

## *Process simulation*

### *Front End of Line Process Models*

*Ion Implantation, Diffusion*

*Epitaxy, Oxidation,*



## *Device simulation*

## *Equipment simulation*

### *Equipment Modeling, Transport Simulation*

*PVD (Monte Carlo, MD (\*))*

*Feature scale, Topography (line of sight))*

*Lithography*

*CMP*

*CVD (\*)*

*ECD*

*Etching (\*)*

*ALD*



## Modeling & Simulation SCOPE & SCALES

### Modeling Overall Goal

- *Support technology development and optimization*
- *Reduce development times and costs*

## ***Challenges: Nano scale device modeling***

Tools for the development of novel nanostructure devices

. quantum transport .spintronics .contacts

- Coupling of optical and electrical systems
- Models for optical interconnects
- Methods, models and algorithms that contribute to prediction of CMOS limits
- Gate stack models
- Models for device impact of statistical fluctuations
- Stress models
- Tools for the design of integrated electrical/optical systems
- Air gap and novel 3D integration

## ***High-frequency device and circuit modeling up to 100 GHz applications***

- Efficient extraction and simulation of full-chip interconnect delay and power consumption
- Accurate and yet efficient 3D interconnect models, especially transmission lines and S-parameters
- Extension of physical models to III/V materials
- High-frequency circuit models including non-quasi static effects, substrate noise, and parasitic coupling
- Parameter extraction assisted by numerical electrical simulation instead of RF measurements
- Scalable active and passive component models for compact circuit simulation
- Co-design between interconnects and packaging

## ***Modeling of chemical, thermomechanical, and electrical properties of new materials***

- Operating behavior for new materials applied in devices and interconnects
- Gate stacks, Predictive modeling of dielectric constant
- Surface states
- Thermomechanical properties
- Optical properties
- Reliability
- Breakdown
- Leakage currents
- Tunneling
  
- Linkage with first principle computation and classical MD and thermodynamic computation
- ULK models

## *Nano scale process modeling*

Process modeling tools for the development of novel nanostructure devices

CNT

nanowires (doped, decorated)

quantum dots, molecular electronics

Process models for optoelectronic devices

- Computer-efficient inclusion of influences of statistics
- Efficient extraction of circuit-level variations from process and device simulation

## ***Front-end process modeling for nanometer structures***

- Diffusion/activation/damage/stress models
- (Si, SiGe:C, Ge, SOI, epilayers, ultra-thin body devices
- Epi-layer modeling (stress, morphology
- Low dopant level characterisation
- Modeling hierarchy from atomistic to continuum for dopants and defects in bulk and at interfaces
- Front-end processing impact on reliability

## ***Integrated modeling of equipment, materials, feature scale processes and influence on devices***

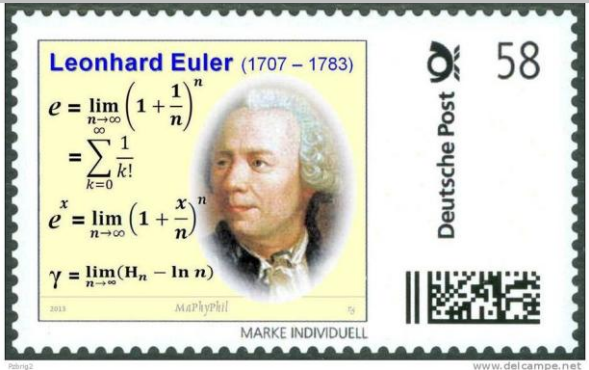
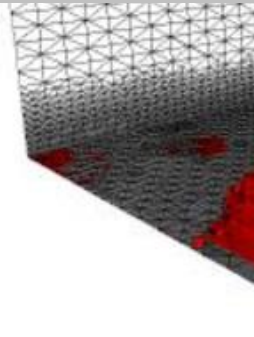
- Fundamental physical data: rate constants, cross sections
- Simplified but physical models for complex chemistry and plasma reaction
- Linked equipment/feature scale models
- CMP, etch, electrochemical polishing ECP, pattern dependent effects
- MOCVD, PECVD, ALD, EP, ELD modeling



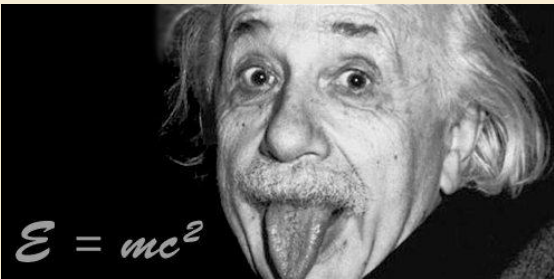
... to find the right parameters

- 1. Parameter of Numerical Method,  
(e.g. discretisation in space and time)
- 2. Parameter of the Physial Model
- 3. Parameter of the Equipment (Dim...)
- 4. Parameter of the Process (T, flow..)

engineer



mathematician

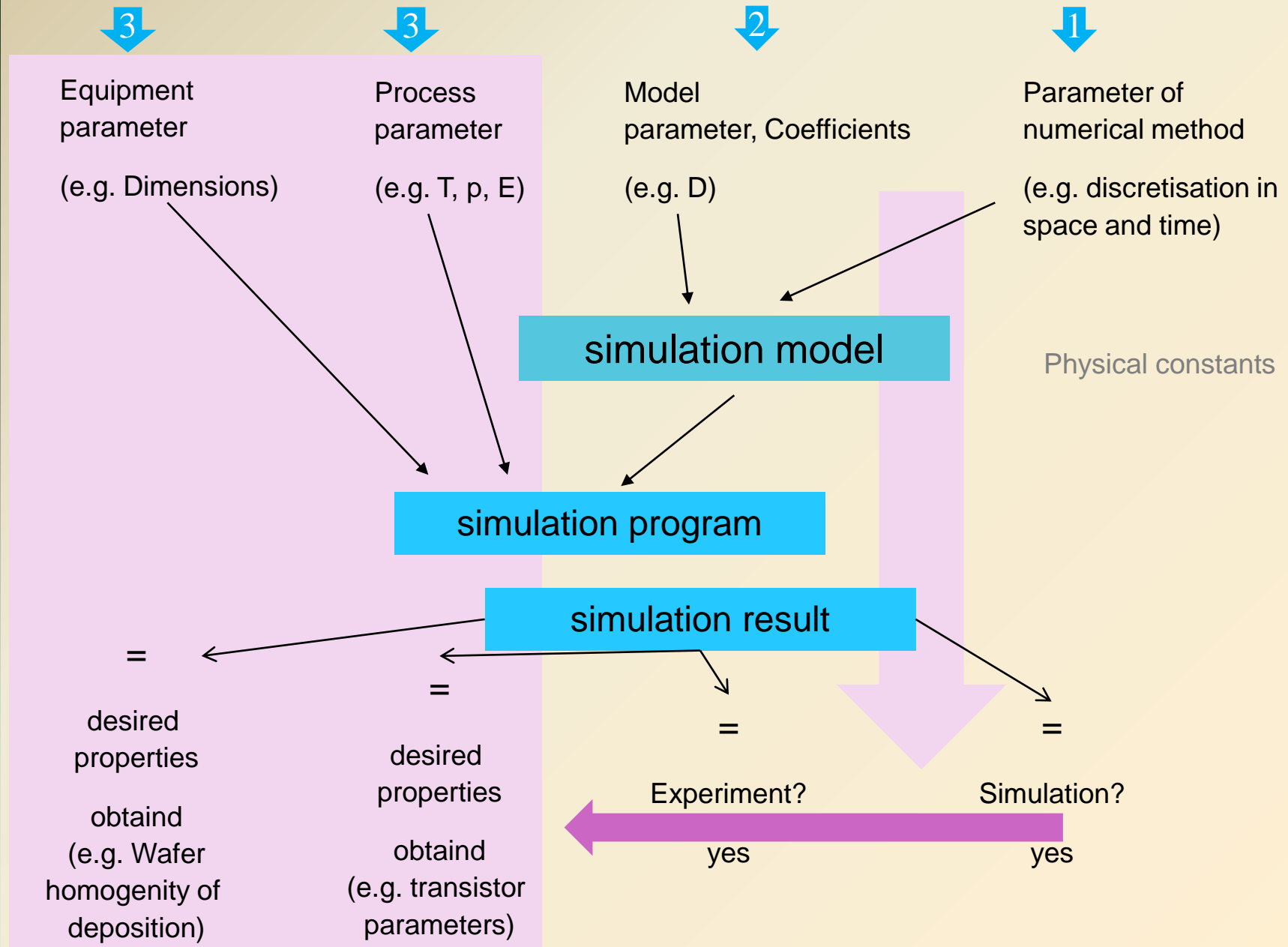


physicist



economist

# Overall goal of simulation: optimization of parameters



# Simulation of Thin Film Deposition

- General Remarks: Properties and Applications of Thin Films
- Small Structures, an Example, The ITRS and one Physical Limit: The Size Effect
- Simulation Models depending on Pressure and Dimensions
- CVD Modeling and Simulation
- ECD
- ALD
- PVD Modeling and Simulation
- Summery



- A **thin film** is a layer of material ranging from fractions of a nanometer (monolayer) to several micrometers in thickness (1  $\mu\text{m}$ !)
- special physical properties like interference, useful for sensitive layers in sensors
- expensive materials can be used economically
  - hard coatings
  - anticorrosion layers

optical coatings



Source: WiKi

- **microelectronics**

CDs/DVDs, hard disks

electronic semiconductor devices / IC (processors, memory..)

optical devices (LEDs)

energy generation (thin film solar cells) and storage (thin-film batteries)

multiferroic materials / superlattices that allow the study of quantum confinement by creating two-dimensional electron states.




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**ZfM**

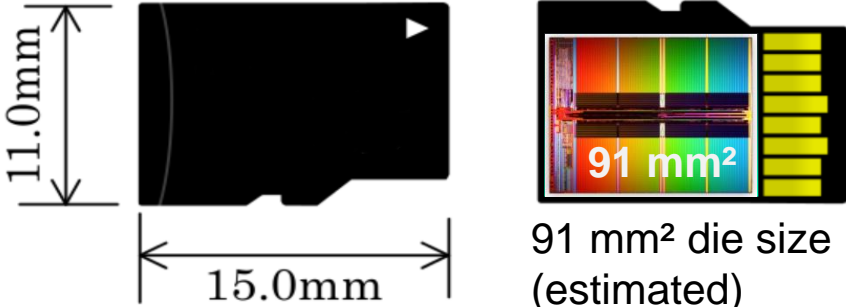
**Fraunhofer**  
ENAS

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# Density of $\mu$ Electronic Structures, Example



**SanDisk**  
200 GByte Micro-SD  
0,7 mm thick  
16 stacked flash dies  
1 controller die



11.0mm  
15.0mm  
91 mm<sup>2</sup> die size (estimated)

Total die area (incl. bus system...)  
 $= 16 \cdot 91 \text{ mm}^2$   
 $= \underline{1456 \text{ mm}^2}$

Space for  
 $\underline{200\,000\,000\,000 \cdot 8}$  memory cells  
per memory cell an area of  
 $A_{\text{cell}} = 1456 \text{ mm}^2 / 1.6\text{e}12 \text{ (Terabit)}$   
 $A_{\text{cell}} = \underline{910 \text{ nm}^2}$

$A_{\text{hair}} / A_{\text{cell}} = 3848 \text{ }\mu\text{m}^2 / 910 \text{ nm}^2$   
 $A_{\text{hair}} / A_{\text{cell}} > 4\,000\,000$

