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- Two prominent types of simulation
  - CFD
    - Resources
    - Basics of the method
    - Examples
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    - Basics
    - Examples
- Conclusions & Summary

Motivation

What is Simulation?

Goal: **Prediction of system behaviour under given 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)

Validiation/ verification : Testing model by comparison with experimental data

Model Generation

- **Determination of system boundaries**
  - Where does system start and end?
  - What belongs to it?
- **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**
  - Reducing complexity
  - **Model reduction**

Process of model generation is essential part of simulation!

A simulation only as good as underlying model!

Solving of Model: Simulation

1. **Analytical solution**

   For some „simple“ cases, analytical solutions can be found

2. **Numerical solution**

   The solution calculated by computers and various numercial techniques

Solution in space & time
„physical simulation“

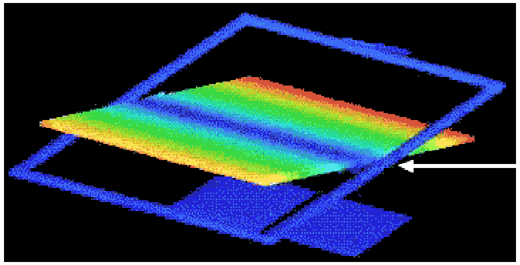
(e.g., finite element method (FEM) for mechanical simulation)

Solution in time
„system simulation“

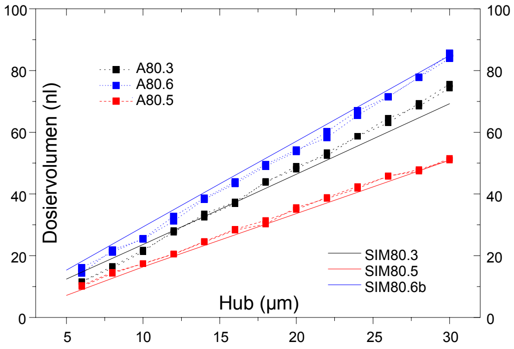
(e.g., electronic circuit simulation)

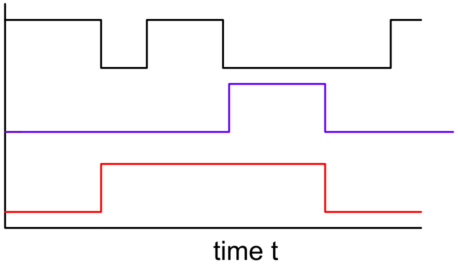
Event oriented
„digital simulation“

(e.g., digital circuit simulation)



Two-axis mirror assembly





What is simulation good for?

- 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

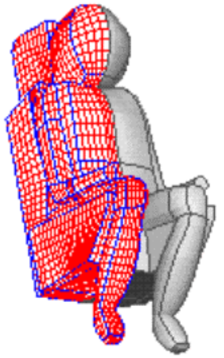
3.A. Simulation

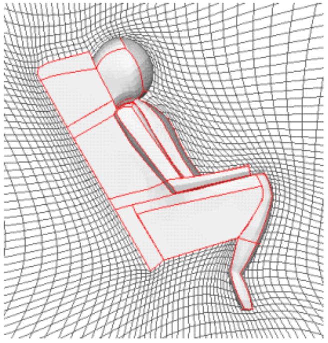
- Motivation: What is simulation good for?
- Two prominent types of simulation: CFD and system simulation
- CFD simulation:
  - Resources
  - Basics of the method
  - Examples
- System simulation
  - Rescources
  - Basics
  - Examples
- Conclusions & Summary

Types of Simulation

Grid-based „physical“ simulation

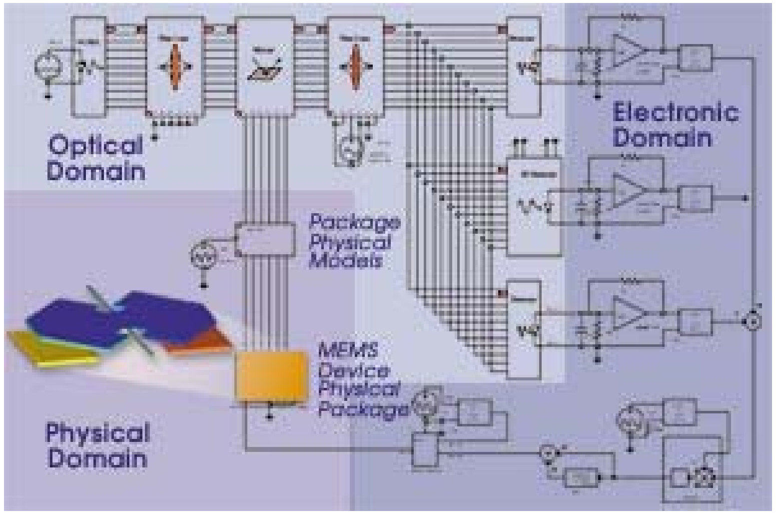
- Simulation of solids (mechanical, electrical, thermal and other domains)
  - ANSYS
  - NASTRAN, ...
- **Simulation of Flow (Computational Fluid Dynamics (CFD))**
  - FLUENT
  - POLYFLOW
  - FLOW-3D
  - ...



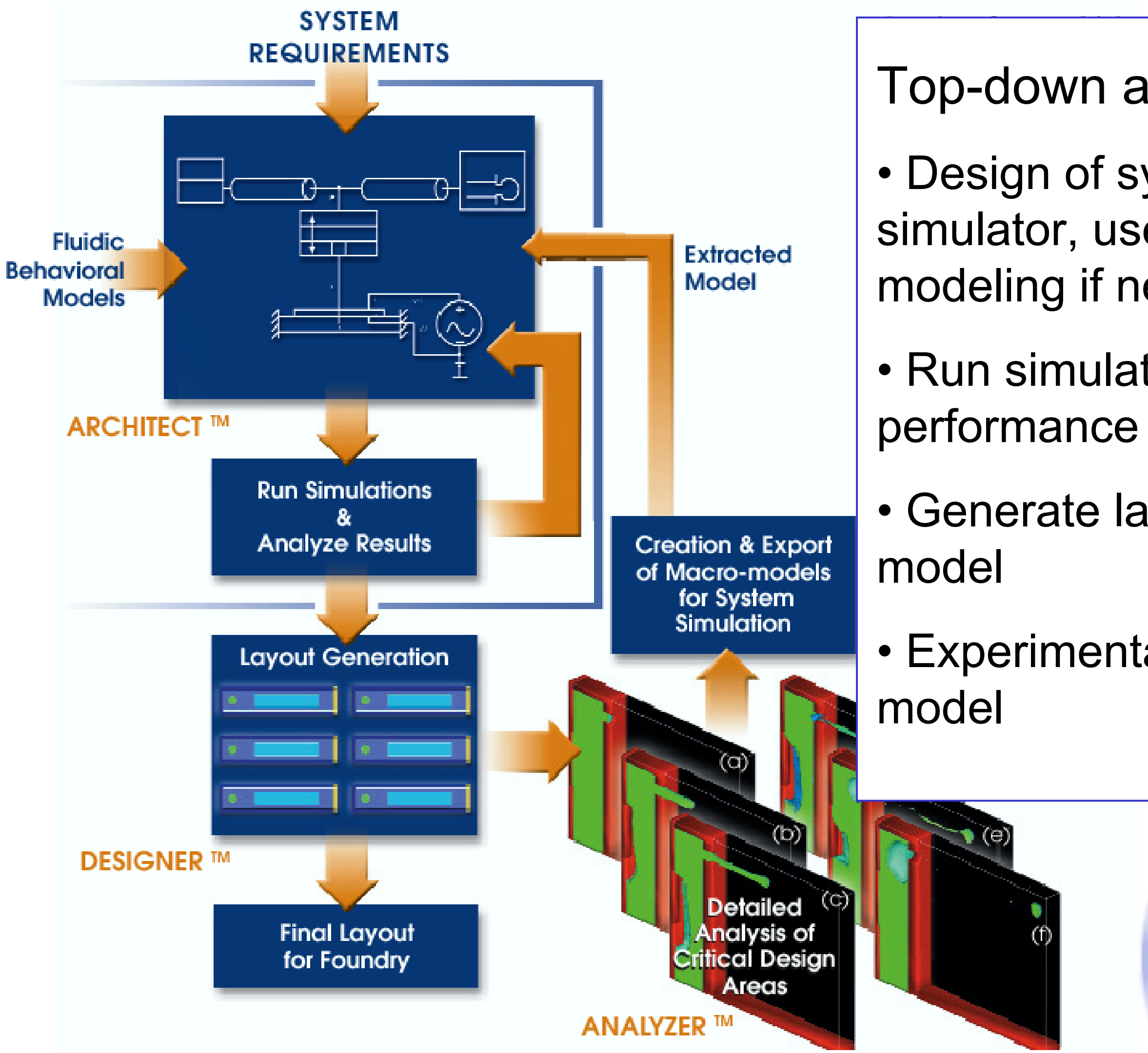


System or network simulation

- 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

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WHAT'S NEXT. AND NEXT. AND NEXT.

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)

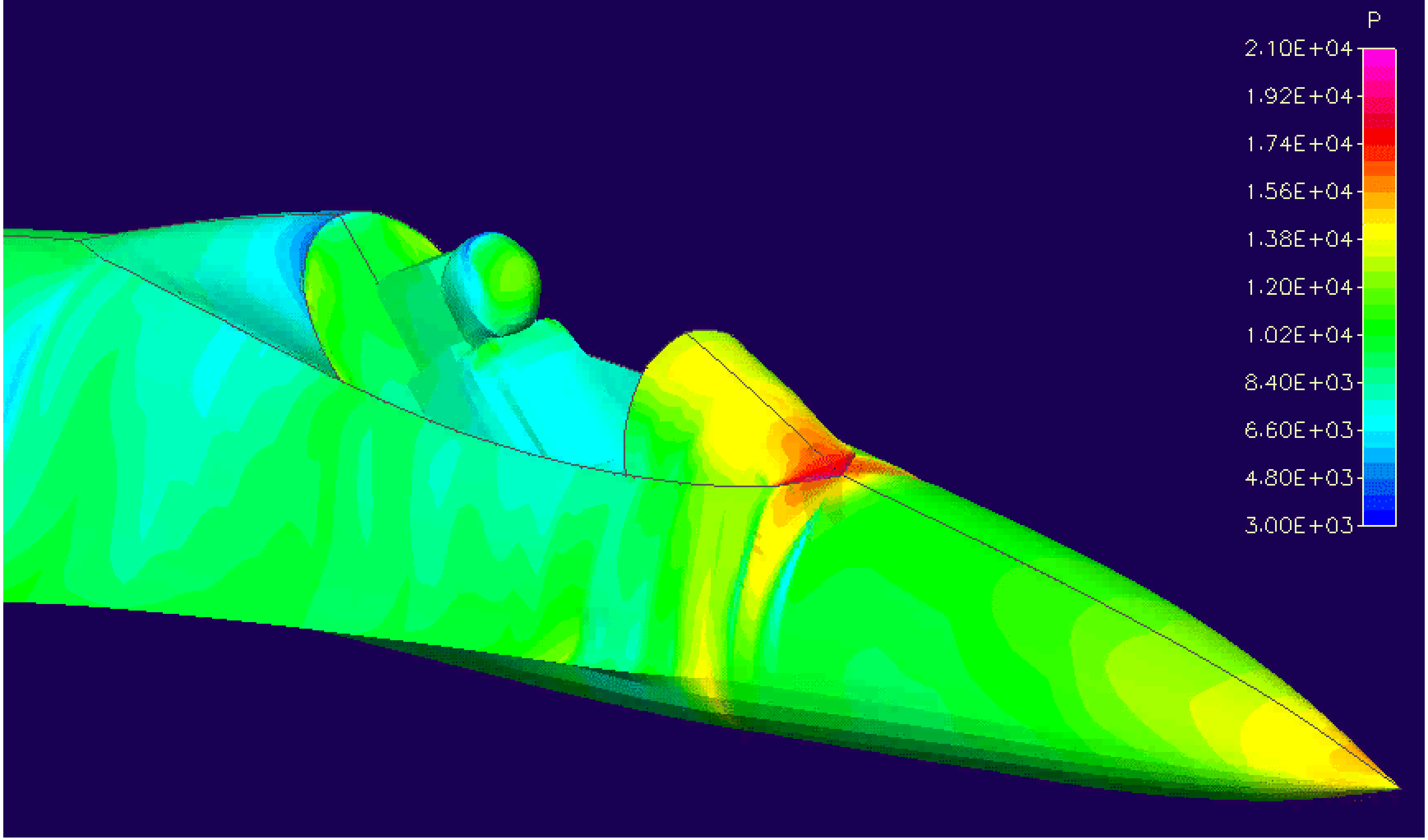
- Multiphysics modeling can be done on „physical“ level as well as on system level
  - Coupling of different grid-based solvers (physical level)
  - Defining different physical domains in network simulations (system level)
  - Coupling of grid-based solvers with network (simulation mixed level)

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
    - Rescources
    - Basics
    - Examples
- Conclusions & Summary

Simulated F–16/ACES–II Ejection

Time = 0.00 sec



Resources

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

- Hompages of commercial suppliers of software
  - http://www.software.aeat.com/cfx
  - http://www.fluent.com
  - http://www.flow-3D.com
  - http://www.cfdrc.com
  - ...

- Service providers for MEMS (not only CFD)
  - http://www.memscap.com
  - http://www.coventor.com
  - ...

Physical Foundations of CFD

Navier-Stokes-Equations

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

$$\nabla \cdot \boldsymbol{v} = 0$$

additional expressions

? Expression for capillary forces (surface tension)

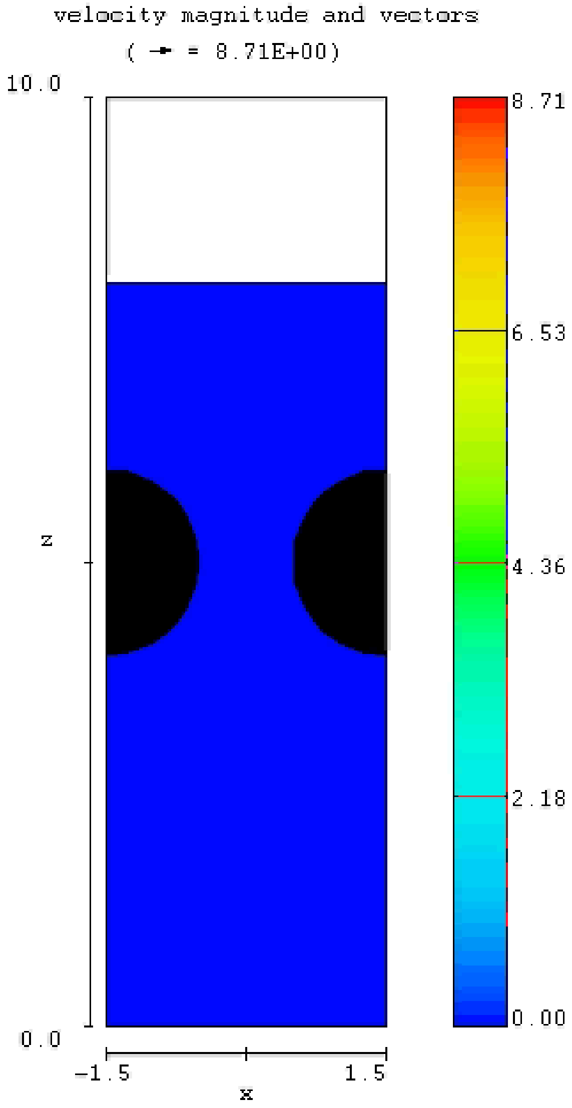
? Expression for electrokinetic effects (electrophoresis, electroosmosis)

? Multi-phase transport $\boldsymbol{v} = \{\boldsymbol{v}_1, \boldsymbol{v}_2, \boldsymbol{v}_3, \ldots\}$

? Chemical reactions $\nabla \cdot \boldsymbol{v} \neq 0$

? Etc.

