Métodos numéricos para escoamentos em nano e microescalas

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Outline

1. *Course structure*
2. *Multiscale molecular simulations*
3. *Complex physical phenomena in Materials (Nano and Microfluidics)*

PME5429

- **Prof. Caetano Rodrigues Miranda**
- **Prof. Julio Romano Meneghini**
- **Prof. Rafael dos Santos Gioria**

- **Período: Diurno**
- **Horário: Terças 09:00h às 12:00h**

RCGI

Home-page:

https://edisciplinas.usp.br/course/view.php?id=82131

Calendário da disciplina (tópicos, cronograma, ...)

- **Atividades**
- **Notas de aula**
- **Conceitos, etc.**

Avaliações

Labs e Projeto: $$Média = \frac{Labs + \Pr oj}{2}$$

Relatórios, apresentação do Projeto

Conceitos:

A	**Média de 9,0 a 10,0**
B	**Média de 7,5 a 9,0**
C	**Média de 5,5 a 7,5**
D	**Média de 4,0 a 5,5**
F	**Reprovado**
O	**Reprovado por faltas (> 6 faltas!)**

Métodos numéricos para escoamentos em nano e microescalas

Objetivos:

Apresentar técnicas avançadas de simulação de fenômenos de transporte e dinâmica dos fluidos em Engenharia (mecânica, aeronáutica, química, naval, civil, petróleo, bio-engenharia, entre outras).

Apresentar métodos de simulação de escoamento com aplicações em nano e micro-fluídica, assim como técnicas de acoplamento dessas escalas para macro escalas nas quais a hipótese do continuo são aplicáveis.

Cobrir métodos em nano e micro-escalas, e.g. atomísticos (Dinâmica Molecular e Método Monte Carlo) e redes de Boltzmann.

Apresentar metodologias de acoplamento desses com métodos convencionais em Dinâmica dos Fluidos Computacional.

Métodos numéricos para escoamentos em nano e microescalas

- Método: Base - Exploração – Aplicação

Métodos em multiescala: atomísticos (Dinâmica Molecular e Método Monte Carlo), redes de Boltzmann, e Dinâmica Computacional de fluídos (volumes / diferenças finitas e elementos finitos).

- Foco na exploração do método
- Ênfase na experimentação dos métodos através de laboratórios computacionais.
- Aplicações na indústria do Petróleo

- Organização: Aulas + Laboratório
- Avaliação: Lab + Projeto

Lab

- Linux / Computação Científica

Micro:

- Dinâmica Molecular

Multiescala:

Acoplando Dinâmica Molecular e Redes de Boltzmann

Macro:

- Métodos do continuo

Projeto e seminário

• Propor um projeto na linha de dinâmica de fluídos a partir de um enfoque em multiescala

Motivação
Importância para indústria
Estudo em micro e macro escalas

Cronograma

	Ter	atividade	Instrutor
set	8		
	15	Apresentação do Curso / Métodos Multiescala	Caetano
	22	Ambientação - Máquina Virtual / Projeto / Linux	Caetano / Kirch
	29	Dinâmica Molecular 1	Caetano / Kirch
out	6	Lab 1 - Dinâmica Molecular -Fluidos bulk (Estrutura e Transporte)	Caetano / Kirch
	13	Dinâmica Molecular 2	Caetano / Kirch
	20	LAB 2 - Dinamica Molecular -Interfaces (Tensão Interfacial) & Viscosidade	Caetano / Kirch
	27	LBM	Julio / Adriano
nov	3	LBM	Julio / Adriano
	10	CFD	Julio / Rafael
	17	CFD	Julio / Rafael
	24	CFD	Julio / Rafael
	1	CFD	Julio / Rafael
dez	8	Projeto - Apresentação	Julio / Rafael / Caetano
	15		

Referências

- Notas de aula
- Artigos relevantes ao método
- Computational Materials Science - Dierk Raabe
- Crystal, Defects and Microstructures - R. Phillips
- Primer on Molecular Dynamics - Ercolessi
- Computer simulations of Liquids - Allen/Tildesley

As referências relevantes serão distribuídas em classe.

PME5429 – Edição 2020

- ***Aulas e laboratórios***

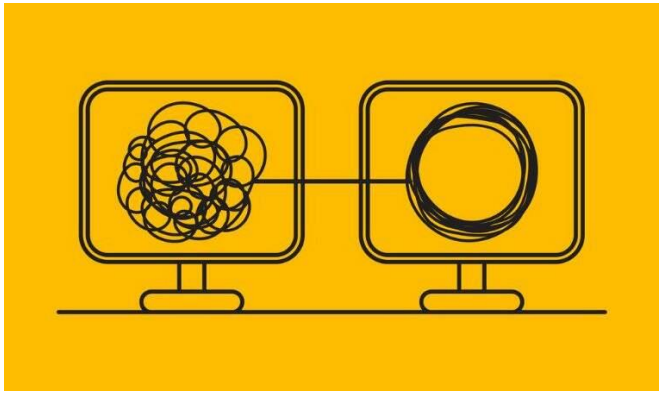
- Síncronas e assincronas (Lives e vídeos de 30 – 60 min)
- Cada aula (3 partes – 45 min com 5 min de intervalo)
- Máquina virtual e/ou acesso remoto
- Engajamento e contato contínuo
- Transmedia (E-disciplinas, Instagram, whatsapp, …)
- Participação importante: atividades coletivas (artigos)
- Gamificação

PME5429 – Edição 2020

- ***Ambientação***
- Montagem das máquinas virtuais e acesso remoto
- Introdução ao Linux, programas de visualização e VR
- Bibliografia a ser distribuída
- Dúvidas: de imediato use ***hotlines***

Tenho dúvidas nas aulas assíncronas … o que fazer ?

Dúvidas use o HOTLINE:
crmiranda@usp.br
Assunto: SCM2020



Todas as dúvidas serão comentadas no inicio das aulas. Projetos e Labs

Seu perfil ?

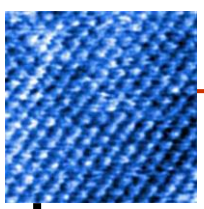
https://docs.google.com/forms/d/e/1FAIpQLSfrv1BXsKjGadnzFDCKM8JjIvfcIXJiNMyZlnE2Xpi4kZG2Tg/viewform

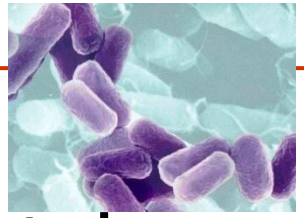
Quem é seu professor ? Experiência Profissional (Nano / porous media / fluidics)

- Do pai poeta, sempre ouvia as palavras de Heráclito, “Tudo flui e nada permanece”.
- Intrigado, voltou-se à Física tendo como alma matter, a Unicamp. Finalizou o doutorado levado a chá preto na Universidade de Cambridge, Inglaterra.
- Como pos-doc, embembeu-se de café no ICTP em Trieste – Itália e coca-cola no MIT explorando simulações moleculares aplicados a materiais sob condições extremas e nanotecnologia.
- Foi professor assistente na Universidade de Kyoto, onde transgrediu percolando água sobre chá verde em alta pressão, enquanto introduzia simulações moleculares para indústria do petróleo.
- Após passagem pela UFABC, é atualmente professor no IFUSP desenvolvendo projetos em dinâmica de fluídos em materiais complexos e design computacional de materiais nanoestruturados para aplicações em energia, combinando realidade virtual e simulações moleculares em multiescala.
- Desenvolve projetos com o setor produtivo e realiza experimentações envolvendo diálogos entre ciência e arte.