Human hair diameter  $d = 70 \text{ }\mu\text{m}$   
Cross section area

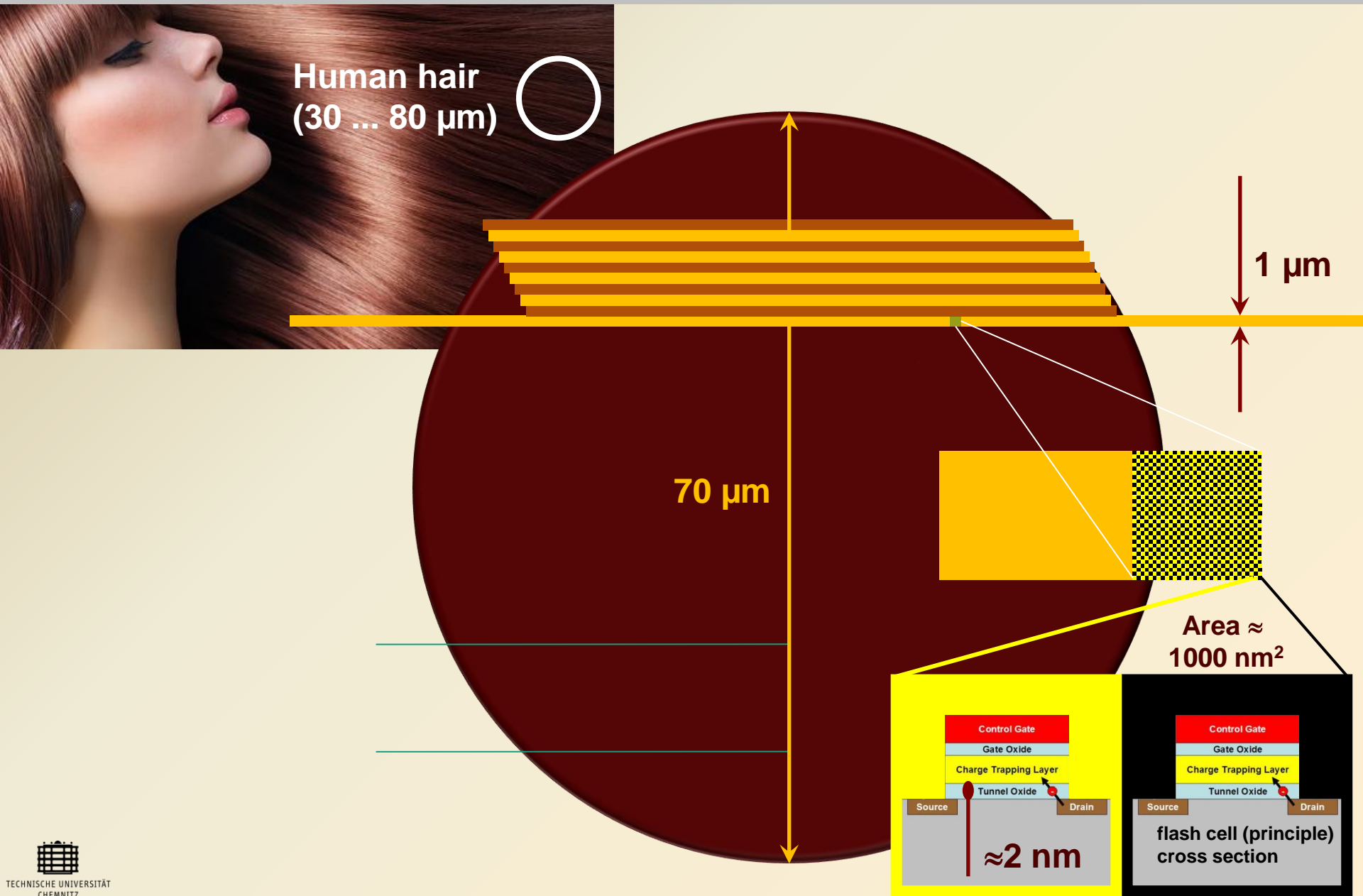
$A_{\text{hair}} = \pi/4 d^2 = \underline{3848 \text{ }\mu\text{m}^2}$

May 2016  
**Samsung**  
256 GByte Micro-SD

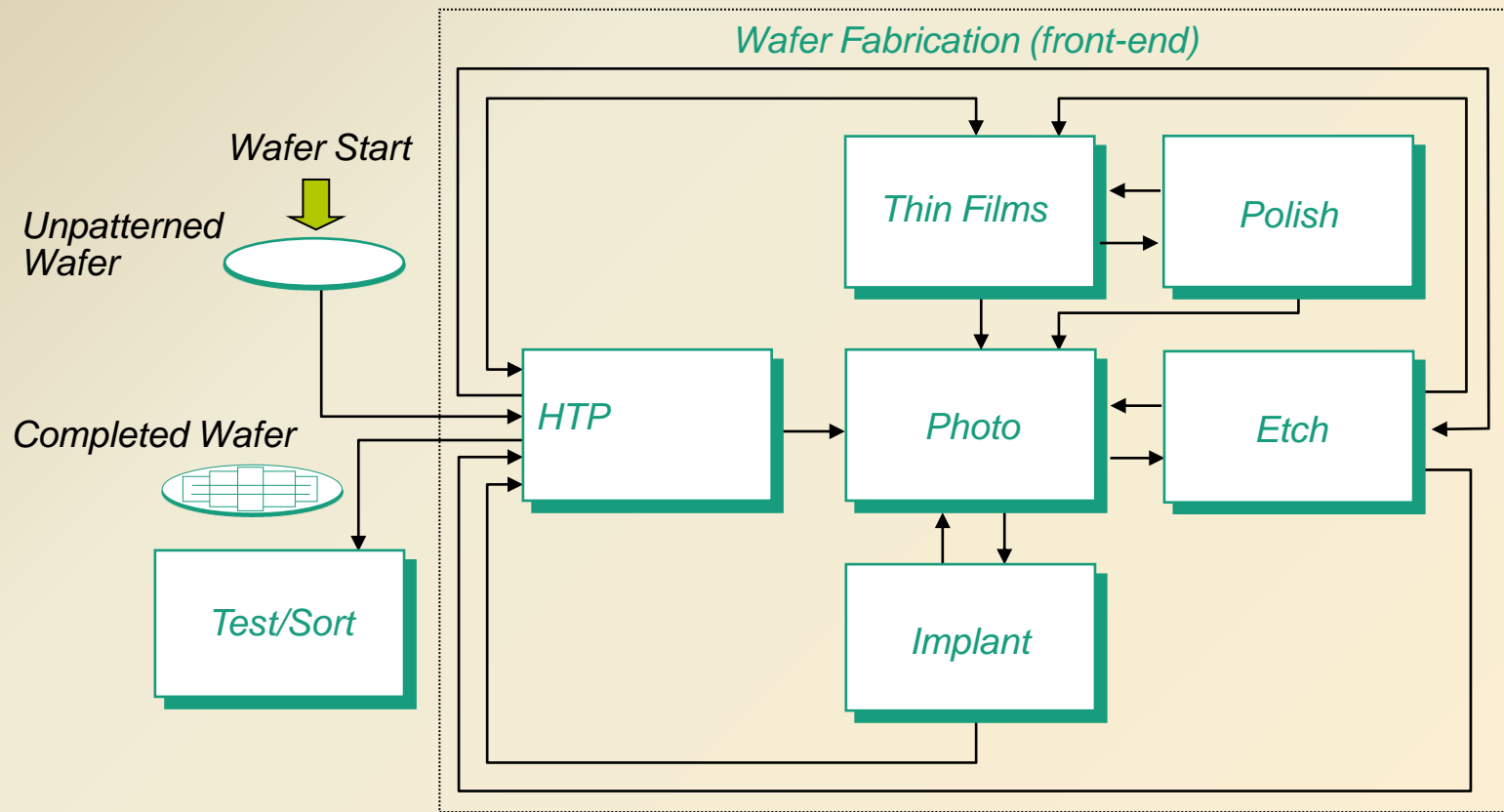




# Density of $\mu$ Electronic Structures, Example



# Model of Typical Wafer Flow in a Sub-Micron CMOS IC Fab



**6 major production areas**

**6 ... 8 weeks involve up to 400 process steps**

**HTP:**  
High Temperature  
Processes: Diffusion,  
Oxidation, Anneal, Epi



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- Cleaning
- Etching
- Packaging
- Waferbonding
- **Thin Film Deposition**
- Lithography
- Doping
- Cleaning
- Measuring Technique



**CVD Chemical Vapour Deposition / Epitaxy**

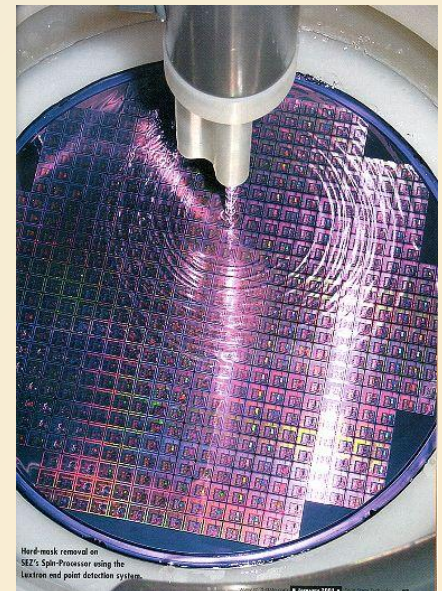
**ALD Atomic Layer Deposition**

**PVD Physical Vapour Deposition(Sputtering/Evaporation)**

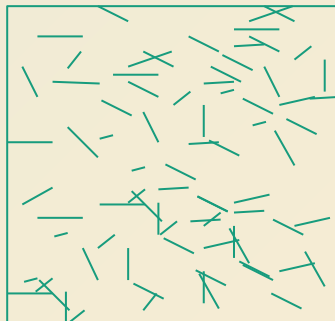
**ECD Electro Chemical Deposition**

**MBE Molecular beam epitaxy**

**spin on**

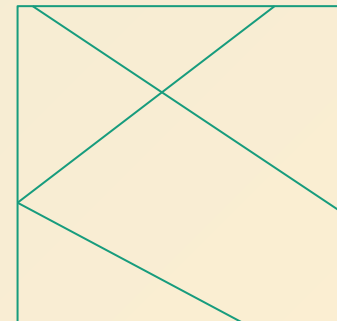


- The **Knudsen number** ( $Kn$ ) is a dimensionless number defined as the ratio of the molecular **mean free path** length to a **representative physical length scale**. This length scale could be, for example, the radius of a layer deposition reactor.
- The Knudsen number helps determine whether **statistical mechanics** or the **continuum mechanics** formulation of **fluid dynamics** should be used to model a situation.
- If the Knudsen number is near or **greater than one**, the mean free path of a molecule is comparable to a length scale of the problem, and the **continuum assumption** of fluid mechanics is no longer a good approximation. In such cases, **statistical methods** should be used.



$$Kn < 1$$

transport is  
determined  
by particle - particle  
interaction



$$Kn > 1$$

transport is  
determined  
by particle - wall  
interaction



# Knudsen number

$$Kn = \frac{\lambda}{L}$$

- $\lambda$  = mean free path [ $L^1$ ],
- $L$  = representative physical length scale [ $L^1$ ].

For a Boltzmann gas, the mean free path may be readily calculated, so that

$$Kn = \frac{k_B T}{\sqrt{2} \pi d^2 p L}$$

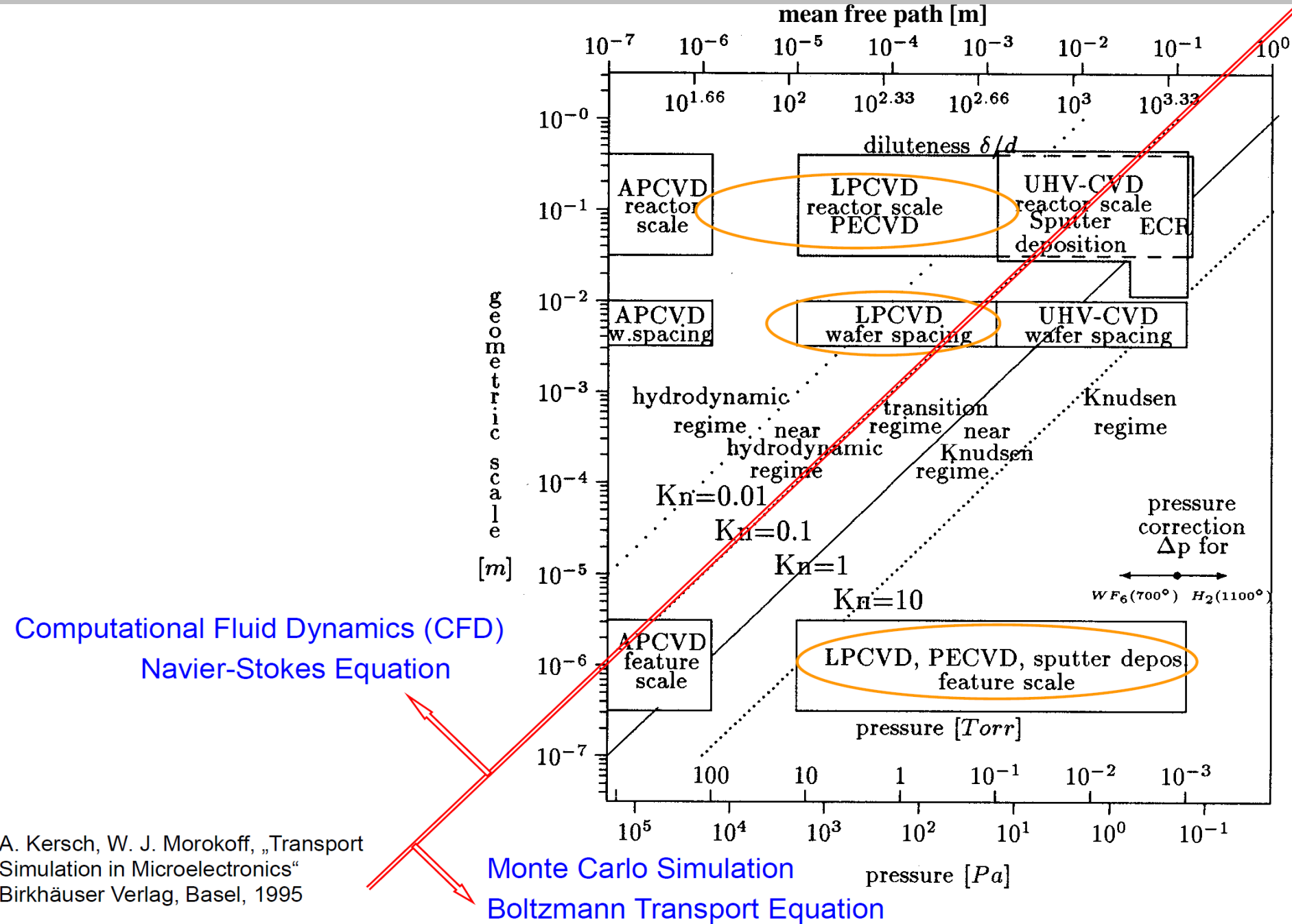
- $k_B$  is the Boltzmann constant ( $1.3806504(24) \times 10^{-23}$  J/K in SI units), [ $M^1 L^2 T^{-2} \theta^{-1}$ ],
- $T$  is the thermodynamic temperature, [ $\theta^1$ ],
- $d$  is the particle hard-shell diameter, [ $L^1$ ],
- $p$  is the total pressure, [ $M^1 L^{-1} T^{-2}$ ].

