| 1. Introduction                                                                 | 9. Liquid Handling                                   |
| 2. Fluids                                                                      | 10. Microarrays                                      |
| 5. Flow Control                                                                | 13. Particle-Laden Fluids                           |
| 7. Sensors                                                                     | b. Fundamentals of Biotechnology                    |
| 8. Ink-Jet Technology                                                          | c. High-Throughput Screening                        |
3.A. Simulation

• Objective for simulation

• Two prominent types of simulation
  
  - CFD
    - Resources
    - Basics of the method
    - Examples
  
  - System
    - Resources
    - Basics
    - Examples

• Conclusions & Summary
Objective for Simulation

Goal: Prediction of system behavior under given temporal and spatial boundary conditions

Approach:

Model generation: Implementation of device or system as „mathematical“ model

Simulation: Determination of performance of system or device by solving model (numerically)

Validation / verification: Testing model by comparison with experimental data
Model Generation

• Determination of system boundaries
  • Where does system start and end?
  • Constituents?

• Identification of relevant effects
  • What physical processes need to be considered?
    • Fluid flow?
    • Heat transfer?
    • Chemical reactions?
    • Etc.

• Determination of model parameters
  • Shape
  • Size
  • Material
  • Actuation
  • Etc.
Model Generation

• **Mathematical formulation of model**
  • In commercial tools usually done by solver
  • User only sets parameters and boundary conditions
  • Taking mutual interactions of components into account
    • **Multiphysics modeling**
  • Reduction of complexity
  • **Model reduction**

Process of model generation is essential part of simulation!

A simulation only as good as underlying model!
1. **Analytical solution**
   For some „simple“ cases, analytical solutions can be found

2. **Numerical solution**
   The solution calculated by computers and various numerical techniques

**Solution in space & time**
„physical simulation“
(e.g., finite element method (FEM) for mechanical simulation)

**Solution in time**
„system simulation“
(e.g., electronic circuit simulation)

**Event oriented**
„digital simulation“
(e.g., digital circuit simulation)
**Objective of Simulation**

- Reduced development time & cost
  - CAD of MEMS devices
  - Automated optimization of designs
  - Less hardware in loop optimizations
  - Virtual prototyping & testing of device
- Gaining insight and understanding
  - Leads to novel ideas
  - Leads to improved concepts
- Easy testing of new concepts & ideas
3.A. Simulation

• Motivation: What is simulation good for?

• Two prominent types of simulation: CFD and system simulation

• CFD simulation:
  ➢ Resources
  ➢ Basics of the method
  ➢ Examples

• System simulation
  ➢ Resources
  ➢ Basics
  ➢ Examples

• Conclusions & Summary
Types of Simulation

Grid-based „physical“ simulation

- Simulation of solids (mechanical, electrical, thermal and other domains)
  - ANSYS
  - NASTRAN, ...

- Simulation of Flow (Computational Fluid Dynamics (CFD))
  - FLUENT
  - POLYFLOW
  - FLOW-3D
  ...

System or network simulation

- Simulation based on equivalent circuit diagrams
  - SPICE
    - Simulation of electric circuits
  - SABER
    - Multi-physics simulation
Design-Flow

Top-down approach

- Design of system in system simulator, use of physical modeling if necessary
- Run simulation, optimize performance
- Generate lay-out from macro model
- Experimental feed-back into model
Multiphysics Modeling

• Multiphysics means that in most cases more than one physical domain has to be considered. For example:
  - Fluidics & heat transfer (e.g., microreactors)
  - Mechanics & electric engineering (e.g., inertial sensors)
  - Fluidics & electrokinetics & chemistry (e.g., lab-on-a-chip)

• Multiphysics modeling can be done on „physical“ level as well as on system level
  - Coupling of different grid-based solvers (physical level)
  - Defining different physical domains in network simulations (system level)
  - Coupling of grid-based solvers with network (simulation mixed level)
3.A. Simulation

- Motivation: What is simulation good for?
- Two prominent types of simulation: CFD and system simulation
- **CFD simulation:**
  - Resources
  - Basics of the method
  - Examples
- System simulation
  - Resources
  - Basics
  - Examples
- Conclusions & Summary
Simulated F–16/ACES–II Ejection
Time = 0.00 sec
Resources

- CFD-Online: Sponsored information service for CFD-users
  
  \[ \text{http://www.cfd-online.com} \]
  
  - \[ \text{http://www.cfd-online.com/Resources/homes.html#Company} \] companies and suppliers
  - \[ \text{http://www.cfd-online.com/Forum/} \] discussion and information forum

- Hompages of commercial suppliers of software
  
  - \[ \text{http://www.software.aeat.com/cfx} \]
  - \[ \text{http://www.fluent.com} \]
  - \[ \text{http://www.flow-3D.com} \]
  - \[ \text{http://www.cfdrc.com} \]
  - ...  