SCALE

Escalas

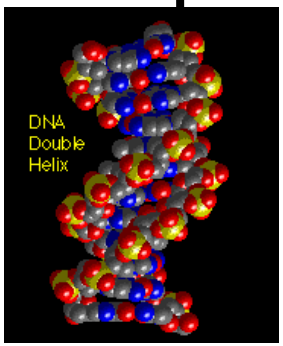


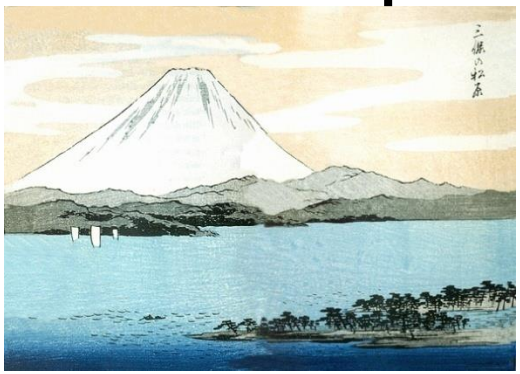


Nanoscale

10^{-10} 10^{-8} 10^{-6} 10^{-4} 10^{-2} 10^{0} 10^{2} 10^{4} 10^{6} 10^{8} 10^{10}

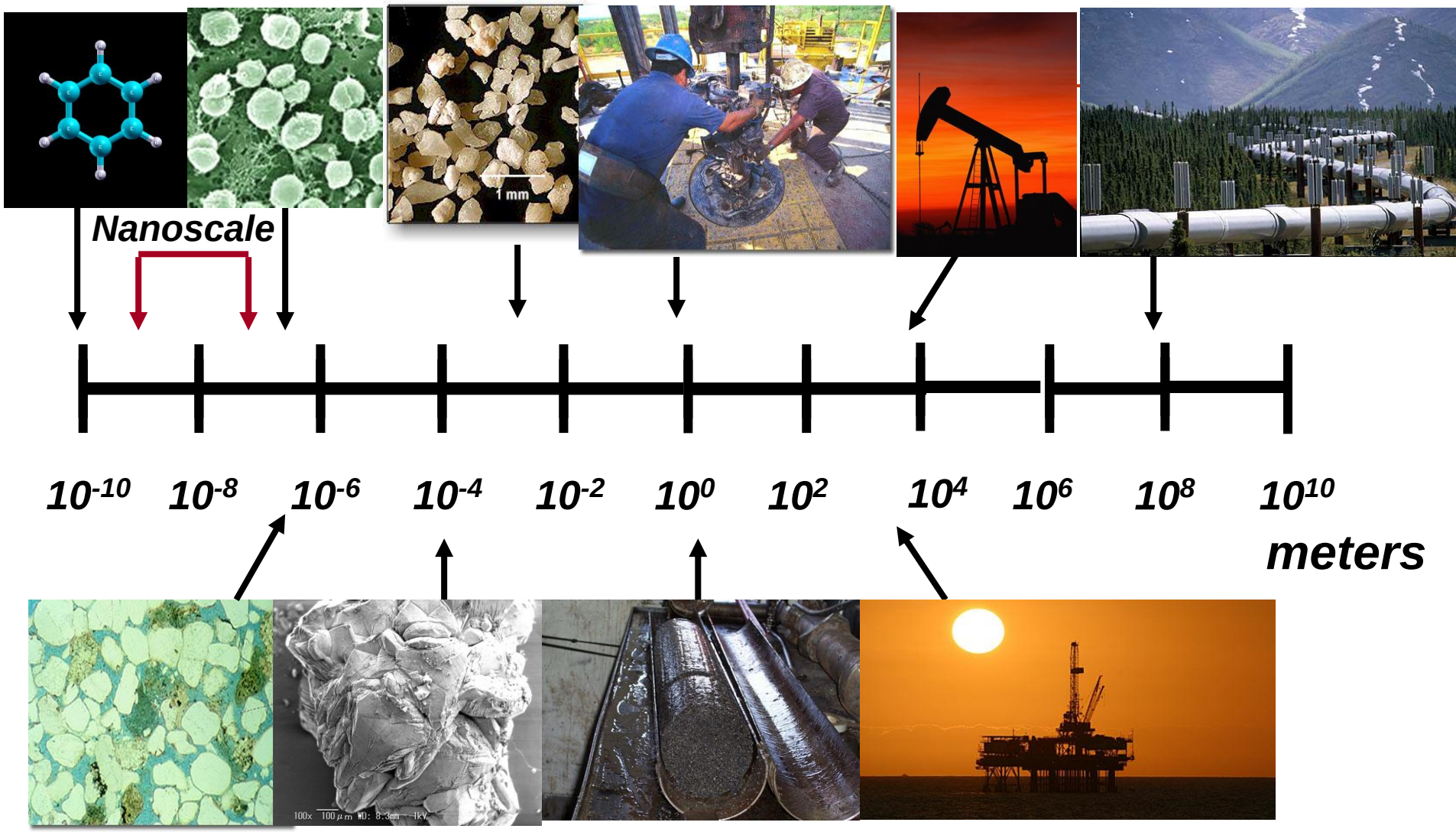
meters





Parte 1 - Nano a Micro **Parte 2 - Meso a Macro**

Crossing scales in Oil & Gas



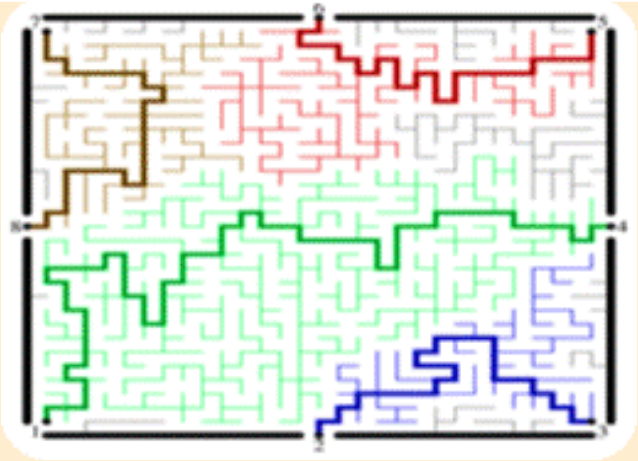
Oil&Gas: How the large can drive small systems ?

Operating conditions (relatively harsh conditions)

- Depths: 1.5 – 4.5 km
- Temperatures: 0 to 180°C
- Pressures: 0 to 8 Kpsi (0 - 550 atm)
- pH: 4-8 (acidic)
- Presence of: complicated fluids, water and clays (heterogenity)
- Salinity: seawater to very concentrated
- Size (pore throats in rock formations): ≤5 μm

- The current average recovery factor from conventional oil reservoirs is ~35%.
- Poor sweep effect in the reservoir & capillary forces

From simple models to solve some problems in industry



"Toy models" in Physics

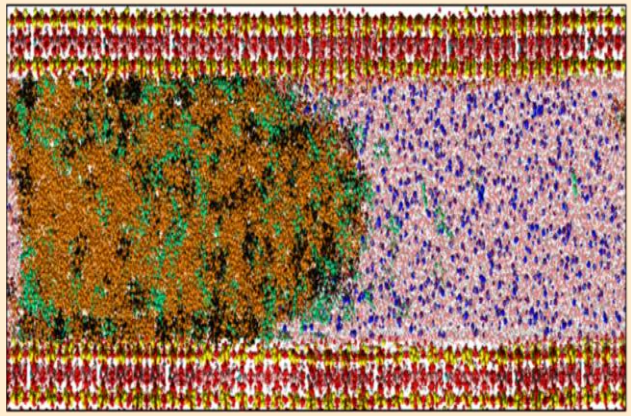
- Simple models
- Strong approximations
- Ideal conditions
- Relative time and length scales
- Searching for analytical solutions or universality classes

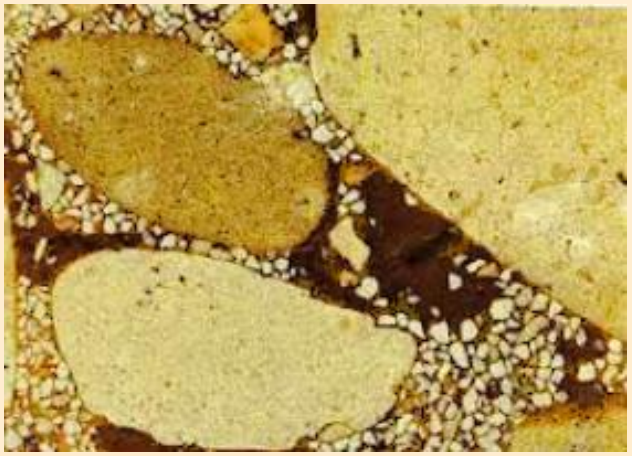
Industry:

- Complex systems
- Heterogeneity
- Real conditions
- "Macroscopic"
- Trial-and-error method

How the knowledge of atomic and molecular interactions can contribute in the development and industrial innovation ?