For particle dynamics in the atmosphere, and assuming standard temperature and pressure, i.e. 25 °C and 1 atm, we have  $\lambda \approx 8 \times 10^{-8}$  m (80 nm).

# Mean Free Path vs. Pressure

Vacuum range	Pressure / hPa	Atoms / cm <sup>3</sup> Molecules / cm <sup>3</sup>	Aver. Dist. Between atoms / molecules	Mean free path
(reference: Silicon, typical doping concentration in Silicon)	-	5·10 <sup>22</sup>  10 <sup>15</sup> ... 10 <sup>20</sup>	<b>L = 0.235 nm</b> (bond length), $L=\frac{1}{4} \sqrt{3}a$ a = 0.543 nm (lattice constant)	-
Ambient pressure	1013	2.7·10 <sup>19</sup>	≈3.3 nm	68 nm
Low vacuum	300 ... 1	10 <sup>19</sup> ... 10 <sup>16</sup>	≈ 5 nm ... 50 nm	0.1 ... 100 μm
Medium vacuum	1 ... 10 <sup>-3</sup>	10 <sup>16</sup> ... 10 <sup>13</sup>	≈ 50 nm ... 0.5 mm	0.1 ... 100 mm
High vacuum	10 <sup>-3</sup> ... 10 <sup>-7</sup>	10 <sup>13</sup> ... 10 <sup>9</sup>	≈ 0.5 mm ... 10 μm	10 cm ... 1 km
Ultra high vacuum	10 <sup>-7</sup> ... 10 <sup>-12</sup>	10 <sup>9</sup> ... 10 <sup>4</sup>	≈ 10 μm... 0.500 mm	1 km ... 10 <sup>5</sup> km
Extremely high vacuum	< 10 <sup>-12</sup>	< 10 <sup>4</sup>	≈ < 0.500 mm	> 10 <sup>5</sup> km

# Transport Simulation in Relation to geometric Scale



A. Kersch, W. J. Morokoff, „Transport Simulation in Microelectronics“  
Birkhäuser Verlag, Basel, 1995



July 28, 2016



Transistors Won't Shrink Beyond 2021, Says Final ITRS Report

Tiffany Trader

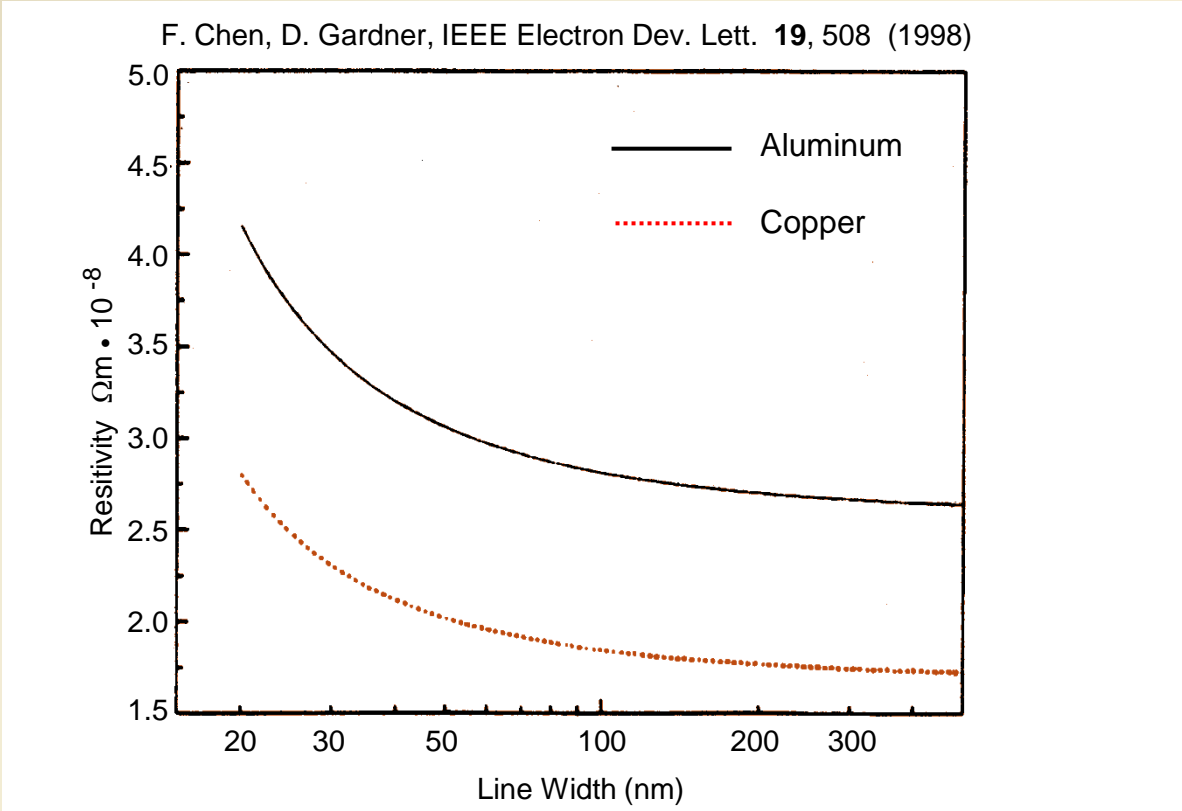
The final International Technology Roadmap for Semiconductors (ITRS) is now out.

**ITRS:** The highly-detailed multi-part report, collaboratively published by a group of international semiconductor experts, offers guidance on the technological challenges and opportunities for the semiconductor industry through 2030.

One of the major takeaways is the insistence that Moore's law will continue for some time even though traditional transistor scaling (through smaller feature sizes) is expected to hit an economic wall in 2021.

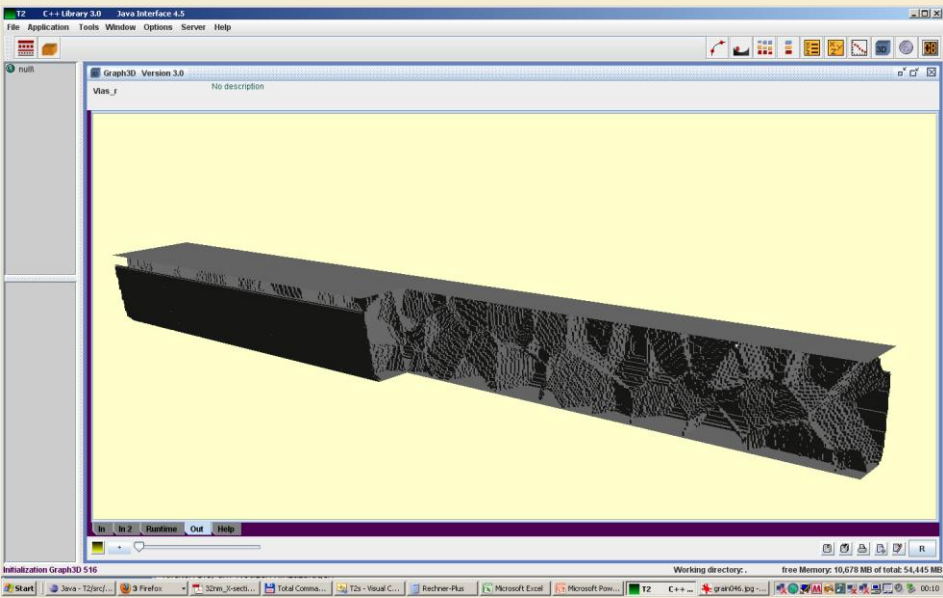


# One Physical Limit: The Size Effect

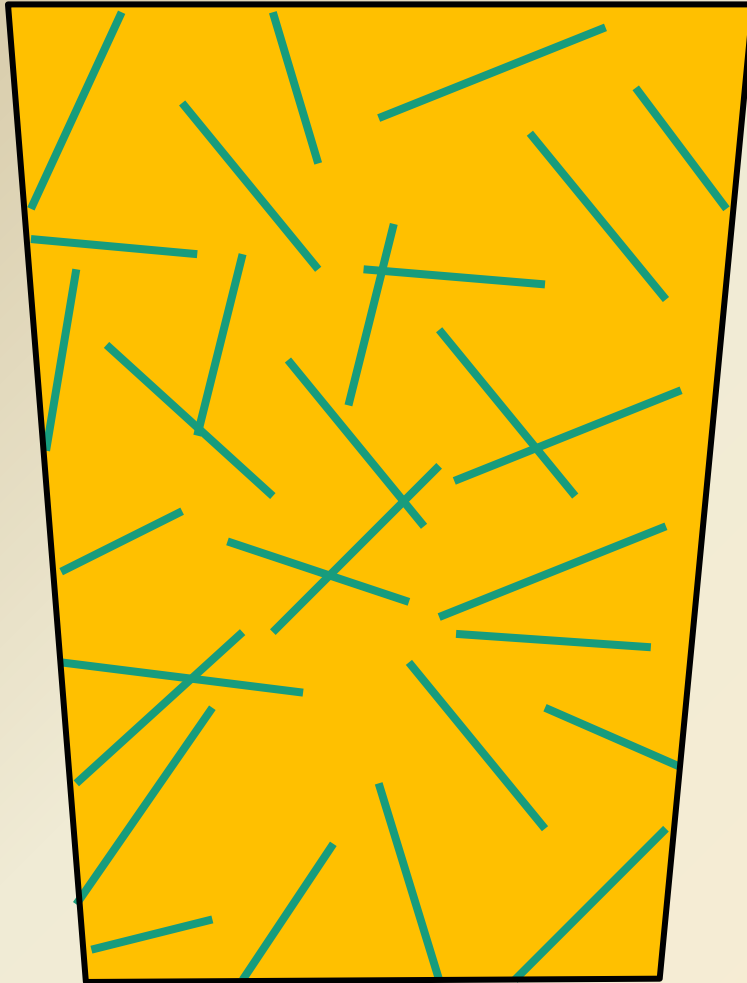


Tech node	Interconnect pitch	Interconnect width (incl. barrier)
10 nm	34	17
7 nm	22	11