- Service providers for MEMS (not only CFD)
  
  - \[ \text{http://www.memscap.com} \]
  - \[ \text{http://www.coventor.com} \]
  - ...
Navier-Stokes-Equations

\[
\rho_{\infty} \left[ \frac{\partial}{\partial t} \mathbf{v} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] = -\nabla p + \eta \nabla^2 \mathbf{v} + \rho_{\infty} g
\]

\[\nabla \cdot \mathbf{v} = 0\]

* Expression for capillary forces (surface tension)
* Expression for electrokinetic effects (electrophoresis, electroosmosis)
* Multi-phase transport \[\mathbf{v} = \{\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3, \ldots\}\]
* Chemical reactions \[\nabla \cdot \mathbf{v} \neq 0\]
* Etc.

additional expressions
Example 1: Discrete Particle Transport

Considered effects:
- Fluid dynamics
- Particle transport
Example 2: Welding

Considered effects:

- Fluid dynamics (two phase flow)
- Heat transfer
- Phase transition
Example 3: Dielectrophoresis

Dielectrophoresis (DEP):
Force acting on non-uniform dielectric materials in non-uniform electric field
Liquid drop can be moved by charging electrode

Considered effects:
• Fluid dynamics (two phase flow)
• Electrodynamic
Droplet in carrier fluid
(Droplet has high dielectric constant)

Potential field
(0 - 100 volts)
Electric Potential @ Time 0.7ms

Droplet in carrier fluid
(Droplet has high dielectric constant)

Potential field
(0 - 100 volts)
Example 4: Bubble-Jet Printhead

Considered effects:

- Fluid dynamics (two phase flow)
- Heat transfer
- Phase transition

Droplet Characteristics by Thermal Bubble Jet

Considered effects:

- Fluid dynamics (two phase flow)
- Heat transfer
- Phase transition
Example 5: Microarraying

Considered effects:

- Fluid dynamics (two phase flow)
- Adhesion & surface tension!

*split-pin fabricated by Brown group in Stanford University, a fine slot is machined into the end of the pin to accommodate liquid sample (courtesy professor Patrick O. Brown, Stanford University).*
Example 6: Dispensing into Well

Considered effects:
- Fluid dynamics (two phase flow)
- Mixing
Example 7: Flap Valve

Considered effects:

- Fluid dynamics
- Fluid-structure interaction
Top-Spot Microarrayer

• Contact-free method
• Maximum 384 different liquids
• Massively parallel printing
• Volumes 100 pl to a a few nl
Simulation of Top-Spot

Simulation of displacement by moving grid

Simplifications

- Simplified pressure profile
- Only one nozzle
- Using symmetry

Questions

- Dosage volume dependent on maximum piston stroke?
- Dependence of droplet generation on piston dynamics?
- Droplet velocity?
Dynamic Simulation

Stroke dynamics: 2 µm / 30 µs

2*10e-6 m Hub, 30*10e-6 s Anstiegszeit
Dynamic Simulation

Stroke dynamics: 2 µm / 50 µs
Dynamic Simulation

Stroke dynamics: 2 µm / 70 µs

2*10e-6 m Hub, 70+10e-6 Anstiegszeit

0.000000s
Results

Standard operation

- Fluid volume / piston stroke approx. linearly dependent
- Direct relation between piston dynamics and droplet velocity

2 µm stroke, within 30 µs resp. 50 µs

Low piston dynamics

- Droplet may return to nozzle
- This has also been observed in experiments!

4 µm stroke, within 60 µs resp. 100 µs
3.A. Simulation

- Motivation: What is simulation good for?
- Two prominent types of simulation: CFD and system simulation
- CFD simulation:
  - Resources
  - Basics of the method
  - Examples
- System simulation
  - Resources
  - Basics
  - Examples
- Conclusions & Summary
System Simulation

**Idea:** Division of complex system into sub-systems, which can be described by **compact (“lumped” or “behavioral”) models**. Interactions between subsystems mediated via **network** of connections.
Resources

• General information on MEMS simulation tools (not only system simulation)
  ➢ http://www.memsnet.org/links/software.html

• Saber Simulator
  ➢ http://www.avanticorp.com/Avant!/SolutionsProducts/Products/Item/1,1500,65,00.html

• Spice Usergroup
  ➢ http://www.seg.iit.nrc.ca/spice/

• Eldo Simulator
  ➢ http://www.mentor.com/eldo/overview.html

• Mathlab
  ➢ http://www.mathworks.com/
Electric Circuit Simulation

• Based on Kirchhoff’s laws
  ➢ Sum of all currents $I_n$ at node is zero
  ➢ Sum of all voltages $U_n$ within closed loop is zero