From simple models to solve some problems in industry





Multiscale comp. methods:

- Complex models
- Controlled approximation
- Real conditions
- Molecular Scale "Microscopic"
- Solutions based on the knowledge acquired

Industry:

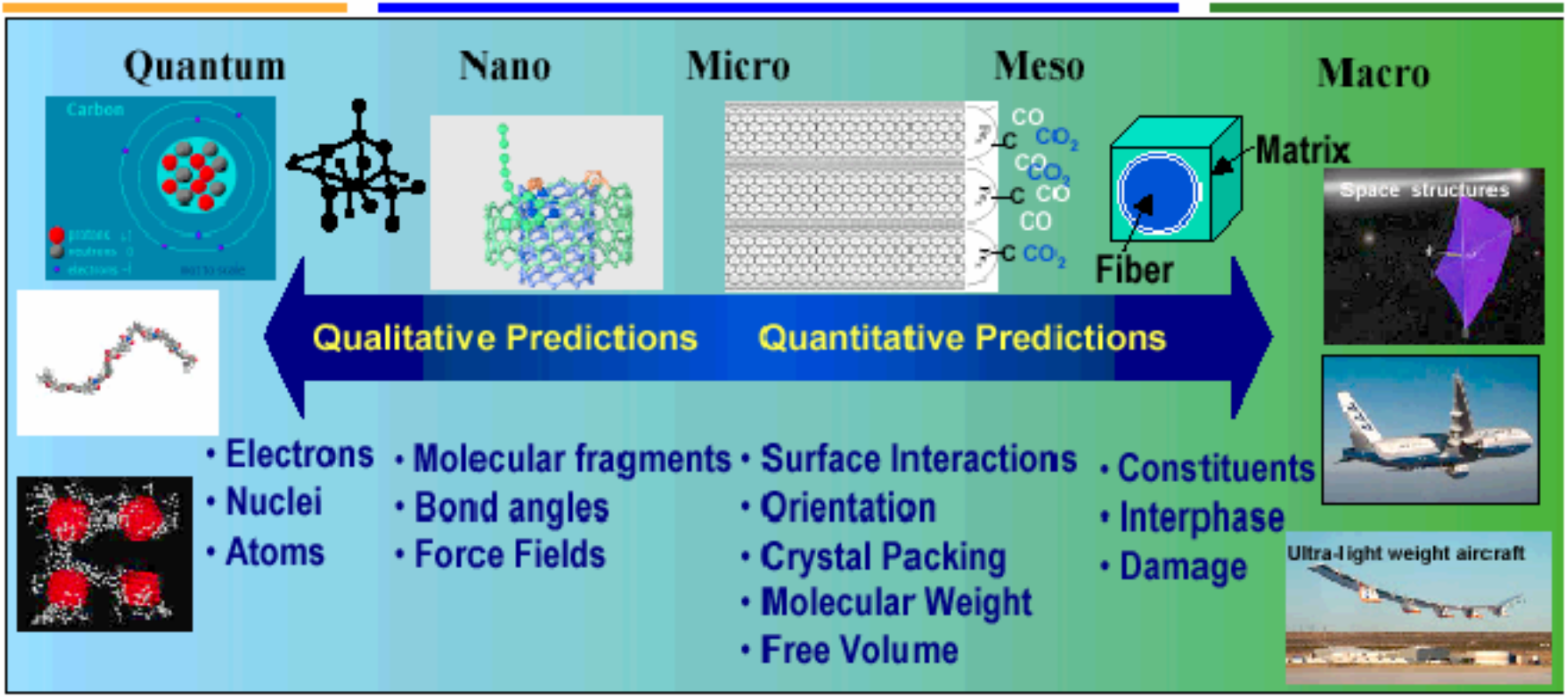
- Complex systems
- Heterogeneity
- Real conditions
- "Macroscopic"
- Trial-and-error method

Length and time scales in materials modeling

NASA Langley Research Center
Hampton, Virginia
Computational Materials - Nanotechnology Modeling and Simulation

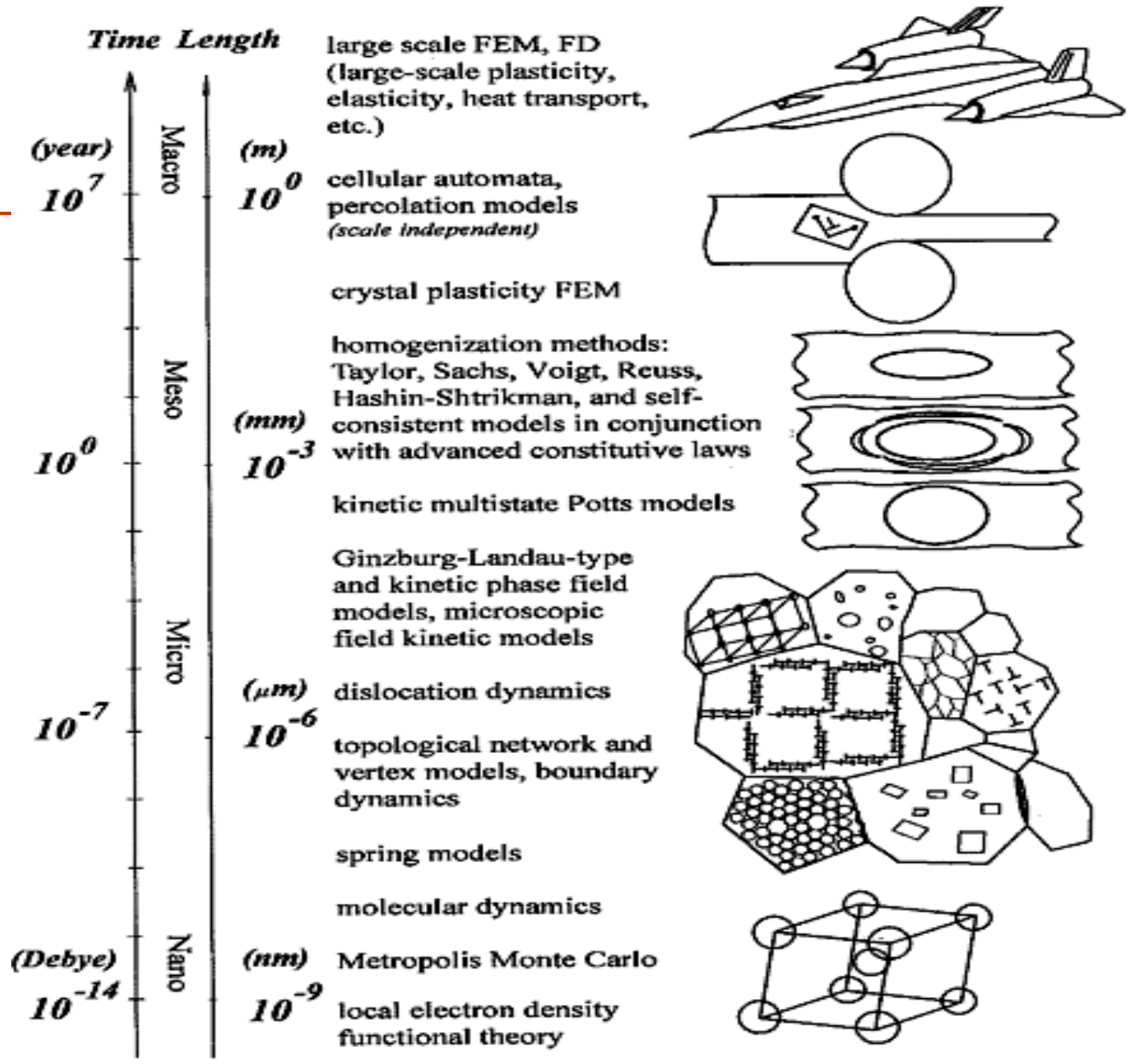
by Greg Odegard, NASA

Computational Chemistry | **Computational Materials** | **Computational Mechanics**



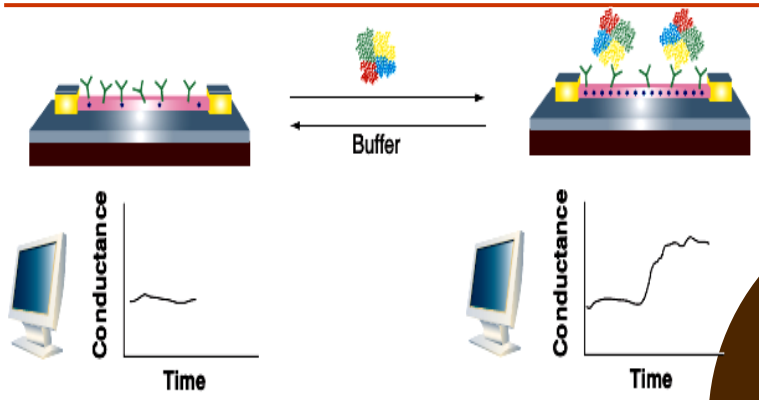
10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0}

