Simulação Computacional dos Materiais

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AULA 2 – 21/08/2020

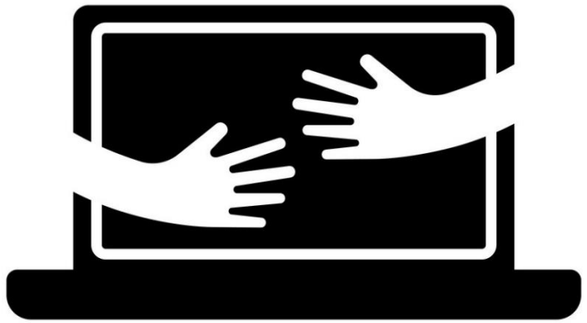
Parte A

Simulação Computacional dos Materiais

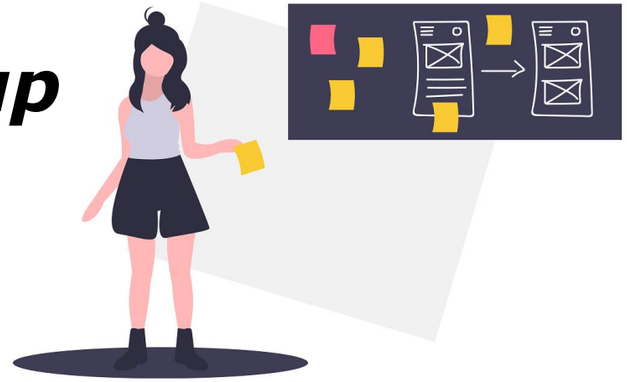
- Método: Base - Exploração - Aplicação
  - Discussão do sistema físico
  - Introdução ao método numérico
  - Modelagem do sistema físico
  - Visualização dos resultados
- Organização: Aulas + Laboratório
- Avaliação: Labs + Projeto

Projeto Acadêmico ou Empreendedorismo ?

Projeto Científico



Start-up



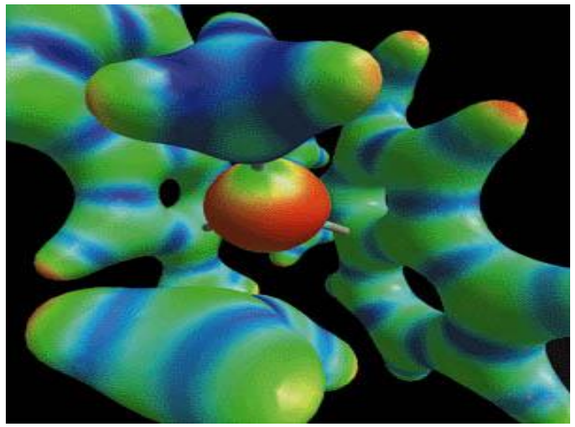
Projetos

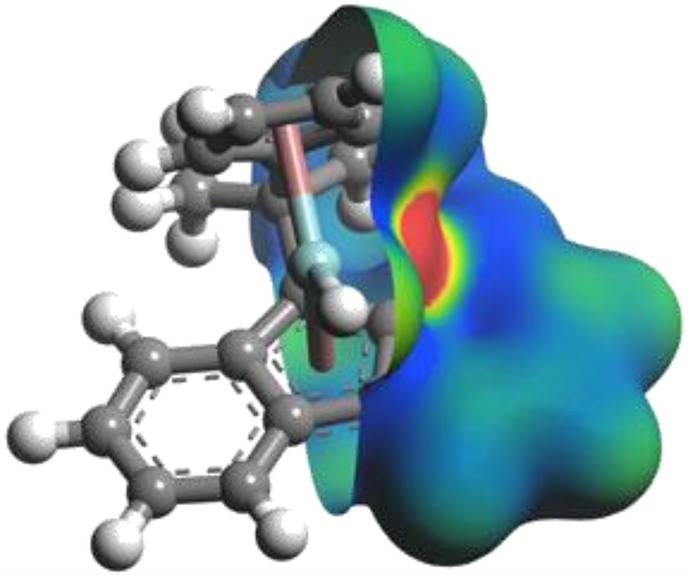
Áreas prioritárias de pesquisa definidas pelo MCTI para o período 2020-2023				
Tecnologias Estratégicas	**Tecnologias Habilitadoras**	**Tecnologias de Produção**	**Tecnologias para o Desenvolvimento Sustentável**	**Tecnologias para Qualidade de Vida**
• Espacial	• Inteligência Artificial	• Indústria	• Cidades inteligentes	• Saúde
• Nuclear	• Internet das coisas	• Agronegócio	• Energias renováveis	• Saneamento básico
• Cibernética	• Materiais avançados	• Comunicações	• Bioeconomia	• Segurança hídrica
• Segurança pública	• Biotecnologia	• Infraestrutura	• Resíduos sólidos	• Tecnologias assistivas
• De fronteira	• Nanotecnologia	• Serviços	• Poluição	
			• Desastres naturais	
			• Preservação ambiental	