Example 1: Discrete Particle Transport



Considered effects:

- Fluid dynamics
- Particle transport

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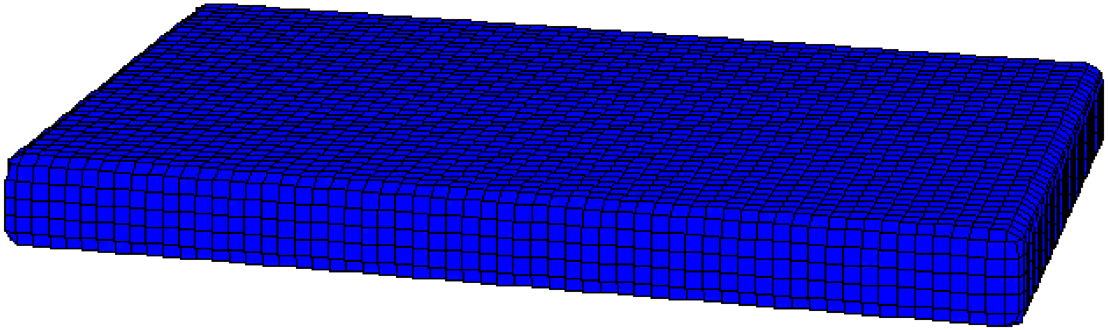
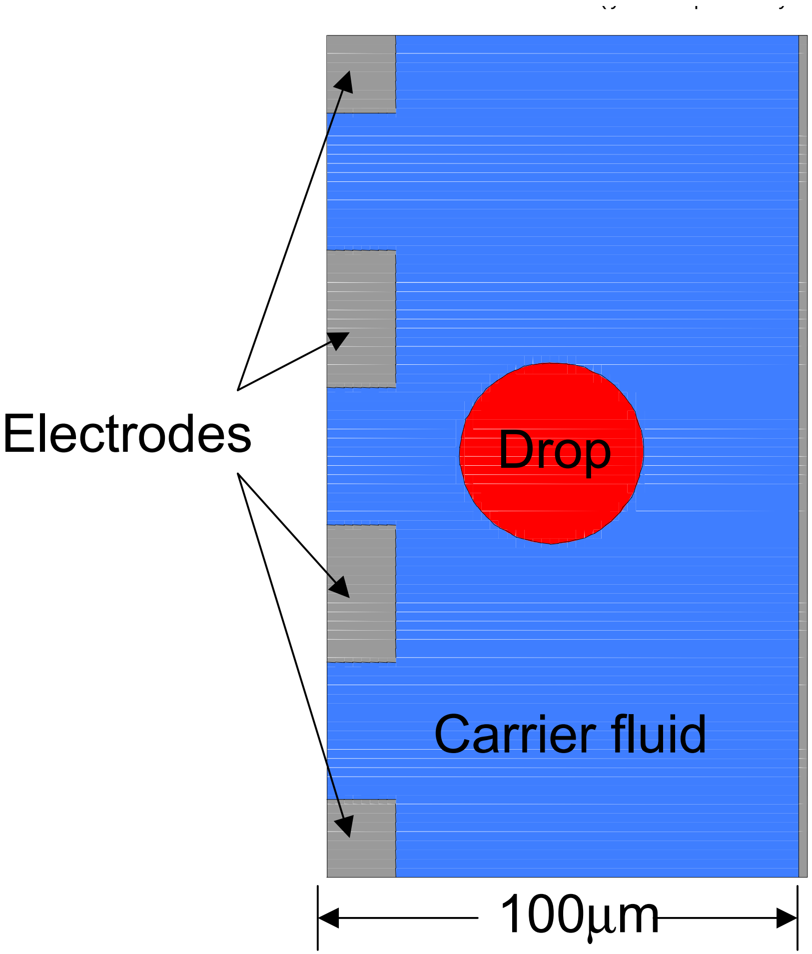
Example 2: Welding



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)
- Electrodynamics

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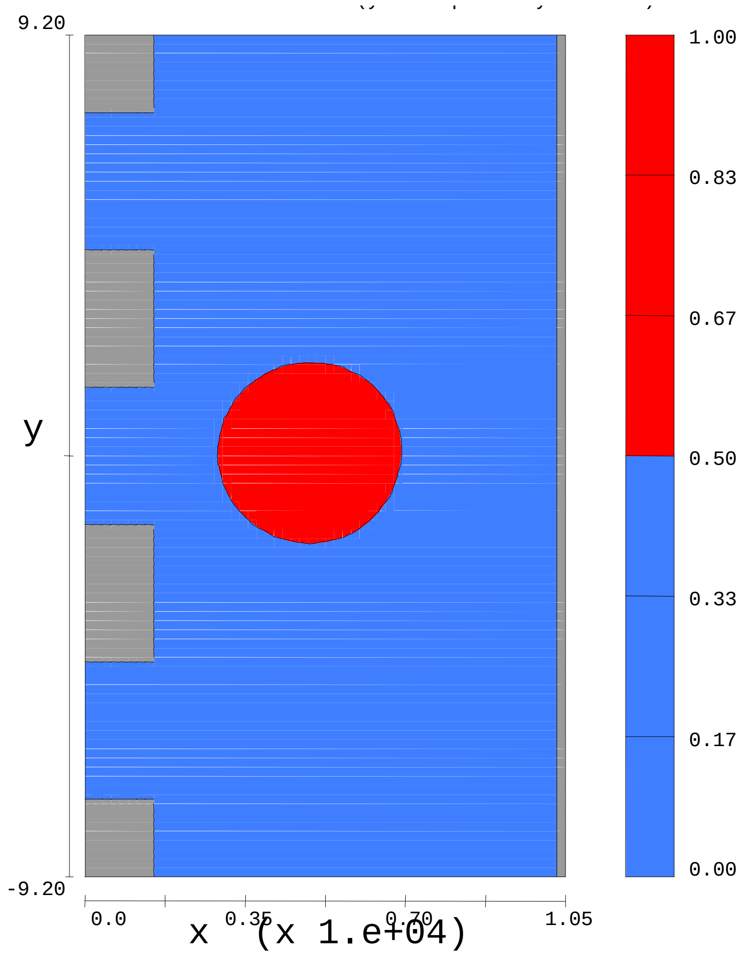
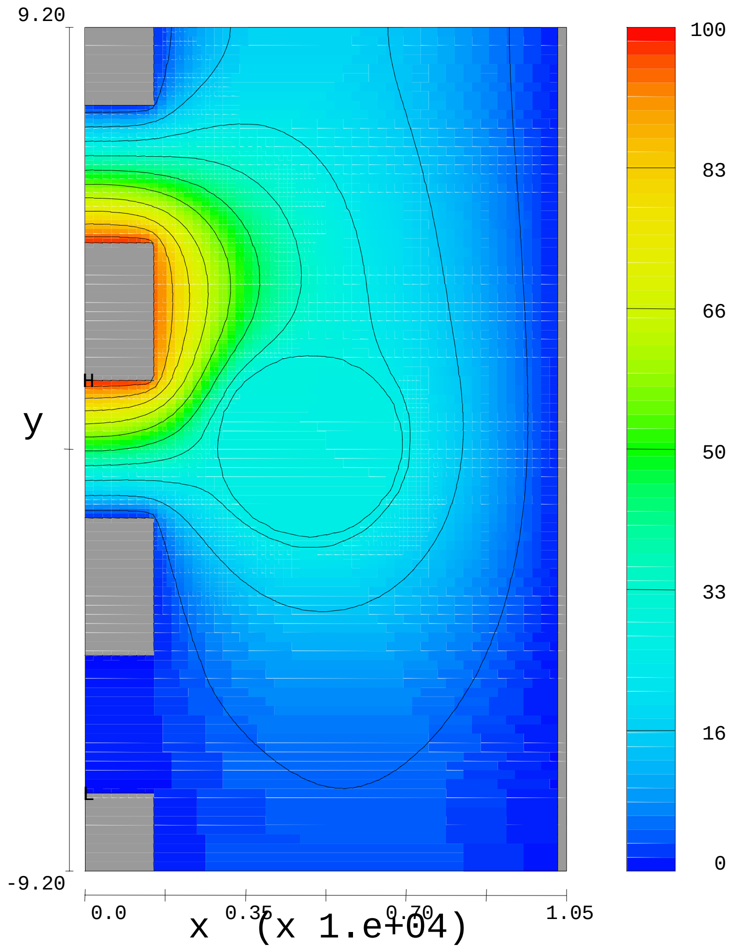
Electric Potential @ Time 0.1ms



Droplet in carrier fluid

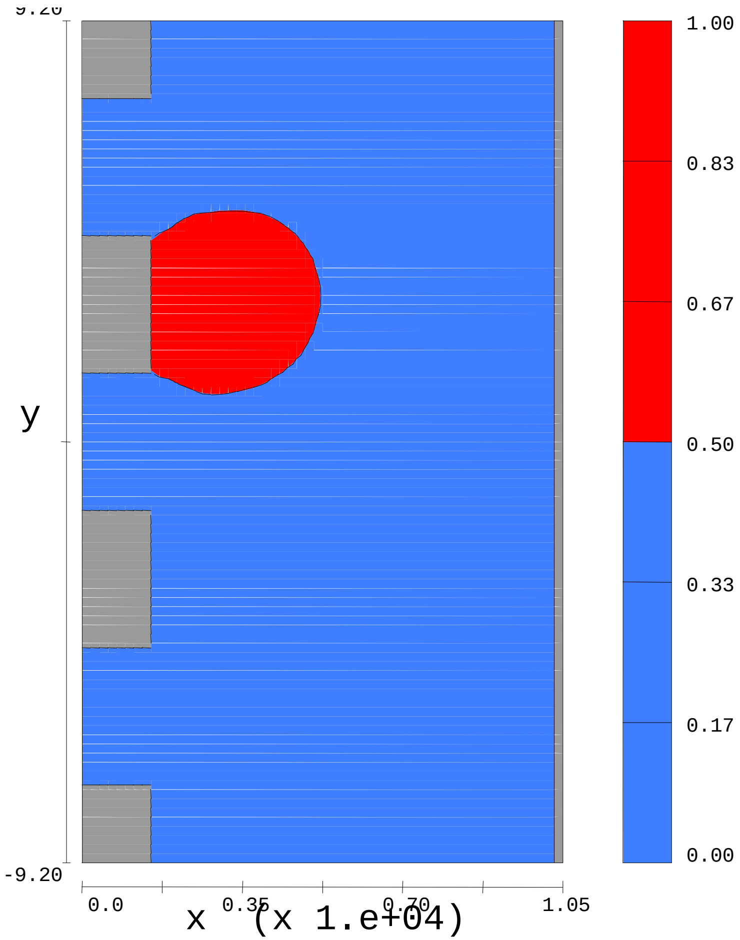
(Droplet has high dielectric constant)



Potential field

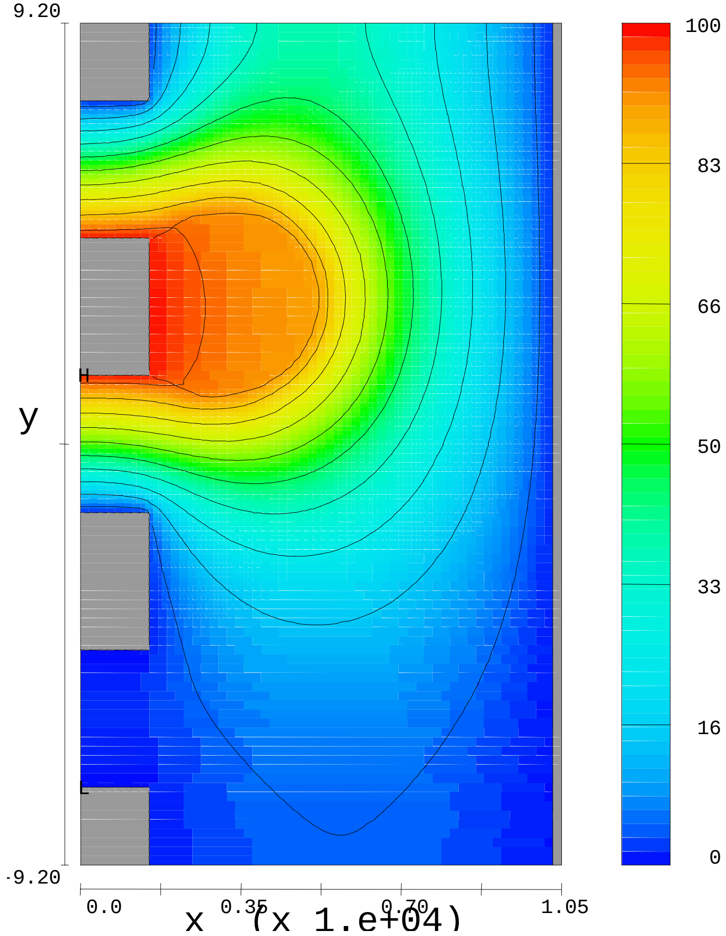
(0 - 100 volts)