• Differential equations derived from “transfer functions“ $U = f(I)$:
  ➢ $U_R = R \cdot I$
  ➢ $U_L = L \cdot \frac{dI}{dt}$
  ➢ $U_{source} = R \cdot I + L \cdot \frac{dI}{dt}$

• Differential equations (DE) solved numerically (time- or frequency domain)
Analogy in Fluidics: $I \Rightarrow q$ and $U \Rightarrow p$

- Completely filled capillary
  - Ohmic resistance $\rightarrow$ fluidic resistance
    - Viscosity
    - Geometry
  - Inductance $\rightarrow$ inertia of fluid
    - Density
    - Geometry

- Transfer functions and DE
  - $p_R = R \cdot q$
  - $p_L = L \cdot \frac{d}{dt} q$
  - $p = R_{fluid} \cdot q + L_{fluid} \cdot \frac{d}{dt} q$

- Numerical solution
Fundamental Principle

“through“ variable + “across“ variable + conservation law = network simulation

Physical system described by field equations

\[ \Psi[f(\mathbf{x}_0, t_0, \mathbf{x}, t)] = 0 \]

Transition from locally dependent variables (e.g., current density) to integral quantities (e.g., current) at selected points in space (nodes)

Through and across variables at discrete points (nodes)

\[ \begin{bmatrix} u_1(t_0, t) \\ \vdots \\ u_n(t_0, t) \end{bmatrix} \begin{bmatrix} i_1(t_0, t) \\ \vdots \\ i_n(t_0, t) \end{bmatrix} \]

Taking into account laws of conservation (e.g., continuity equation, conservation of energy) and modelling the transfer function (e.g., \( R = U / I \))

Netlist & transfer functions

\[ \begin{bmatrix} u_1(t_0, t) \\ \vdots \\ u_n(t_0, t) \end{bmatrix} = M(t) \times \begin{bmatrix} i_1(t_0, t) \\ \vdots \\ i_n(t_0, t) \end{bmatrix} \]

\( \Rightarrow \) Differential equation for network simulation
## Analogy in Many Physical Domains

![Table showing analogies between different physical domains](image)

How to obtain transfer functions?

- Analytical solution of fundamental differential equation, e.g.,
  - Ohmic resistance
  - Inductance
  - Empirical compact models, e.g.,
    - Diode models
    - Tubular flow
- Experimental or simulation data (grid-based simulations), e.g.,
  - Look-up tables
  - Couple simulations
- Automated model reduction techniques, example on next slide
Model Reduction Techniques

Reduction of degrees of freedom (DOF) e.g., with singular value decomposition (SVD) or modal analysis, etc.

Approximation of solution obtained from physical modeling e.g., with nonlinear fit or neural networks, etc.

$\text{f(x)}$

Microfluidics - Jens Ducrée

Physics: Simulation
Example 1: Capillary Model

- **Capillary states**
  - *empty*: only air flow considered
  - Transition state: *wet1dry2* (filling from one end); *wet2dry1* (vice versa)
  - *Full*: resistance according to tube flow

- **Nozzle states**
  - *empty* and *wet2dry1* identical
  - Additional consideration of *meniscus state* \( (p < 2p_{cap}) \)
  - In *eject*-state \( (p > 2p_{cap}) \) approximation of pressure drop by Toricelli’s formula

---

1. end  \[ \rightarrow \]  I  \[ \rightarrow \]  2. end
Capillary Channel

Capillary channel with circular cross section (\( \varnothing d \), length \( l \)):

Capillary pressure \( p_{\text{cap}} \), laminar flow resistance \( R \), fluidic inductance \( L \) and position of meniscus are considered

\[
R = \frac{8 \eta l}{\pi^2 \left( \frac{d}{2} \right)^4}; \quad L = \frac{l}{\pi \left( \frac{d}{2} \right)^2 \rho}; \quad p_k = \frac{\sigma}{d}; \quad p_i = \frac{d}{dt}(Lq)
\]

Logical pin input

Logical pin output

Fluidic line

\[ p = Rq + p_k + p_i \]
Capillary Nozzle

Capillary nozzle with circular cross section ($\varnothing d$, length $l$):

Capillary pressure $p_{\text{cap}}$, laminar flow resistance $R$, fluidic inductance $L$ and free jet ejection are considered

- logical pin input
- logical pin output
- fluidic line

$q = \begin{cases} 
0 & ; \quad p < \frac{8\sigma}{d} \\
\frac{\mu \pi d^2}{4} \sqrt{\frac{2p}{\rho}} & ; \quad p \geq \frac{8\sigma}{d} 
\end{cases}$