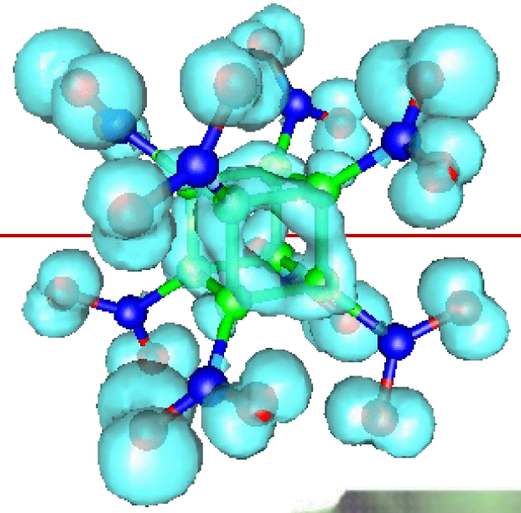
SIMULAÇÃO COMPUTACIONAL DOS MATERIAIS

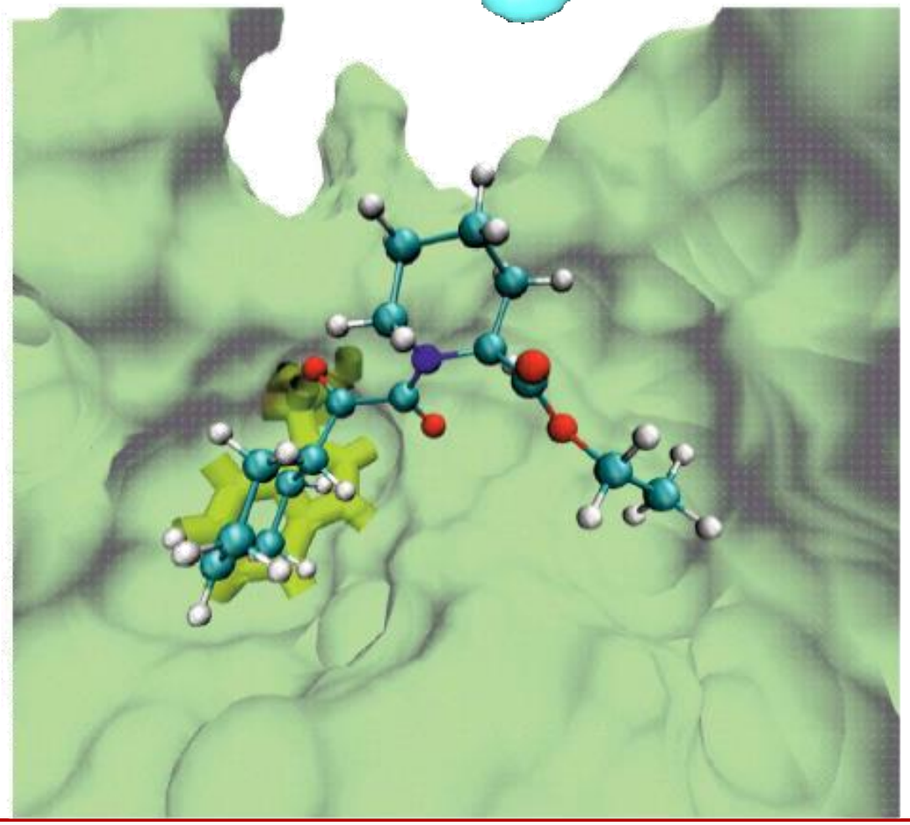
Filosofia do curso

Filosofia do curso



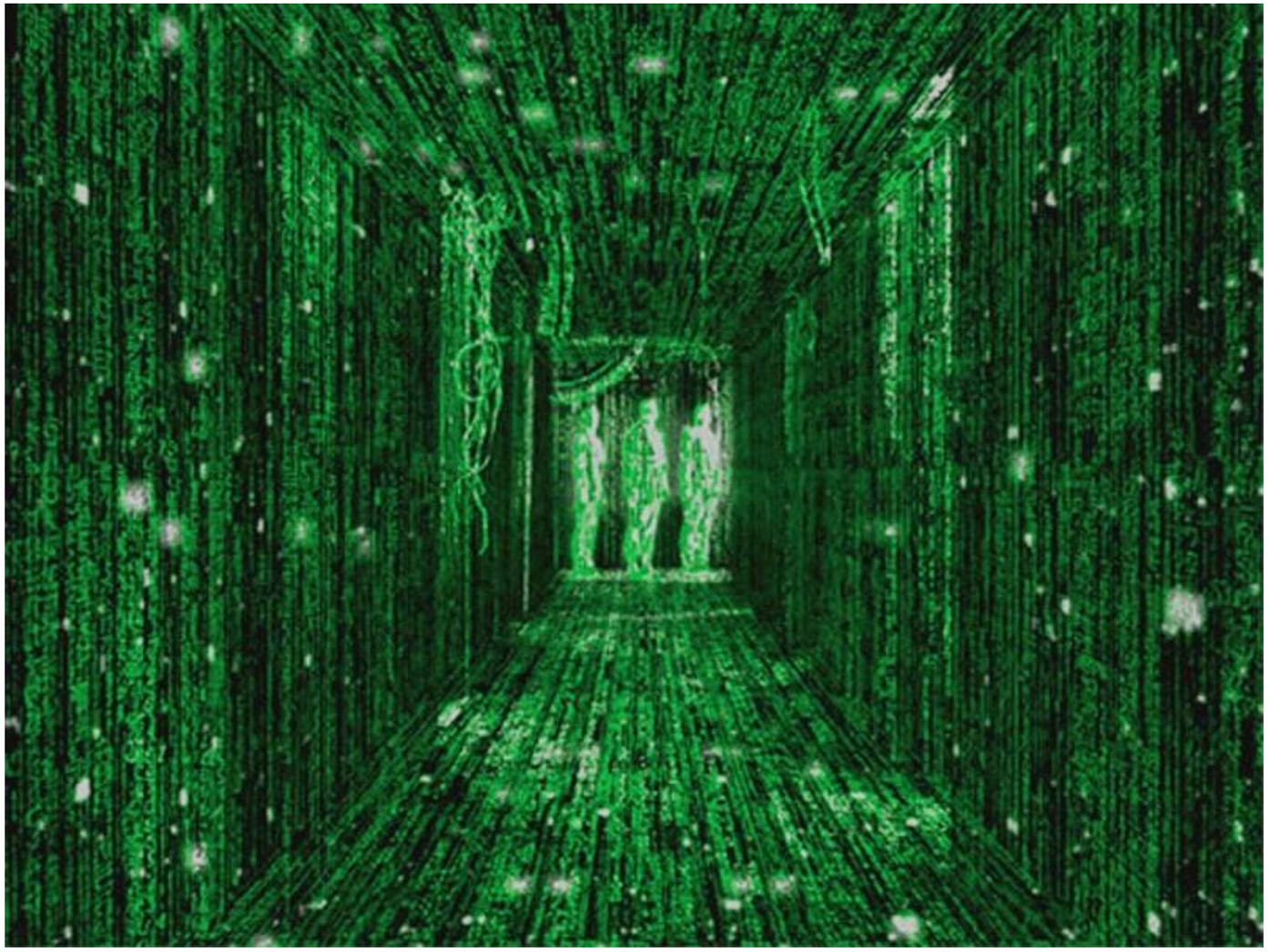






SIMULAÇÃO COMPUTACIONAL DOS MATERIAIS

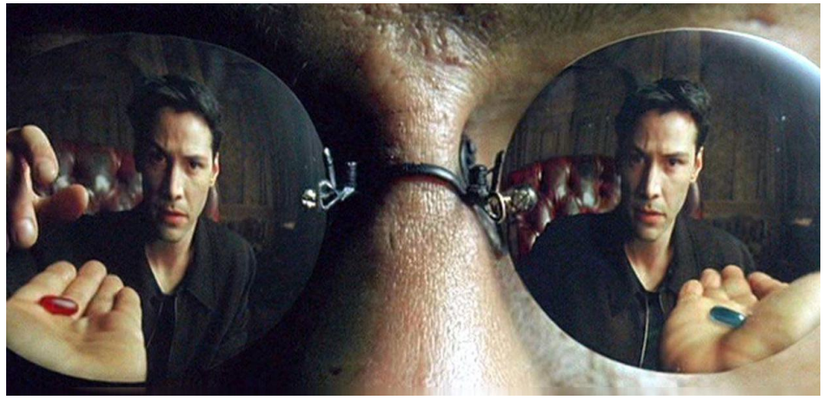
Simulacros e Simulação



Baseado em Jean Baudrillard

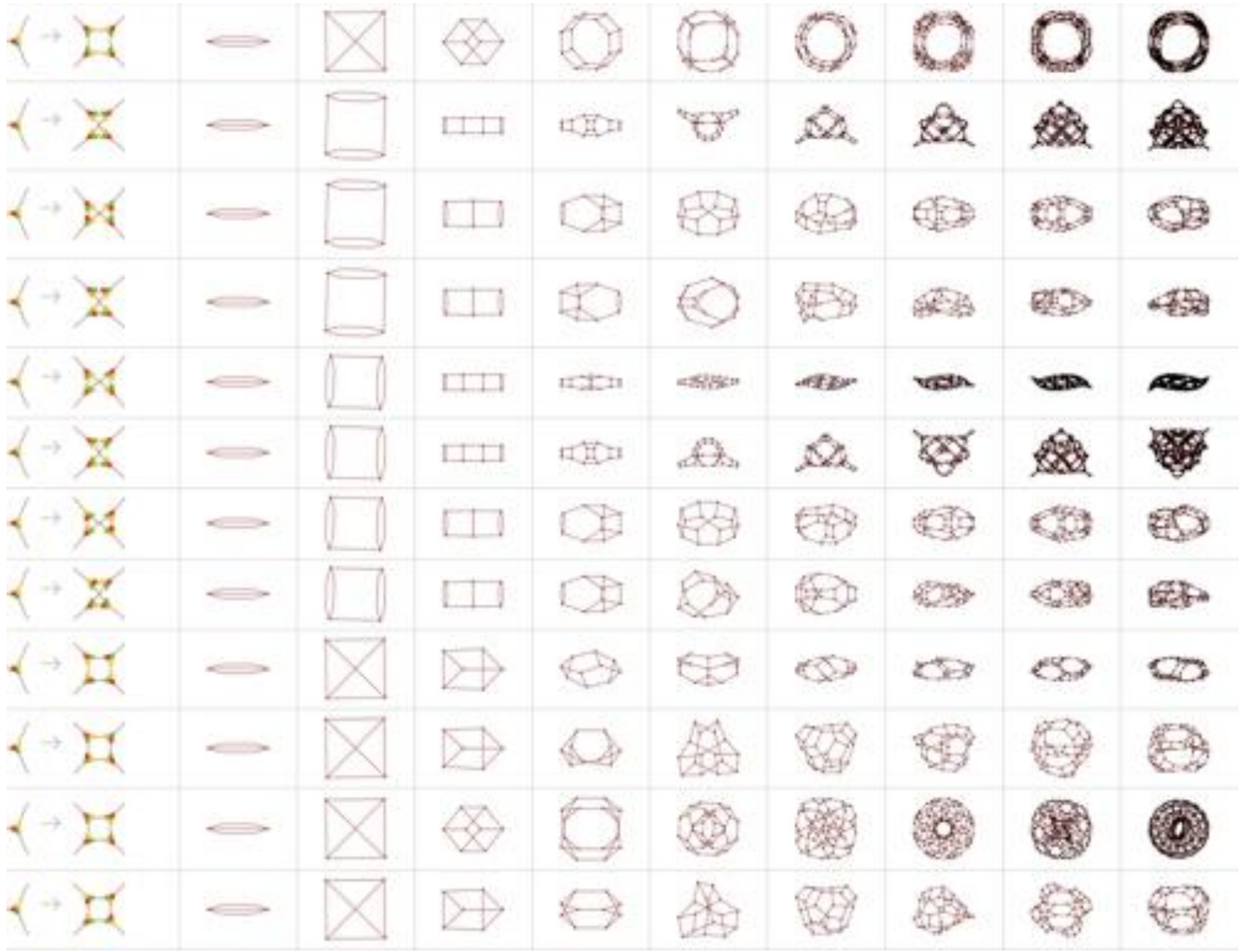
Extraído do filme – Matrix (1999)

Simulacros e Simulação



Simulação tornou-se uma forma de experimentação em um universo de teorias – Gary Flake (The computational Beauty of Nature – MIT press)

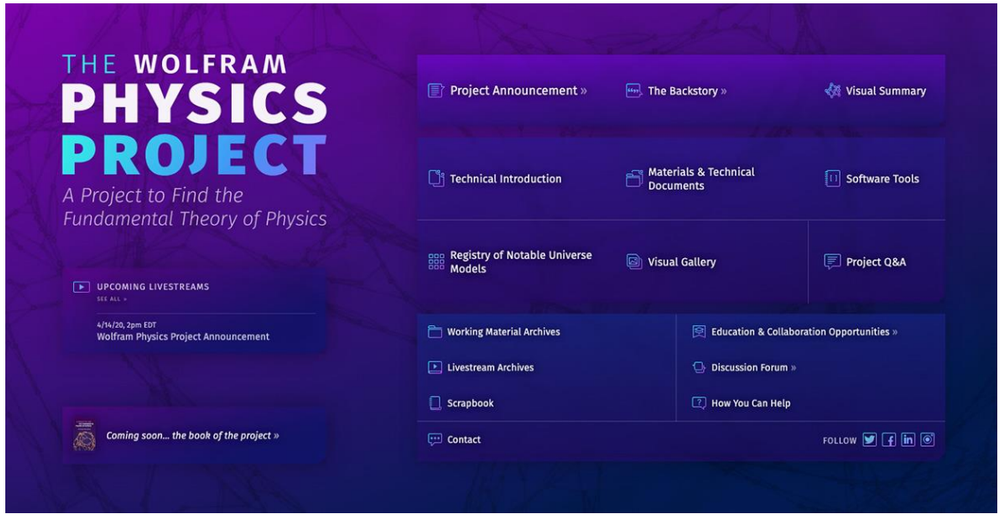
Seria possível simular o universo em um computador ?



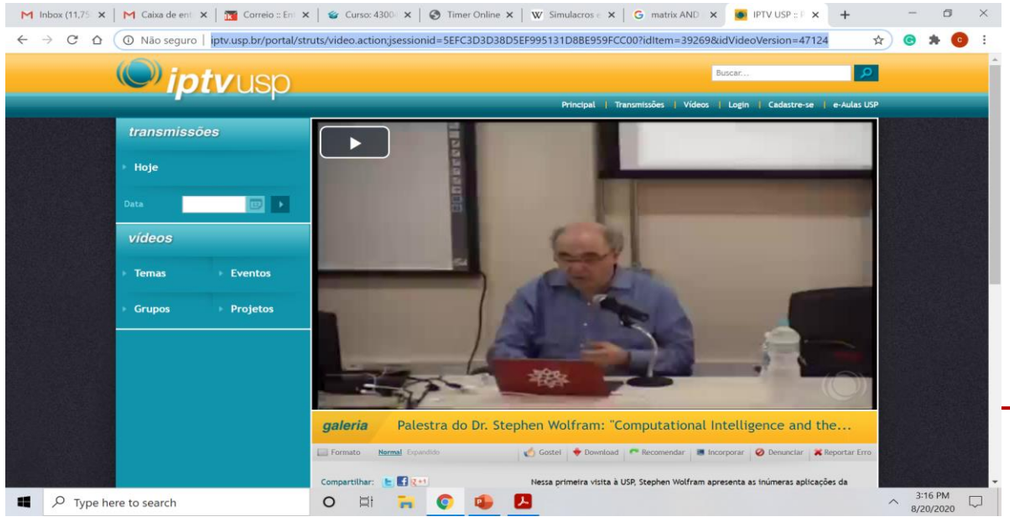
Stephen Wolfram desenvolveu o Mathematica e Wolfram Alpha. Agora ele quer simular o "universo".