# The Size Effect: Conductivity Dependence on Mean Free Path



Number of  
electrons with  
Fermi-energy

elementary charge

relaxation time

$$\sigma = \frac{N_f e^2 \tau}{m_{eff}}$$

effective mass of electrons

relaxation time ..mean free path of  
electrons (Copper 39 nm)

resistivity = 1.6  $\mu\text{Ohm cm}$



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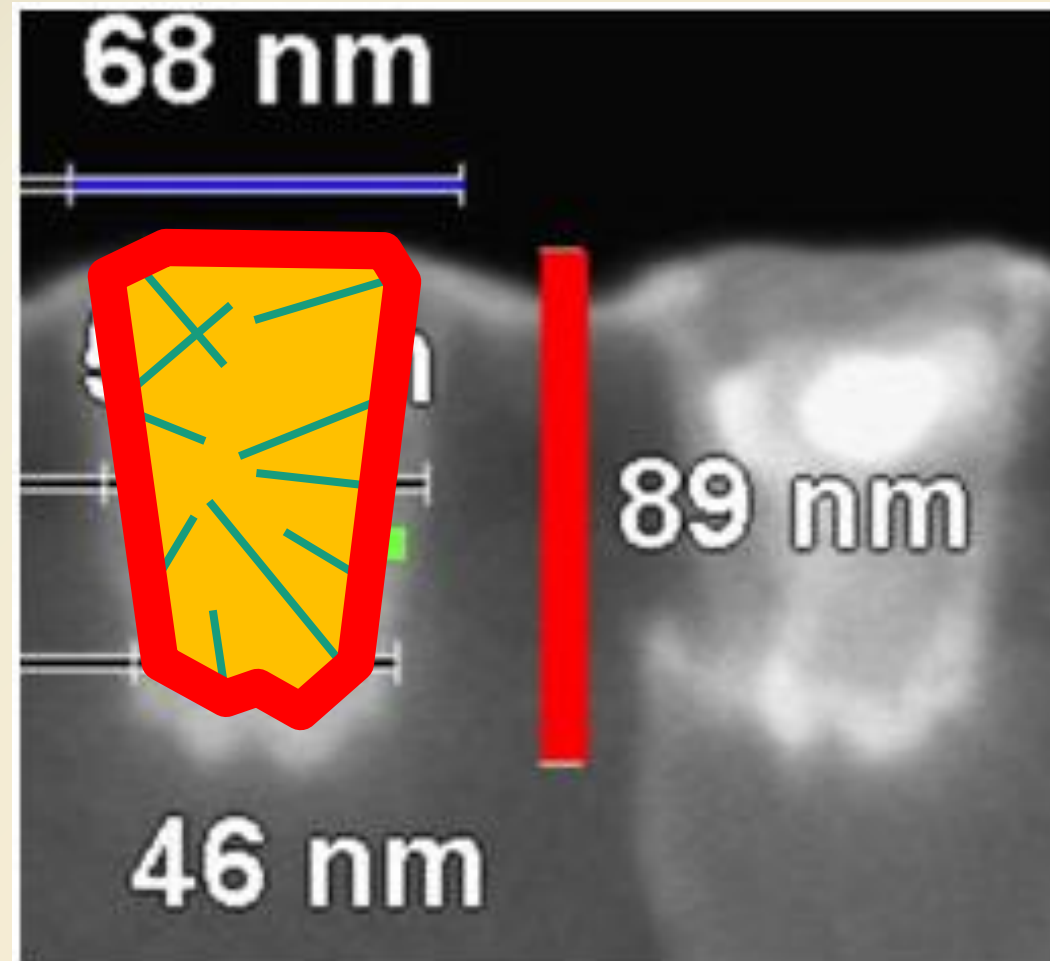
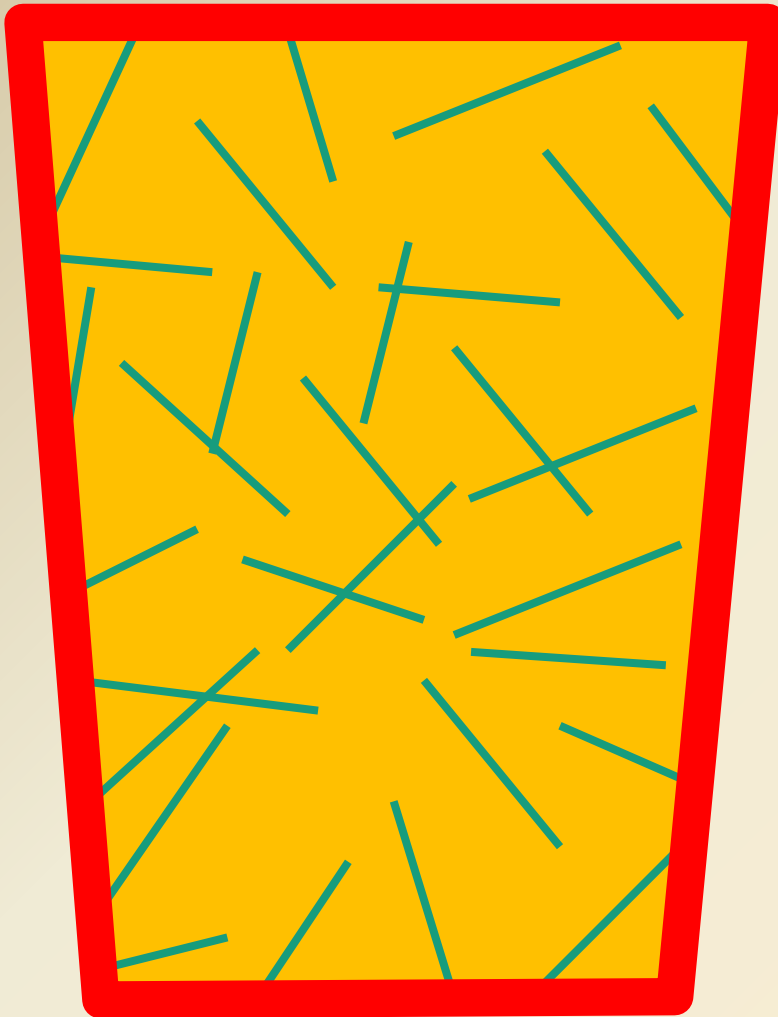
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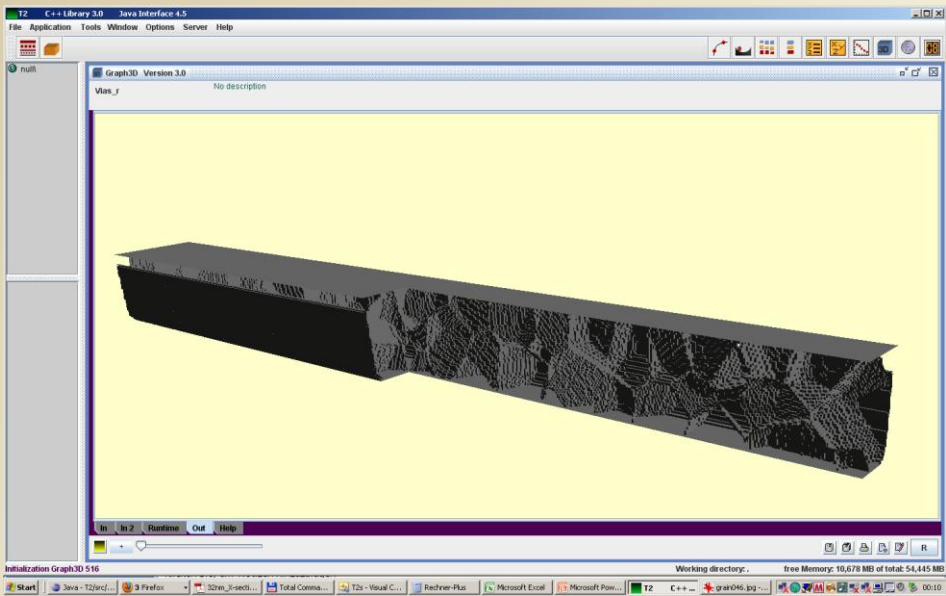
## The Size Effect

*copper interconnects*



To inhibit the detrimental **diffusion of copper into silicon devices**, an effective barrier is strongly demanded.

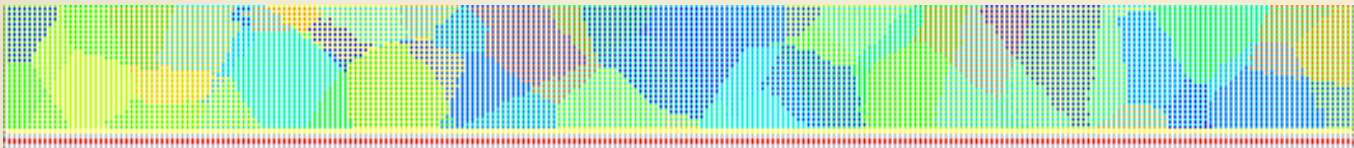
# The Size Effect: Structure Generation with Simulator T2 for Size Effect Simulation



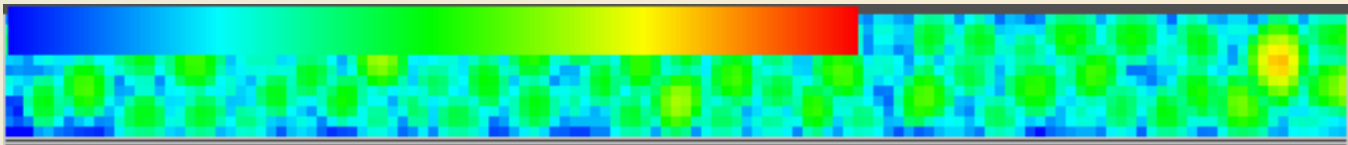
Grain structure, randomly generated

Lattice resolution = 1nm

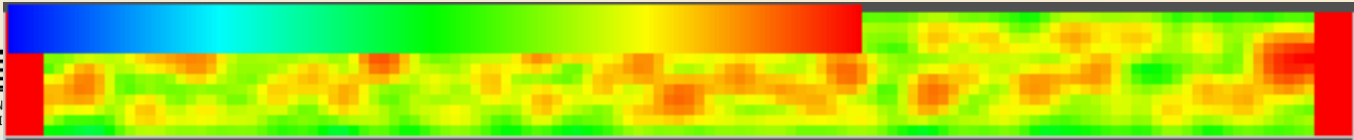
$\tau(x,y,z)$        $\sigma(x,y,z)$  Poisson eq.



Grain Structure



Local relaxation time

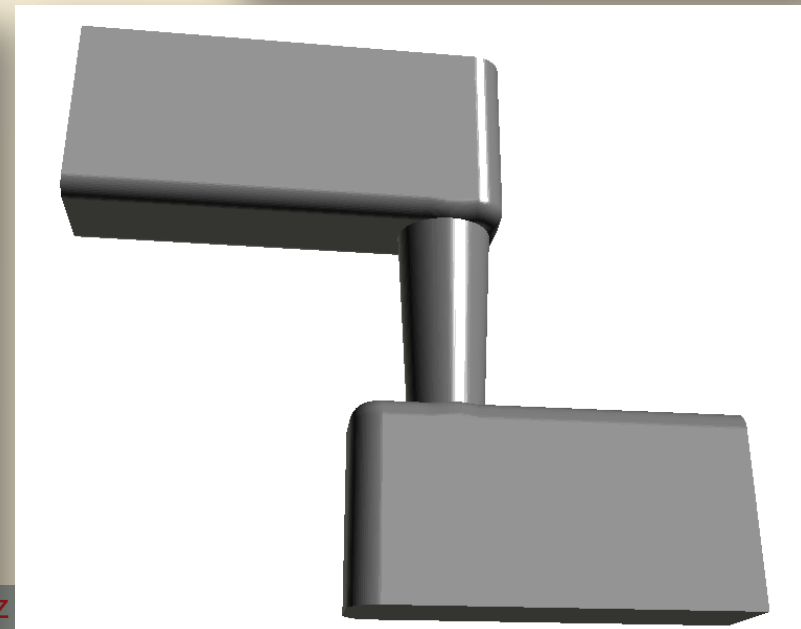
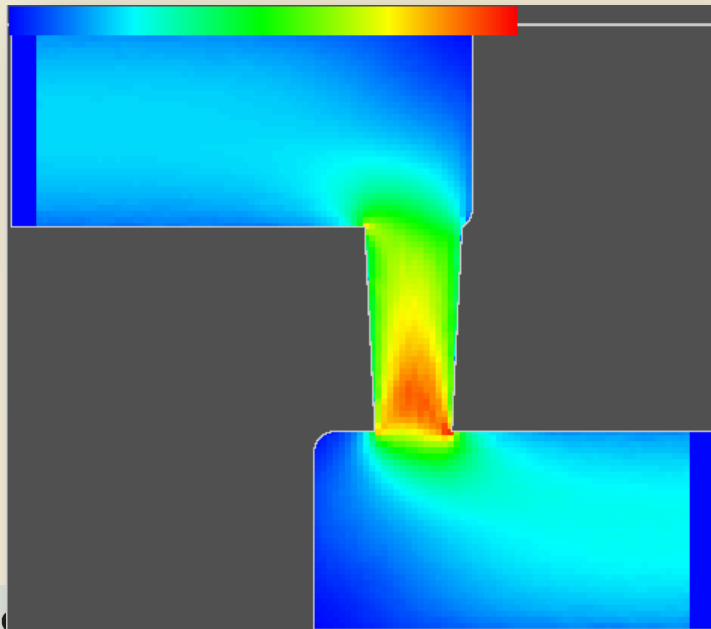
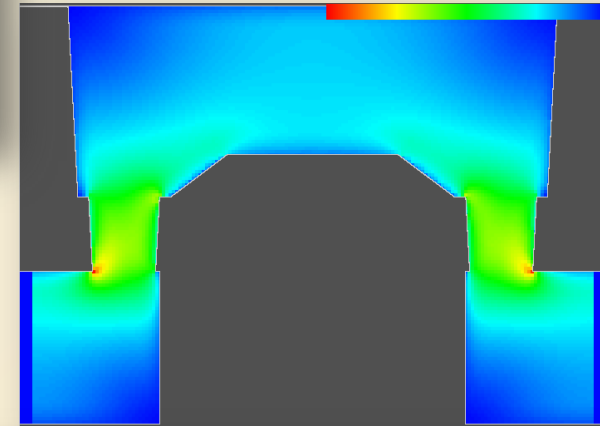
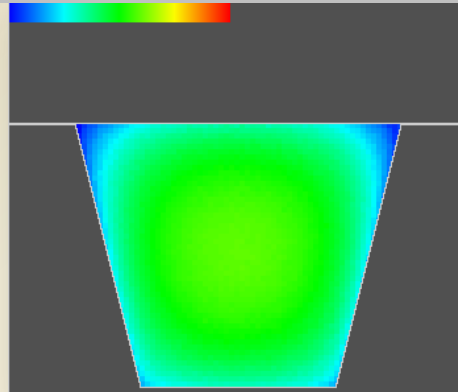