Length, (m)

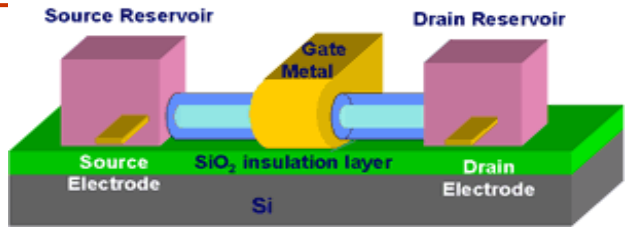

Time Length
(year)
10^{7}
Macro
(m)
10^{0}
large scale FEM, FD (large-scale plasticity, elasticity, heat transport, etc.)
cellular automata, percolation models
(scale independent)
crystal plasticity FEM
homogenization methods: Taylor, Sachs, Voigt, Reuss, Hashin-Shtrikman, and self-consistent models in conjunction with advanced constitutive laws
Meso
(mm)
10^{0}
10^{-3}
kinetic multistate Potts models
Ginzburg-Landau-type and kinetic phase field models, microscopic field kinetic models
Micro
(μm)
10^{-7}
10^{-6}
dislocation dynamics
topological network and vertex models, boundary dynamics
spring models
molecular dynamics
(Debye)
10^{-14}
Nano
(nm)
10^{-9}
Metropolis Monte Carlo
local electron density functional theory

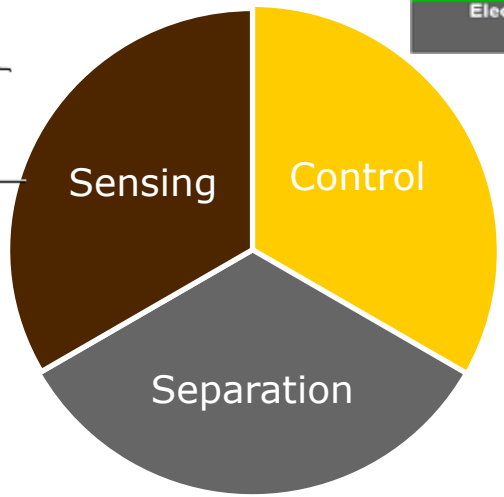
NANOFLUIDICS

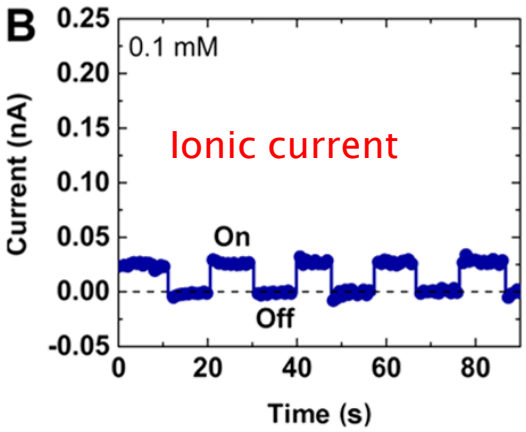
Nanofluidics



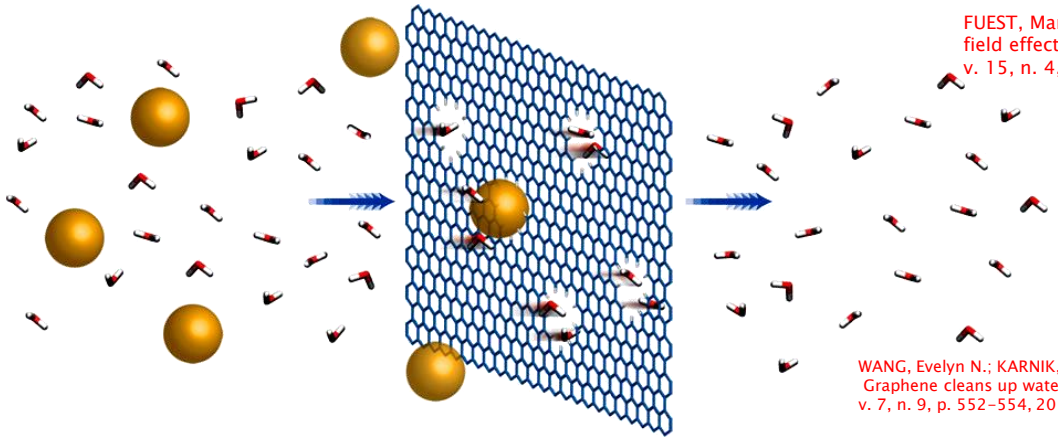
PATOLSKY, Fernando; ZHENG, Gengfeng; LIEBER, Charles M. Nanowire sensors for medicine and the life sciences. 2006.





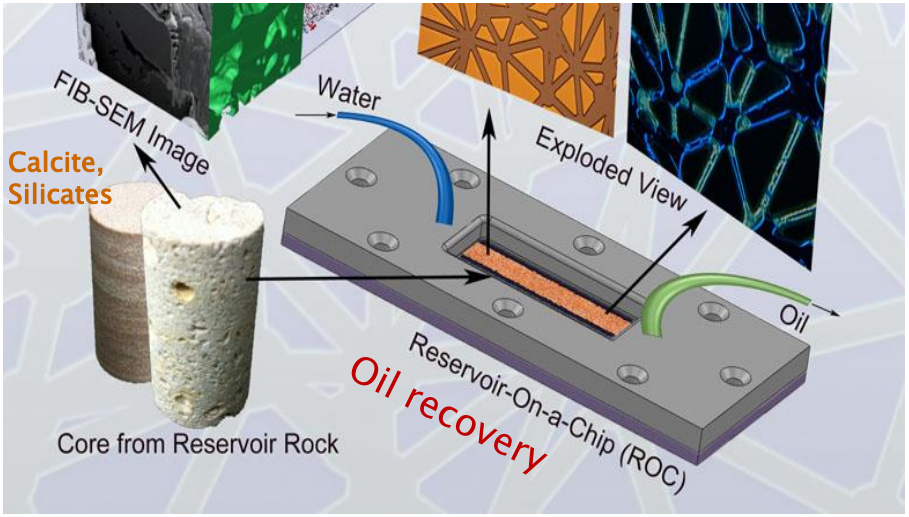


FUEST, Marie et al. A three-state nanofluidic field effect switch. **Nano letters**, v. 15, n. 4, p. 2365-2371, 2015.

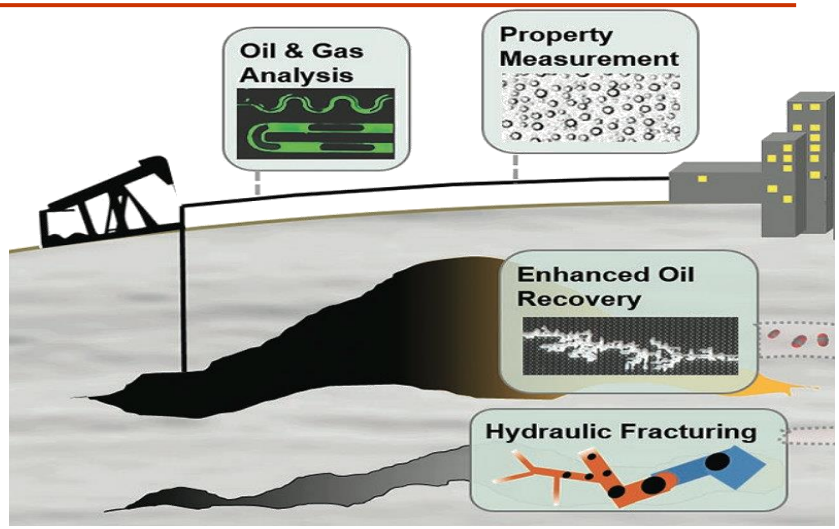


WANG, Evelyn N.; KARNIK, Rohit. Water desalination: Graphene cleans up water. **Nature nanotechnology**, v. 7, n. 9, p. 552-554, 2012.