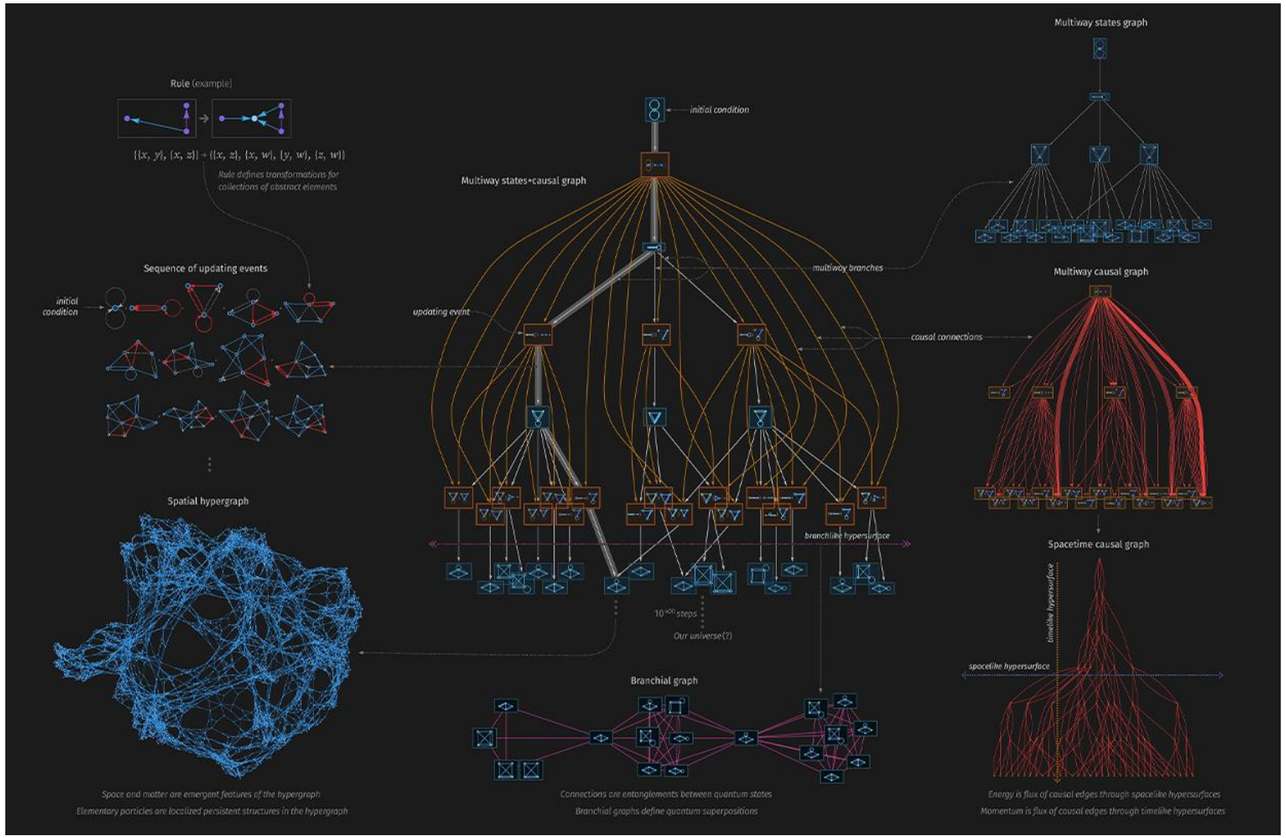
The Wolfram Physics Project
Abril 2020

Wolfram



https://www.wolframphysics.org/



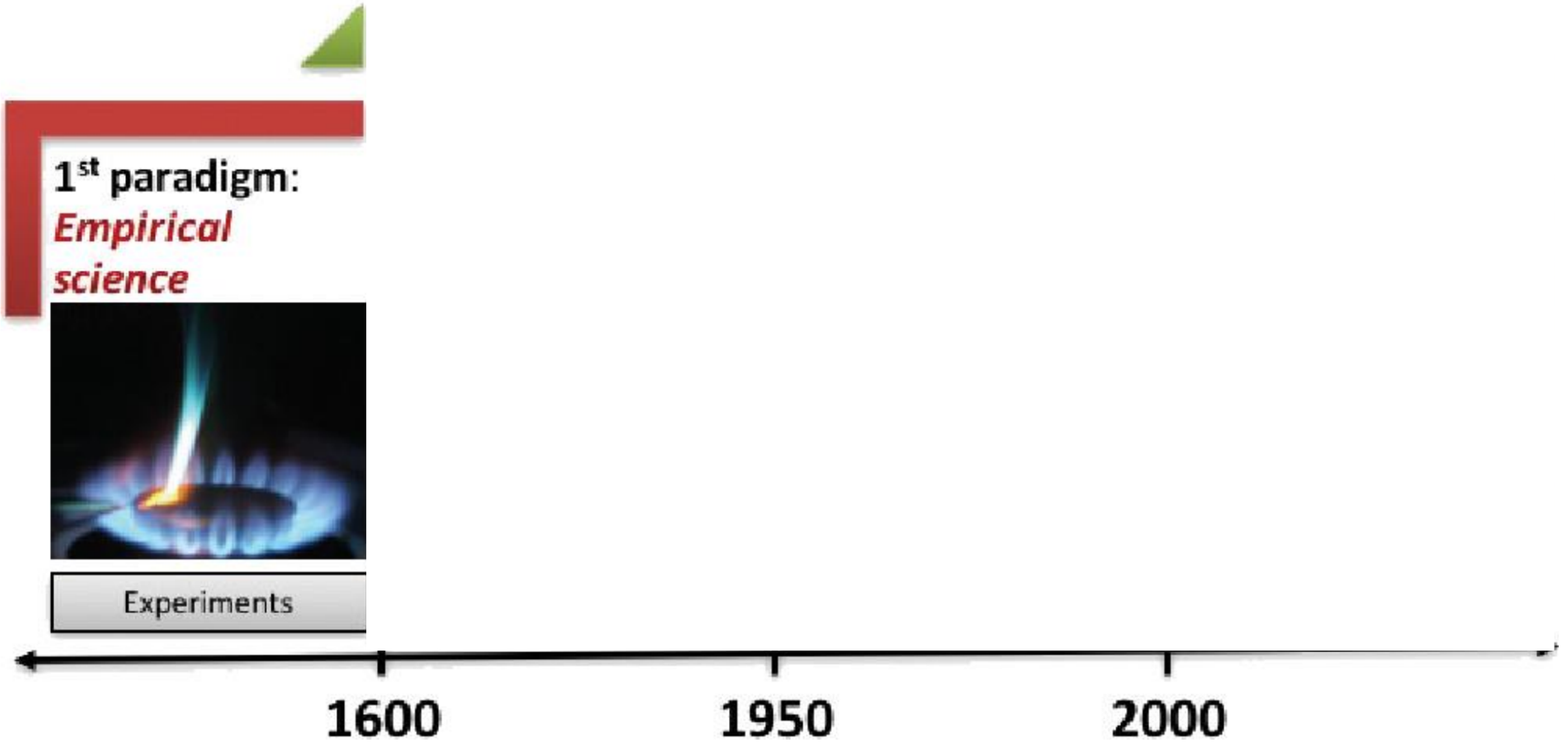


SIMULAÇÃO **COMPUTACIONAL** DOS MATERIAIS

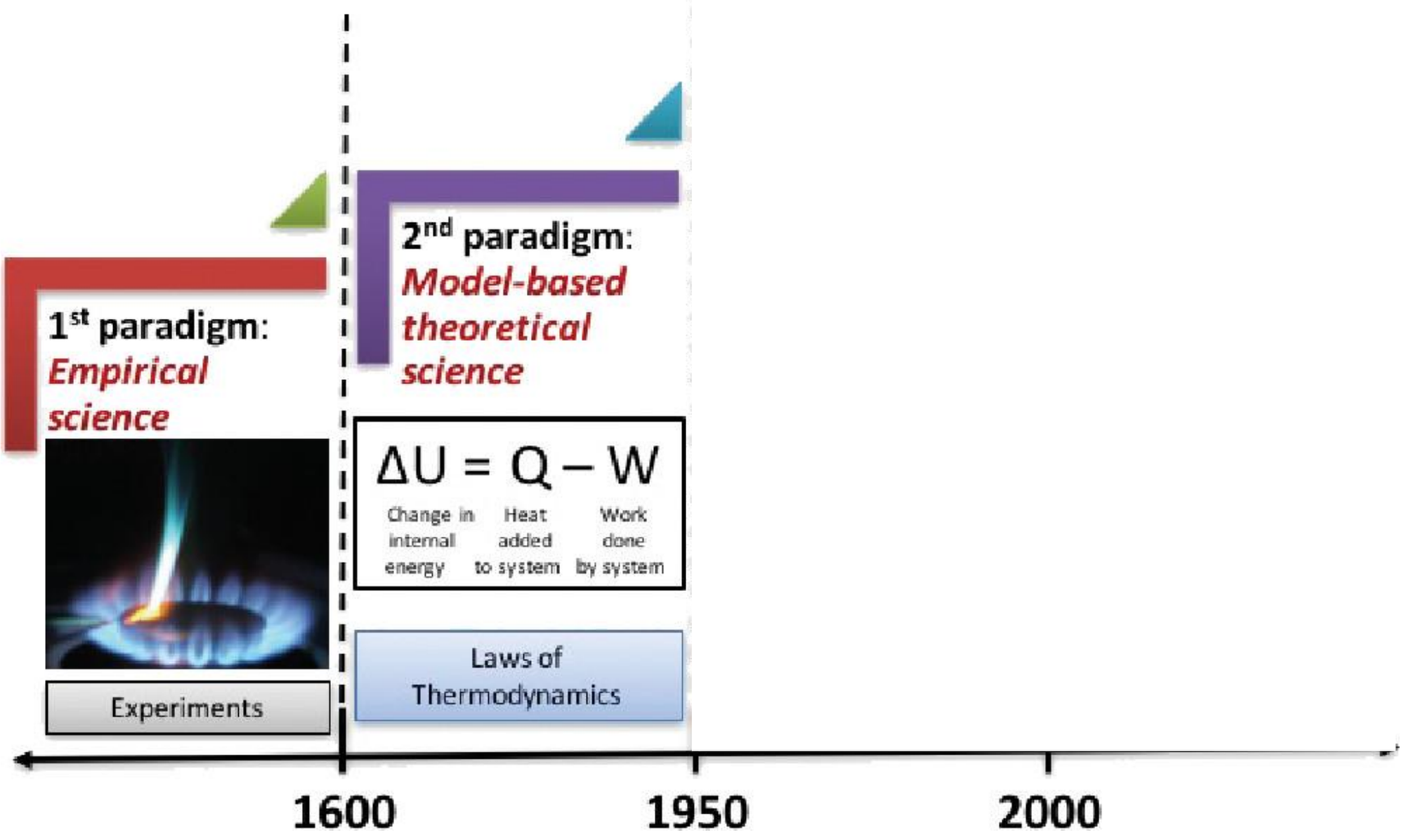
Do sonho de Laplace …

Uma *inteligência* que pode, a qualquer momento, compreender *todas as forças* pelas quais a natureza é animada e as *respectivas posições* dos seres que o compõem, e além disso, se essa inteligência fosse abrangente o suficiente para submeter esses *dados à análise*, abrangeria nessa fórmula ambos os movimentos dos *maiores corpos* no universo e aqueles dos *átomos* mais leves: para ele nada seria ser incerto, e o futuro, assim como o passado, seria presente aos seus olhos. A mente humana nos oferece, *na perfeição que deu à astronomia*, um esboço tênue dessa inteligência.

P. S. de Laplace. Oeuvres Completes de Laplace. Thiorie Analytique des ProbabiliUs, volume VII. Gauthier-Villars, Paris, France, third edition, 1820.

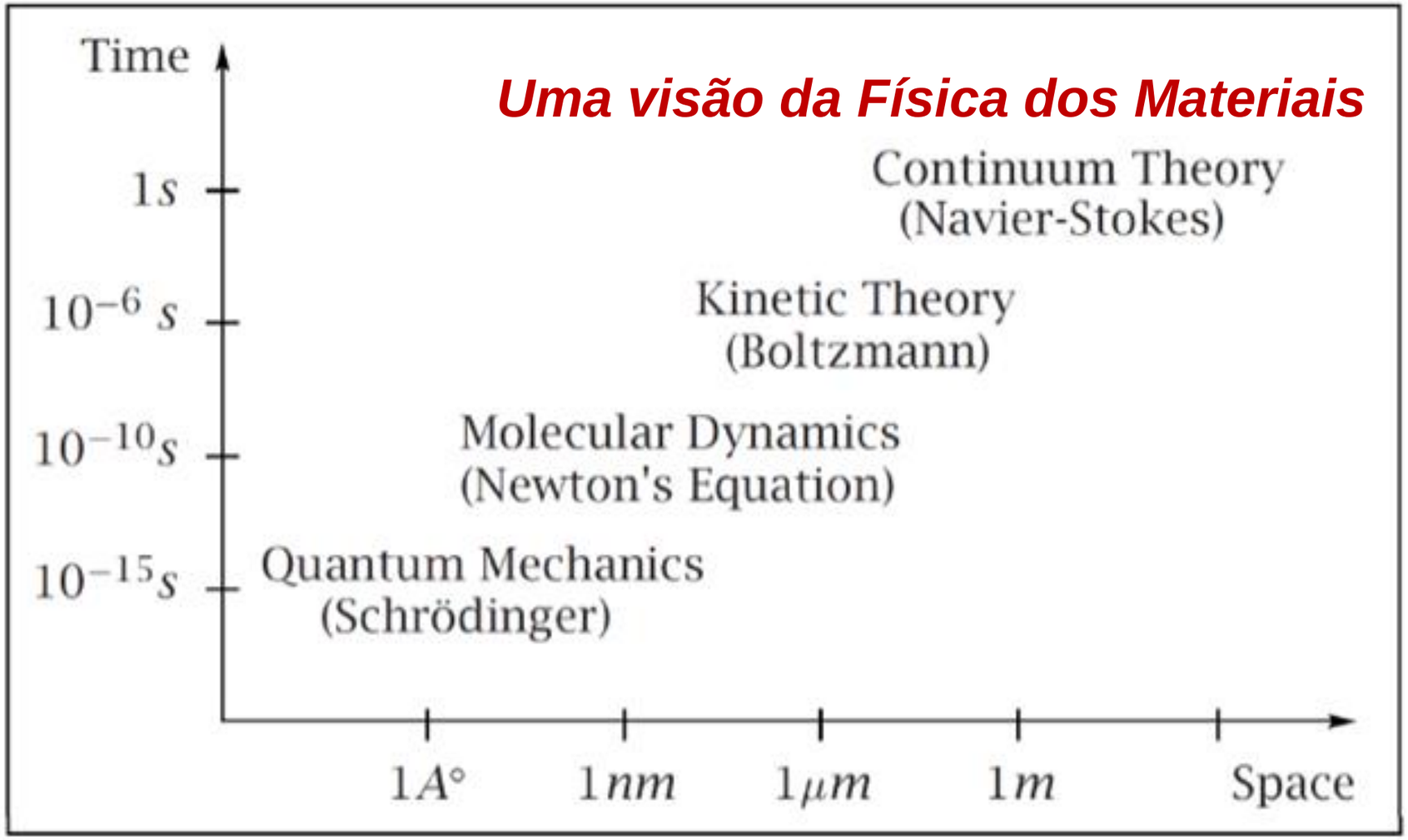


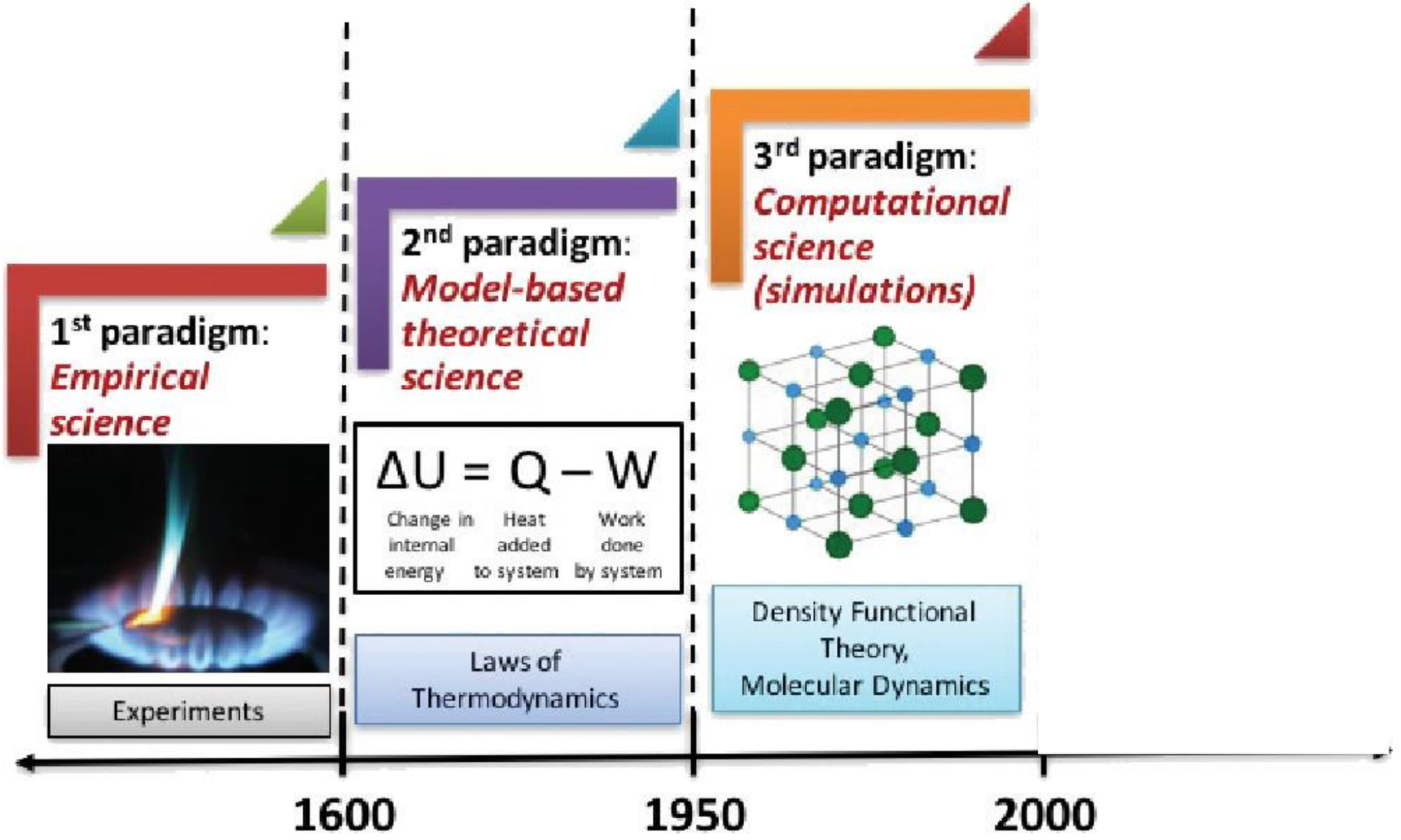
Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
DOI: 10.1063/1.4946894



Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
DOI: 10.1063/1.4946894

Multiescala nas leis da Física





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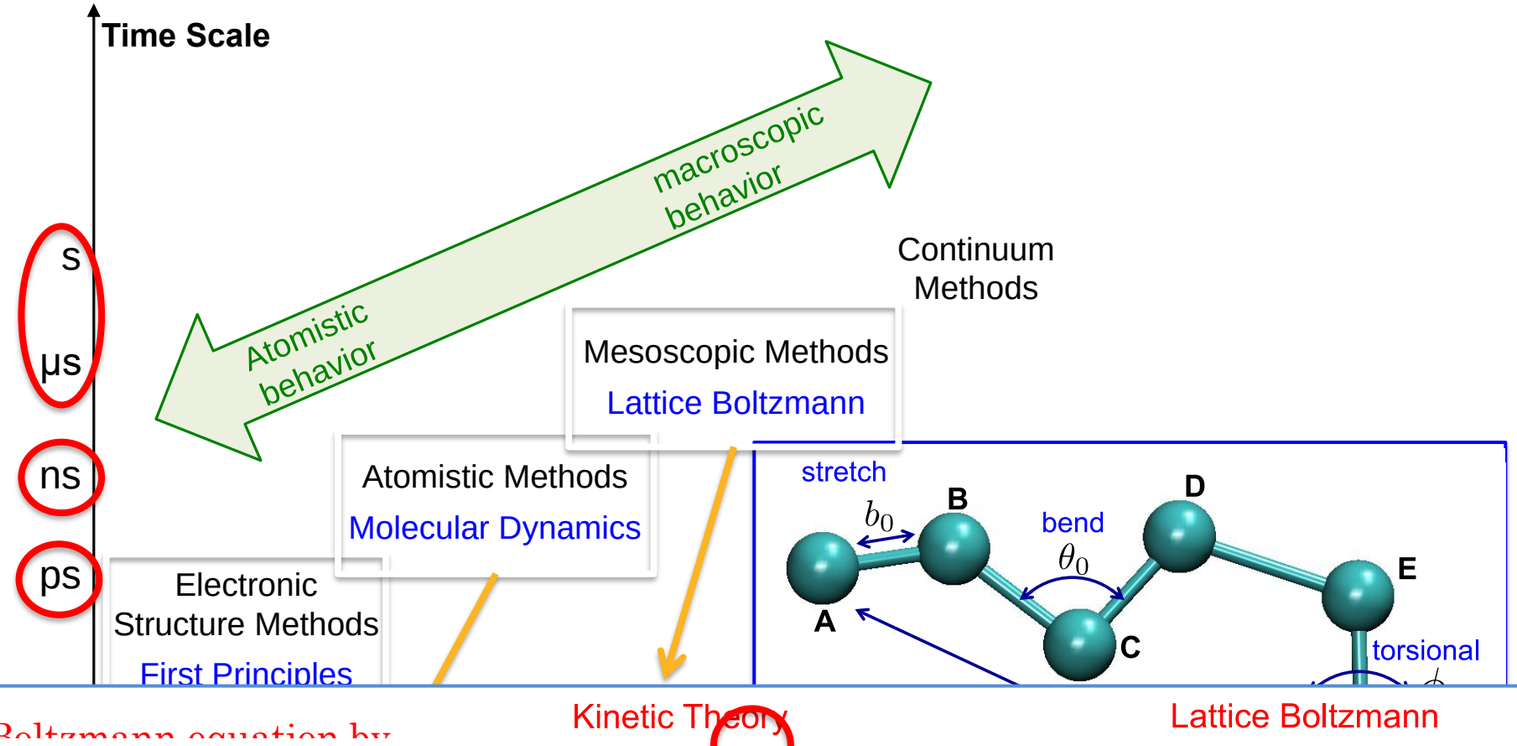
Multiscale computational approach