Electric Potential @ Time 0.7ms



Droplet in carrier fluid

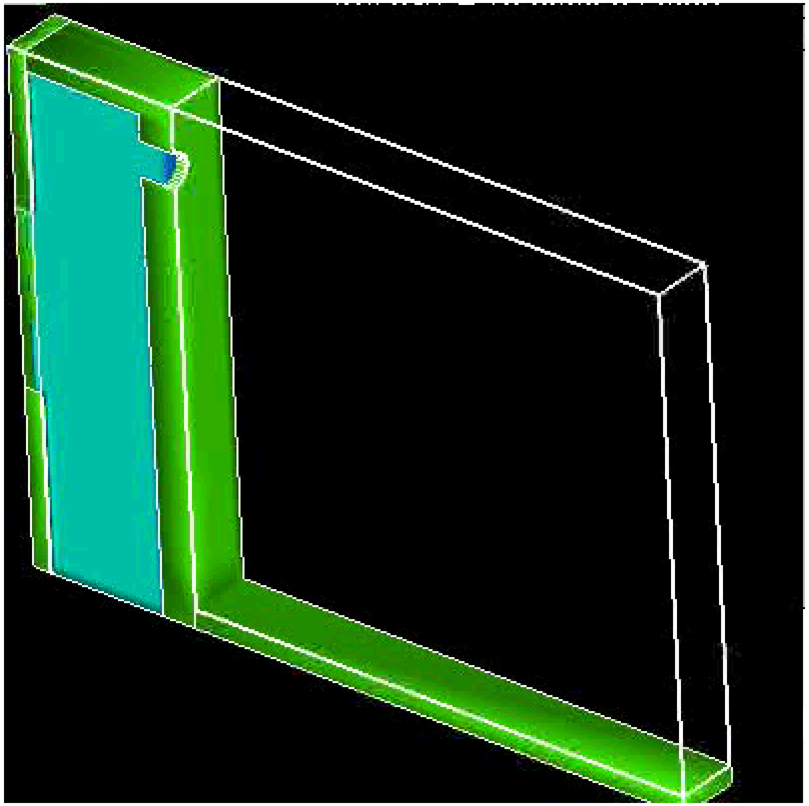
(Droplet has high dielectric constant)



Potential field

(0 - 100 volts)

Example 4: Bubble-Jet Printhead



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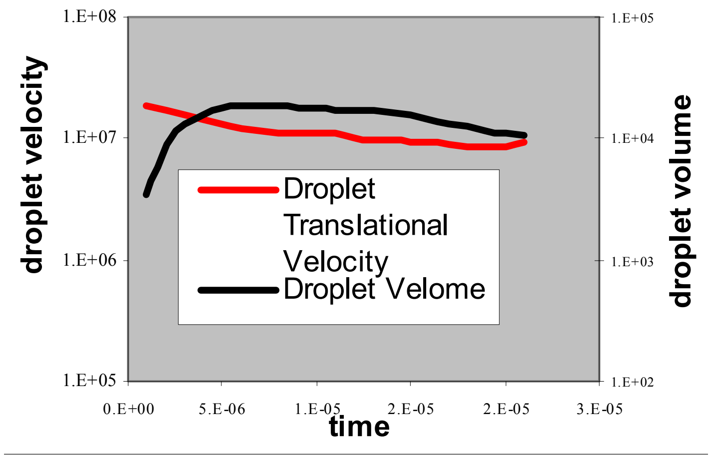
Considered effects:

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

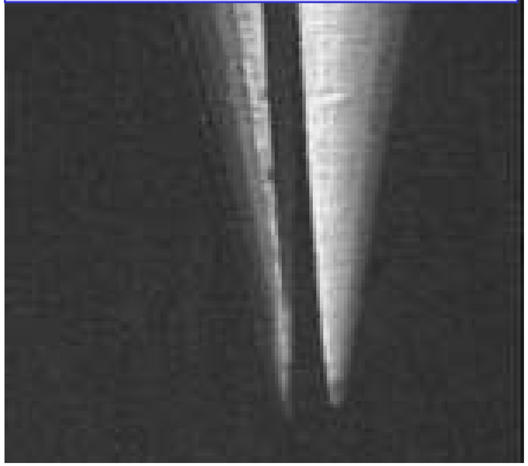
Droplet Characteristics by Thermal Bubble Jet

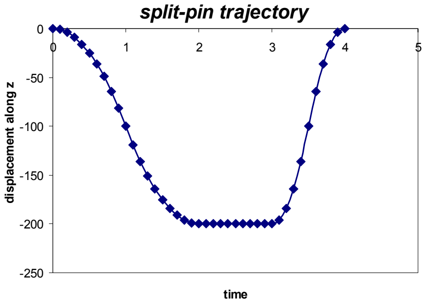


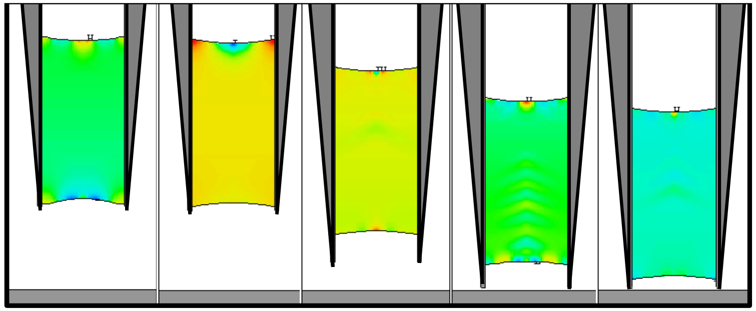
Example 5: Microarraying

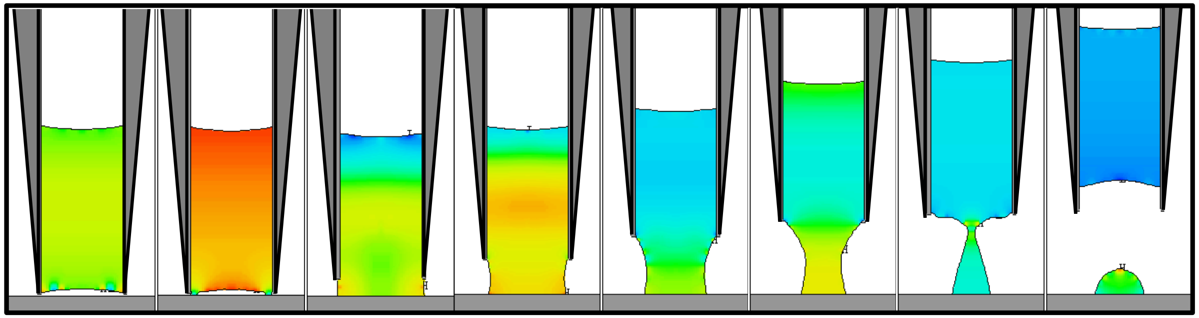
Considered effects:

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









a 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).

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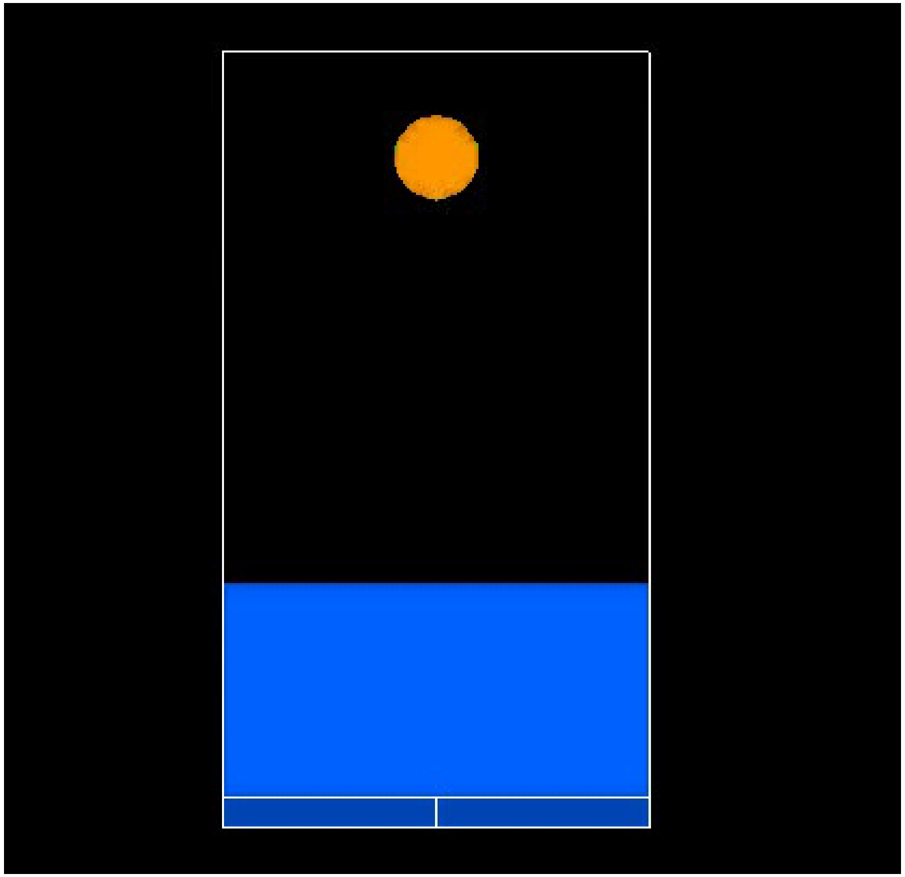
WHAT'S NEXT. AND NEXT. AND NEXT.

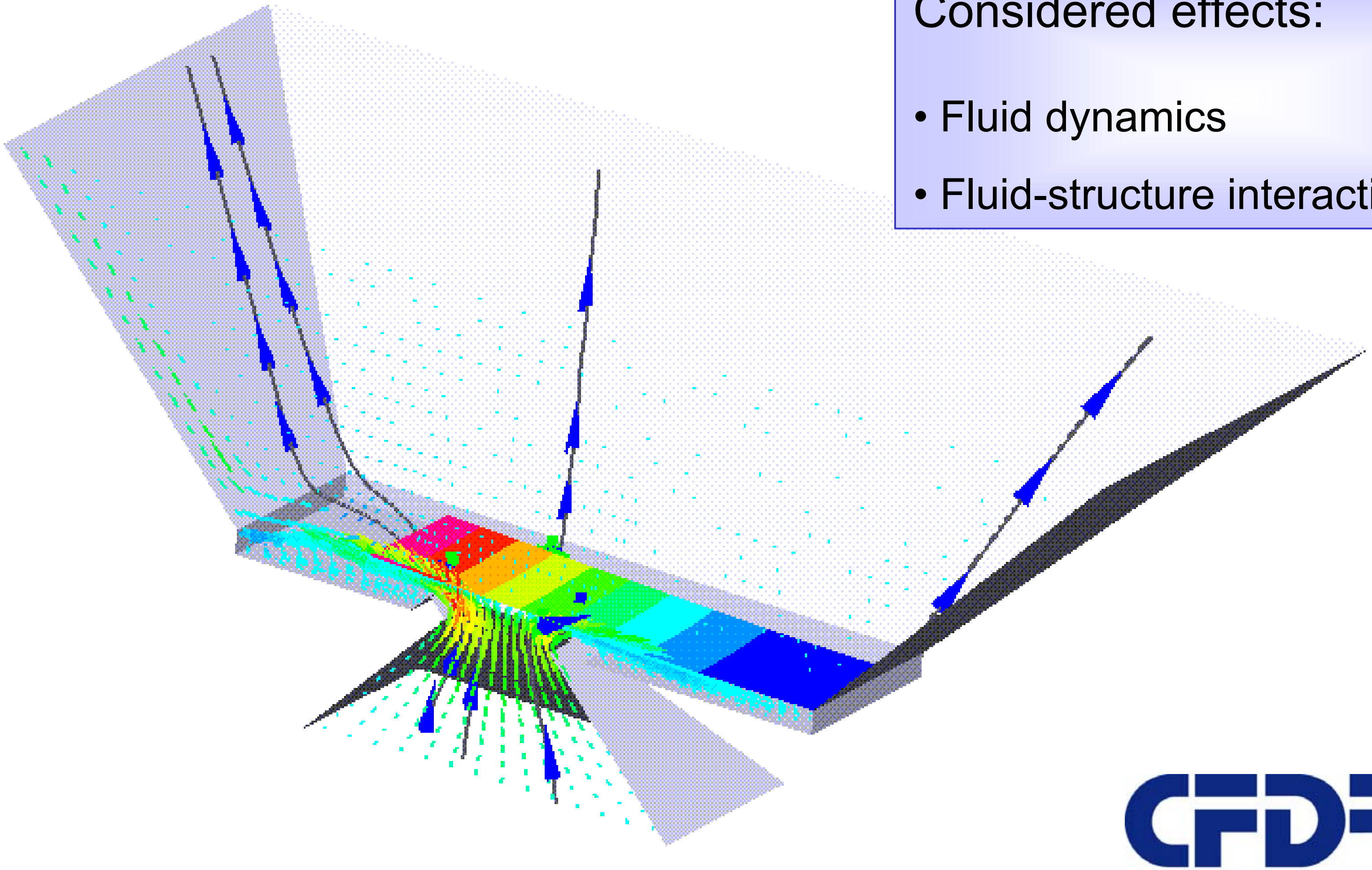
Example 6: Dispensing into Well



Considered effects:

- Fluid dynamics (two phase flow)
- Mixing

Example 7: Flap Valve

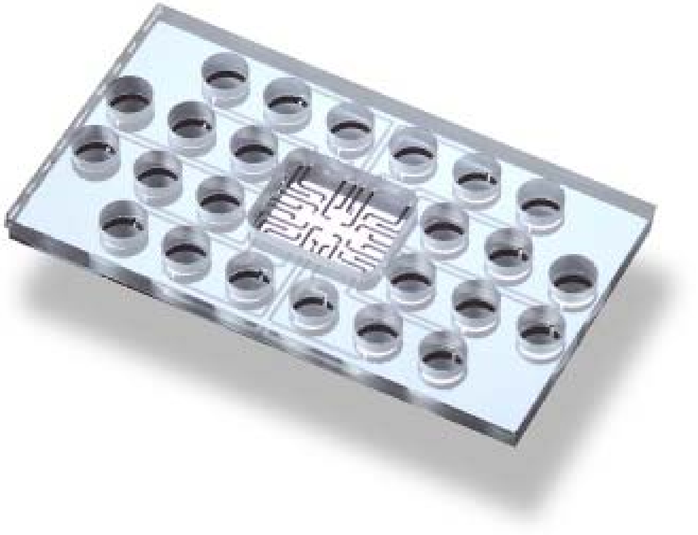


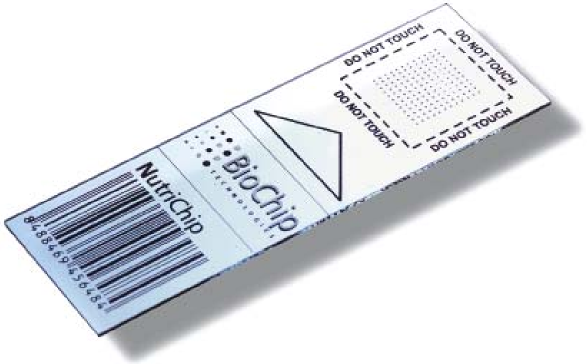
Considered effects:

- Fluid dynamics
- Fluid-structure interaction

Top-Spot Microarrayer

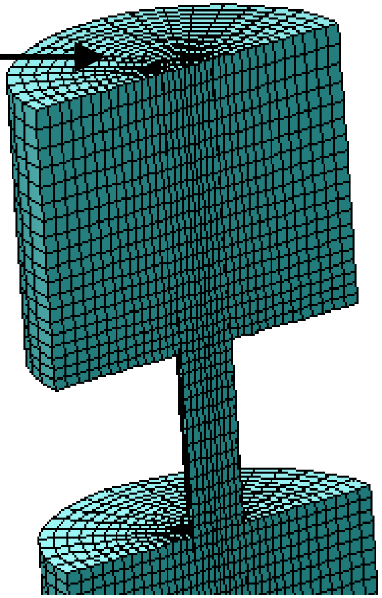
- Contact-free method
- Maximum 384 different liquids
- Massive parallel printing
- Volumes 100 pl to a a few nl





Simulation of Top-Spot

Simulation of displacement by moving grid

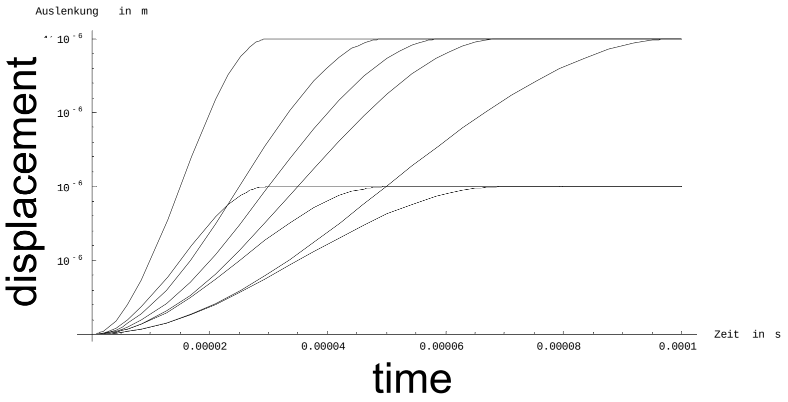


Simplifications

- Simplified pressure profile
- Only one nozzle
- Using symmetry

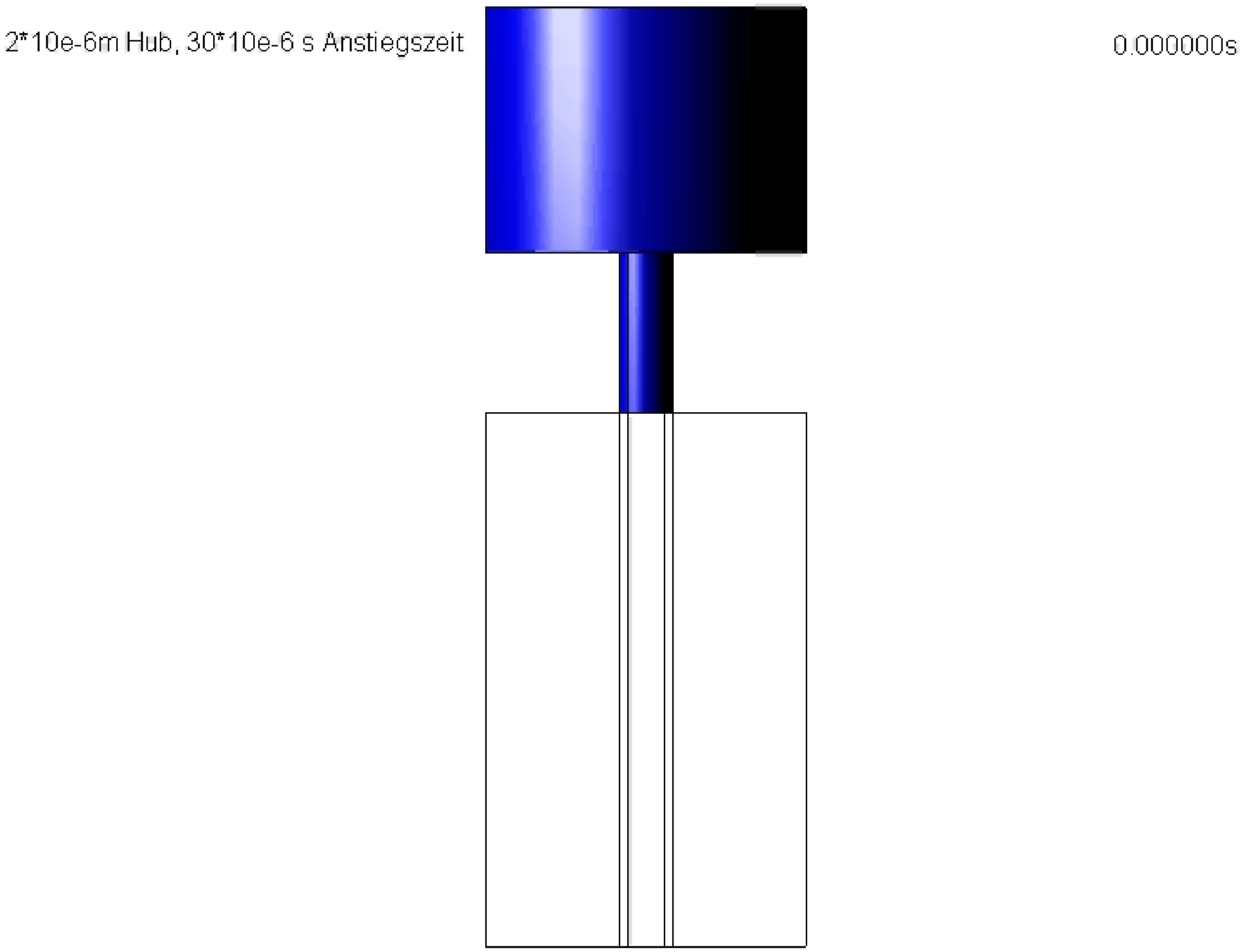
Questions

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



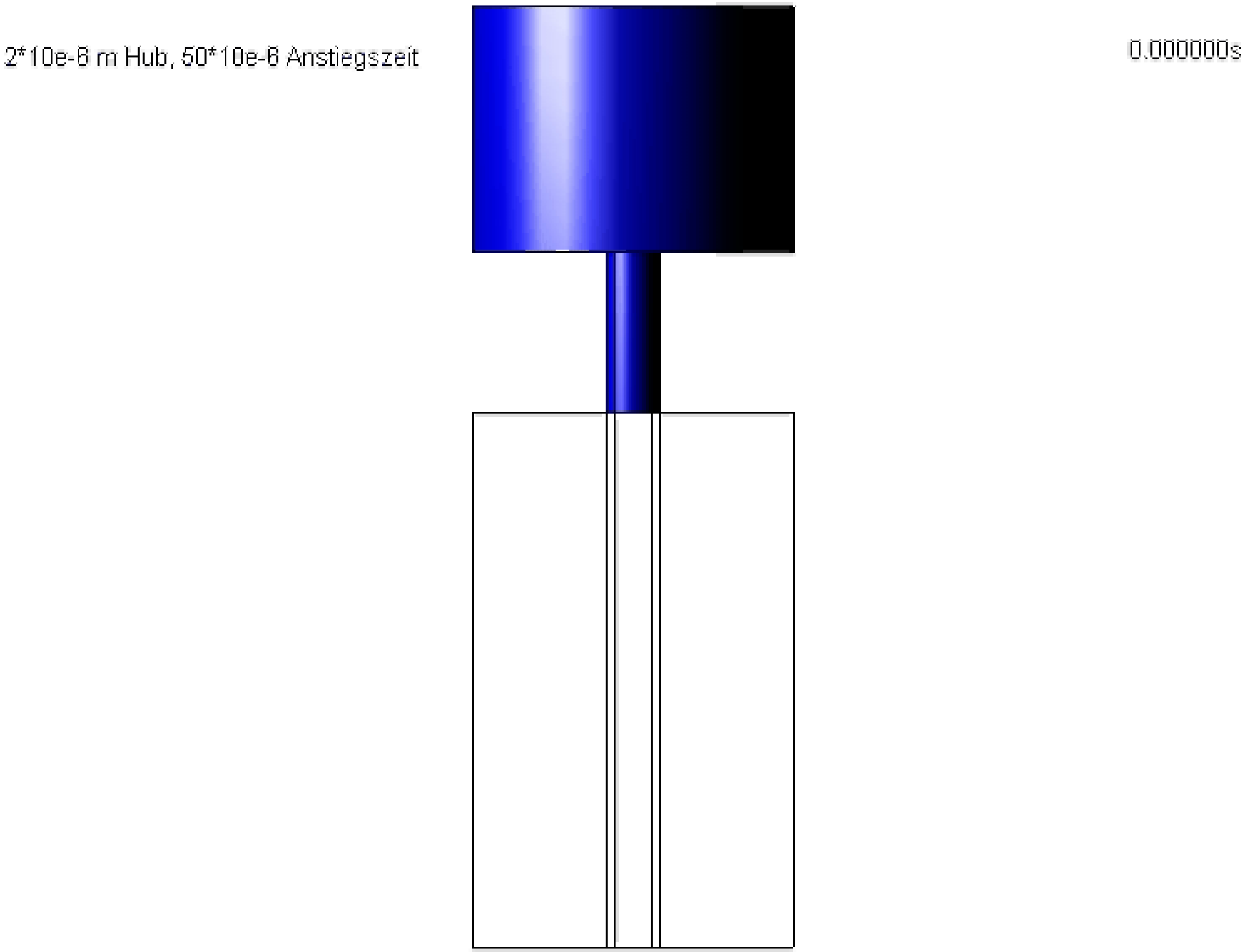
Dynamic Simulation

Stroke dynamics: 2 µm / 30 µs



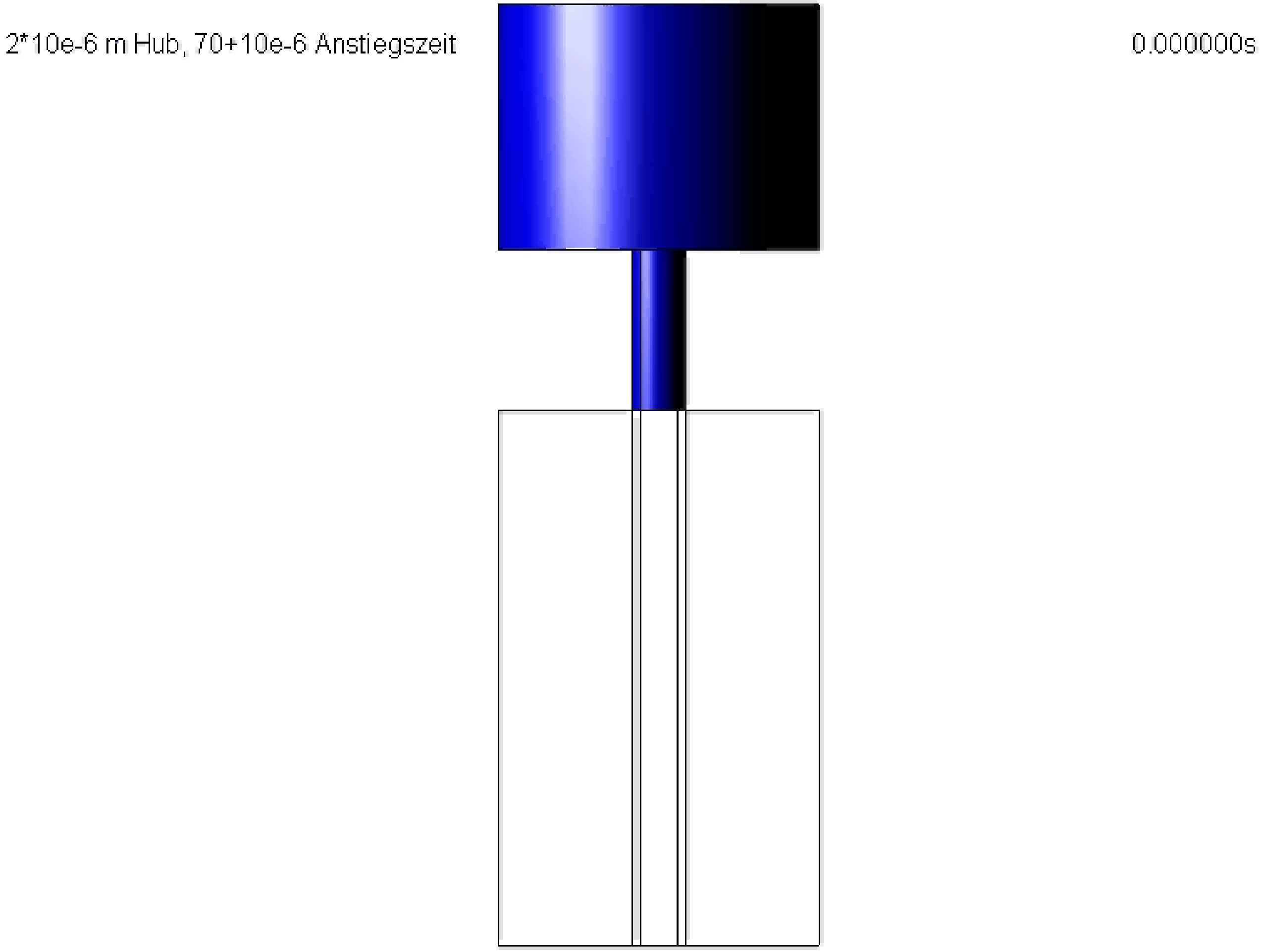
Dynamic Simulation

Stroke dynamics: 2 µm / 50 µs



Dynamic Simulation

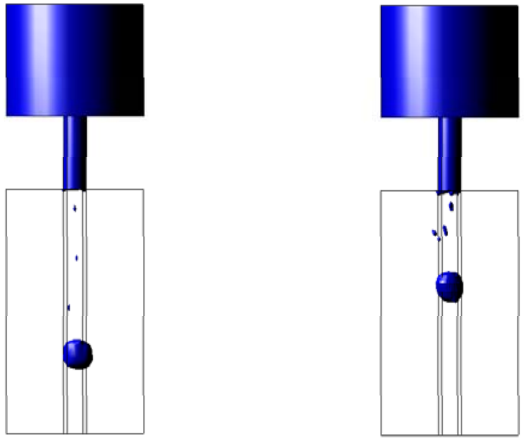
Stroke dynamics: 2 µm / 70 µs



Results

Standard operation

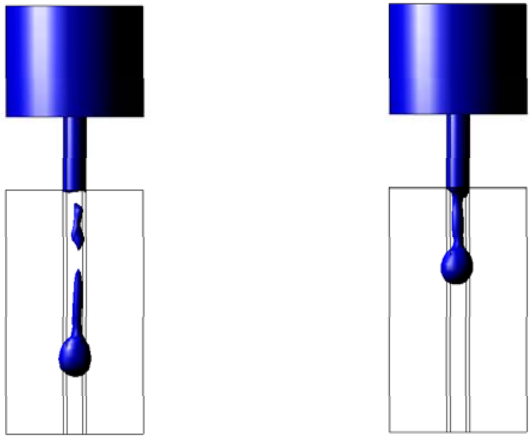
- Fluid volume / piston stroke approx. linearly dependent
- Direct relation between piston dynamics and droplet velocity