Current density

# The Size Effect: Simulation Results

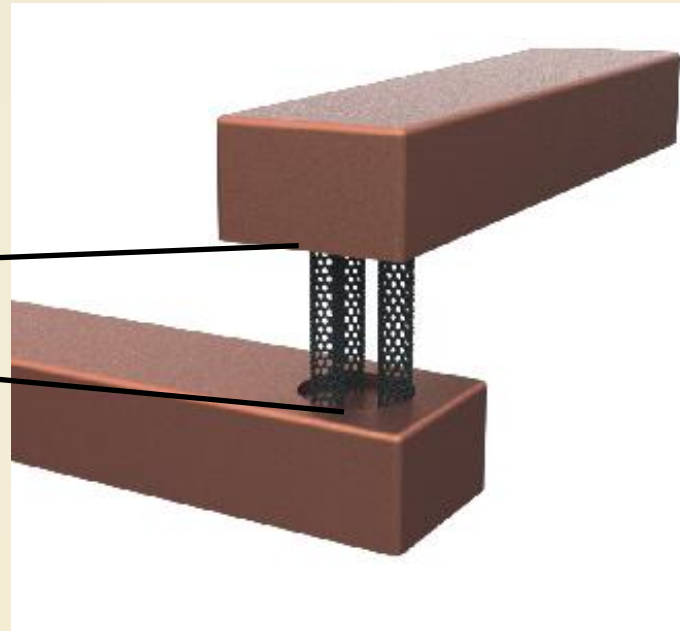
Technology optimization improves conductivity (grain structure and surface quality, e-reflection).

Simulation can help to understand the transport in complex structures.



## ***Solution: Replacement of metal interconnects with Carbon Nanotubes ?***

- ✓ No electromigration issues
- ✓ High current carrying capacity
- ✓ Thermal management



CNT-Via/Metal-  
Hybridstructure





# CVD Chemical Vapour Deposition / Epitaxy

ALD Atomic Layer Deposition

PVD Physical Vapour Deposition

ECD Electro Chemical Deposition

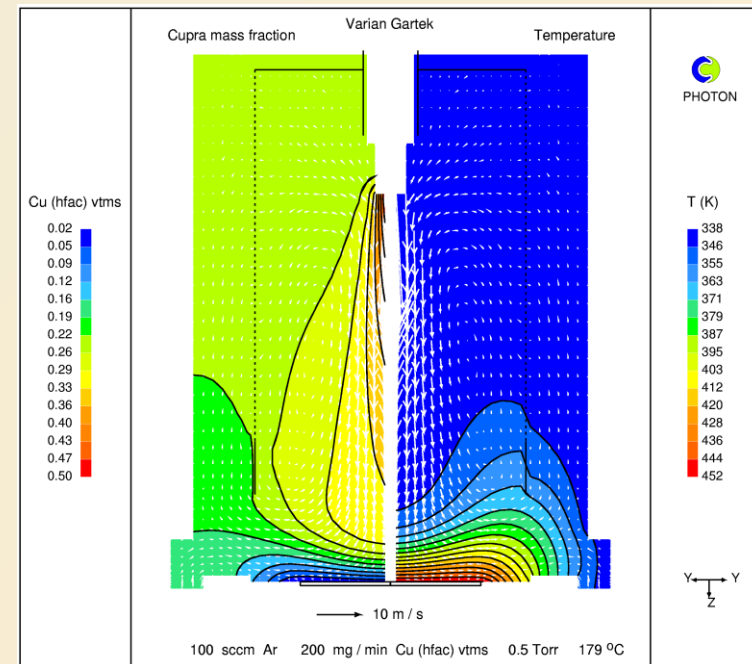
MBE Molecular beam epitaxy

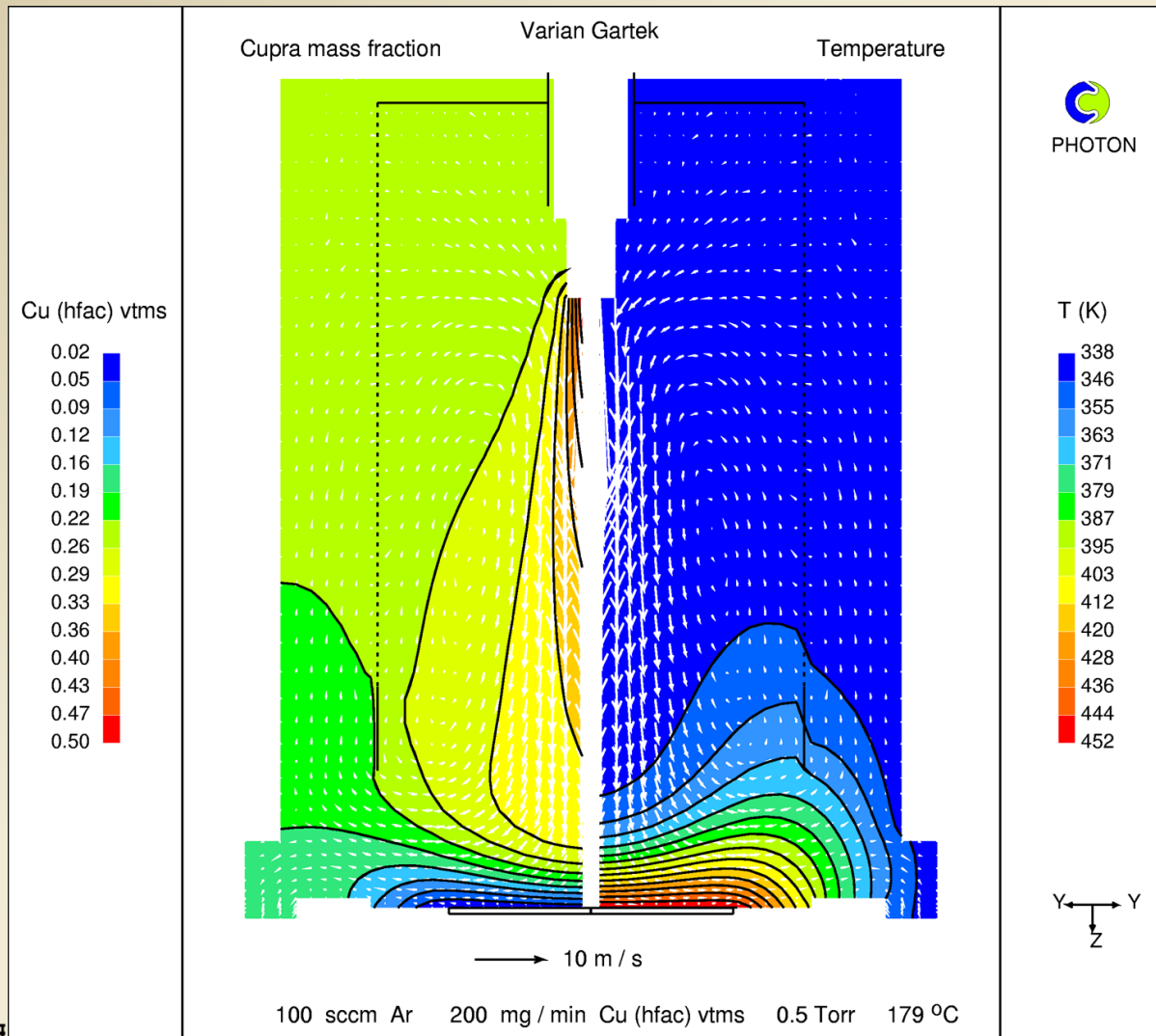
spin on

...Modeling and Simulation

Transport Simulation

1. Particles to wafer





## Improvement of

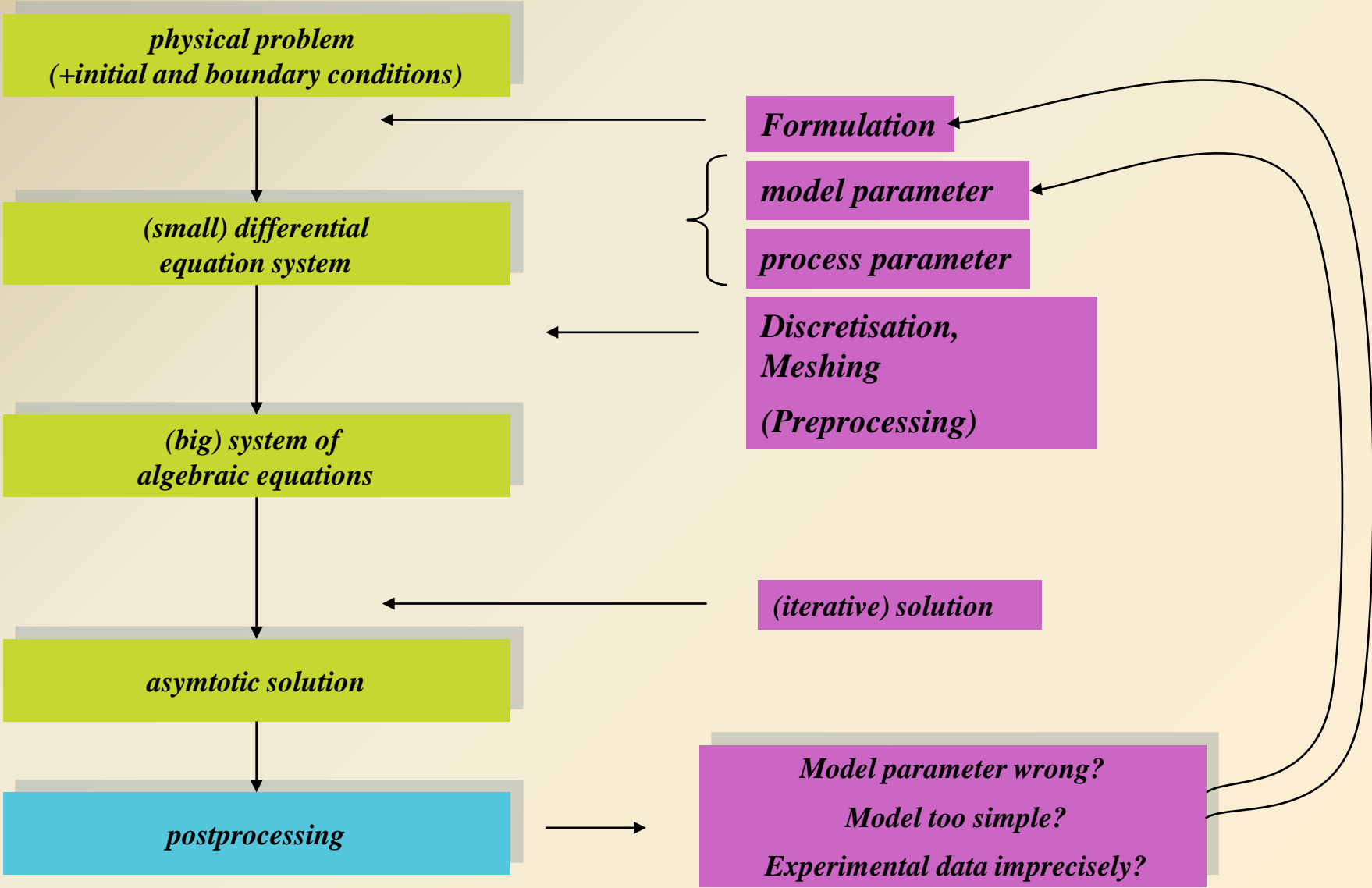
- deposition rates
- uniformity
- fill behavior of vias and trenches