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

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

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

Passo 1 – Da quântica a simulações atomísticas

Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

MD ab initio and classical X LBM: a soccer perspective

Ab initio MD

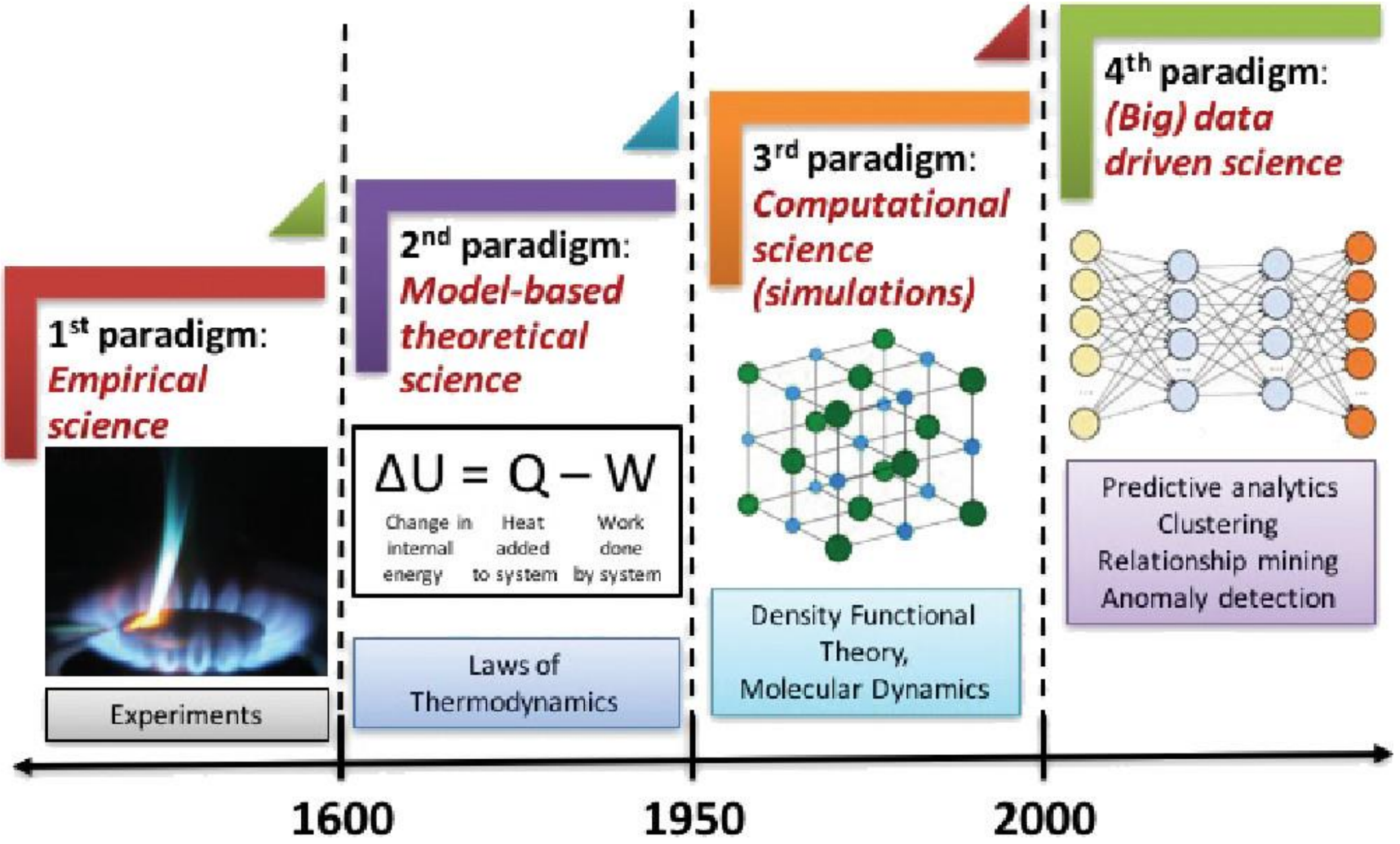
- Tactical formation or random
- Collisions
- Interactions between players result in a goal

Classical MD

foosball

Simple way to describe the movement of players during a game

LBM



Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
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Processamento-estrutura-propriedade-desempenho (PSPP)

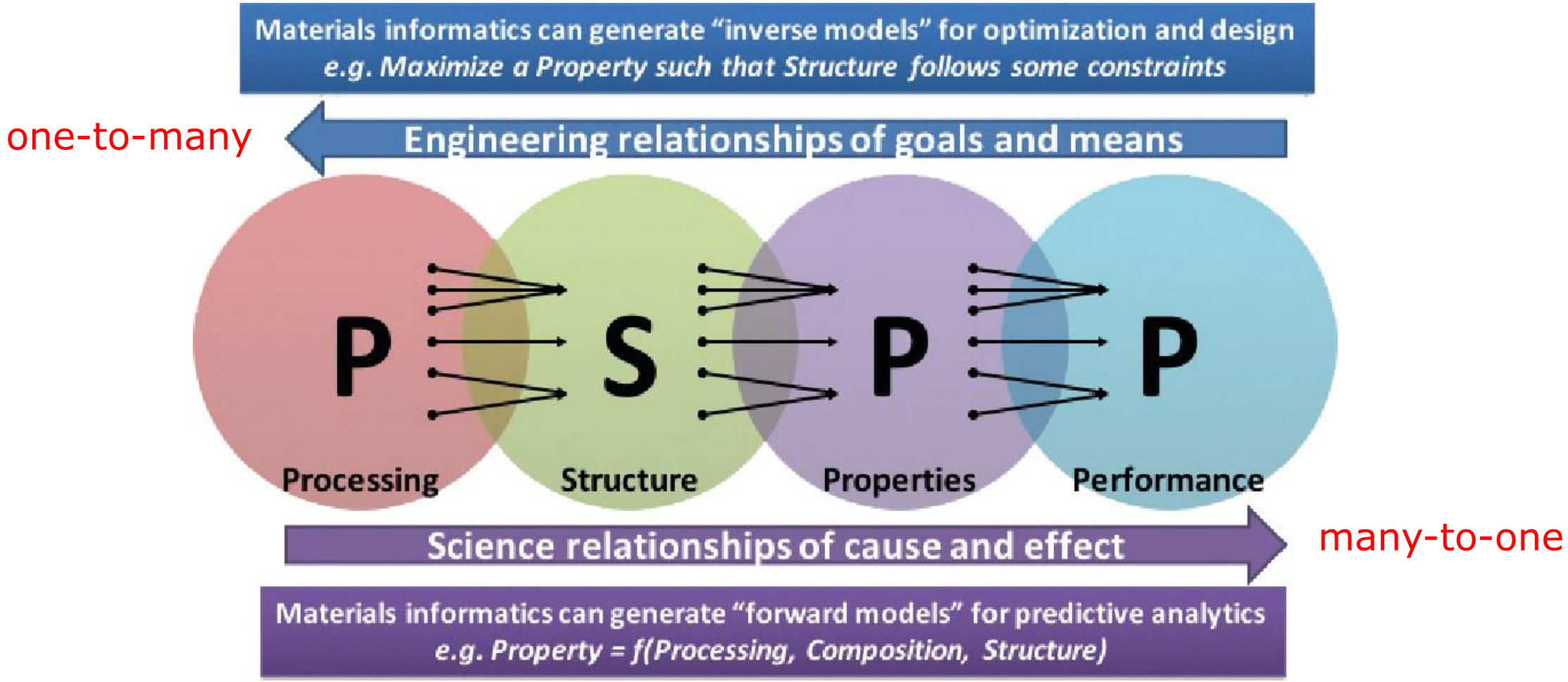


FIG. 2. The processing-structure-property-performance relationships of materials science and engineering, and how materials informatics approaches can help decipher these relationships via forward and inverse models.

Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
DOI: 10.1063/1.4946894

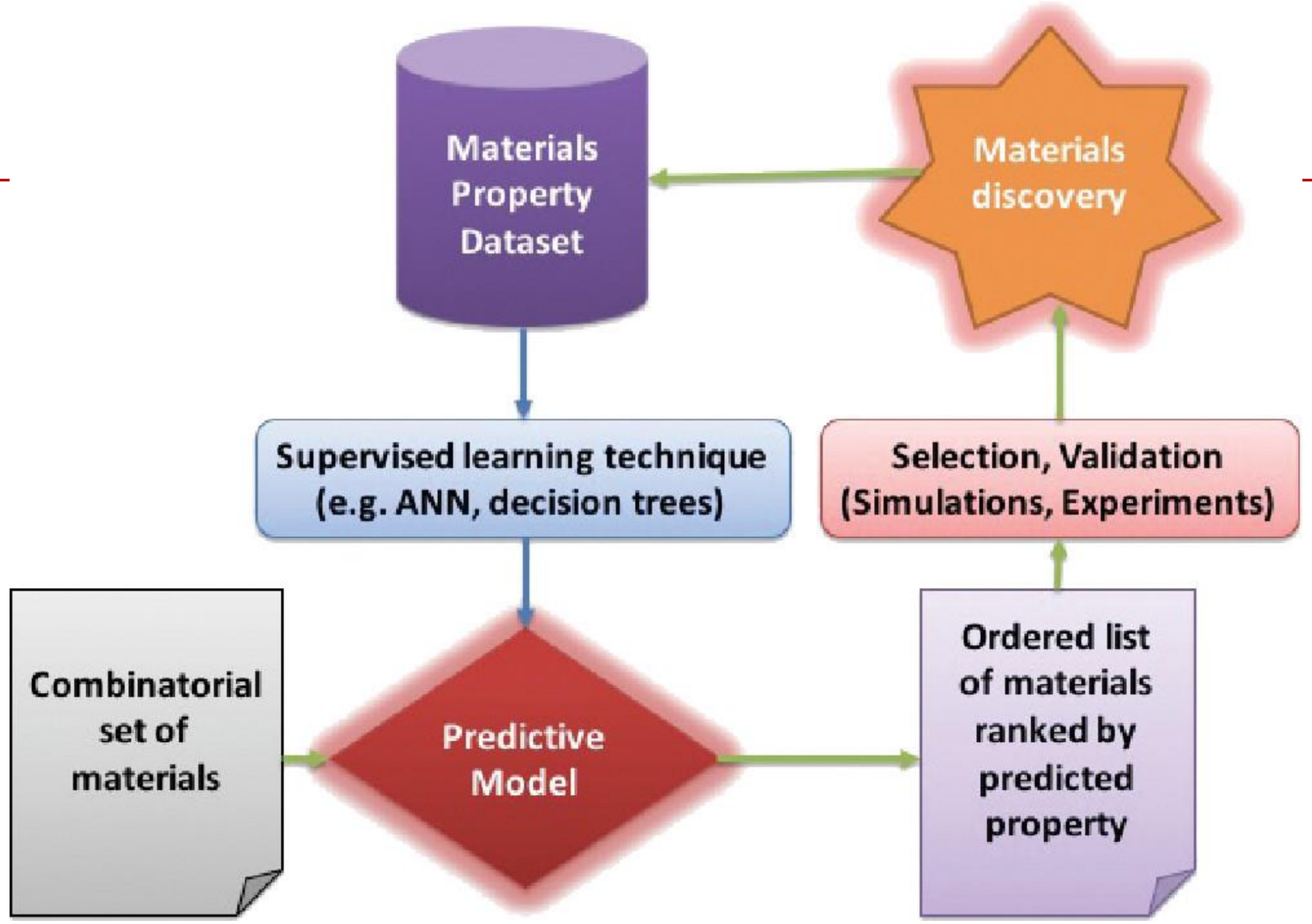


FIG. 4. A simple realization of the inverse models for PSPP relationships. The forward predictive model built using a supervised learning technique on a labeled materials dataset can be used to scan a combinatorial set of materials and thus convert this set to a ranked list, ordered by the predicted property. This can be followed by one or more screening steps to select and validate the predictions using simulation and/or experiments, thereby enabling data-driven materials discovery, which can in turn be fed back into the materials dataset to derive improved models, and so on. Blue arrows denote the forward model construction process, and green arrows denote the materials discovery process via inverse models.

Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
DOI: 10.1063/1.4946894

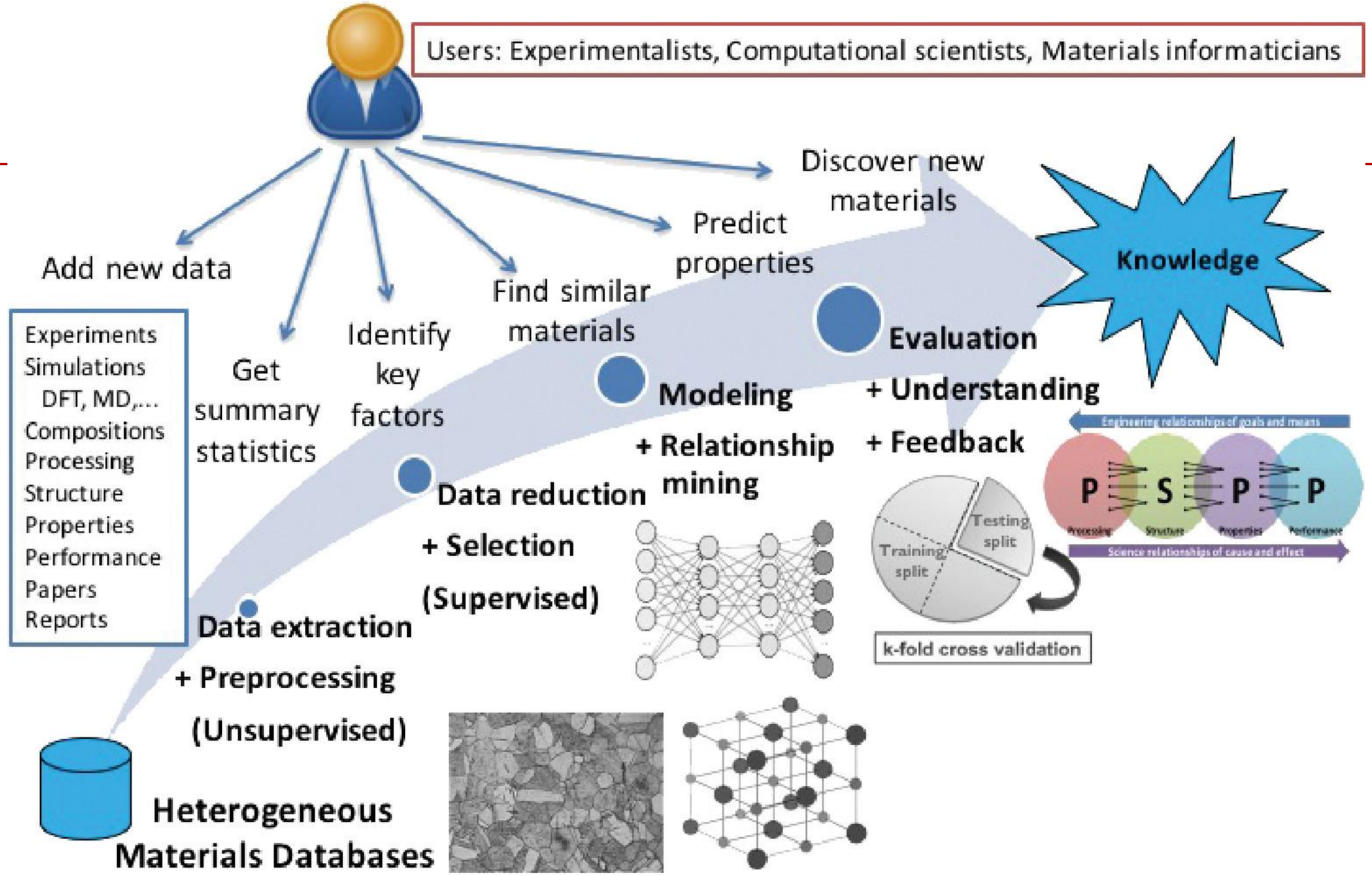
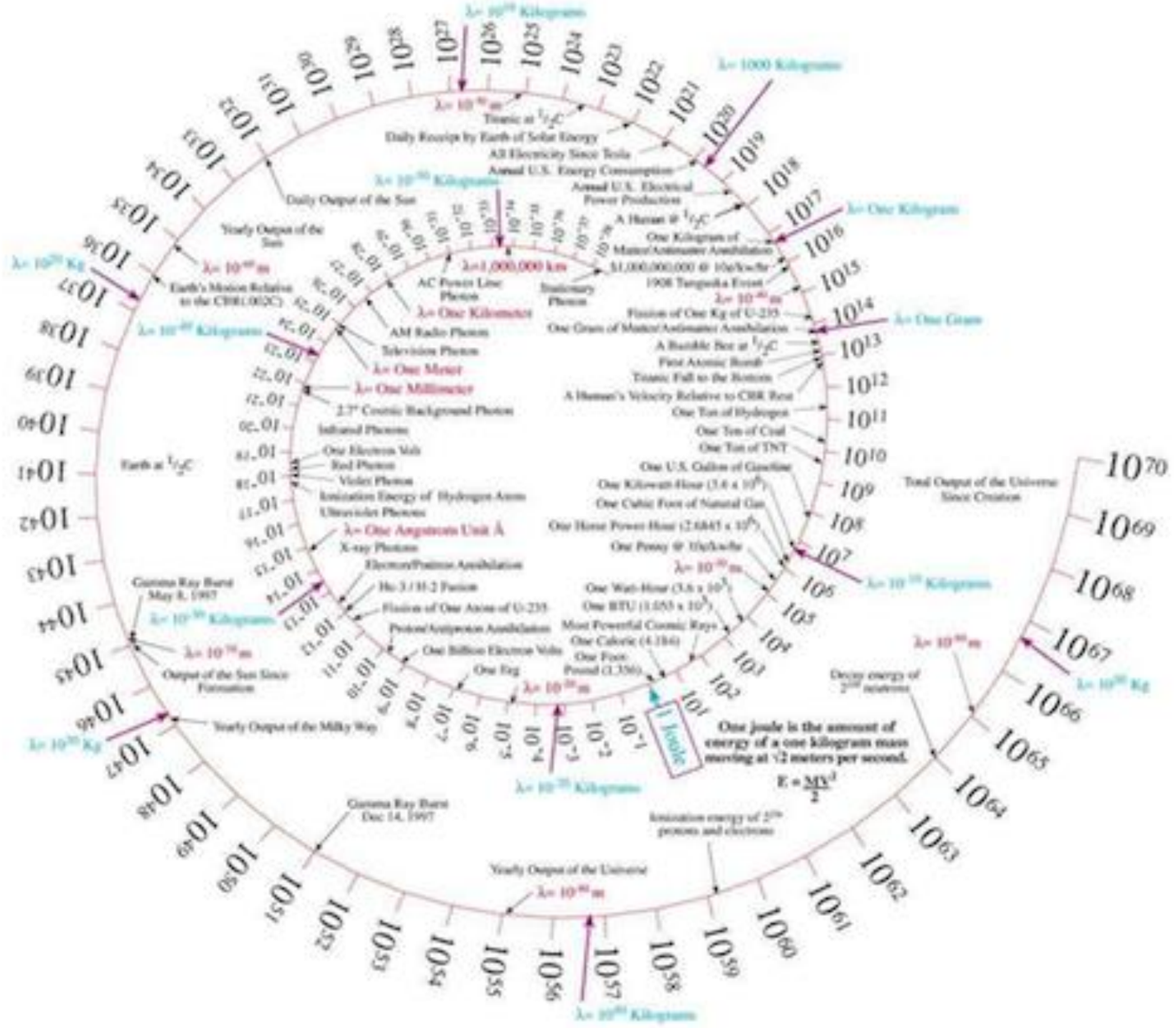


FIG. 3. The knowledge discovery workflow for materials informatics. The overall goal is to mine heterogenous materials databases and extract actionable PSPP linkages to enable data-driven materials discovery and design.

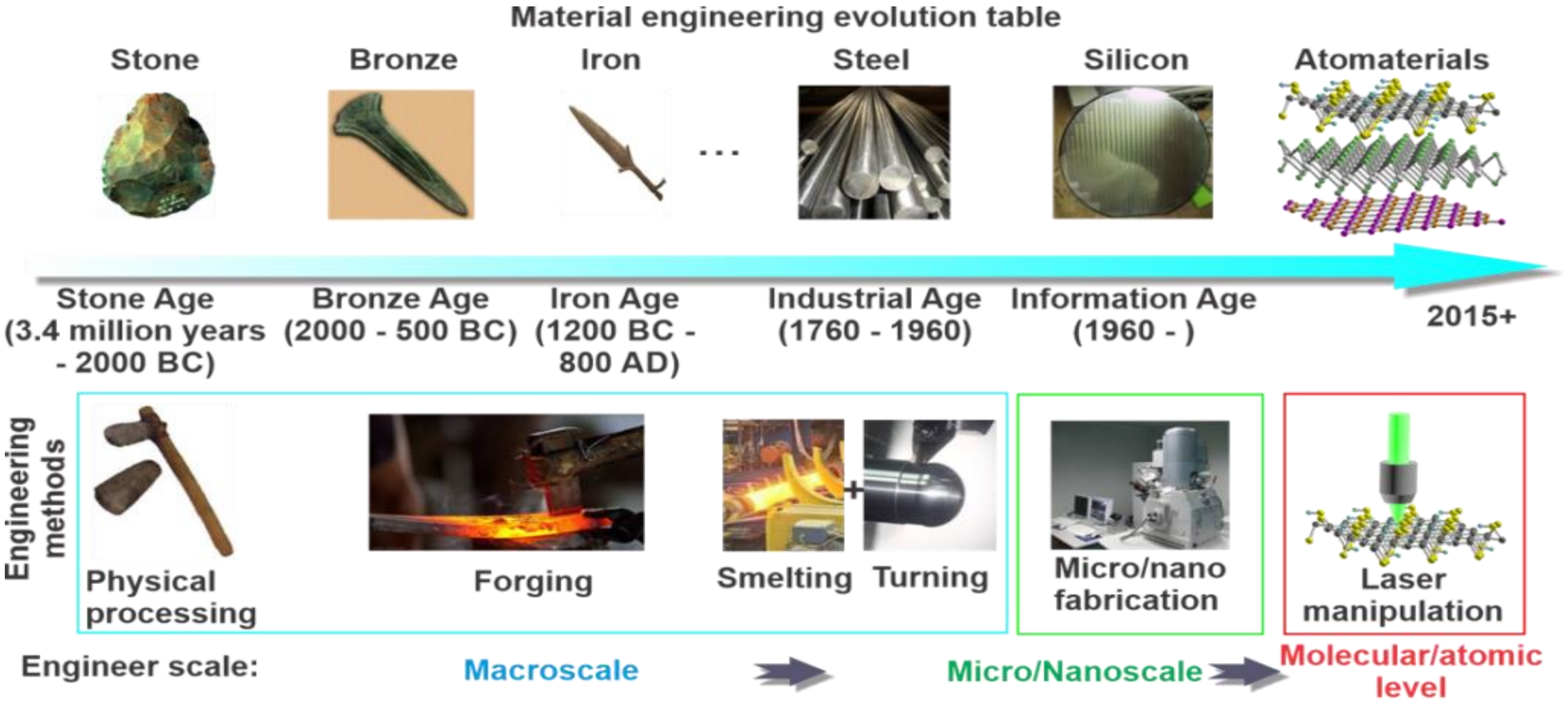
Published in: Ankit Agrawal; Alok Choudhary; *APL Materials* **4,** 053208 (2016)
DOI: 10.1063/1.4946894