2 µm stroke, within 30 µs resp. 50 µs

Low piston dynamics

- Droplet may return to nozzle
- <u>This has also been observed in experiments!</u>



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
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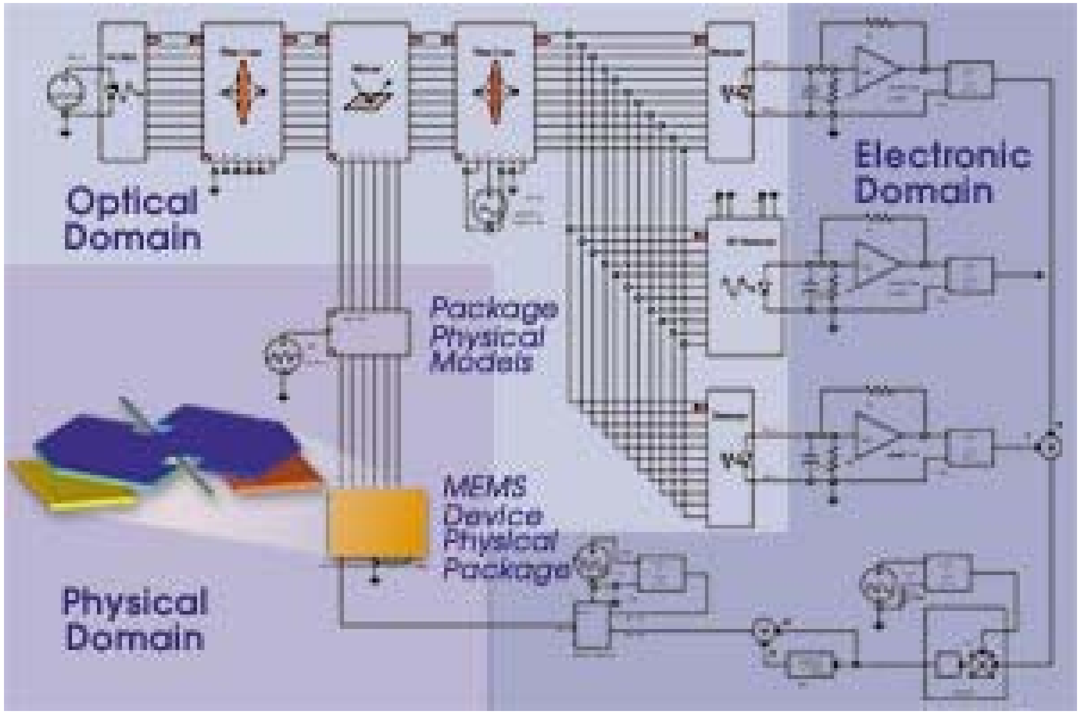
System Simulation

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

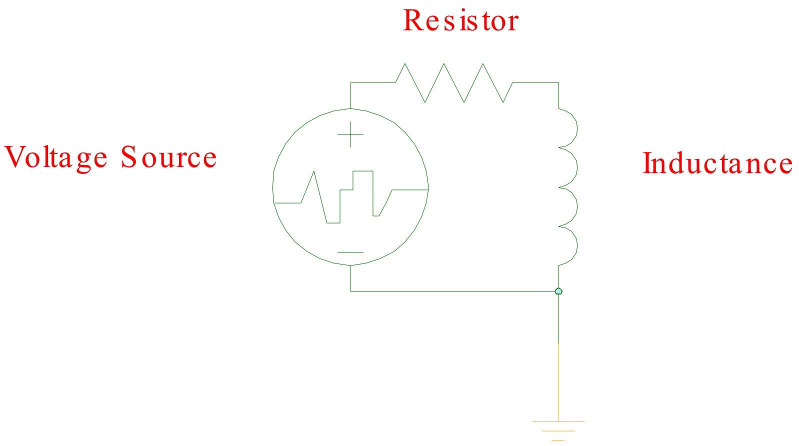


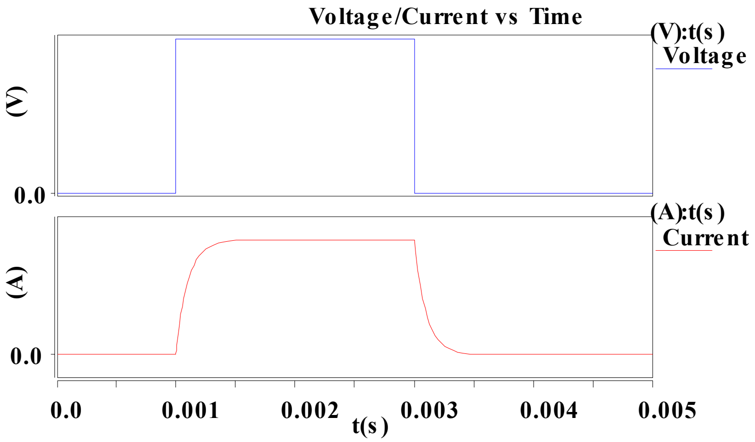
Resources

- 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

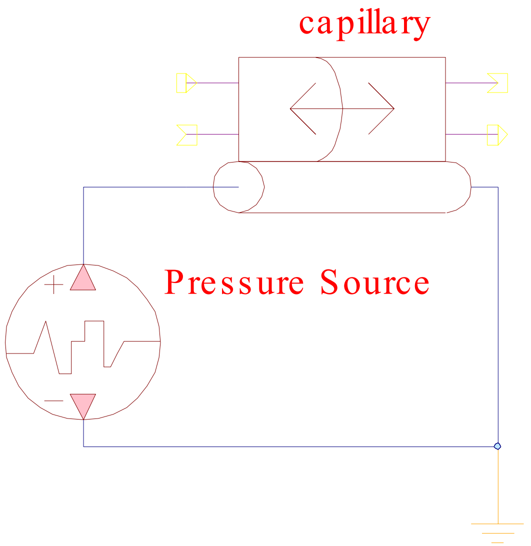
- Based on Kirchhoff‘s laws
  - Sum of all currents I_n at node is zero
  - Sum of all voltages U_n within closed loop is zero
- Differential euqations derived from „transfer functions“ $U = f(I)$:
  - $U_R = R \cdot I$
  - $U_L = L \cdot \mathrm{d}I / \mathrm{d}t$
  - $U_{\mathrm{source}} = R \cdot I + L \cdot \mathrm{d}I / \mathrm{d}t$
- Differential equations (DE) solved numerically (time- or frequency domain)



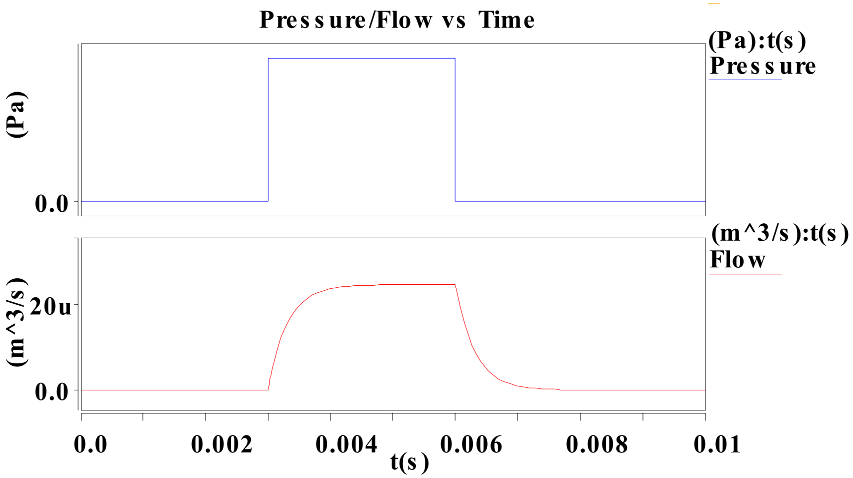


Analogy in Fluidics: $I \Rightarrow q$ and $U \Rightarrow p$

- Completely filled capillary
  - Ohmic resistance → fluidic resistance
    - Viscosity
    - Geometry
  - Inductance → inertia of fluid
    - Density
    - Geometry



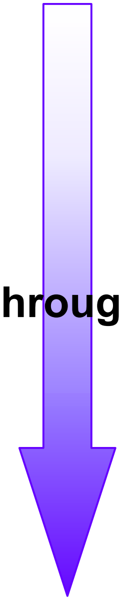
- Transfer functions and DE
  - $p_R = R \bullet q$
  - $p_L = L \bullet dq / dt$
  - $p = R_{fluid} \bullet q + L_{fluid} \bullet dq / dt$



- Numerical solution

Fundamental Principle

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



Physical system described by field equations

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

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

Through and across variables at discret points (nodes)

$$\left\{\begin{pmatrix}u_1(t_0,t)\\ \vdots\\ u_n(t_0,t)\end{pmatrix},\begin{pmatrix}i_1(t_0,t)\\ \vdots\\ i_n(t_0,t)\end{pmatrix}\right\}$$

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

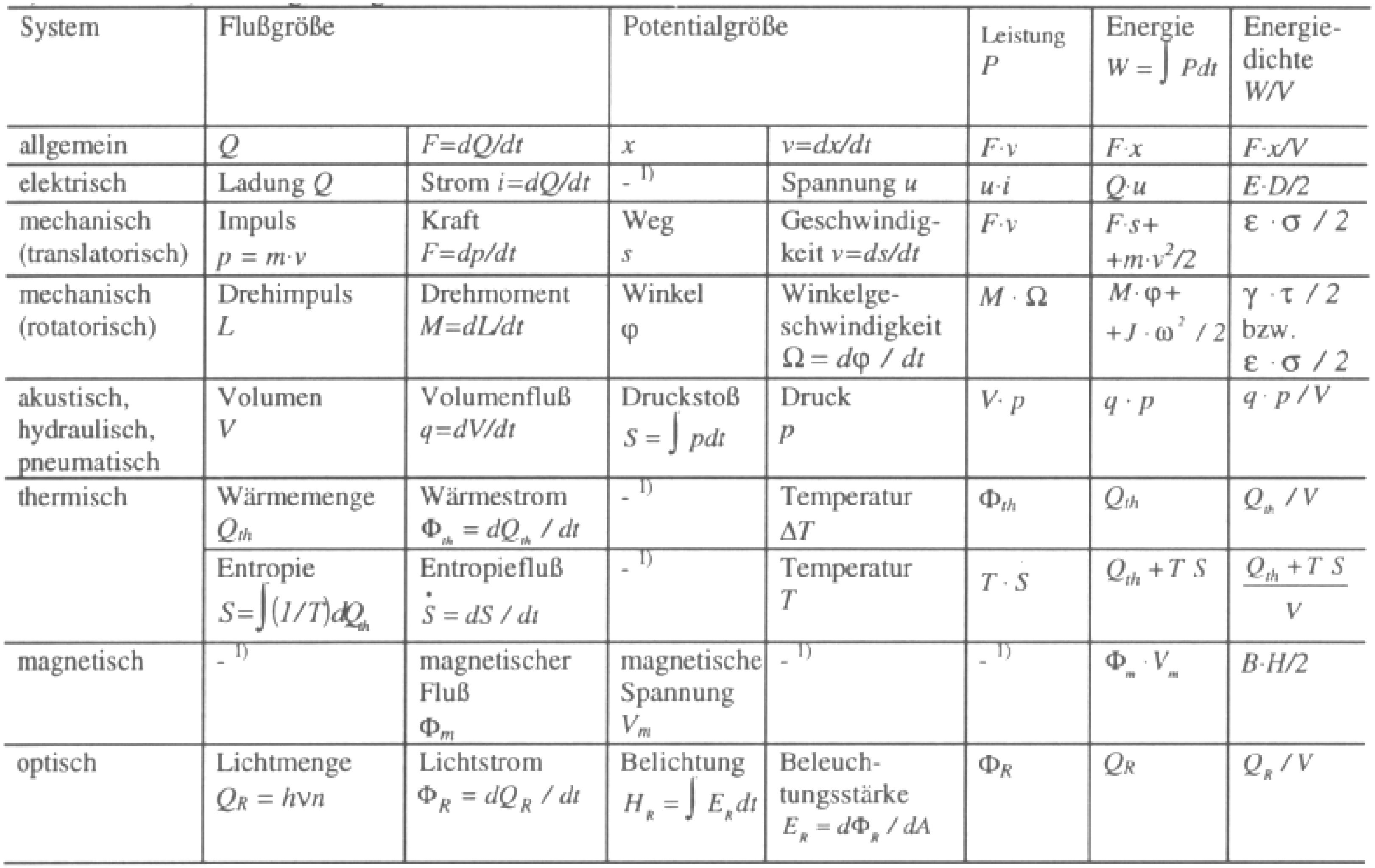
Netlist & transfer functions

➔Differential equation for network simulation

$$\begin{pmatrix}u_1(t_0,t)\\ \vdots\\ u_n(t_0,t)\end{pmatrix}=\underline{\underline{M}}(t)\times\begin{pmatrix}i_1(t_0,t)\\ \vdots\\ i_n(t_0,t)\end{pmatrix}$$

Analogy in Many Physical Domains

[G.Gerlach, W.Dötzel, „Grundlagen der Mikrosystemtechnik“, Hanser Lehrbuch (1997)], S. 81