## by optimization of

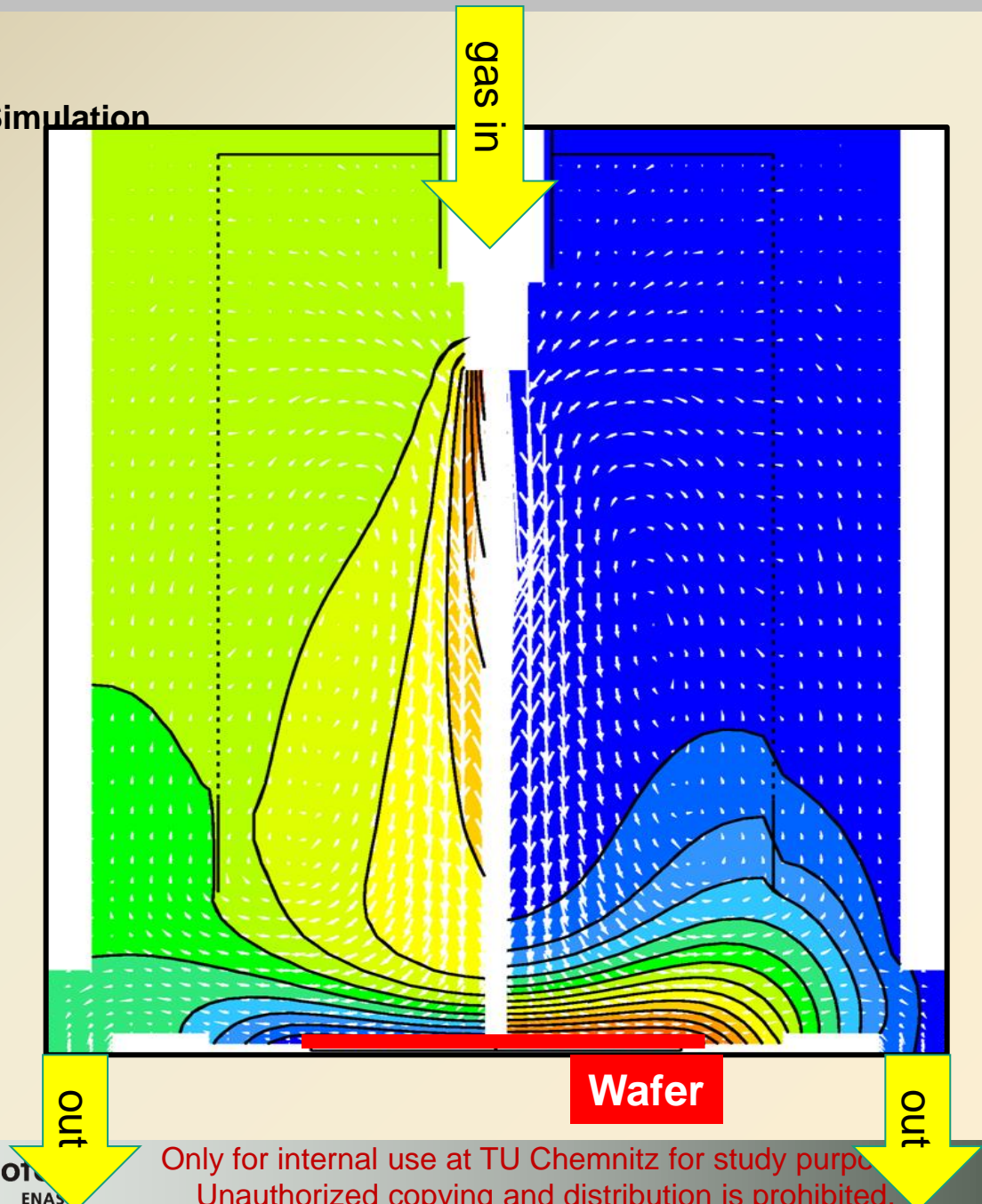
- process conditions
- reactor configuration