Nanofluidics



Naga Siva Kumar Gunda, Bijoyendra Bera, Nikolaos K. Karadimitriou, Sushanta K. Mitra and S. Majid Hassanizadeh (2011) Reservoir-on-a-Chip (ROC): A new paradigm in reservoir engineering. *Lab Chip*, 11, 3785-3792



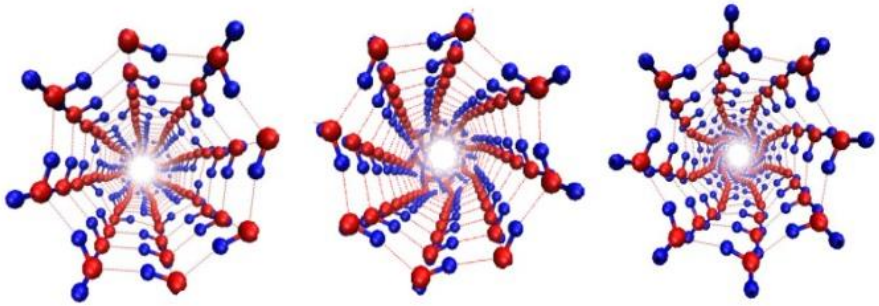
Sinton, D., 2014. Energy: The Microfluidic Frontier. *Lab on a Chip*, 14 (17): 3127-3134. Available on http://www.spe.org

- Low reagent volumes;
- Low cost;
- Excellent control of environment conditions;
- Fluidic-based analysis and separations tools for applications in the chemical industry;
- Better fluid property measurement and fluid analysis;
- Understand pore-scale process in reservoirs

Nanofluidics

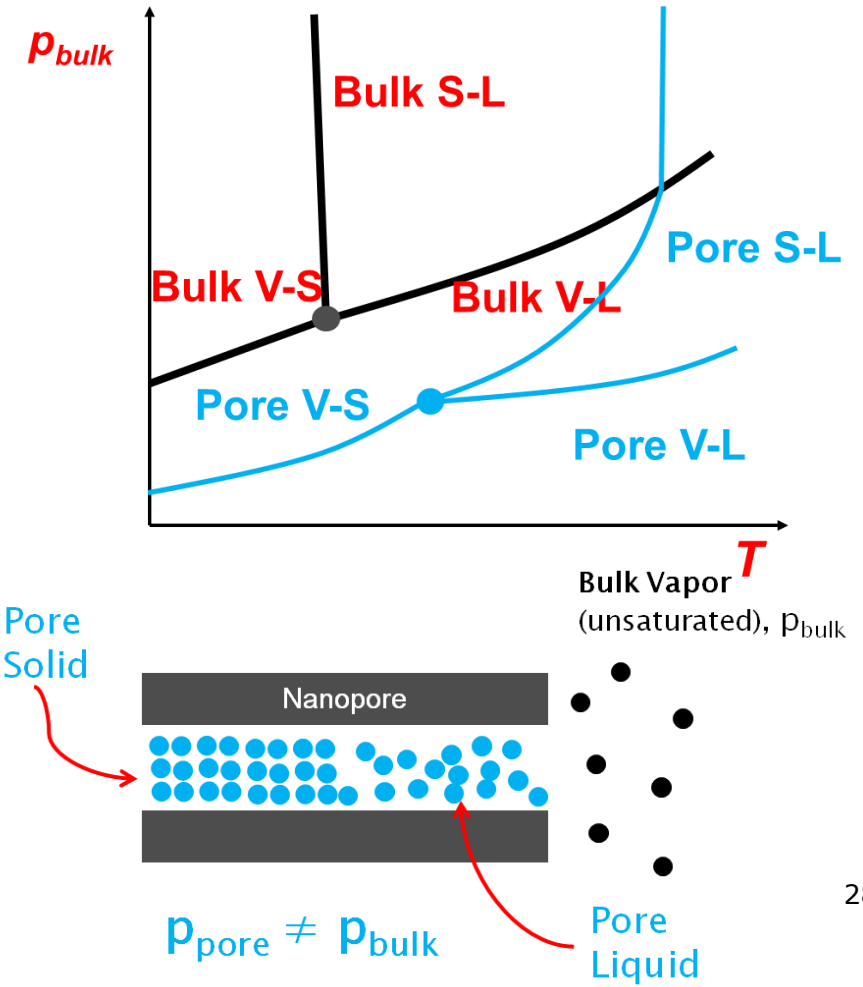
Water structuring

300K, 1atm



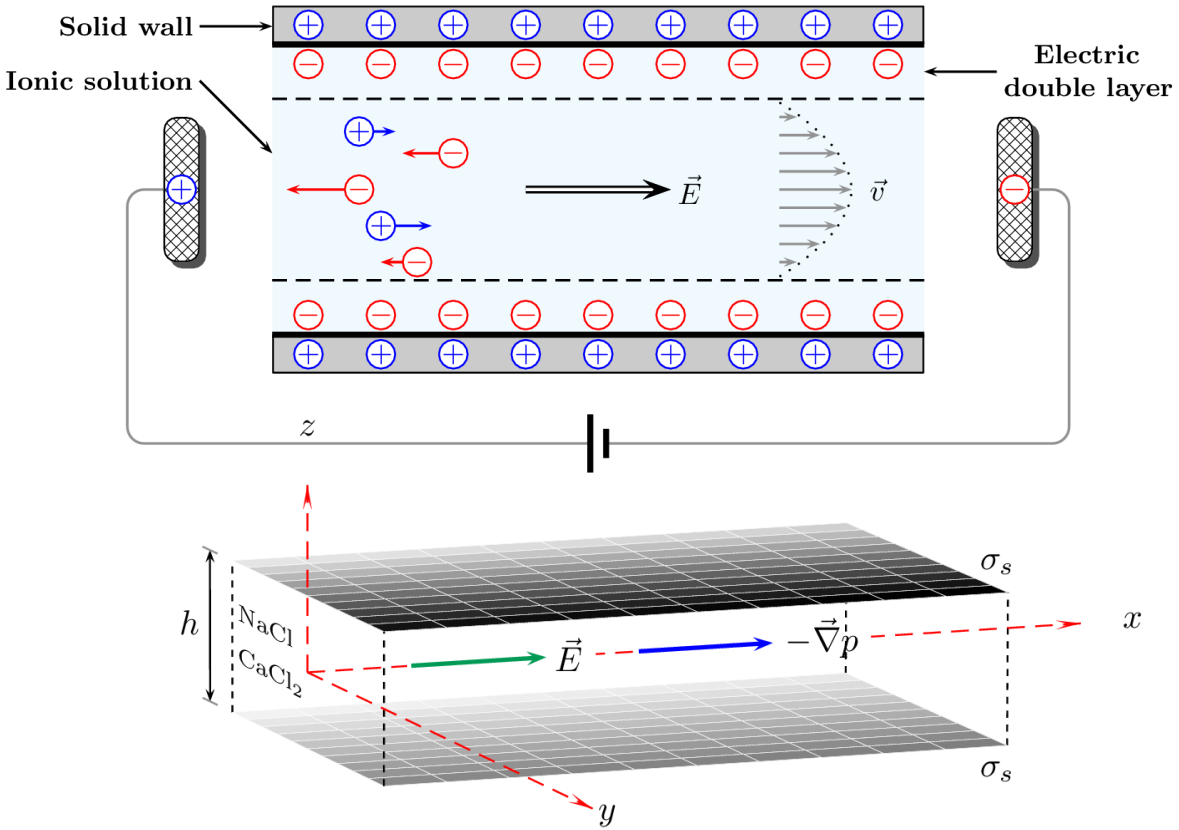
Phys. Chem,2015,17,7303

Phase Diagram



LIMITS ATOMISTIC AND CONTINUUM

Phenomenon of Electroosmosis



Electroosmosis

- Electrostatic (Ion concentration)
- Hydrodynamic (Velocity profile)

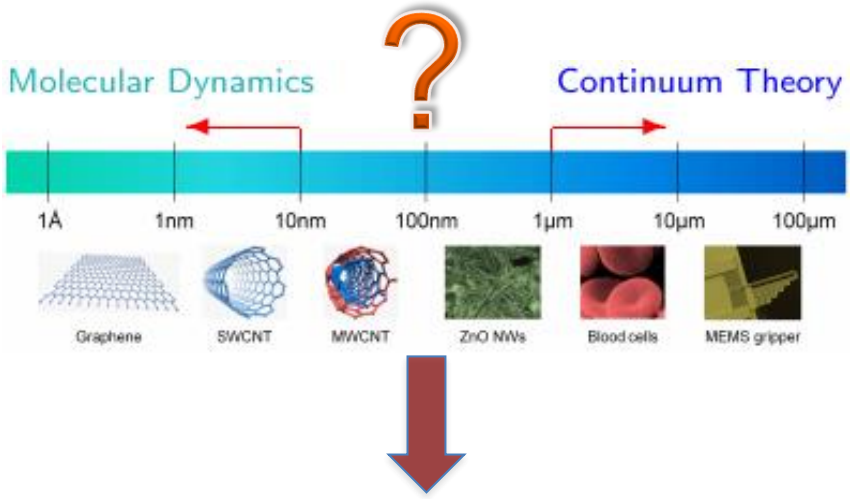
Phenomenon of Electroosmosis at nanoscale