System	Flußgröße		Potentialgröße		Leistung P	Energie $W = \int P dt$	Energiedichte W/V
allgemein	Q	$F=dQ/dt$	x	$v=dx/dt$	$F \cdot v$	$F \cdot x$	$F \cdot x/V$
elektrisch	Ladung Q	Strom $i=dQ/dt$	- 1)	Spannung u	$u \cdot i$	$Q \cdot u$	$E \cdot D/2$
mechanisch (translatorisch)	Impuls $p = m \cdot v$	Kraft $F=dp/dt$	Weg s	Geschwindigkeit $v=ds/dt$	$F \cdot v$	$F \cdot s + m \cdot v^2/2$	$\varepsilon \cdot \sigma / 2$
mechanisch (rotatorisch)	Drehimpuls L	Drehmoment $M=dL/dt$	Winkel φ	Winkelgeschwindigkeit $\Omega = d\varphi / dt$	$M \cdot \Omega$	$M \cdot \varphi + J \cdot \omega^2 / 2$	$\gamma \cdot \tau / 2$ bzw. $\varepsilon \cdot \sigma / 2$
akustisch, hydraulisch, pneumatisch	Volumen V	Volumenfluß $q=dV/dt$	Druckstoß $S = \int p dt$	Druck p	$V \cdot p$	$q \cdot p$	$q \cdot p / V$
thermisch	Wärmemenge Q_{th}	Wärmestrom $\Phi_{th} = dQ_{th} / dt$	- 1)	Temperatur ΔT	Φ_{th}	Q_{th}	Q_{th} / V
	Entropie $S = \int (1/T) dQ_{th}$	Entropiefluß $\dot{S} = dS / dt$	- 1)	Temperatur T	$T \cdot \dot{S}$	$Q_{th} + T S$	$\frac{Q_{th} + T S}{V}$
magnetisch	- 1)	magnetischer Fluß Φ_m	magnetische Spannung V_m	- 1)	- 1)	$\Phi_m \cdot V_m$	$B \cdot H/2$
optisch	Lichtmenge $Q_R = h \nu n$	Lichtstrom $\Phi_R = dQ_R / dt$	Belichtung $H_R = \int E_R dt$	Beleuchtungsstärke $E_R = d\Phi_R / dA$	Φ_R	Q_R	Q_R / V

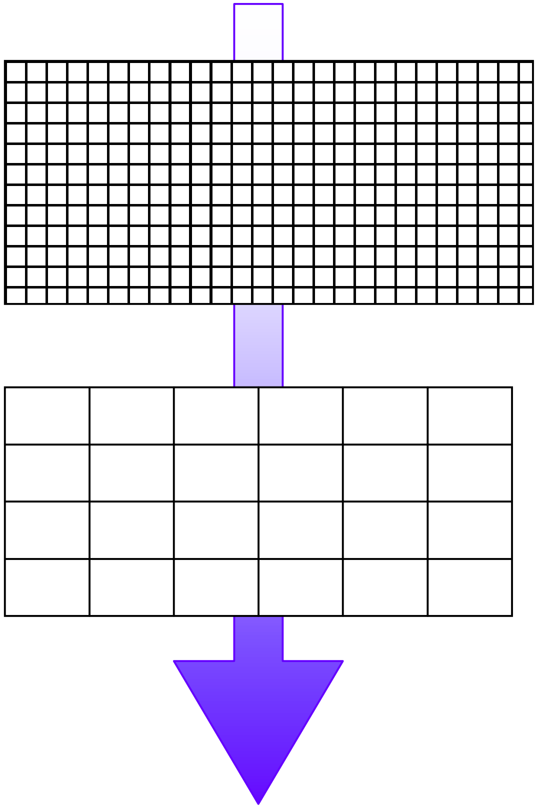
How to obtain transfer functions?

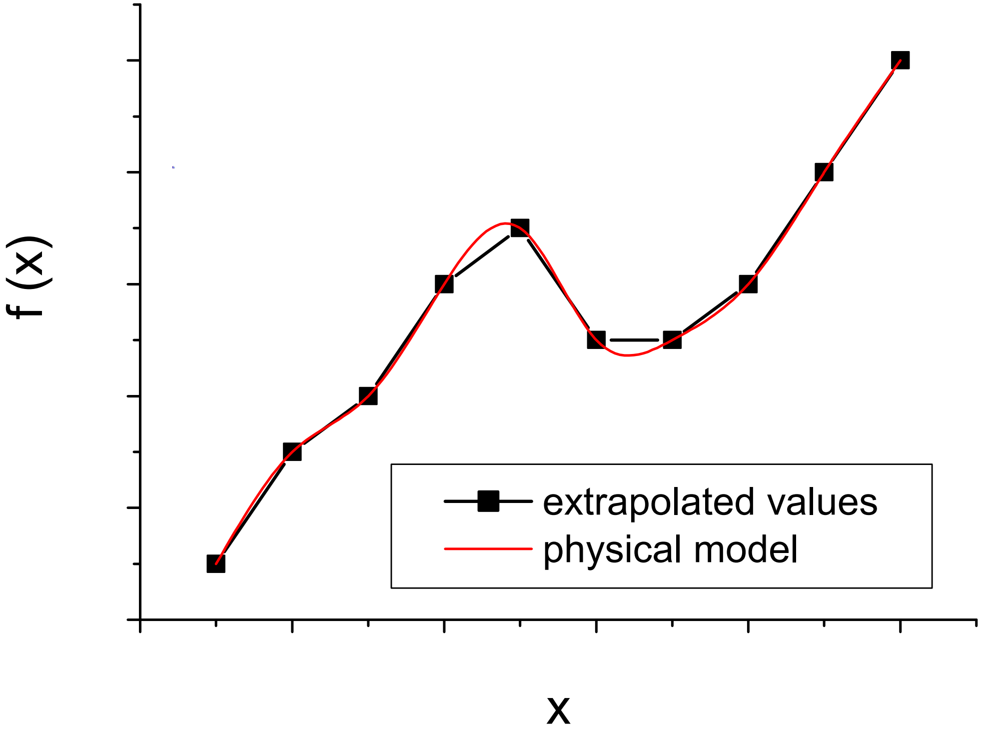
- Analytical solution of fundamental differential equation, e.g.,
  - Ohmic resistance
  - Inductance
  - Empirical compact models, e.g.,
  - Diode models
  - Tubular flow
- Experimental or simulation data (grid-based simulations), e.g.,
  - Look-up tables
  - Couple simulations
- Automated model reduction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

Model Reduction Techniques

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

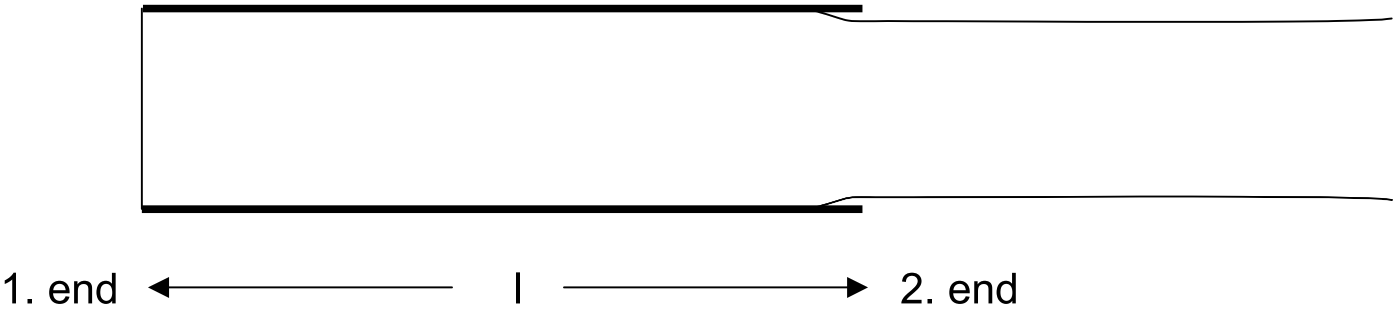
Approximation of solution obtained from physical modeling e.g., with nonlinear fit or neural networks, etc.





Example 1: Capillary Model

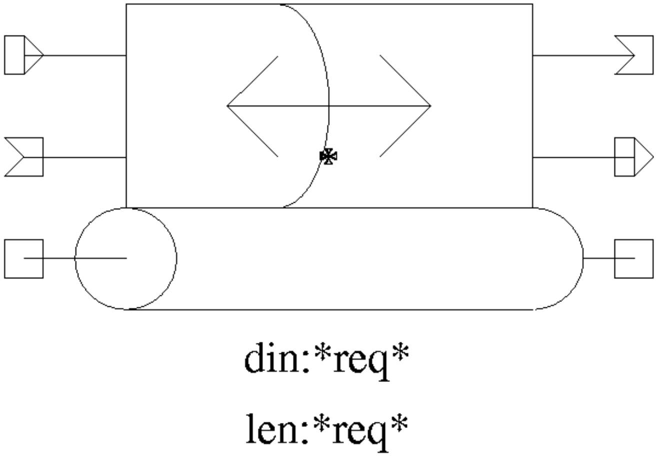
- Capillary states
  - *empty:* only air flow considered
  - Transition state: *wet1dry2* (filling from one end); *wet2dry1* (vice versa)
  - *Full:* resistance according to tube flow
- Nozzle states
  - *empty* and *wet2dry1* identical
  - Additional consideration of *meniscus state* ($p < 2\, p_{cap}$)
  - In *eject*-state ($p > 2\, p_{cap}$) approximation of pressure drop by Toricelli's formula



Capillary Channel

Capillary channel with circular cross section (∅ *d*, length *l*):

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



logical pin input

logical pin output

fluidic line

$$\mathrm{p} = \mathrm{R}\mathrm{q} + \mathrm{p}_\mathrm{k} + \mathrm{p}_\mathrm{i}$$

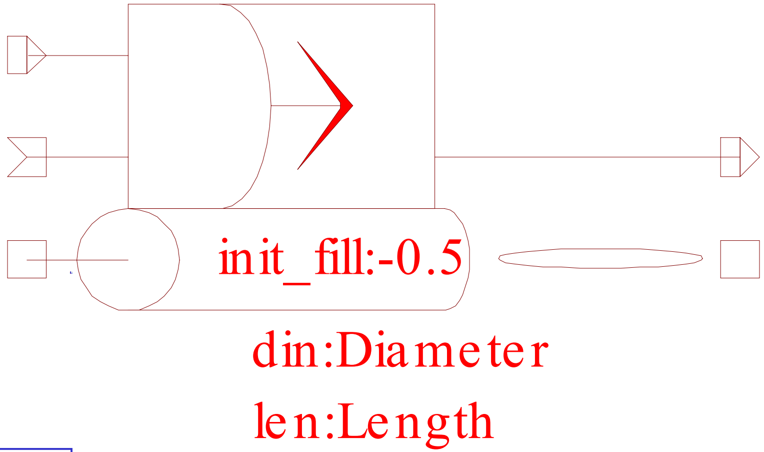
resistance capillary pressure inertia

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

Capillary Nozzle

Capillary nozzle with circular cross section (∅ *d*, length *l*):