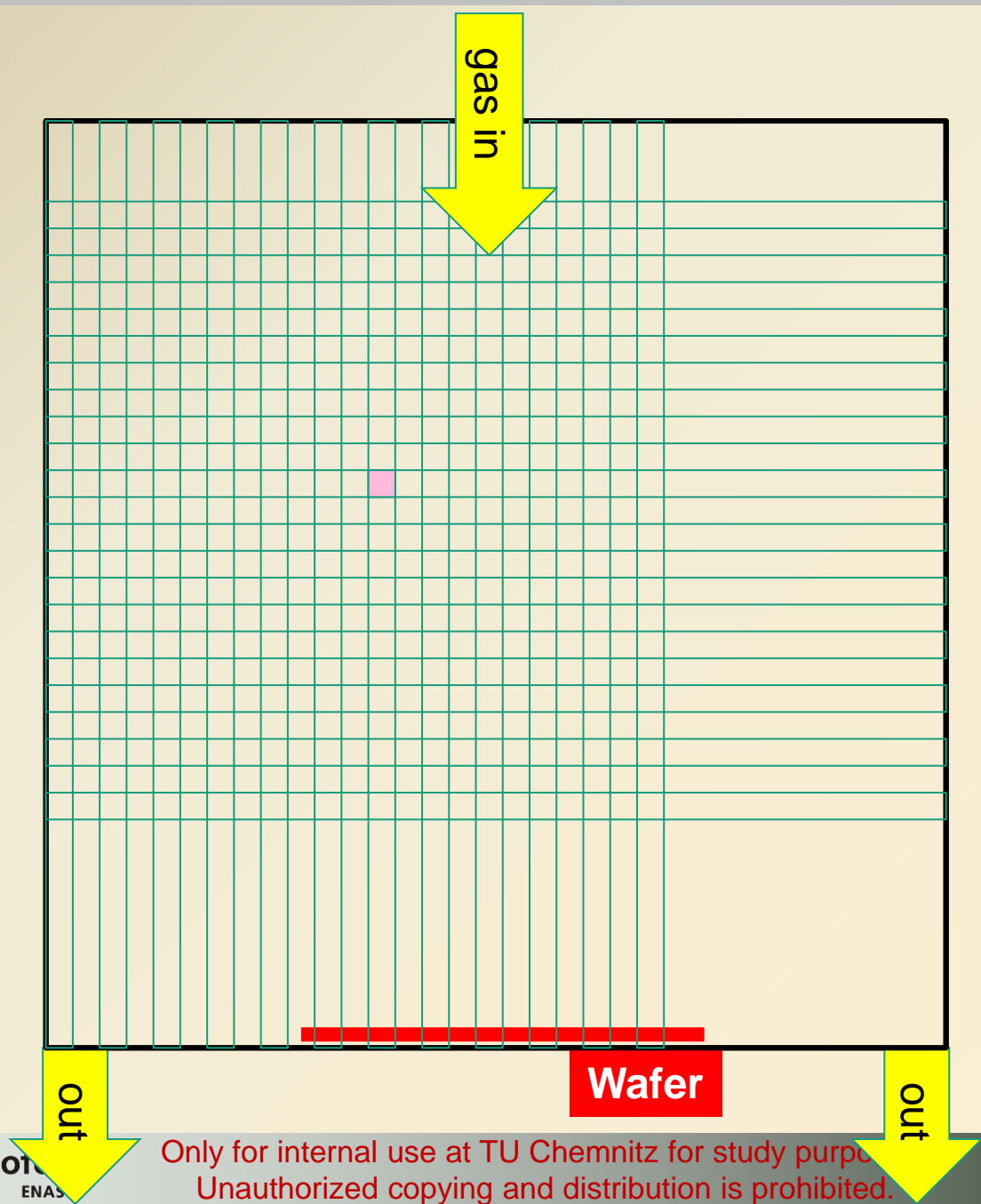




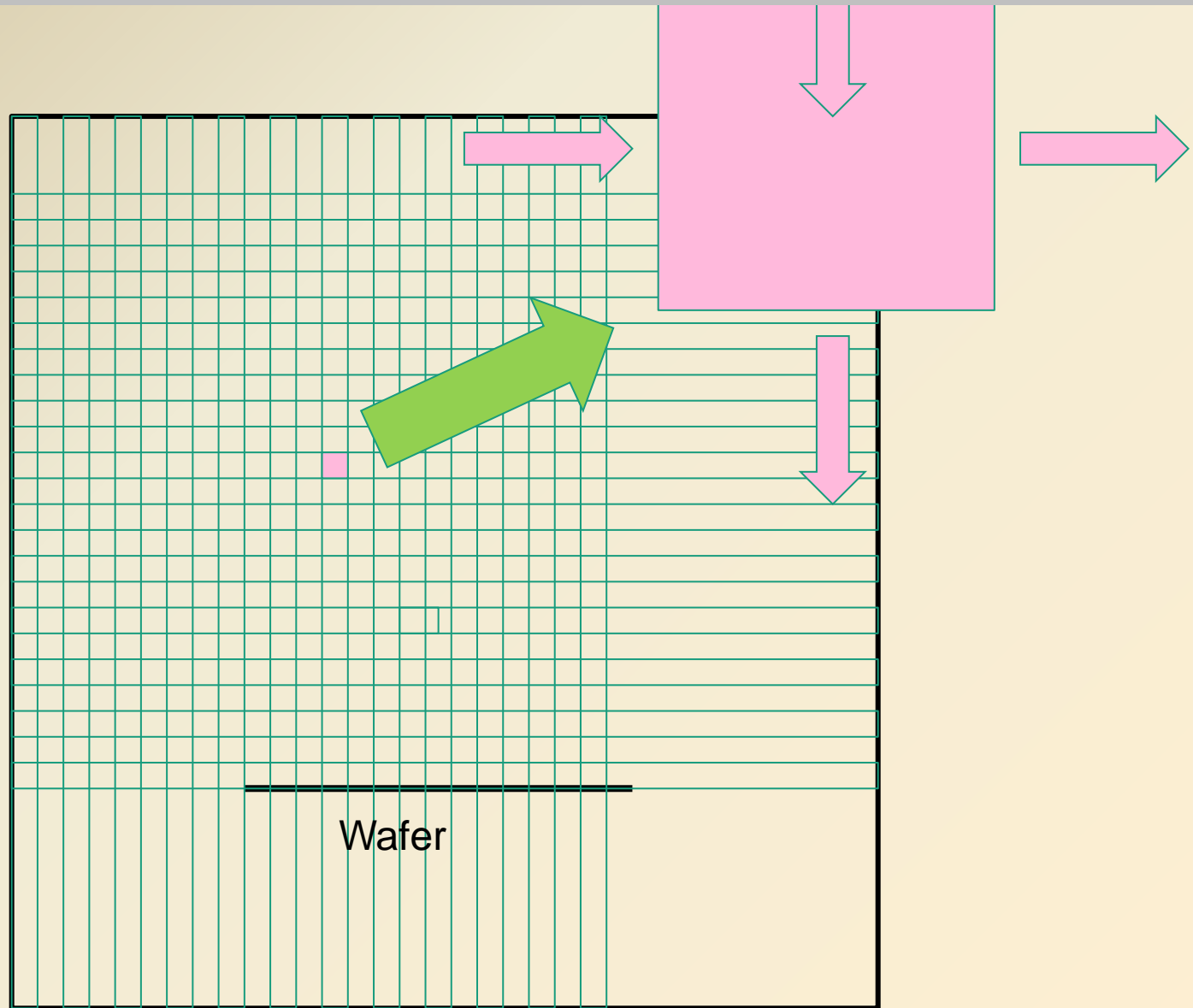


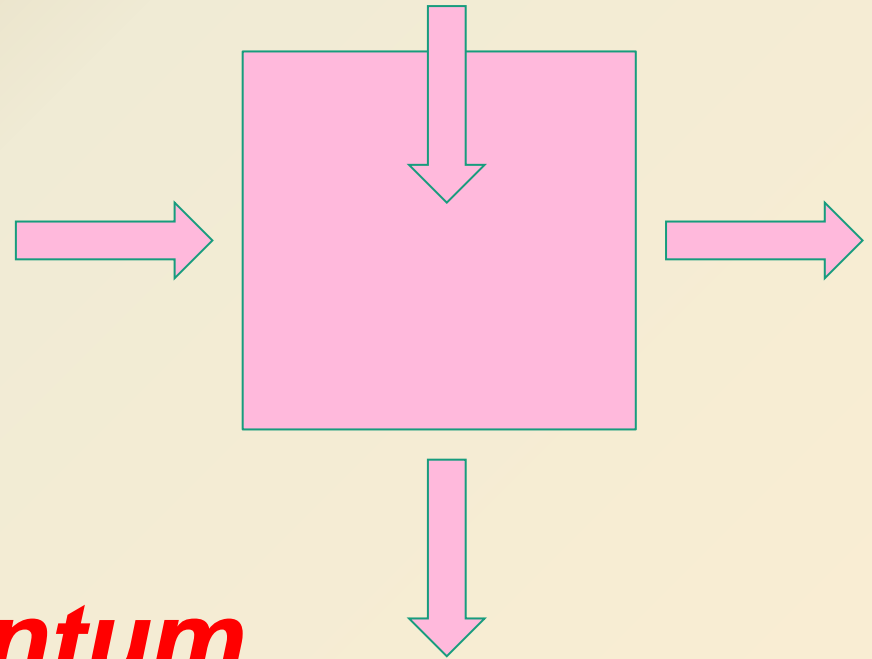
Reactor  
1 Transport Simulation





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***Mass***

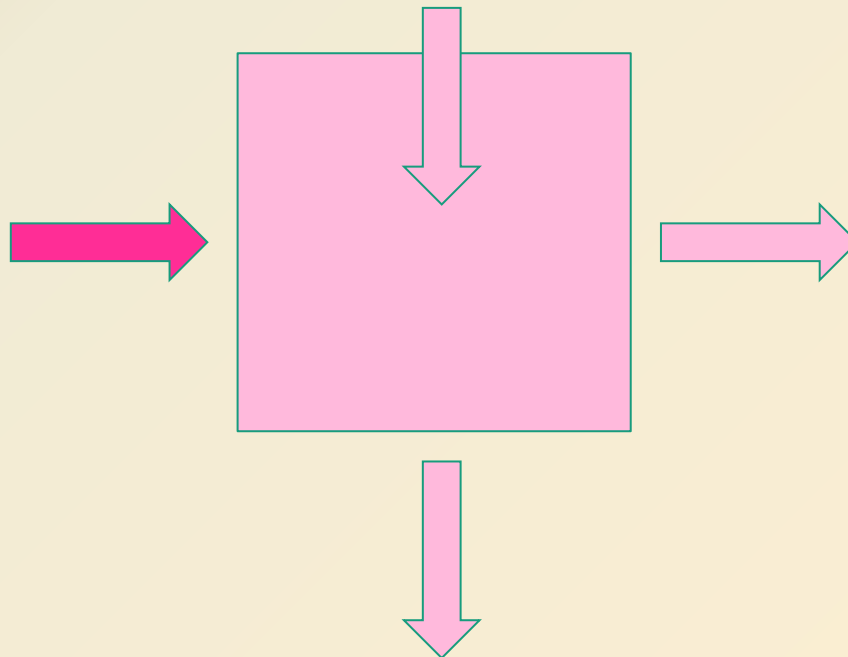
***Momentum***

***Energy***

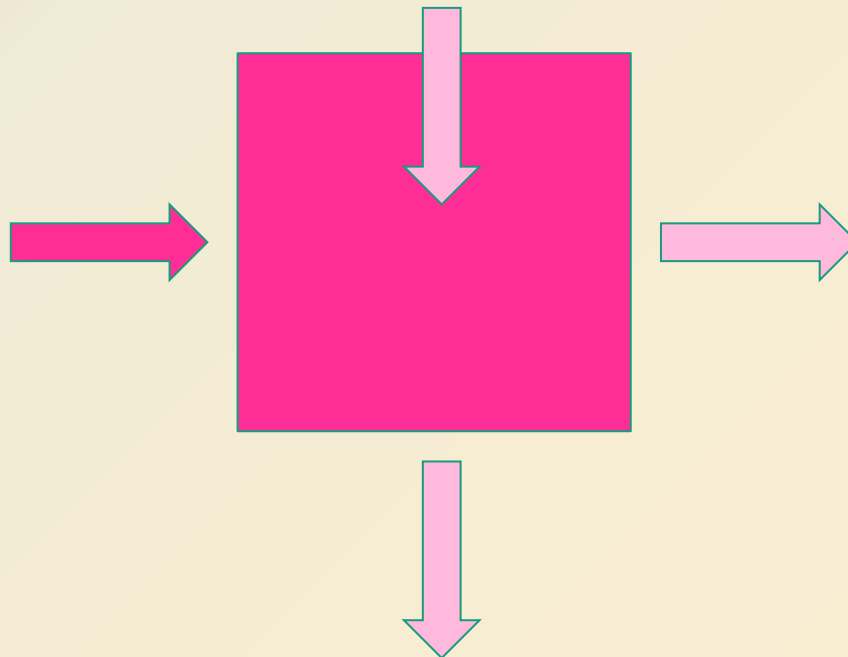
***Species***  $i = 1 \dots n$



$$\overset{\text{transient}}{\xi \frac{d}{dt} (\rho \phi)} = - \overset{\text{convection}}{\xi \nabla (\rho \underline{v} \phi)} + \overset{\text{diffusion}}{\nabla (\Gamma \nabla \phi)} + \overset{\text{source}}{\mathbf{S}}$$



$$\overset{\text{transient}}{\xi \frac{d}{dt} (\rho \phi)} = - \overset{\text{convection}}{\xi \nabla (\rho \underline{v} \phi)} + \overset{\text{diffusion}}{\nabla (\Gamma \nabla \phi)} + \overset{\text{source}}{\mathbf{S}}$$



$$\begin{array}{ccccccc} \text{transient} & & \text{convection} & & \text{diffusion} & & \text{source} \\ \xi \frac{d}{dt} (\rho \phi) = & - & \xi \nabla (\rho \underline{v} \phi) & + & \nabla (\Gamma \nabla \phi) & + & S \end{array}$$

**Continuity**

**Momentum**

**Energy**

**Species**  $i = 1 \dots n$





$$\begin{array}{ccccccc} \text{transient} & & \text{convection} & & \text{diffusion} & & \text{source} \\ \xi \frac{d}{dt} (\rho \phi) = & - & \xi \nabla (\rho \underline{v} \phi) & + & \nabla (\Gamma \nabla \phi) & + & S \\ \underset{=1}{} & & \underset{=1}{} & & \underset{=0}{} & & \underset{=0}{} \end{array}$$

$$\frac{d}{dt} (\rho) = - \nabla (\rho \underline{v})$$

## Continuity



*transient*  
 $\xi \frac{d}{dt} (\rho \phi) =$   
<sub>=1</sub>

*convection*  
 $- \xi \nabla (\rho \underline{v} \phi)$   
<sub>=1</sub>

*diffusion*  
 $+ \nabla (\Gamma \nabla \phi)$   
<sub>=  $\mu$       =  $\underline{v}$</sub>

*source*  
 $+ S$

$$\frac{d}{dt} (\rho \underline{v}) = - \nabla (\rho \underline{v} \underline{v}) + \nabla (\mu \nabla \underline{v}) + S$$

Momentum

S=

$$\nabla \cdot \left( \mu (\nabla \underline{v})^\dagger + \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \underline{v}) \underline{\underline{I}} \right) - \nabla P + \rho \underline{g}$$

**S=**

dynamic viscosity of the gas mixture,  $kg\ m^{-1}\ s^{-2}$

velocity vector,  $m\ s^{-1}$

transposed vector

volume viscosity,  $kg\ m^{-1}\ s^{-1}$

unity tensor

pressure,  $Pa$

$$\nabla \cdot \left( \mu (\nabla \underline{v})^\dagger + \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \underline{v}) \underline{\underline{I}} \right) - \nabla P + \rho \underline{g}$$

$$\nabla \left( \mu (\nabla \underline{v}) \right)^\dagger + \left( k - \frac{2}{3} \mu \right) (\nabla \cdot \underline{v}) \underline{\underline{I}} - \nabla P - \rho \underline{g}$$

gravity vector,  $(g_z = -9.81\ m\ s^{-2})$

density,  $kg\ m^{-3}$



$$\begin{matrix} \text{transient} \\ \xi \end{matrix} \frac{d}{dt} (\rho \phi) = - \begin{matrix} \text{convection} \\ \xi \end{matrix} \nabla (\rho \underline{v} \phi) + \nabla \cdot \begin{matrix} \text{diffusion} \\ \Gamma \end{matrix} \nabla \phi + S$$

$\underset{=c}{\phantom{\xi}} \quad \quad \quad \underset{=T}{\phantom{\phi}} \quad \quad \quad \underset{=c}{\phantom{\xi}} \quad \quad \quad \underset{=\lambda}{\phantom{\Gamma}} \quad \quad \quad \underset{=T}{\phantom{\phi}}$

Energy

$$c \frac{d}{dt} (\rho T) = - c \nabla (\rho \underline{v} T) + \nabla (\lambda \nabla T) + S$$

S=

$$\nabla \cdot \left( RT \sum_{i=1}^N \frac{D_i^T}{m_i} \nabla (\ln f_i) \right) + \sum_{i=1}^N \left( \frac{H_i}{m_i} \nabla \cdot \underline{j}_i - \sum_{k=1}^K H_i \nu_{ik} (\mathcal{R}_k^g - \mathcal{R}_{-k}^g) \right)$$

universal gas constant =  $8.314 \text{ J mole}^{-1} \text{ K}^{-1}$

Temperature,  $K$

number of gaseous species

multicomponent thermal diffusion coefficient  
of species  $i$ ,  $\text{kg m}^{-1} \text{ s}^{-1}$

mole mass of species  $i$

species  $i$  mole fraction

S=

$$\nabla \cdot \left( RT \sum_{i=1}^N \frac{\mathbf{D}_i^T}{m_i} \nabla (\ln f_i) \right) + \sum_{i=1}^N \left( \frac{H_i}{m_i} \nabla \cdot \underline{j}_i - \sum_{k=1}^K H_i \nu_{ik} (\mathcal{R}_k^g - \mathcal{R}_{-k}^g) \right)$$

diffusive mass  
flux vector,  
 $\text{kg m}^{-2} \text{ s}^{-1}$

reverse reaction rate of the  
 $k^{\text{th}}$  gas phase reaction,  $\text{mole m}^{-3} \text{ s}^{-1}$

forward reaction rate of the  
 $k^{\text{th}}$  gas phase reaction,  $\text{mole m}^{-3} \text{ s}^{-1}$

molar enthalpy,  $\text{J mole}^{-1}$

stoicmetric coefficient of the  $i^{\text{th}}$  gaseous species  
in the  $k^{\text{th}}$  gas phase reaction

number of gas phase reactions

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# General Transport Equation for Species

$$\begin{array}{ccccccc}
 \text{transient} & & \text{convection} & & \text{diffusion} & & \text{source} \\
 \xi \frac{d}{dt} (\rho \phi) = & - & \xi \nabla (\rho \underline{v} \phi) & + & \nabla (\Gamma \nabla \phi) & + & S \\
 \underset{=1}{} & & \underset{=1}{} & & \underset{=\rho D_i}{} & & \underset{=T}{}
 \end{array}$$

**Species**  $i = 1 \dots n$

$$\frac{d}{dt} (\rho \omega_i) = - \nabla (\rho \underline{v} \omega_i) + \nabla (\rho D_i \nabla \omega_i) + S$$

**S=**

$$\begin{aligned}
 & \nabla \cdot (\mathbb{D}_i^T \nabla (\ln T)) + \nabla \cdot (\rho \omega_i \mathbb{D}_i \nabla (\ln m)) \\
 & - \nabla \cdot \left( m \omega_i \mathbb{D}_i \sum_{j=1}^N \frac{j_j}{m_j D_{ij}} \right) \\
 & + m_i \sum_{k=1}^K \nu_{ik} \left( k_k \prod_{i=1}^N c_i^{\|\nu_{ik}\|} - k_{-k} \prod_{i=1}^N c_i^{\|\nu_{ik}\|} \right)
 \end{aligned}$$

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**ZfM**

**Fraunhofer**  
ENAS

S=

multicomponent thermal diffusion coefficient  
of species  $i$ ,  $\text{kg m}^{-1} \text{s}^{-1}$

species  $i$  mass fraction

effective multicomponent diffusion  
coefficient of species  $i$ ,  $\text{kg m}^2 \text{s}^{-1} \text{kg}$

Temperature, K density,  $\text{kg m}^{-3}$

average mole mass, kg

$$\nabla \cdot (\mathbb{D}_i^T \nabla (\ln T)) + \nabla \cdot (\rho \omega_i \mathbb{D}_i \nabla (\ln m)) - \nabla \cdot \left( m \omega_i \mathbb{D}_i \sum_{j=1}^N \frac{j_j}{m_j D_{ij}} \right) + m_i \sum_{k=1}^K \nu_{ik} \left( k_k \prod_{i=1}^N c_i^{\|\nu_{ik}\|} - k_{-k} \prod_{i=1}^N c_i^{\|\nu_{ik}\|} \right)$$