Molecular Dynamics

- **Euler – Lagrange equations**
- **Interatomic potential**

Continuum Theory

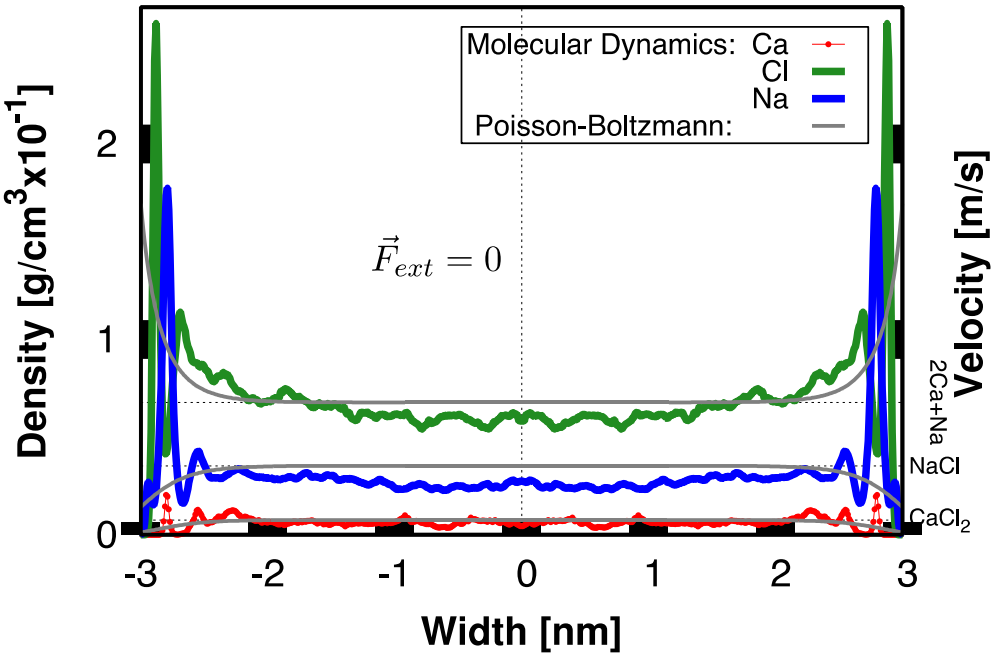
- **Electrostatic (Poisson – Boltzmann)**
- **Hydrodynamic (Navier – Stokes)**



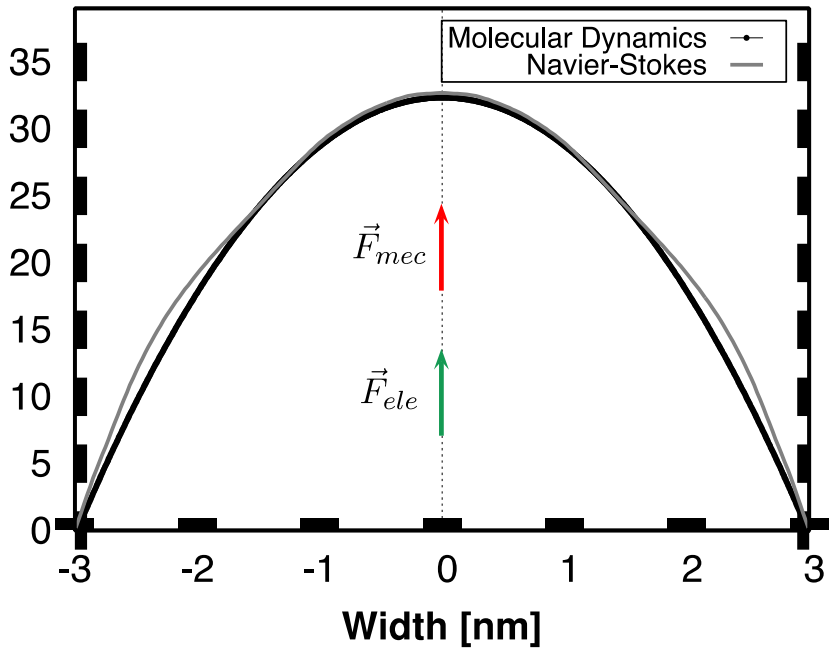
- **Modified Poisson – Boltzmann equation**
- **Embending Velocity MD (in Navier – Stokes)**

Limitations at nanoscale

Ion concentration



Velocity profile



MD (h > 10 nm)

High

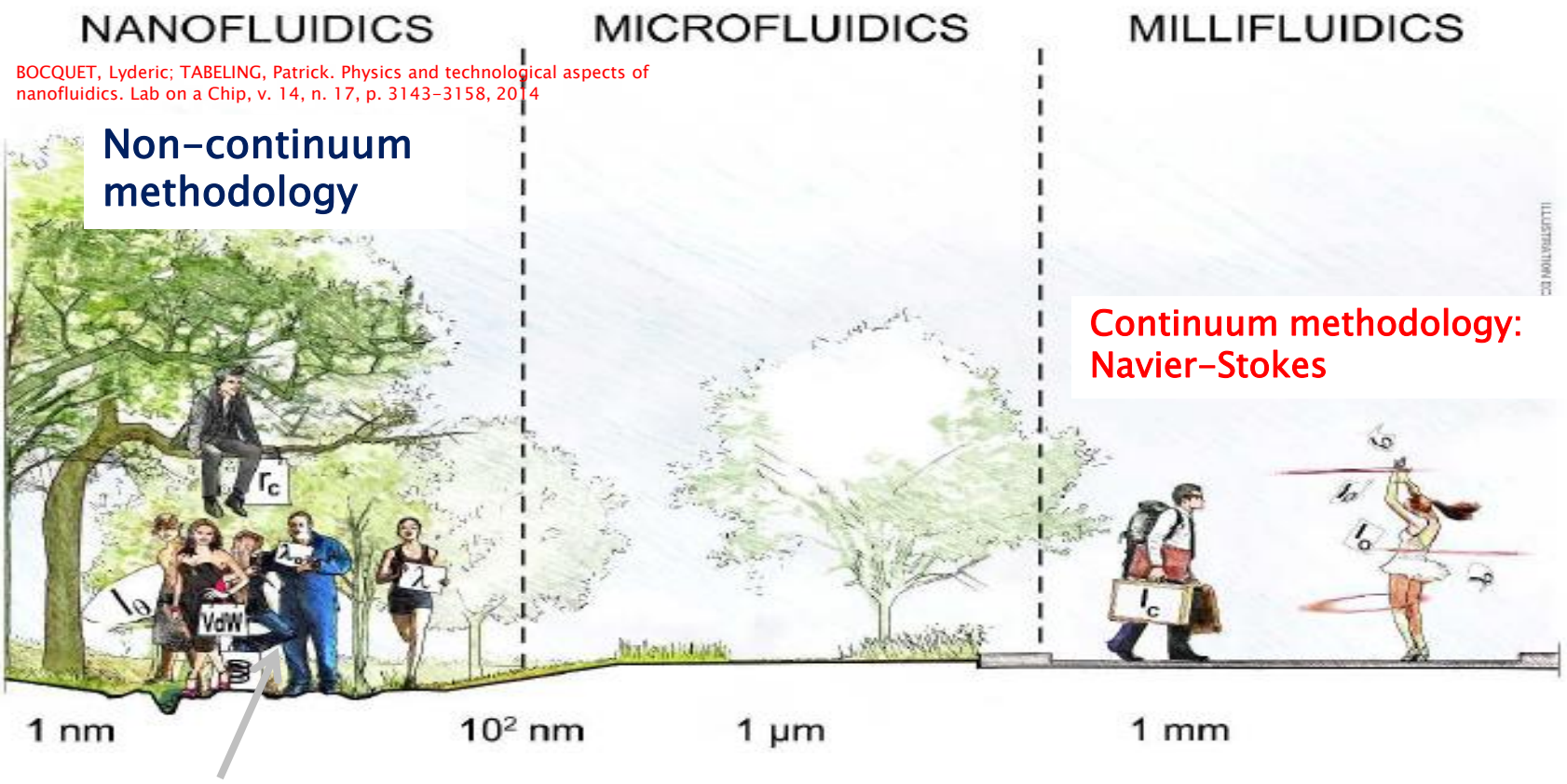
- Computational cost
- Simulation time

CT (h < 1000 nm)

Neglects

- Atomic interaction
- Variable viscosity

Nanofluidics



- Noncontinuum description
- Surface-dominated
- Low Reynolds number
- Multiscale and multiphysics

How the characteristic scales pertaining to the 1-100 nm range interfere with the system size ?