SIMULAÇÃO COMPUTACIONAL DOS **MATERIAIS**

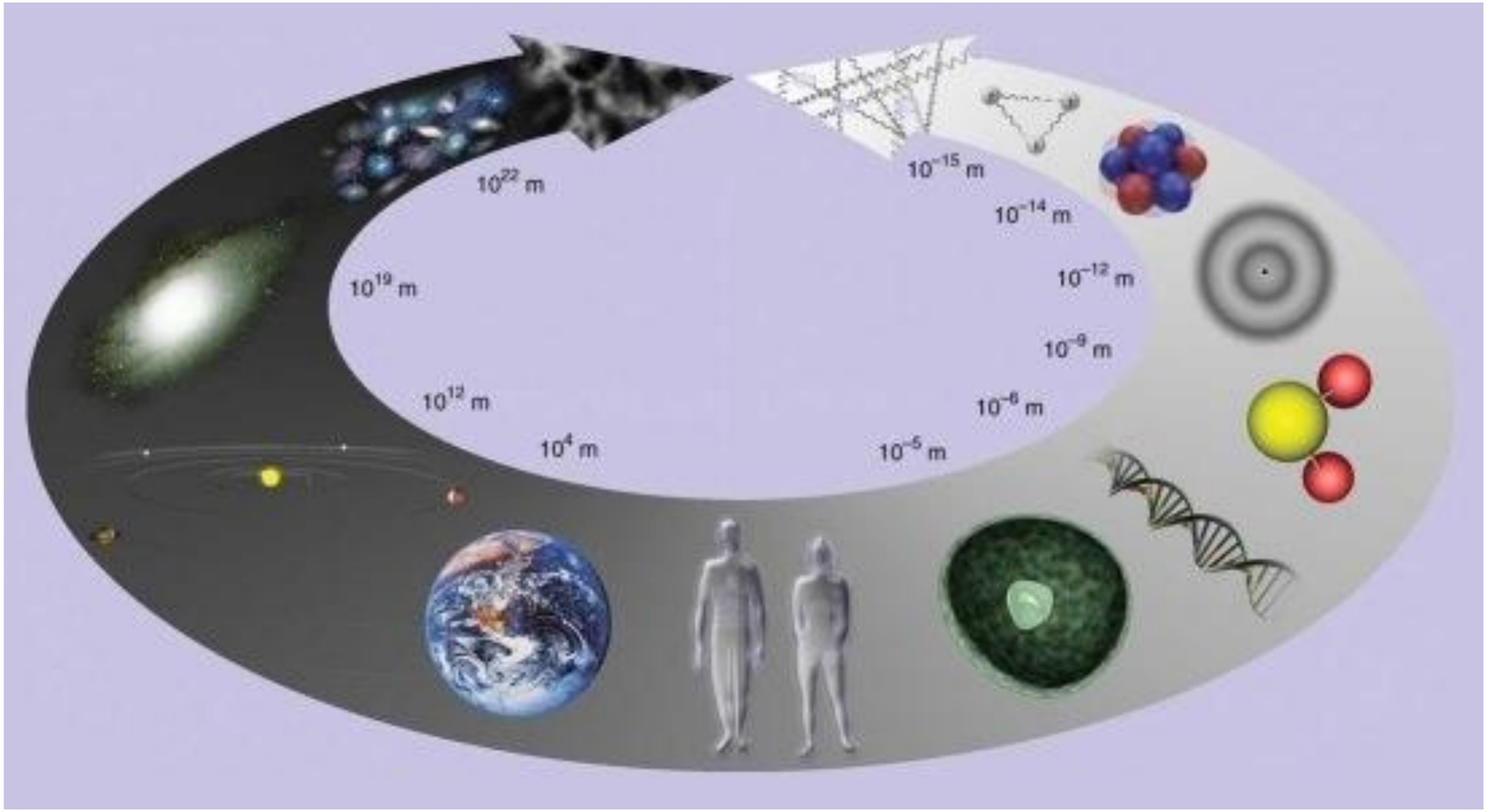
Escalas de energia



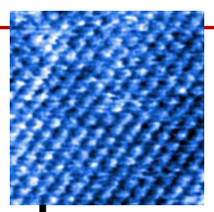
A eras através dos materiais



Escalas de comprimento



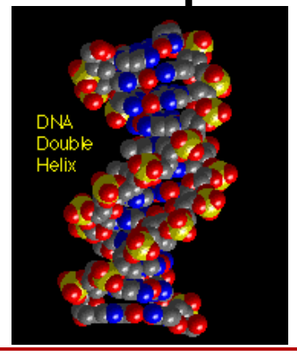
Escalas

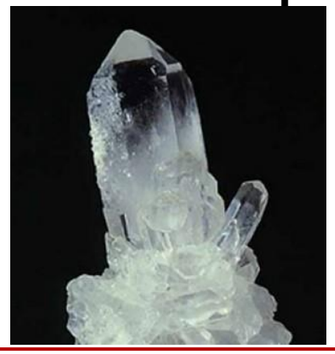


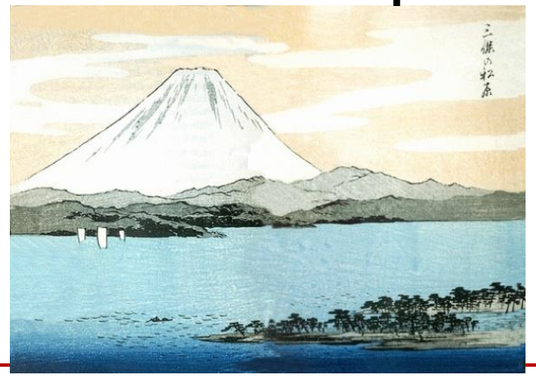
Nanoscale

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

meters

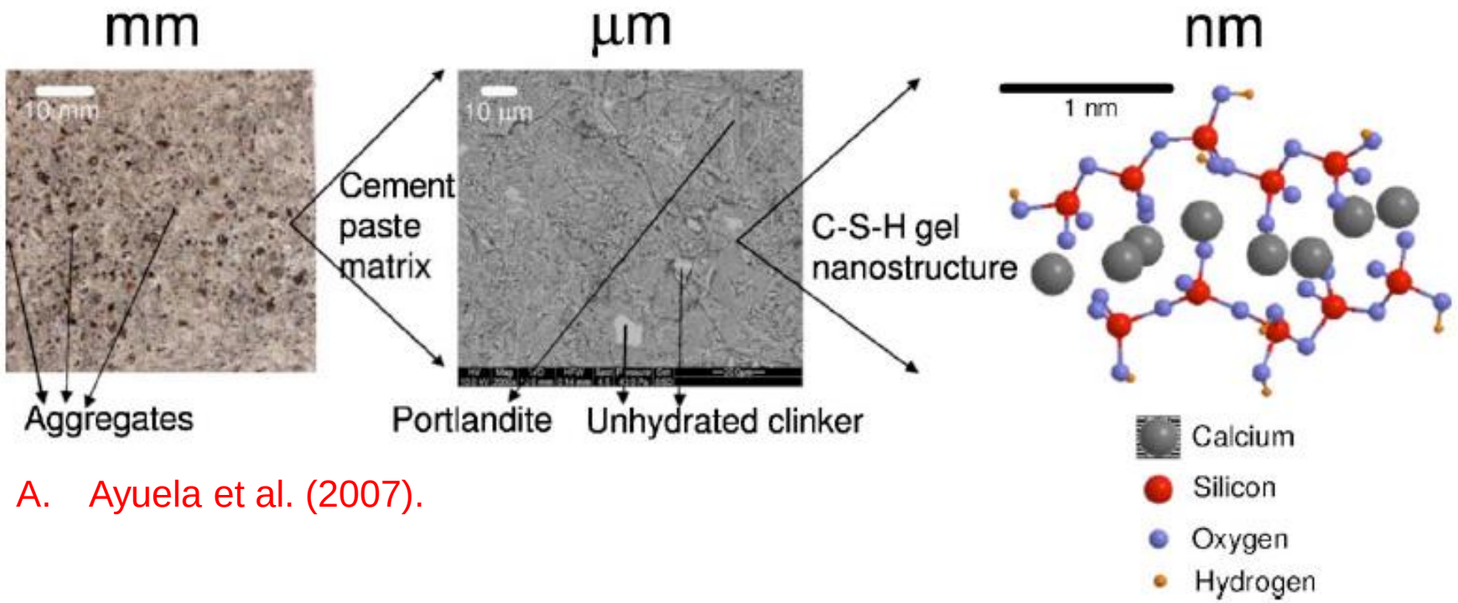




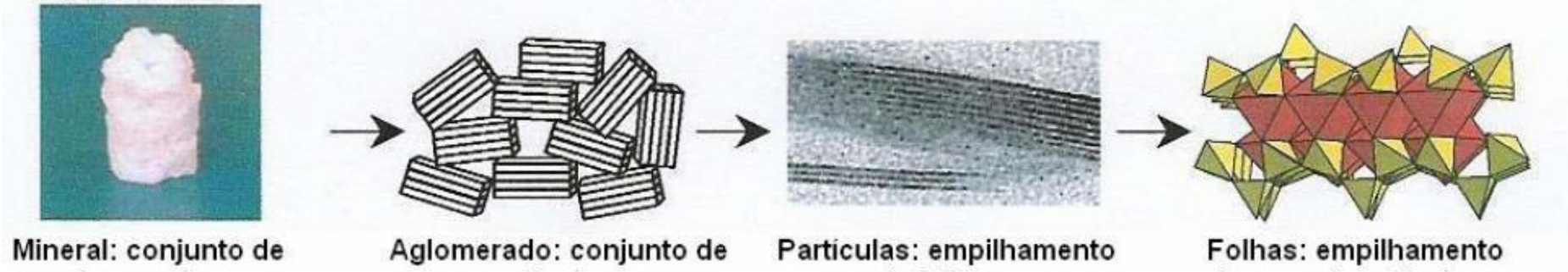


Parte 1 - Nano a Micro **Parte 2 - Meso a Macro**

Escalas em materiais à base de cimento



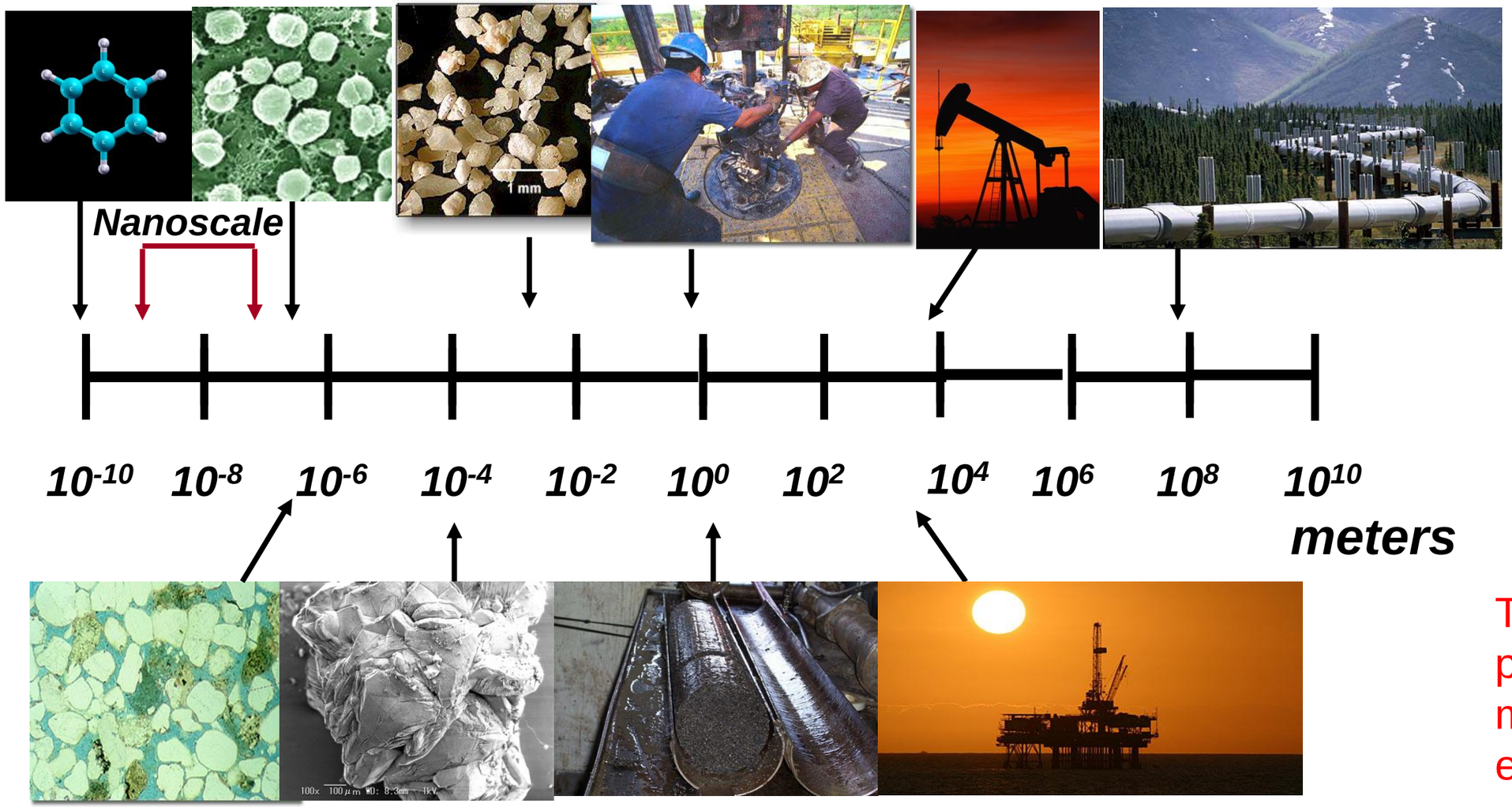
A. Ayuela et al. (2007).



Calcium Silicate Hydrate – different length scales

MINET, J. PhD thesisFrança, 2003.

Escalas em materiais para indústria de O&G



Temperatura, pressão, salinidade, meios heterogêneos e multifásicos

Fenômenos físicos complexos em materiais

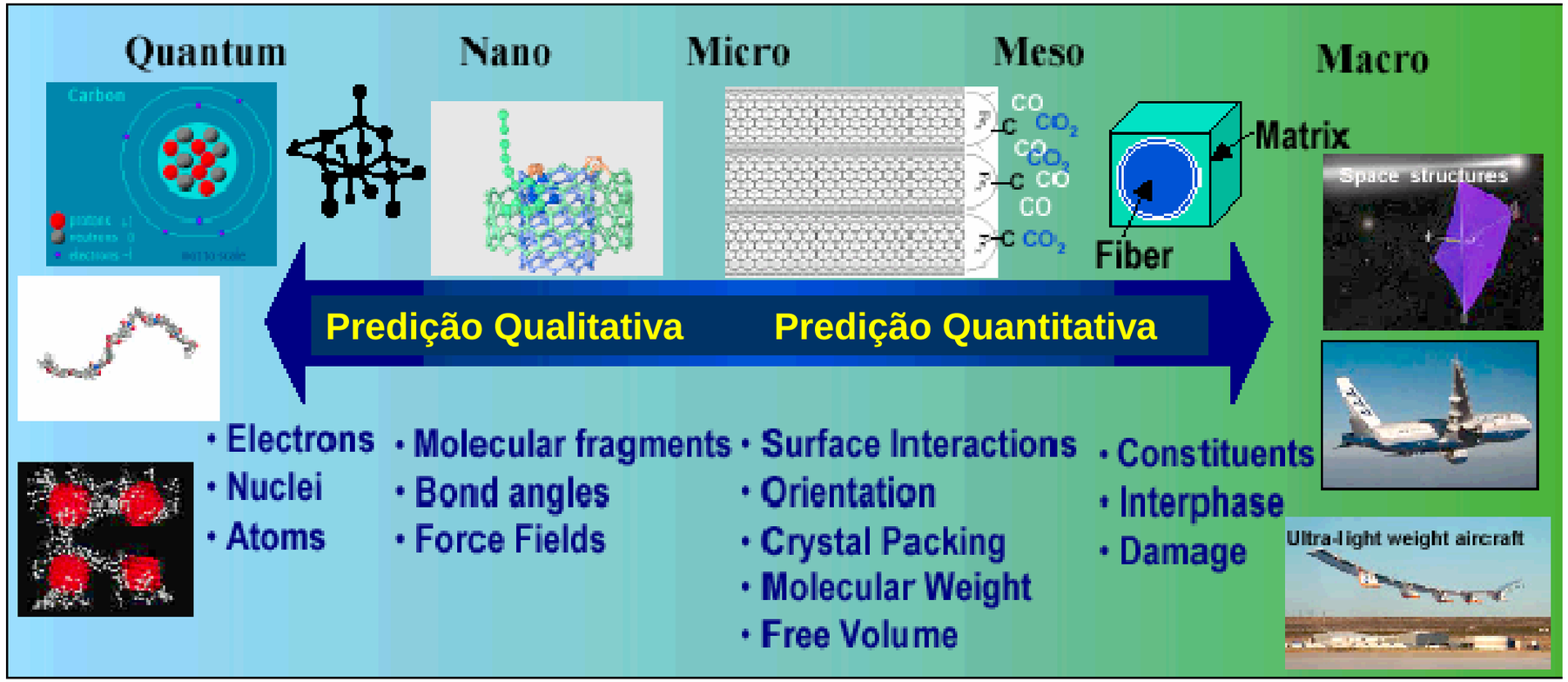
O&G: Como os grandes podem induzir os sistemas pequenos?