number of  
gaseous species

specific heat of the  
gas mixture,  $\text{J kg}^{-1} \text{K}^{-1}$

molar mass of  
species  $i$ ,  
 $\text{kg mole}^{-1}$

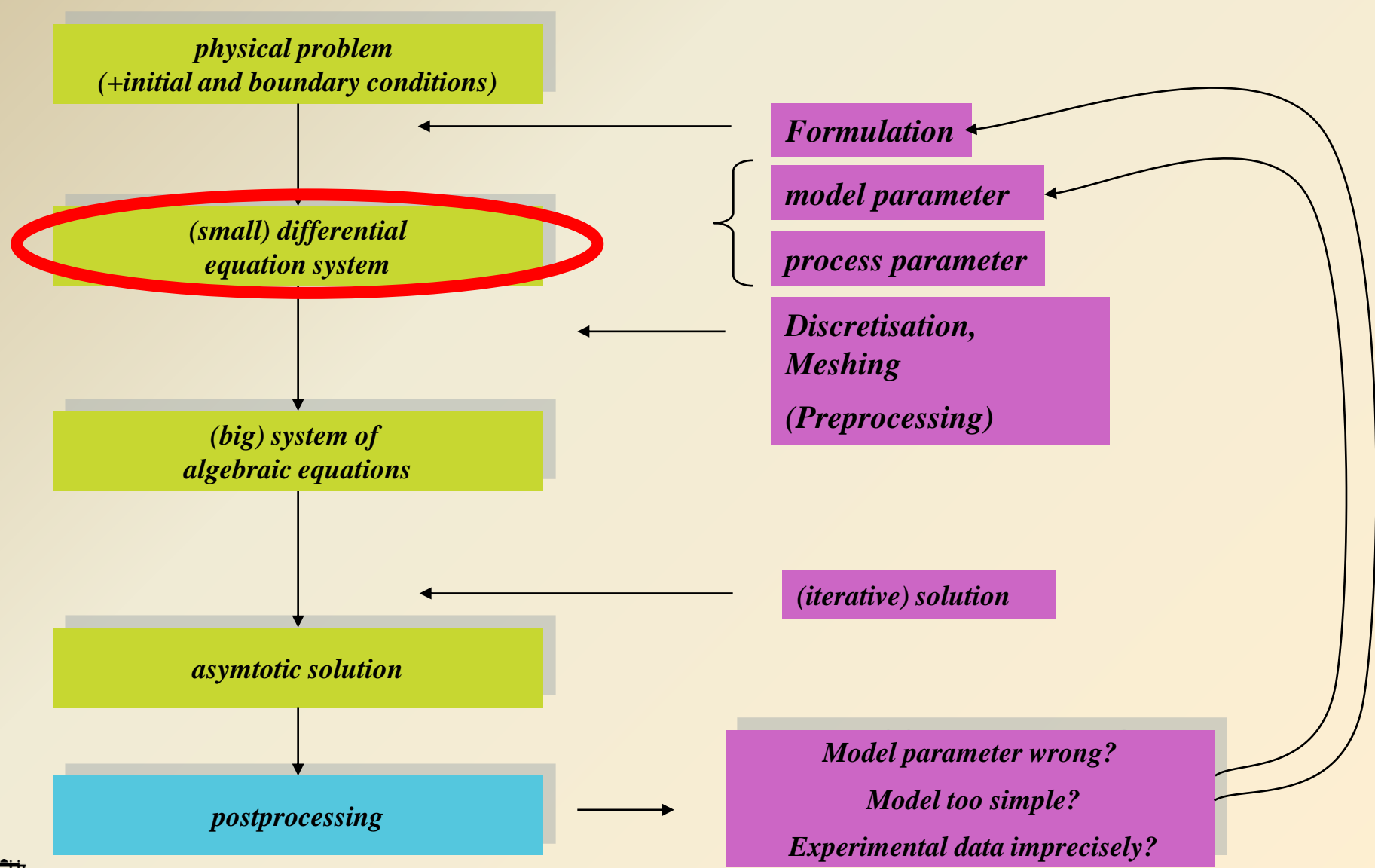
reverse reaction rate constant for the of the  
 $k^{\text{th}}$  homogeneous in  $\text{m}^3$ , mole and s dep. on  
the reaction order

number of gas  
phase reactions

foreward reaction rate constant for the of the  
 $k^{\text{th}}$  homogeneous in  $\text{m}^3$ , mole and s dep. on the reaction order

stoicmetric coefficient of the  $i$ th gaseous species  
in the  $k^{\text{th}}$  gas phase reaction





# General Transport Equation

*transient*  $\xi \frac{d}{dt} (\rho \phi) =$  *convection*  $- \xi \nabla (\rho \underline{v} \phi)$  *diffusion*  $+ \nabla (\Gamma \nabla \phi)$  *source*  $+ S$

$\frac{d}{dt} (\rho) = - \nabla (\rho \underline{v})$  *Continuity*

$\frac{d}{dt} (\rho \underline{v}) = - \xi \nabla (\rho \underline{v} \underline{v}) + \nabla (\mu \nabla \underline{v}) + S$

*c*  $\frac{d}{dt} (\rho T) = - c \nabla (\rho \underline{v} T) + \nabla (\lambda \nabla T) + S$

$\frac{d}{dt} (\rho \omega_i) = - \nabla (\rho \underline{v} \omega_i) + \nabla (\rho D_i \nabla \omega_i) + S$

*Momentum*  $S =$

$$\nabla \cdot \left( \mu (\nabla \underline{v})^\dagger + \left( \kappa - \frac{2}{3} \mu \right) (\nabla \cdot \underline{v}) \underline{\underline{I}}} \right) - \nabla P + \rho \underline{g}$$

*Energy*  $S =$

$$\nabla \cdot \left( RT \sum_{i=1}^N \frac{D_i^T}{m_i} \nabla (\ln f_i) \right) + \sum_{i=1}^N \left( \frac{H_i}{m_i} \nabla \cdot \underline{j}_i - \sum_{k=1}^K H_i \nu_{ik} (\mathcal{R}_k^g - \mathcal{R}_{-k}^g) \right)$$

*Species*  $S =$

$$\nabla \cdot (\text{ID}_i^T \nabla (\ln T) + \nabla \cdot (\rho \omega_i \text{ID}_i \nabla (\ln m) - \nabla \cdot \left( m \omega_i \text{ID}_i \sum_{j=1}^N \frac{j_j}{m_j D_{ij}} \right) + m_i \sum_{k=1}^K \nu_{ik} \left( k_k \prod_{i=1}^N c_i^{\|-\nu_{ik}\|} - k_{-k} \prod_{i=1}^N c_i^{\|\nu_{ik}\|} \right))$$

Example: Iterative Solution of 2D Diffusion equation based on FDM

$\xi \frac{d}{dt} (\rho \phi) = - \xi \nabla (\rho \underline{v} \phi) + \nabla (\Gamma \nabla \phi) + S$   
 $\frac{d}{dt} (C) = \nabla (D \nabla C)$

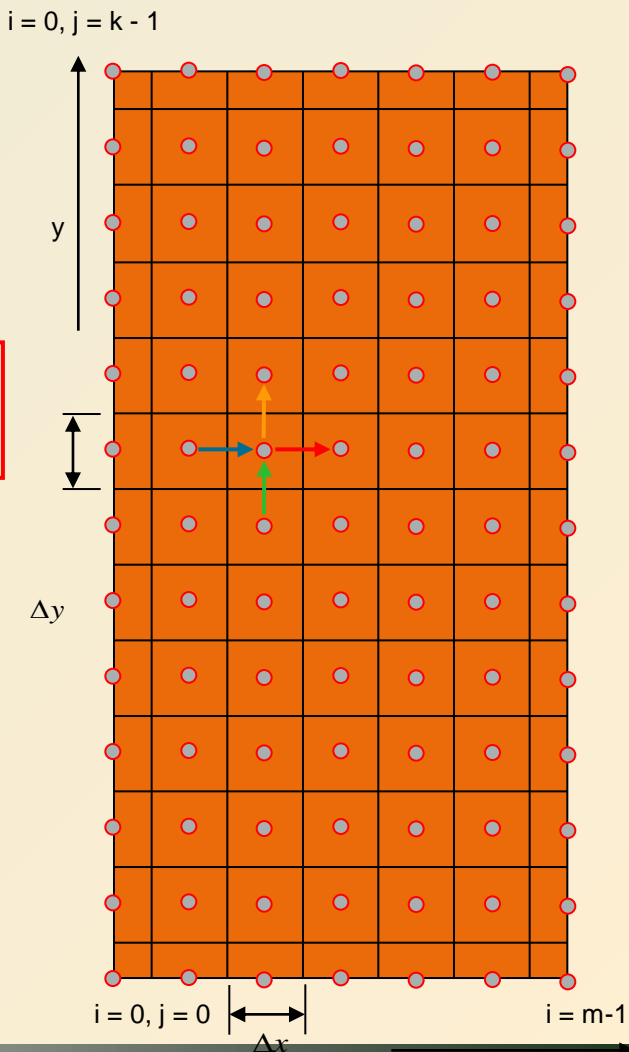
2 Dim:  $D \nabla C = D (dC/dx + dC/dx)$

$j = - \frac{D(C_{i,j+1}^n - C_{i,j}^n)}{\Delta y}$

$j = - \frac{D(C_{i,j}^n - C_{i-1,j}^n)}{\Delta x}$   $\rightarrow$   $j = - \frac{D(C_{i+1,j}^n - C_{i,j}^n)}{\Delta x}$

$j = - \frac{D(C_{i,j}^n - C_{i,j-1}^n)}{\Delta y}$

$div(\vec{j}) = \frac{\oint \vec{j} ds}{A} = \frac{(\boxed{j} - \boxed{j})\Delta y + (\boxed{j} - \boxed{j})\Delta x}{\Delta x \Delta y}$



$$\frac{\partial C}{\partial t} = -\text{div}(j) = D \left( \frac{(C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}))}{\Delta x^2} + \frac{(C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}))}{\Delta y^2} \right)$$

5-points equation

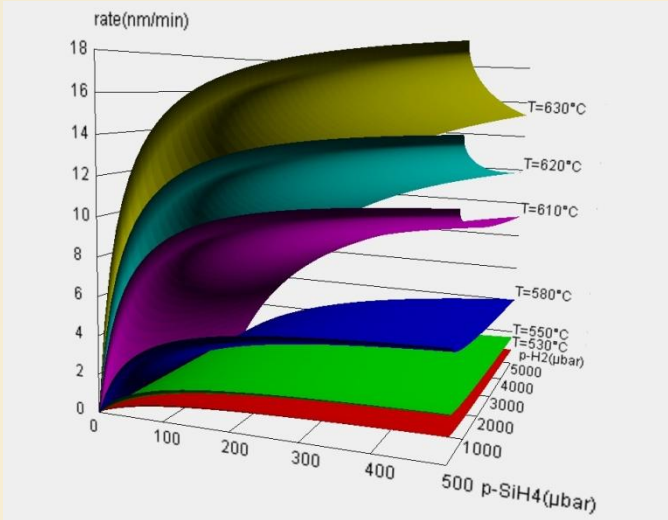
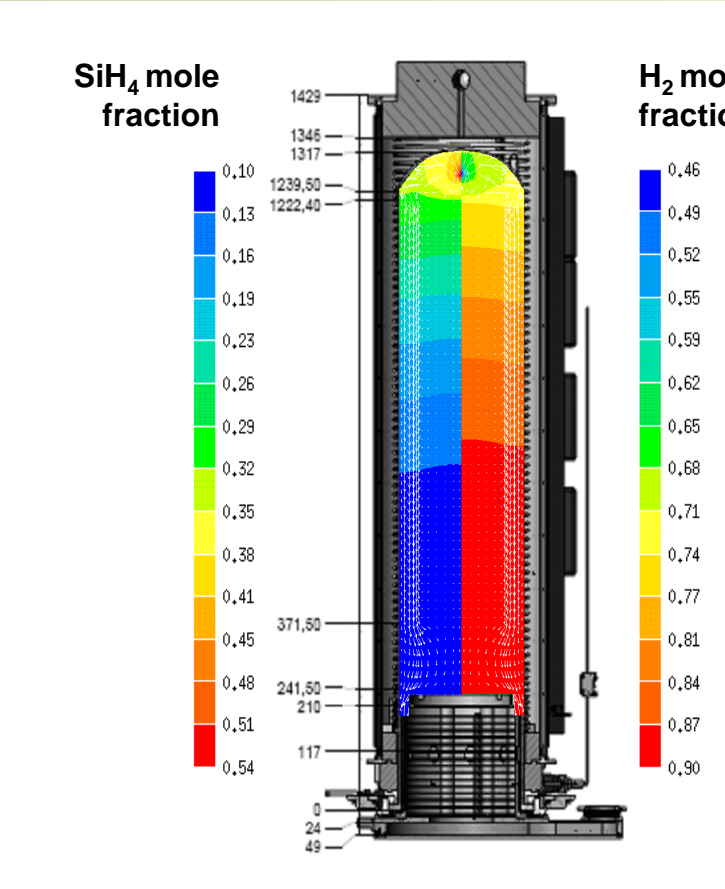
$$C_{i,j}^{n+1} = C_{i,j}^n + \Delta t \cdot D \left( \frac{(C_{i+1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i-1,j}^{n+1}))}{\Delta x^2} + \frac{(C_{i,j+1}^{n+1} - 2C_{i,j}^{n+1} + C_{i,j-1}^{n+1}))}{\Delta y^2} \right)$$

1d: tri diagonal mx

$$\begin{bmatrix} & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \end{bmatrix} = \begin{bmatrix} C_{0,0}^{n+1} \\ C_{0,k}^{n+1} \\ \\ \\ \\ \\ \\ \\ C_{m-1,k}^{n+1} \end{bmatrix} = \begin{bmatrix} R_{0,0} \\ \cdot \\ \cdot \\ \cdot \end{bmatrix}$$

## Improvement of

- deposition rates
  - uniformity
- by **optimization** of
- process conditions
  - reactor configuration



Flow pattern and distributions of  $\text{SiH}_4$  and  $\text{H}_2$  mole fractions inside the reactor for silicon deposition at  $630^\circ\text{C}$ ,  $200\ \mu\text{bar}$ ,  $200\ \text{sccm}\ \text{SiH}_4$ ,  $0\ \text{sccm}\ \text{H}_2$ .

Dependence of deposition rates on the local partial pressures of  $\text{SiH}_4$  and  $\text{H}_2$  for different deposition temperatures

# Reactor Scale: Deep trenches (Multi-step trench filling with As doped poly)

