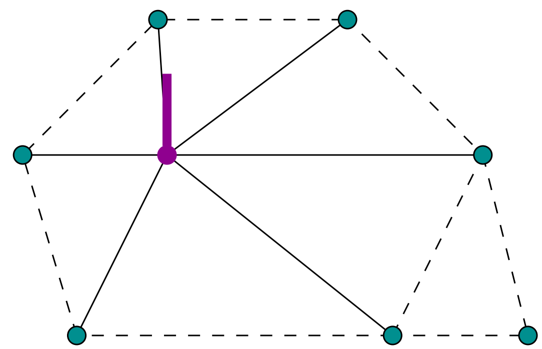


Non-transient Problem (i.e., stationary): $\frac{\partial \Psi}{\partial t} \equiv 0$

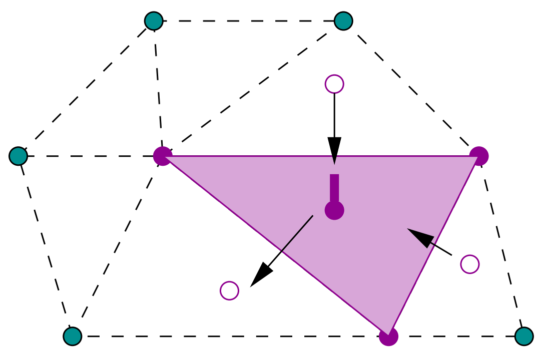
Non-linear Problem: e.g., $S = \mathcal{S}(\Psi) = a \cdot \Psi + b \cdot \Psi^2$

Numerical Methods

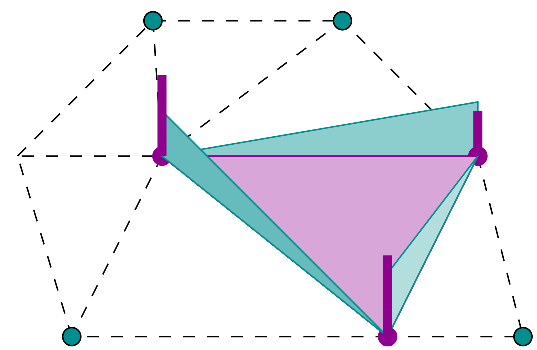
Finite Difference (FD):



Finite Volume (VF):

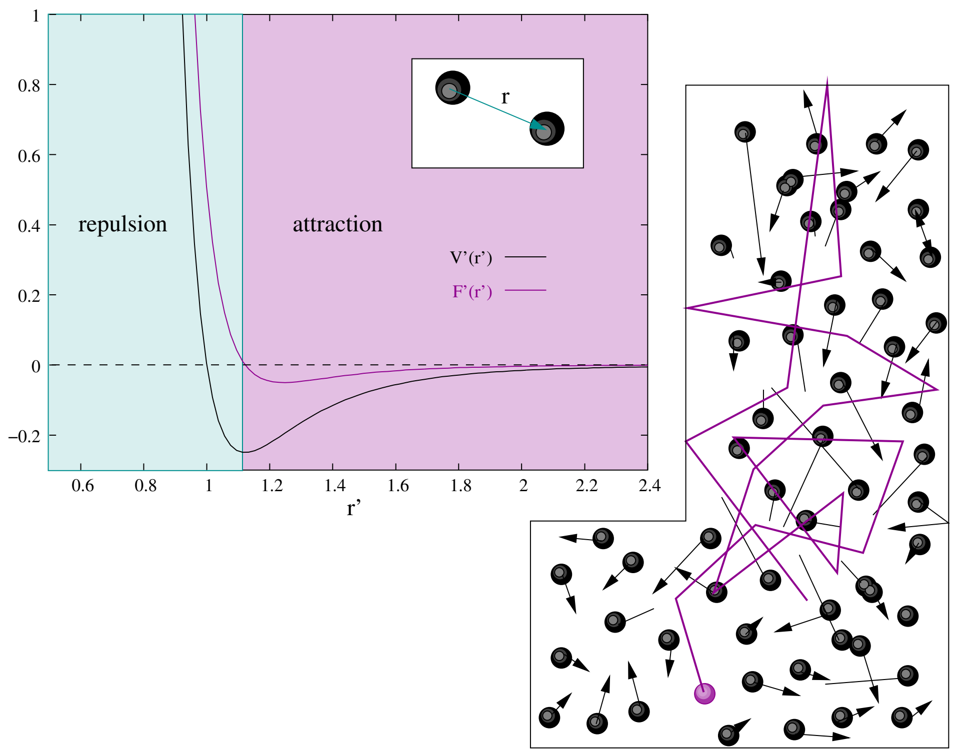


Finite Element (FE):



Molecular Approaches

Molecular Dynamics

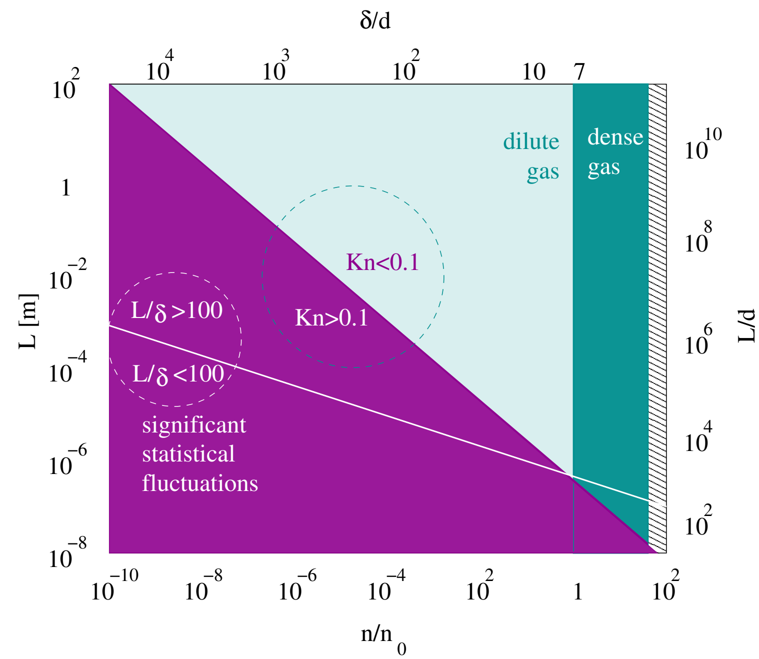


$$m_i \cdot \frac{d^2 r_i}{d t^2} = \sum_{j=1, j \neq i}^{N} F_{ij}$$

N molecules

Direct Simulation Monte Carlo

- particles consist of thousands of molecules $10^{14} - 10^{18}$
- molecular motion of particles treated deterministically
- collisions are treated statistically (kinetic theory)
- good for $0.1 <$ Kn < 10, i.e., transitional regime



- moving particles → indexing → particle collisions → sampling
- limitations in cell size, timestep size
- difficulties for boundary conditions