Escalas de tempo e espaço em modelagem

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

by Greg Odegard, NASA

Química Computacional | Ciência dos Materiais Computational | Mecânica Computational

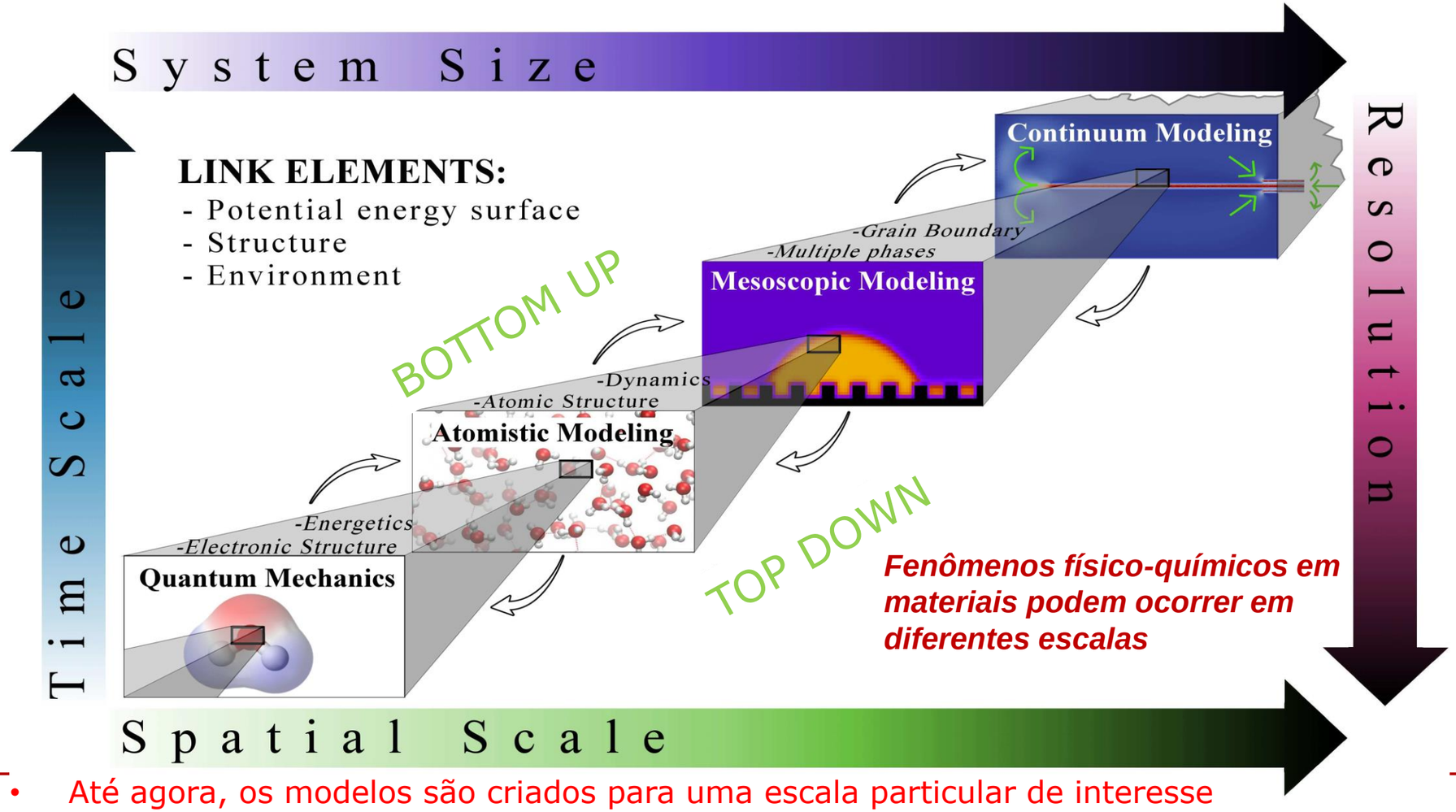


10^{-12} 10^{-9} 10^{-6} 10^{-3} 10^{0}

Comprimento (m)

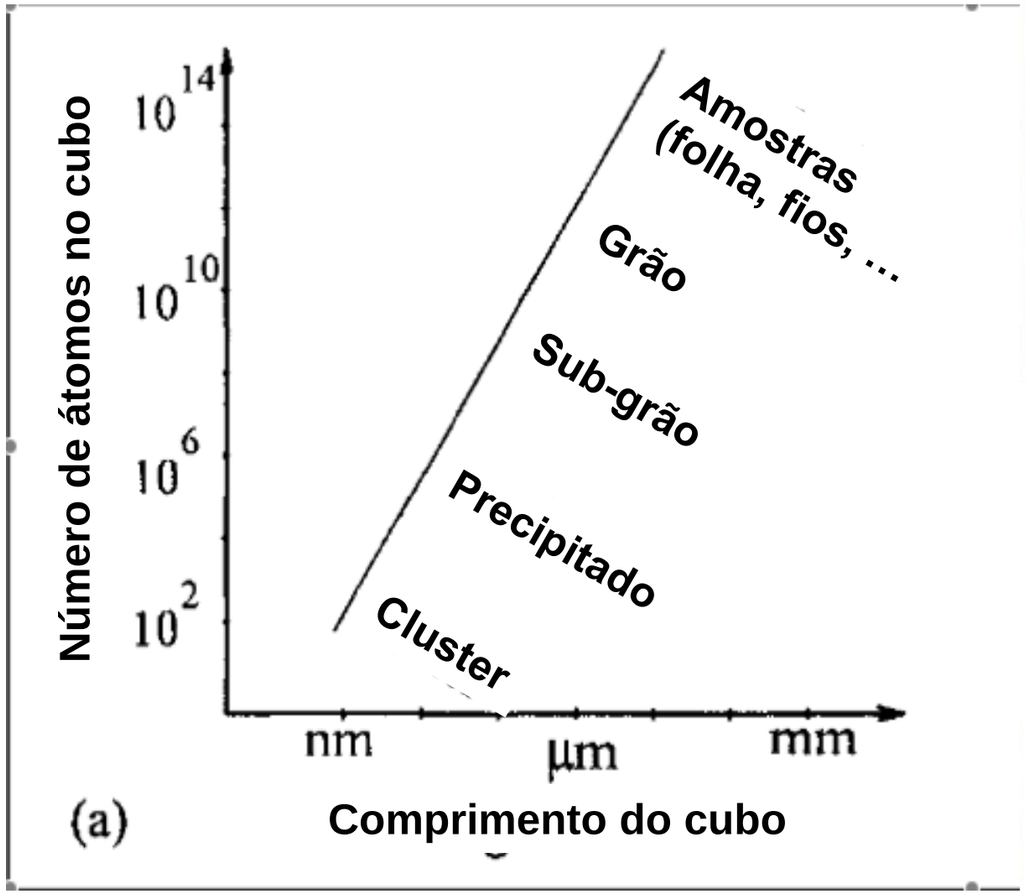
Abordagem em multiescala

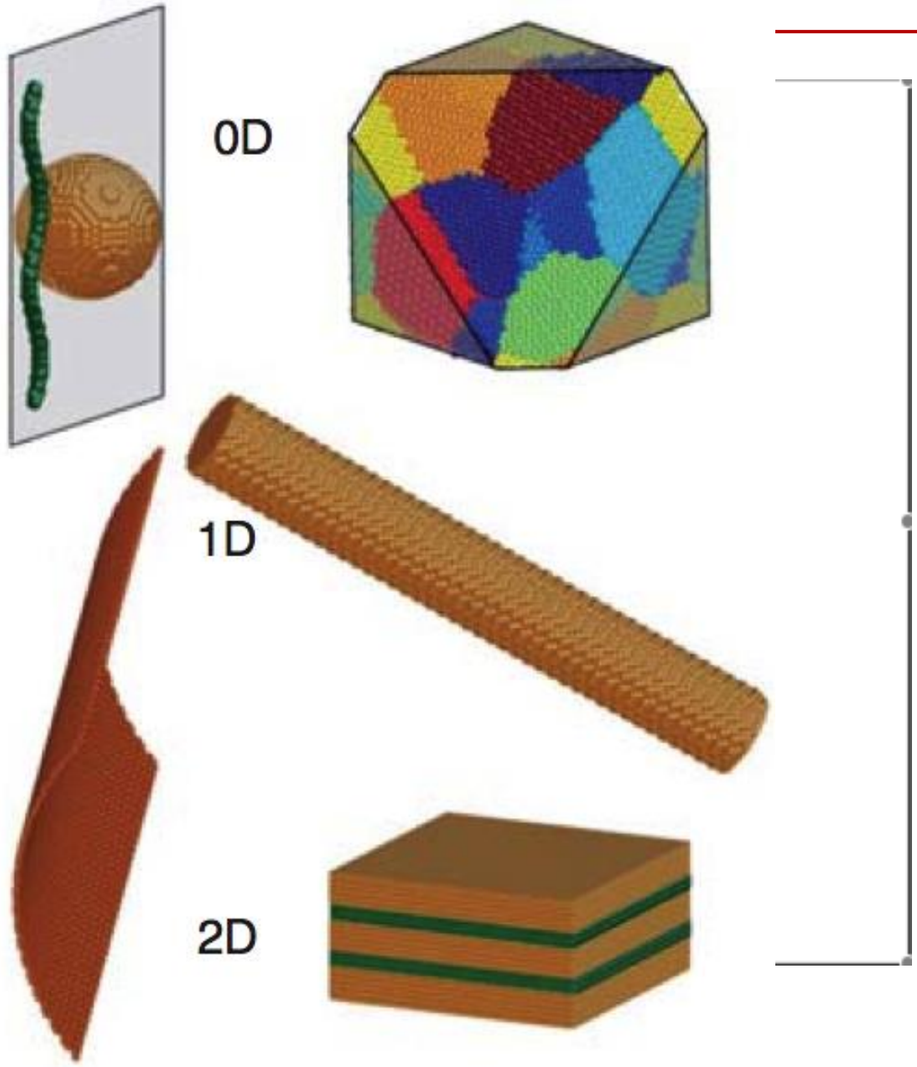
Desafio: modelar fenômenos físicos que variam de escalas moleculares a micro e macro.



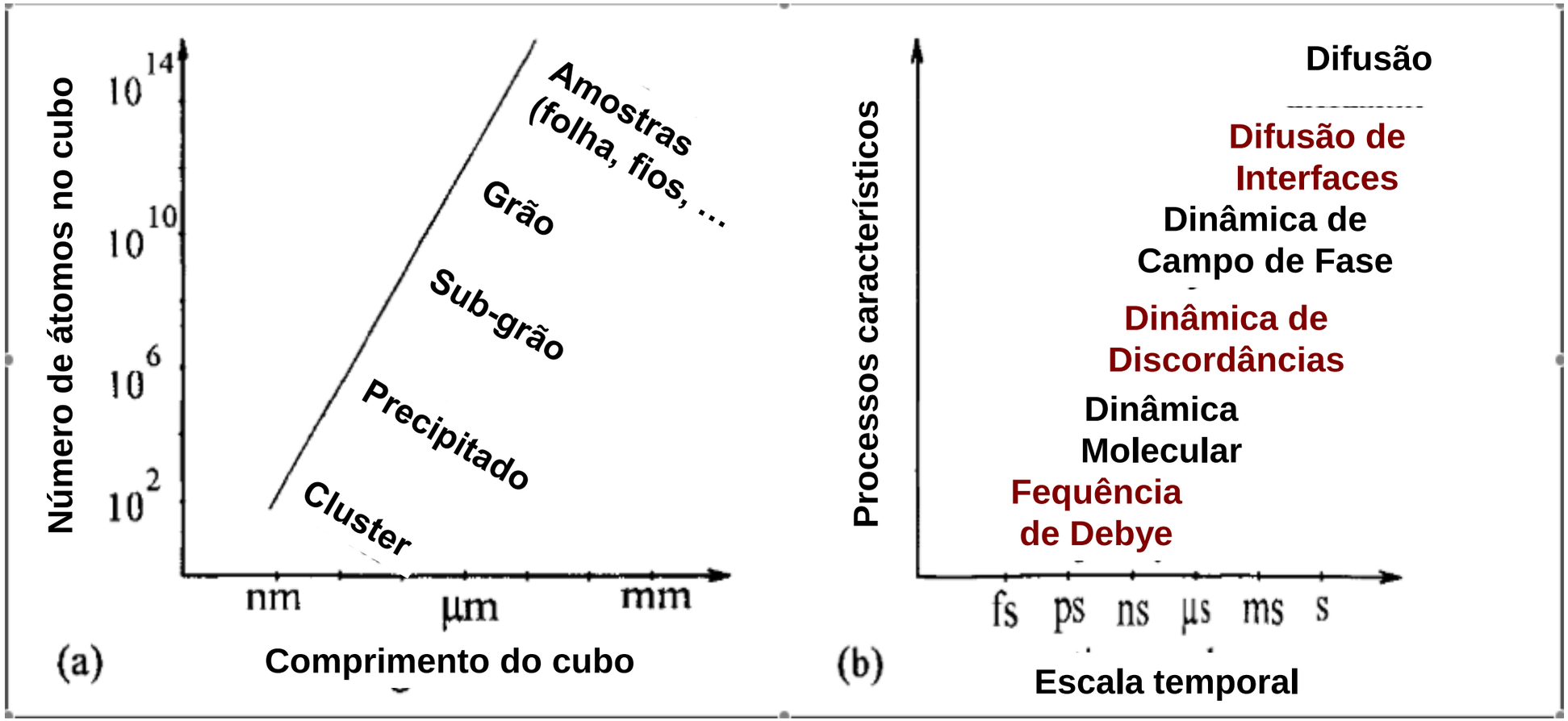
- Até agora, os modelos são criados para uma escala particular de interesse