- No ejection: pressure smaller than $2p_{\text{cap}}$
- Ejection: Torcelli’s formula
Validation of Capillary Model

by priming of meandering capillaries

experiment

system model

[Sesterhenn et.al MSM conference 1999, 538-541 Cambridge, MA]
Comparison with Measurements

![Graph showing comparison between simulation and measurements. The graph plots distance (d) in millimeters against time (t) in seconds. The axes range from 0 to 350 on the y-axis and from 0 to 25 on the x-axis. The graph includes lines for both simulation and measurements, with data points marked at specific intervals. The reference is Sesterhenn et al. at the MSM conference 1999, pages 538-541, Cambridge, MA.]
Validation of Nozzle Model

Simple multi channel test system
- Representing simple dispenser
- Micromachined in silicon
- Well suited for validation
System Model

- Pressure source
  - Ideal, piecewise linear profile
- Reservoir
  - Capillary with 1500 μm diameter and 425 μm length
- Nozzle
  - 100 μm diameter, 100 μm length
- Integrator
  - Selective to fluid
Simulation Results in Time Domain

Progression vs time

- Pressure: \( \text{(N/m}^2\) : t(s) \)
- Flow through nozzle: \( \text{(m}^3/\text{s}) : t(s) \)
- Dispensed Volume: \( \text{(liters}) : t(s) \)

Microfluidics - Jens Ducrée

Physics: Simulation
Comparison with Measurements

Dispensed Volume [nL] vs. Max. Pressure [kPa]

- Calibration point: calibration factor $\mu = 0.905$
- $t_{\text{pulse}} = 11.5\text{ms}$
- $t_{\text{pulse}} = 15\text{ms}$
- $t_{\text{pulse}} = 21\text{ms}$
- $t_{\text{pulse}} = 26\text{ms}$

- $d = 100 \mu m$
- $d = 50 \mu m$
Example 2: Systemmodel for VAMP

Micro valve & micro diaphragm pump
(Valve And Micro Pump (VAMP))
[HSG-IMIT, Villingen-Schwenningen]

---

Piezo-Biegewandler

Dichtfläche

Anschluß 1  Anschluß 2

Grundplatte

---

Microfluidics - Jens Ducrée
Physics: Simulation
49
Network model of VAMP

mechanical domain

piezo-bimorph

valve

electrical domain

capillary channels

fluidic domain

reservoir
Simulation of Valve Operation

opening and closing cycle

force on valve seat
deflection of the membran
pressure
flow
Micro Valve Characteristics

![Graph showing Micro Valve Characteristics](image)

**Actuation Voltage**

- 160V
- 120V
- 100V
- 80V
- 60V
- 40V
- 20V
- 0V

**Microfluidics - Jens Ducrée**

Physics: Simulation
3.A. Simulation

- Motivation: What is simulation good for?
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- CFD simulation:
  - Resources
  - Basics of the method
  - Examples
- System simulation
  - Resources
  - Basics
  - Examples
- Conclusions & Summary
## Comparison: CFD & Network Simulation

<table>
<thead>
<tr>
<th>CFD $\rightarrow \Phi(x,t)$ (continuous in space and time)</th>
<th>network $\rightarrow \Phi_n(t)$ (discrete in space, continuous in time)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>DE known</strong>: Navier-Stokes-equations (including required “special effects”). DE is fundamental, universal</td>
<td><strong>DE unknown</strong>, calculated on basis of netlist and transfer functions DE only valid for actual system</td>
</tr>
<tr>
<td><strong>To do</strong>: geometry, boundary conditions and material properties have to be specified</td>
<td><strong>To do</strong>: Division of the system in sub-systems, modeling of transfer functions and determining model parameters</td>
</tr>
<tr>
<td><strong>Simulation</strong>: Solving 3-D partial DE on grid by approximate methods in space and time (mesh generation, solver, post processing)</td>
<td><strong>Simulation</strong>: Solving time dependent ordinary DE at discrete points (nodes) (linearization, matrix methods)</td>
</tr>
<tr>
<td><em>Time consuming &amp; accurate</em></td>
<td><em>Fast &amp; especially suited for large systems</em></td>
</tr>
</tbody>
</table>
Conclusions

Numerical Simulations of microfluidic systems ...

• Can be carried out with various methods
  ➢ CFD => computation costly, however accurate
  ➢ Network simulation => fast, however challenging due to model generation (few compact models available)

• Methods have to be appropriately chosen
  ➢ CFD => problem for which geometry plays crucial role
  ➢ Network simulation => system simulations with many „simple“ strongly interacting components

• Have different methodical & numerical background
  ➢ CFD => solution in time- and space; complete, fundamental physical description
  ➢ Network simulation => solution in time at discrete nodes; behavioral modeling using compact models