Introduction to Microfluidics Modeling:
Part II - Simulation Techniques

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CFD in a Nutshell

*Colorfull? Fluid Dynamics*

- **Computational Fluid Dynamics**
- numerical solution of continuum equation for fluidic material
- is not as trivial as it sometimes might appear
- preprocessing $\Rightarrow$ computation $\Rightarrow$ 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 post-processing 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 $\Rightarrow$ numerical $\Rightarrow$ postprocessing solution

THINK! $\Rightarrow$ PRAY! $\Rightarrow$ GET EXITED!

or GET A CLUE!

$\Leftarrow$ and GET IT FIXED!
Numerics

Conservation Laws

local change $= \text{convection} + \text{diffusion} + \text{production}$
Partial Differential Equations

\[
\rho \cdot \frac{\partial \Psi}{\partial t} = -\rho \cdot u \cdot \frac{\partial \Psi}{\partial x} + D \cdot \frac{\partial^2 \Psi}{\partial x^2} + \rho \cdot S
\]
Partial Differential Equations

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

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

\[ + \quad \rho \cdot S \]

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

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

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

\[ + \quad \rho \cdot S \]

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

Non-linear Problem: e.g., \[ S = S(\Psi) = a \cdot \Psi + b \cdot \Psi^2 \]
Numerical Methods

Finite Difference (FD):

Finite Volume (VF):

Finite Element (FE):
Molecular Approaches

Molecular Dynamics

\[ \sum_{j=1, j \neq i}^{N} F_{ij} = \frac{m_i}{d^2} \frac{d^2 r_i}{dt^2} \]

\( N \) 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 $\rightarrow$ indexing $\rightarrow$ particle collisions $\rightarrow$ sampling
- limitations in cell size, timestep size
- difficulties for boundary conditions