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



logical pin input

logical pin output

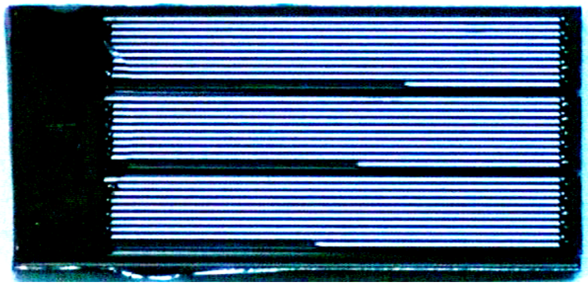
fluidic line

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

← No ejection: pressure smaller than 2 p_{cap}

← Ejection: Torcelli‘s formula

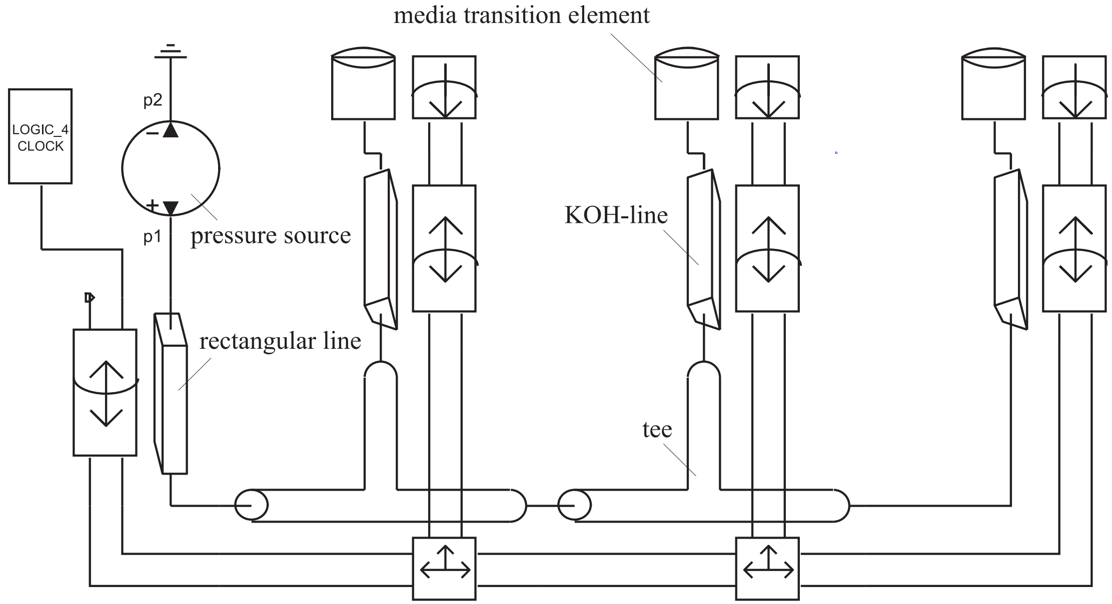
Validation of Capillary Model



by priming of meandering capillaries

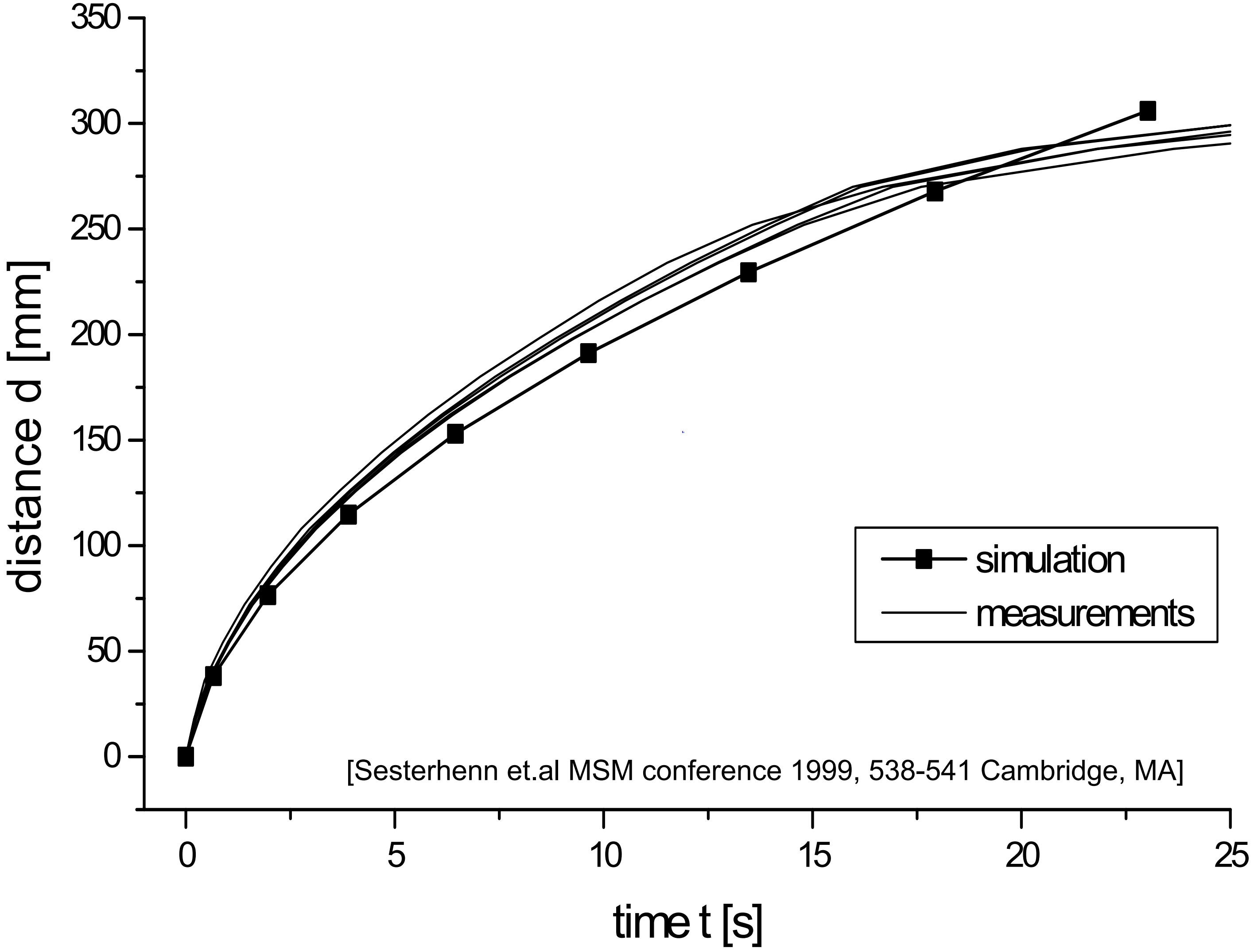
← experiment

system model



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

Comparison with Measurements

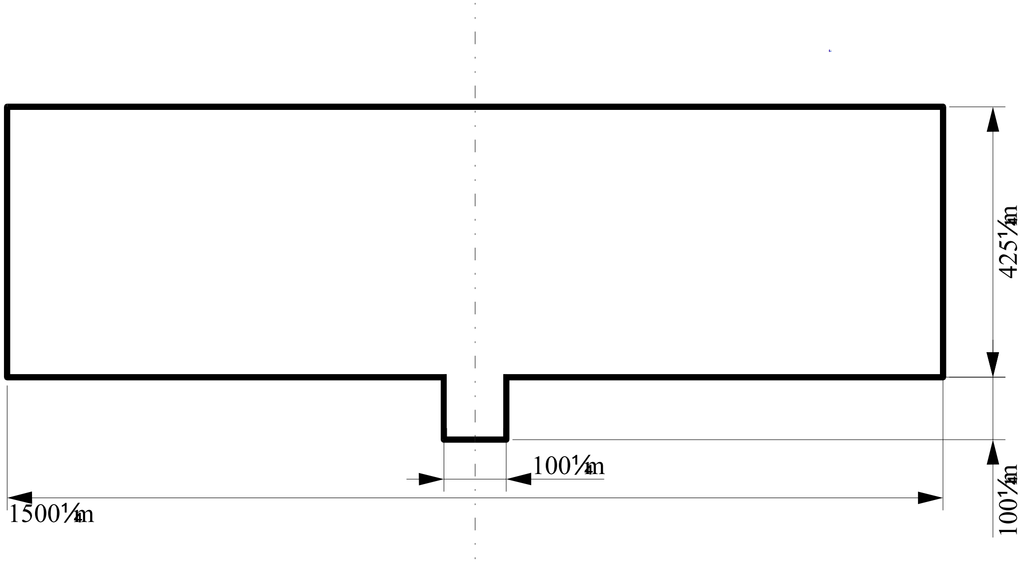


[Sesterhenn et.al MSM conference 1999, 538-541 Cambridge, MA]

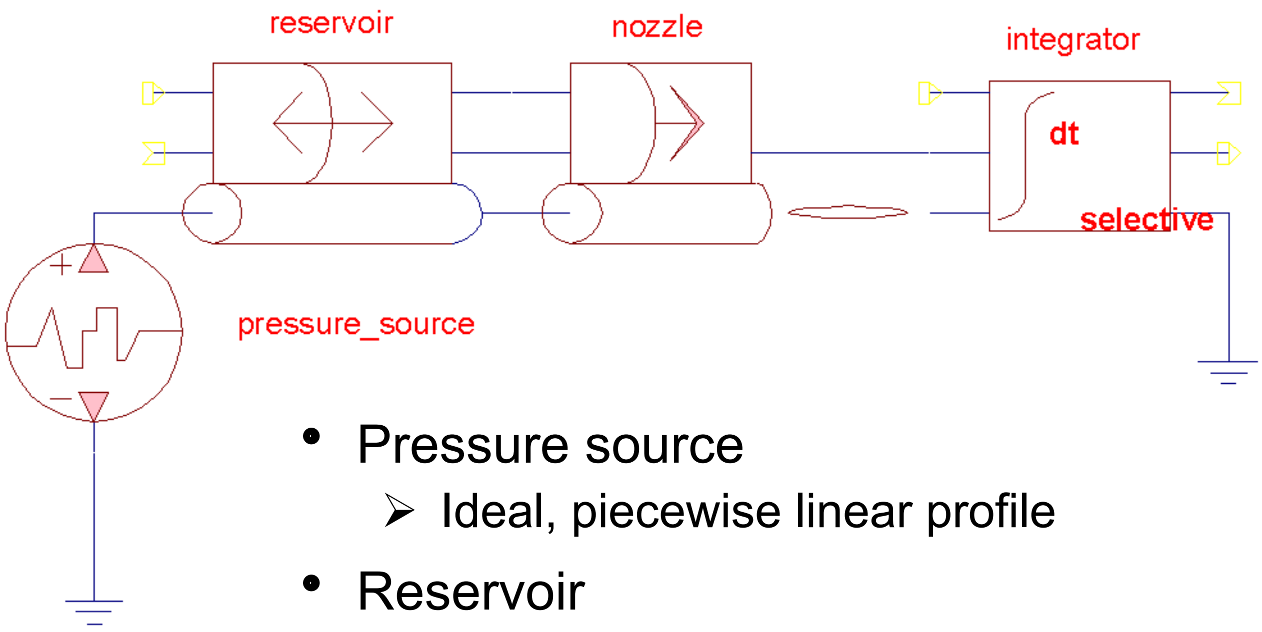
Validation of Nozzle Model

Simple multi channel test system

- Representing simple dispenser
- Micromachined in silicon
- Well suited for validation

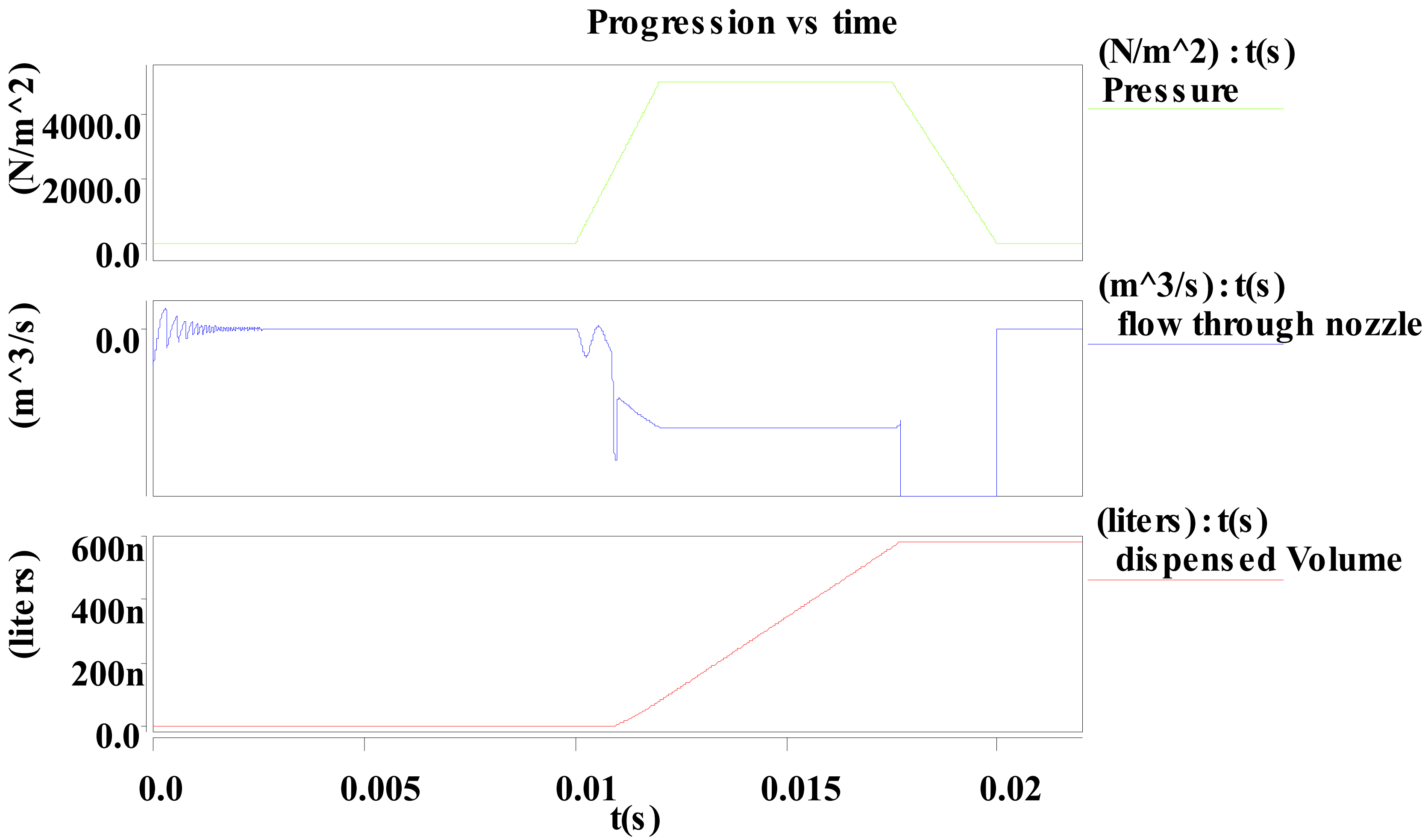


System Model

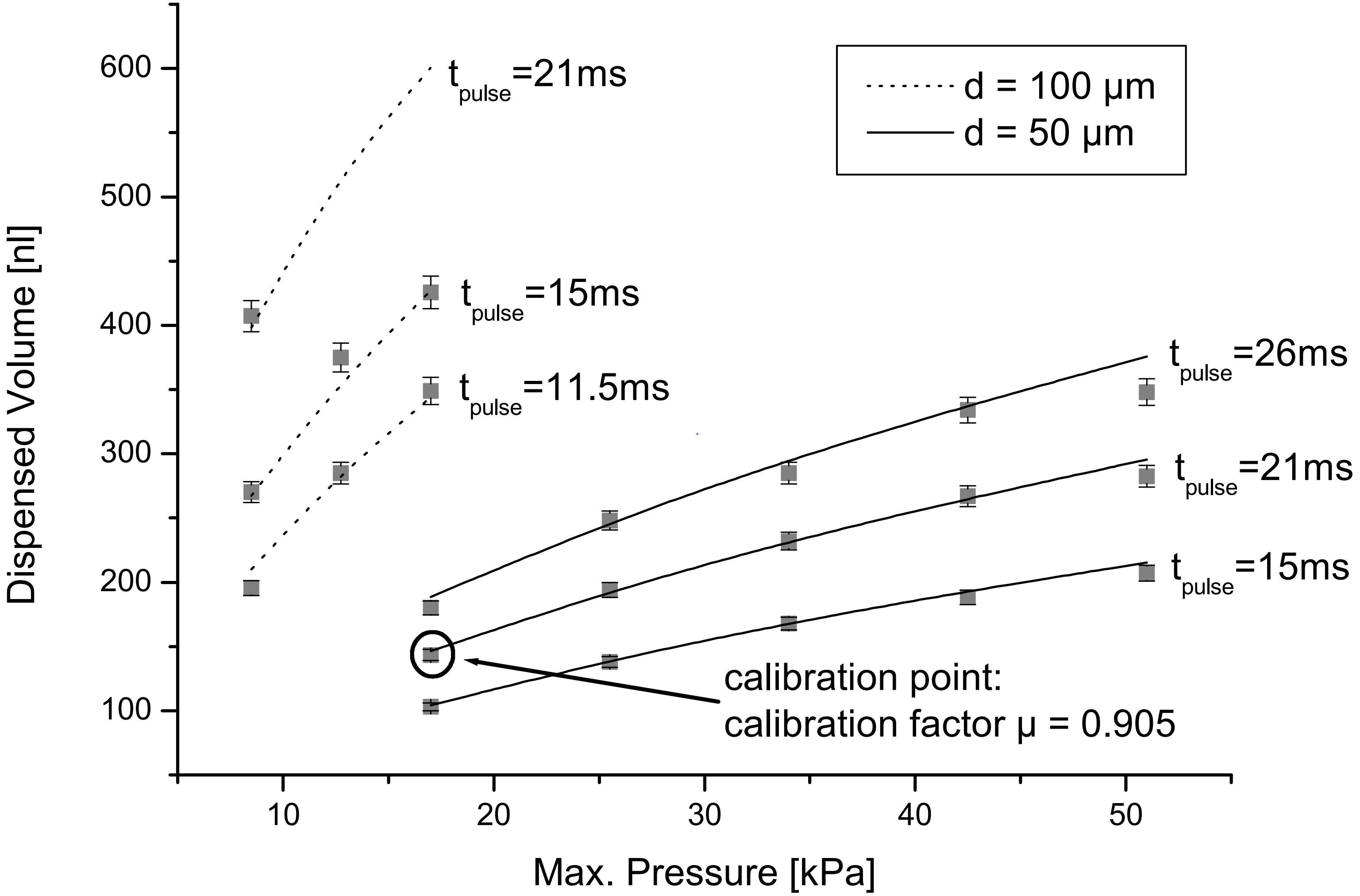


- Pressure source
  - Ideal, piecewise linear profile
- Reservoir
  - Capillary with 1500 µm diamter and 425 µm length
- Nozzle
  - 100 µm diameter, 100 µm length
- Integrator
  - Selective to fluid