Can they combine together to produce new physical effects ?

MULTISCALE APPROACHES

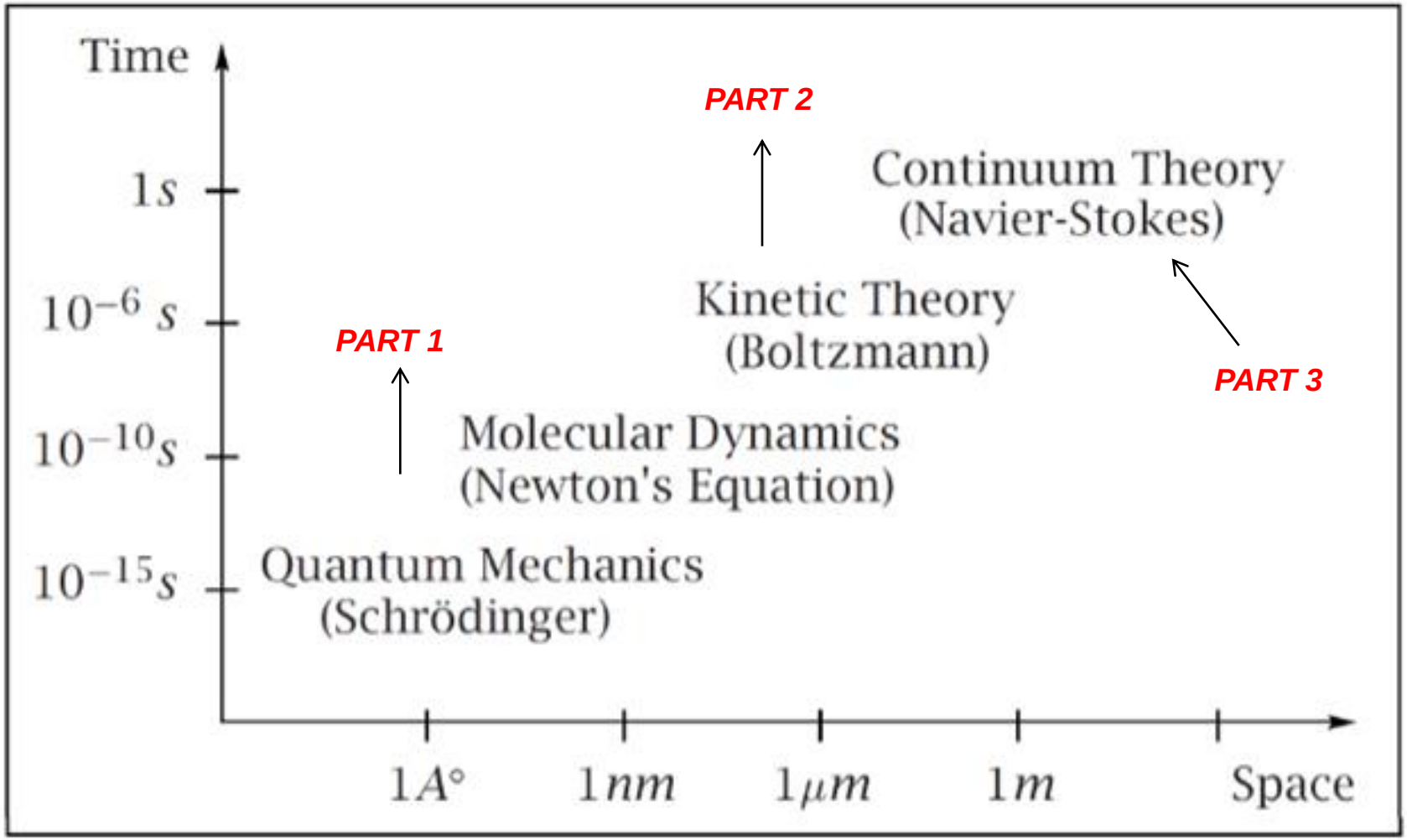
What is multiscale modeling and why do we need it ?

- Physical-chemistry phenomena in materials can occur in different scales
- **Challenge:** modeling a physical phenomena ranging from micro to macro
- So far, models are created for particular scale of interest

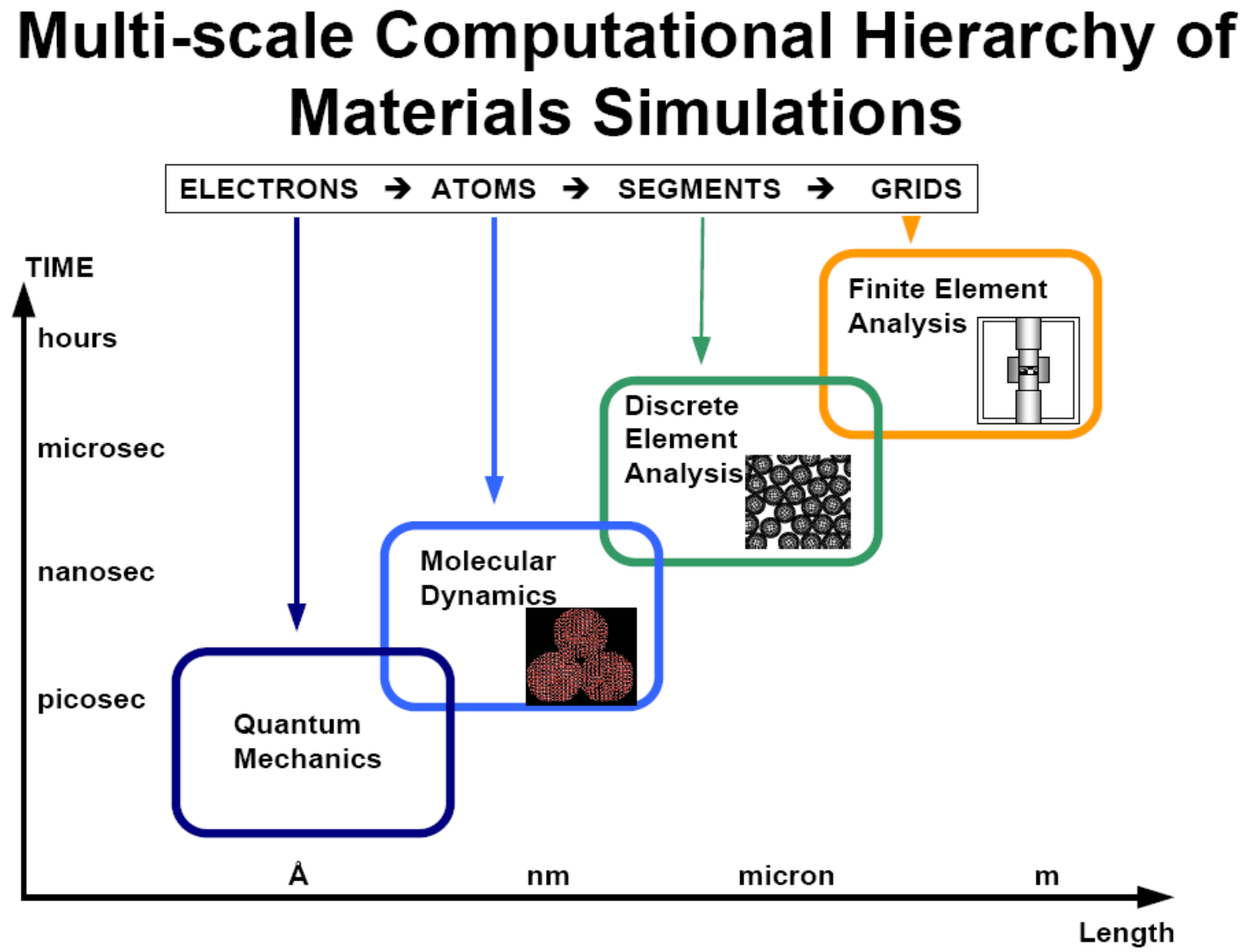
- ***Finer*** scale processes often govern processes seen at ***coarser*** scales and vice versa

- **Multiscale Modeling:** combination of models from different scales.

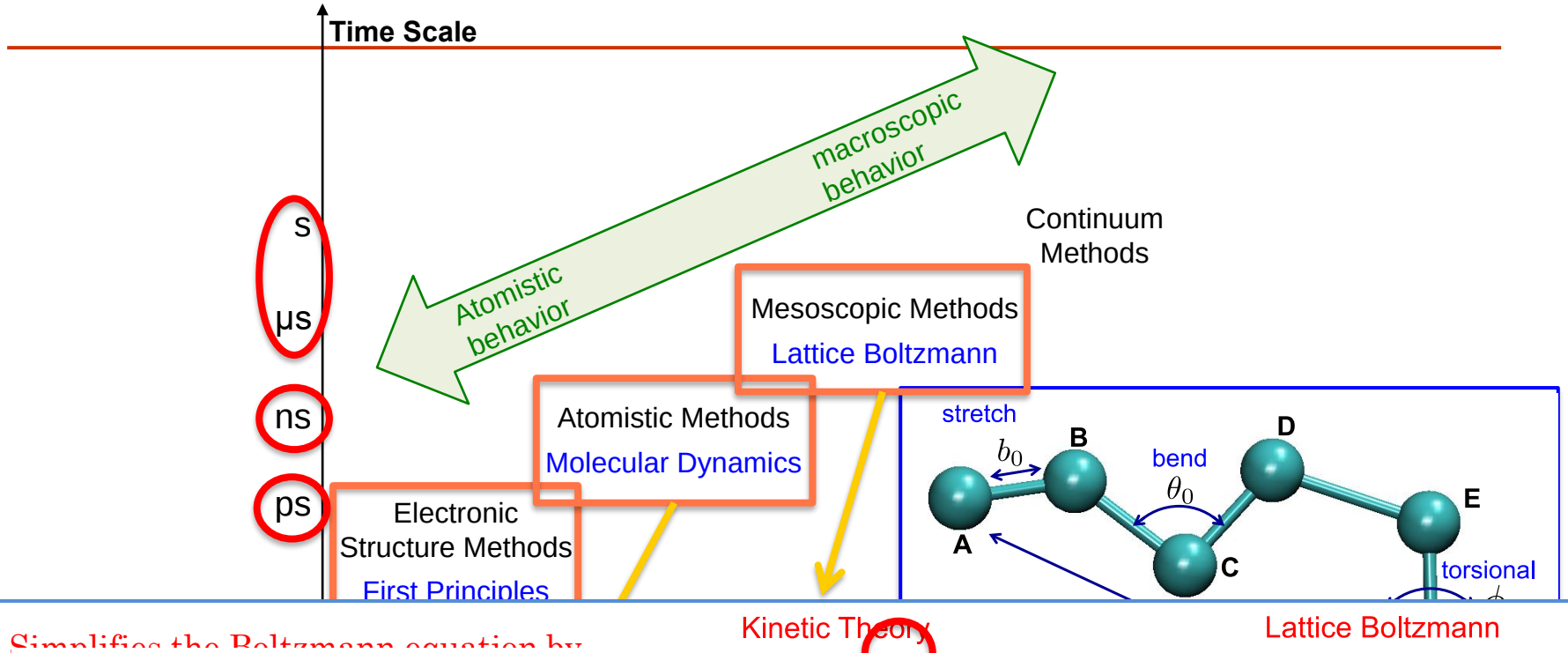
Multiscale in the laws of Physics



Modeling across scales



Multiscale computational approach



- Understanding of fluid behavior at the microscale
- Phase separation, interface instability, bubble/droplet dynamics and wetting effects

$$\mathbf{v}\nabla_{\mathbf{x}} f + \mathbf{F}\nabla_{\mathbf{p}} f + \frac{\partial f}{\partial t} = \Omega$$

$$f_i(\mathbf{x} + \mathbf{e}_i \Delta t, t + \Delta t) = f_i(\mathbf{x}, t) + \Omega_i(\mathbf{x}, t)$$

MD ab initio and classical X LBM: a soccer perspective

Ab initio MD

- Tactical formation or random
- Collisions
- Interactions between players result in a goal

Classical MD

foosball

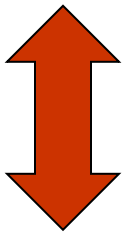
Simple way to describe the movement of players during a game

LBM

How to combine the scales ?

- Goal: to obtain **constitutive laws** and **physical properties** of a given system, whose parameters can be determined from a **finer/coarser** scale models:

Microscopic $M(p, m_1, m_2, \ldots, m_n) = 0$



Continuum $C(p, c_1, c_2, \ldots, c_p) = 0$

Linking levels of resolution: energies, time and length

- ***Coarse graining methods*** are characterized by the physical quantities, which the **models of different levels** are supposed to **reproduce** as ***accurate*** as possible.

- The link between levels of resolution can be based on:

i) Potential energy surface (energy and forces)
ii) Structure (characteristic time and length scales)
iii) Environment (electrostatic, hydrodynamics, elastic, …)

- "The first ***ansatz*** directly allows for a forward and backward mapping of the investigated systems."

Multiscale Modeling strategies

- Different ways to combine each levels of resolution (energy, time and/or length):

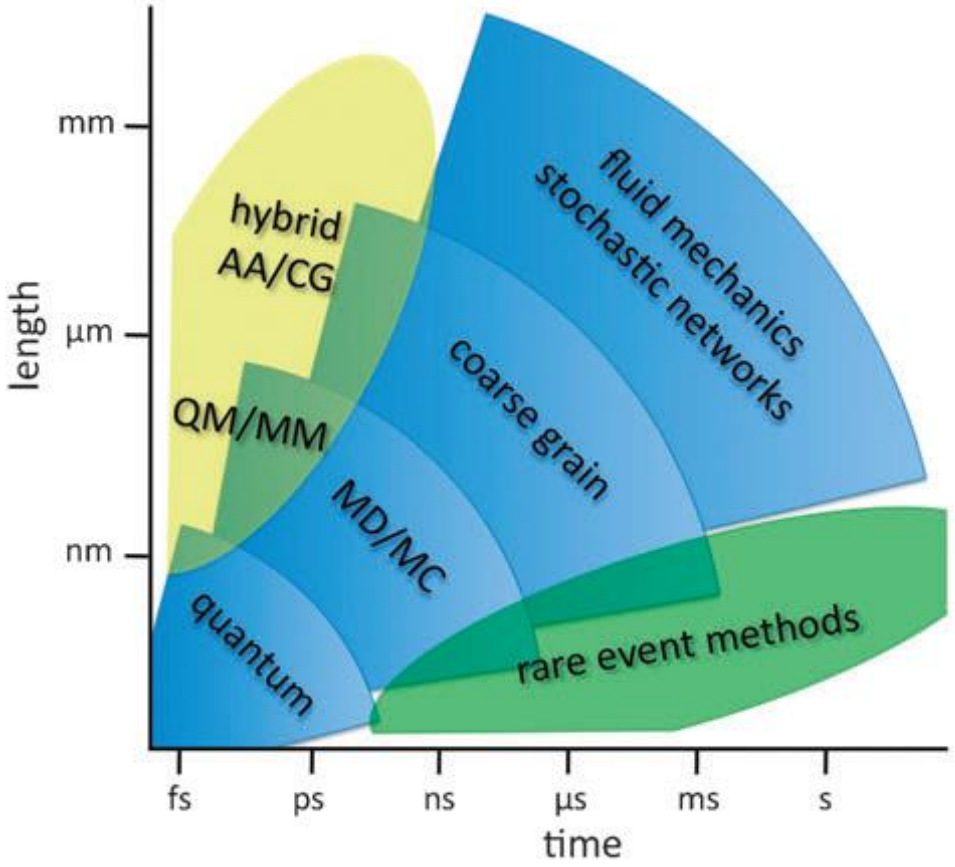
(i) ***Sequential***: the simulation models on different scales are treated separately by simply transfer information between levels of resolution. (mature)

(ii) ***Hybrid:*** different levels of resolution are running simultaneously with a direct link between them, (developed)

(iii) ***Adaptive:*** switch between resolution levels on the fly (work in progress – problem specific)

Which one choose ?

- The size and time scale of the problem,
- the accuracy of the method,
- the desired resolution,
- the available computing resources.



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S. O. Nielsen, R. E. Bulo,P. B. Moore and B. Ensing,
Phys. Chem. Chem. Phys., 2010, 12, 12401