Simulation Results in Time Domain



Comparison with Measurements

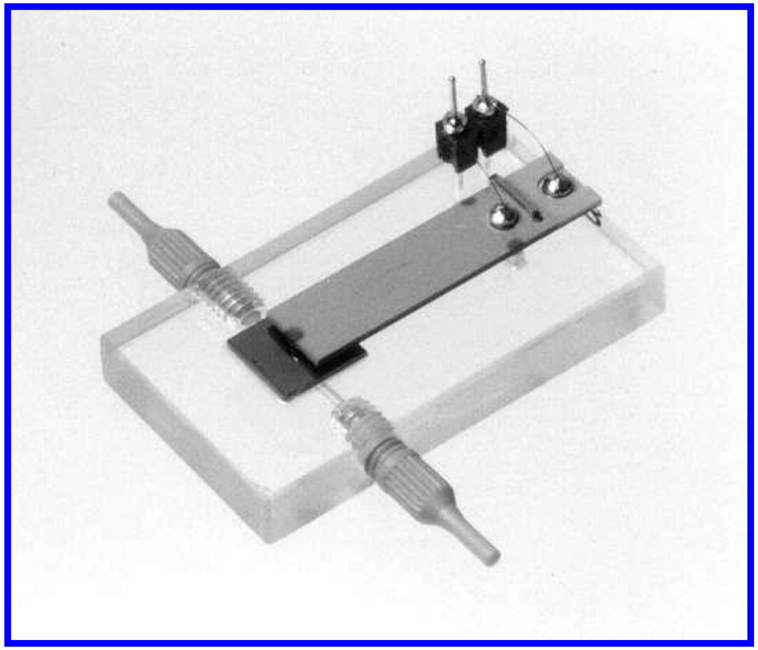


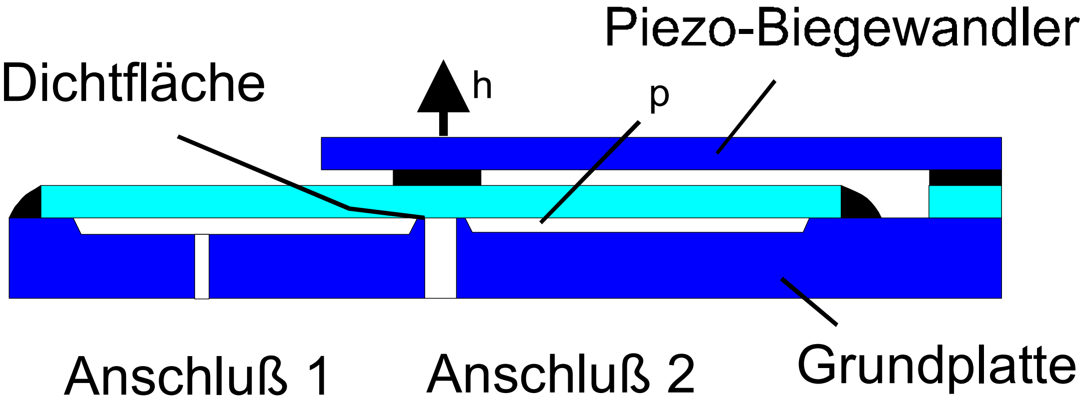
calibration point:
calibration factor µ = 0.905

Example 2: Systemmodel for VAMP

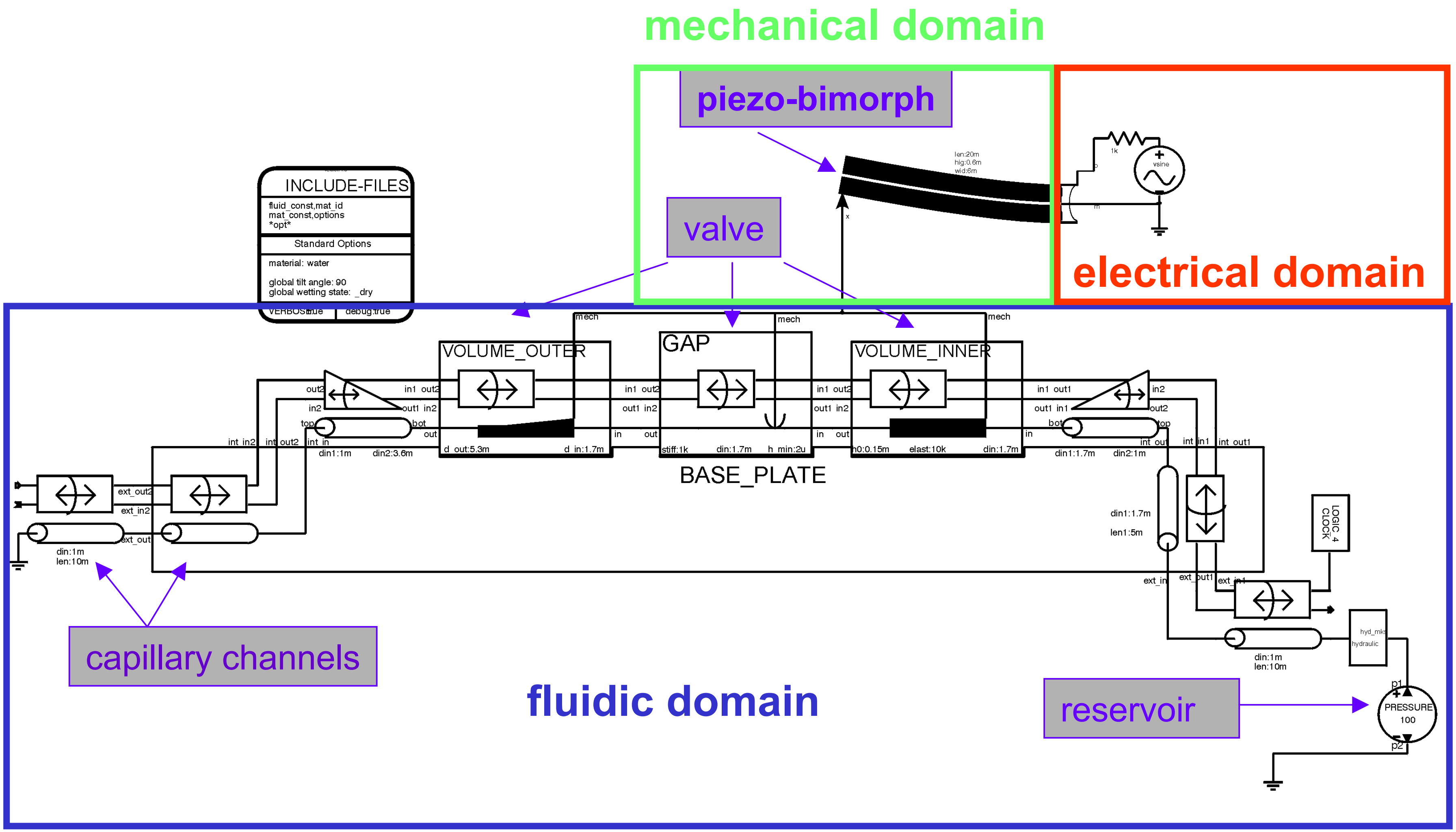
Micro valve & micro diaphragm pump
(Valve And Micro Pump (VAMP))

[HSG-IMIT, Villingen-Schwenningen]





Network model of VAMP



mechanical domain

piezo-bimorph

valve

electrical domain

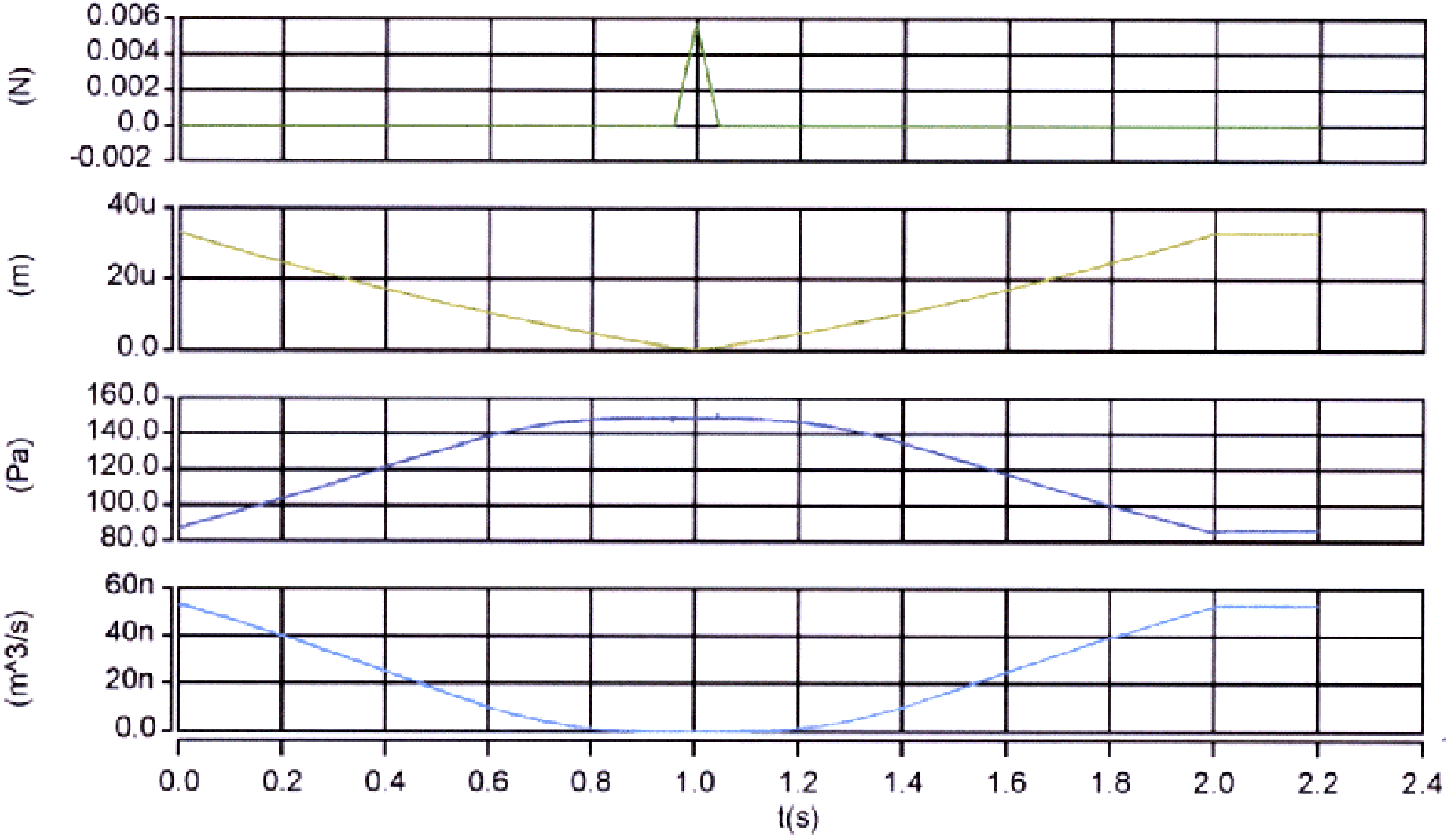
capillary channels

fluidic domain

reservoir

Simulation of Valve Operation

opening and closing cycle



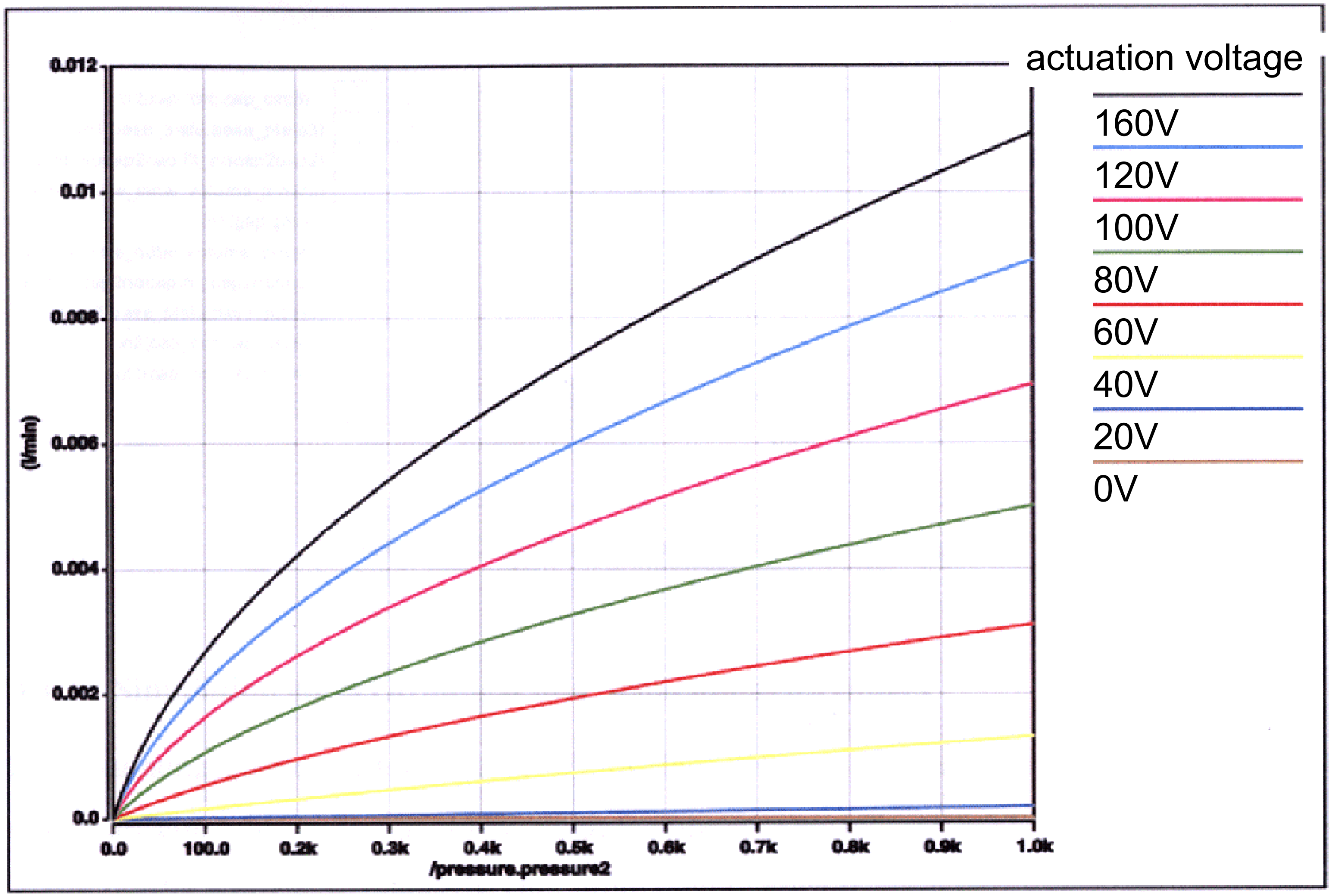
force on valve seat

deflection of the membran

pressure

flow

Micro Valve Characteristics



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
  - Rescources
  - Basics
  - Examples
- Conclusions & Summary

Comparison: CFD & Network Simulation

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

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