Escalas

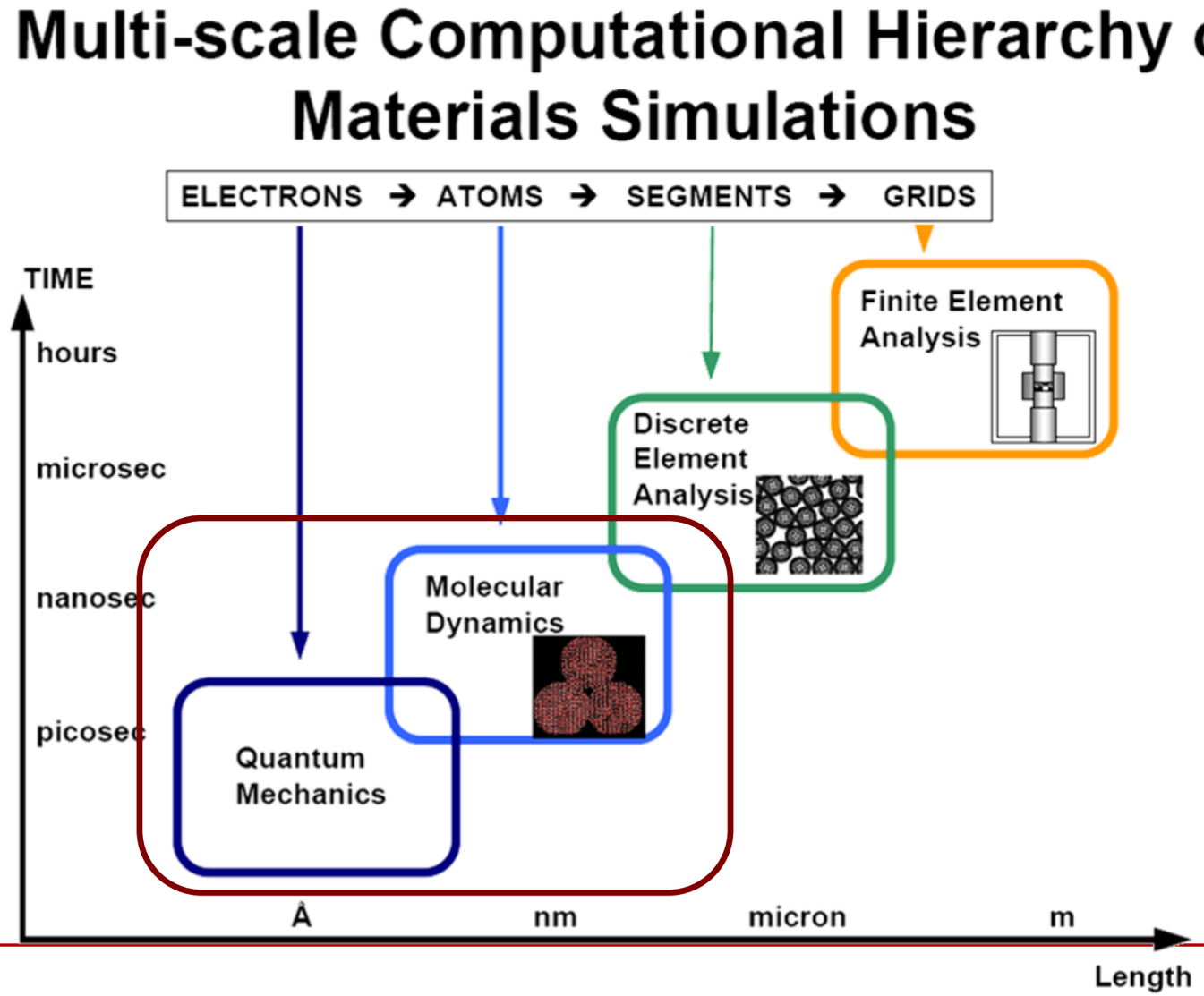

Número de átomos no cubo
10^{14}
10^{10}
10^{6}
10^{2}
Amostras (folha, fios, ...
Grão
Sub-grão
Precipitado
Cluster
nm
µm
mm
(a)
Comprimento do cubo


0D
1D
2D

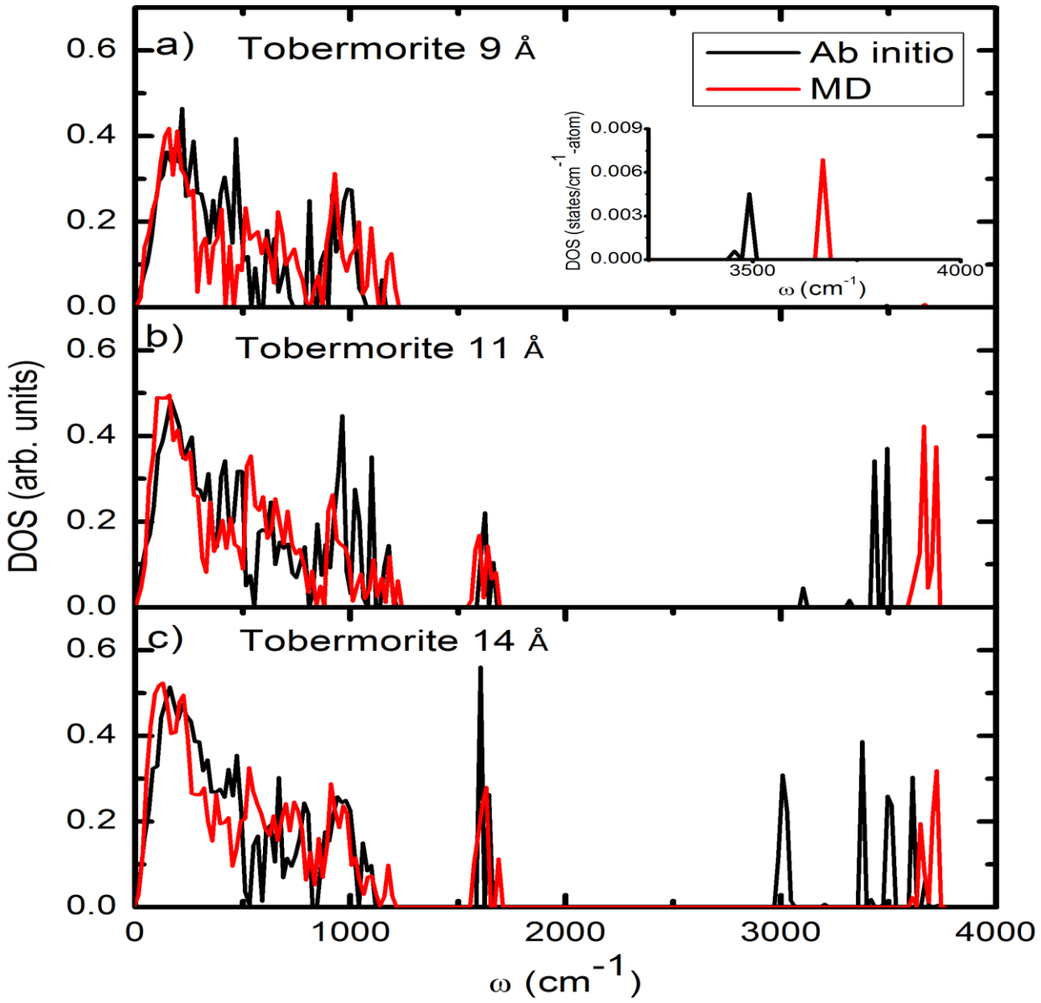
Escalas

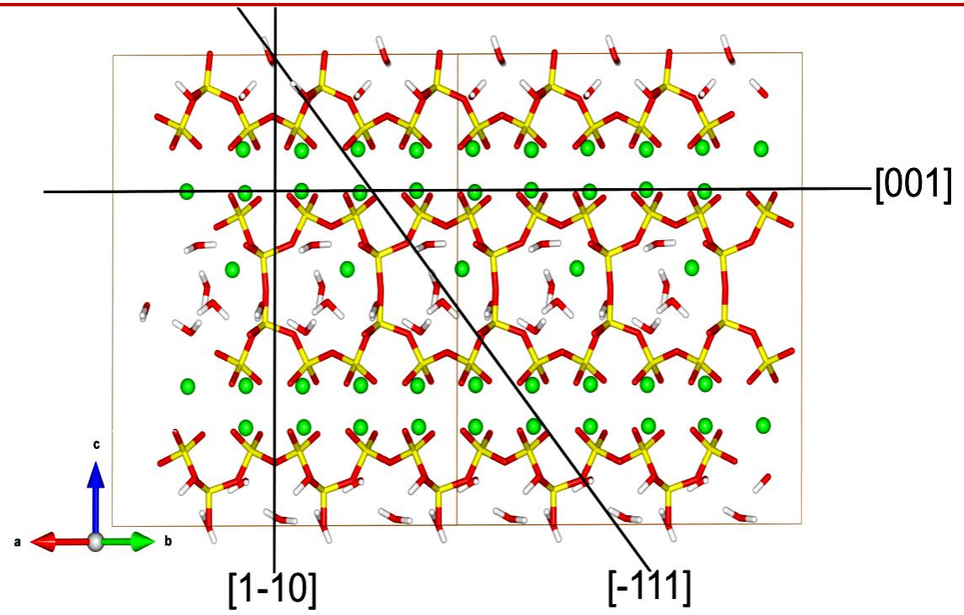

Número de átomos no cubo
10^{14}
10^{10}
10^{6}
10^{2}
Amostras (folha, fios, ...
Grão
Sub-grão
Precipitado
Cluster
nm
µm
mm
(a)
Comprimento do cubo
Processos característicos
Difusão
Difusão de Interfaces
Dinâmica de Campo de Fase
Dinâmica de Discordâncias
Dinâmica Molecular
Fequência de Debye
fs
ps
ns
µs
ms
s
(b)
Escala temporal

Introdução – Métodos de partículas



Cimento por primeiros princípios

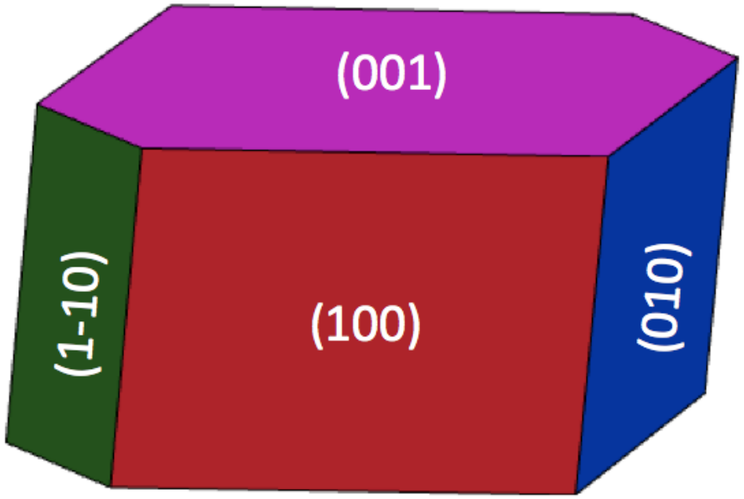




Surface termination	Surface energy (J/m^2)
(001)	0.46
(010)	0.88
(100)	0.69
(1$\bar{1}$0)	1.05
(1$\bar{1}\bar{1}$)	1.73
(10$\bar{1}$)	1.22
(0$\bar{1}$1)	1.35

Cimento por primeiros princípios

Morfologia- Tobermorite 11 Å



Tobermorite 11 Å baseado nos cálculos de primeiros princípios

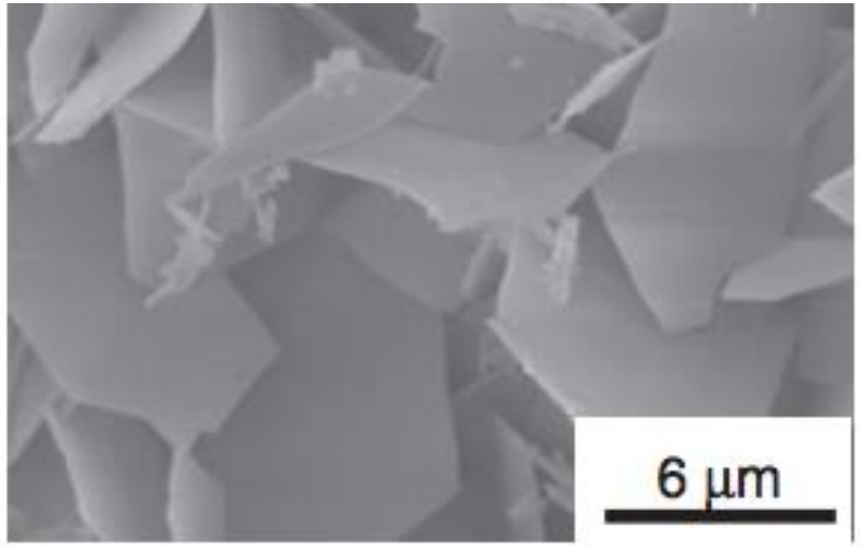
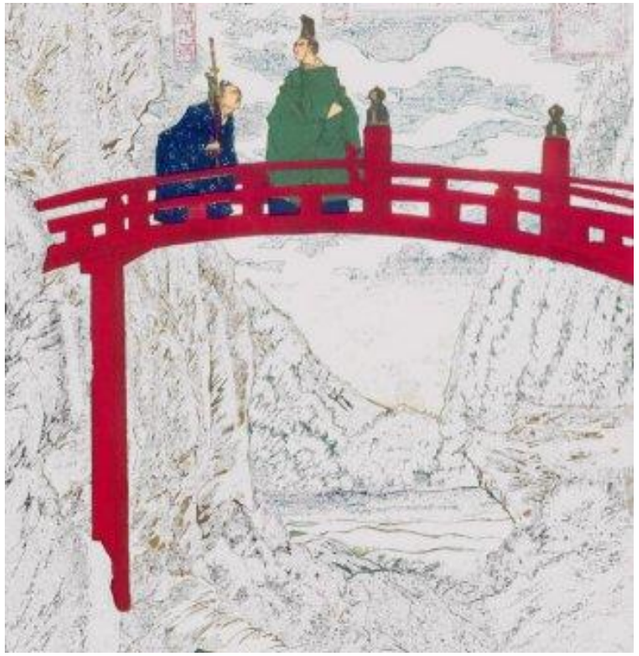


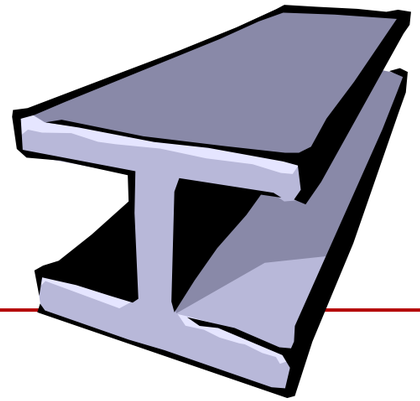
Imagem de Microscopia (SEM) da tobermorita.

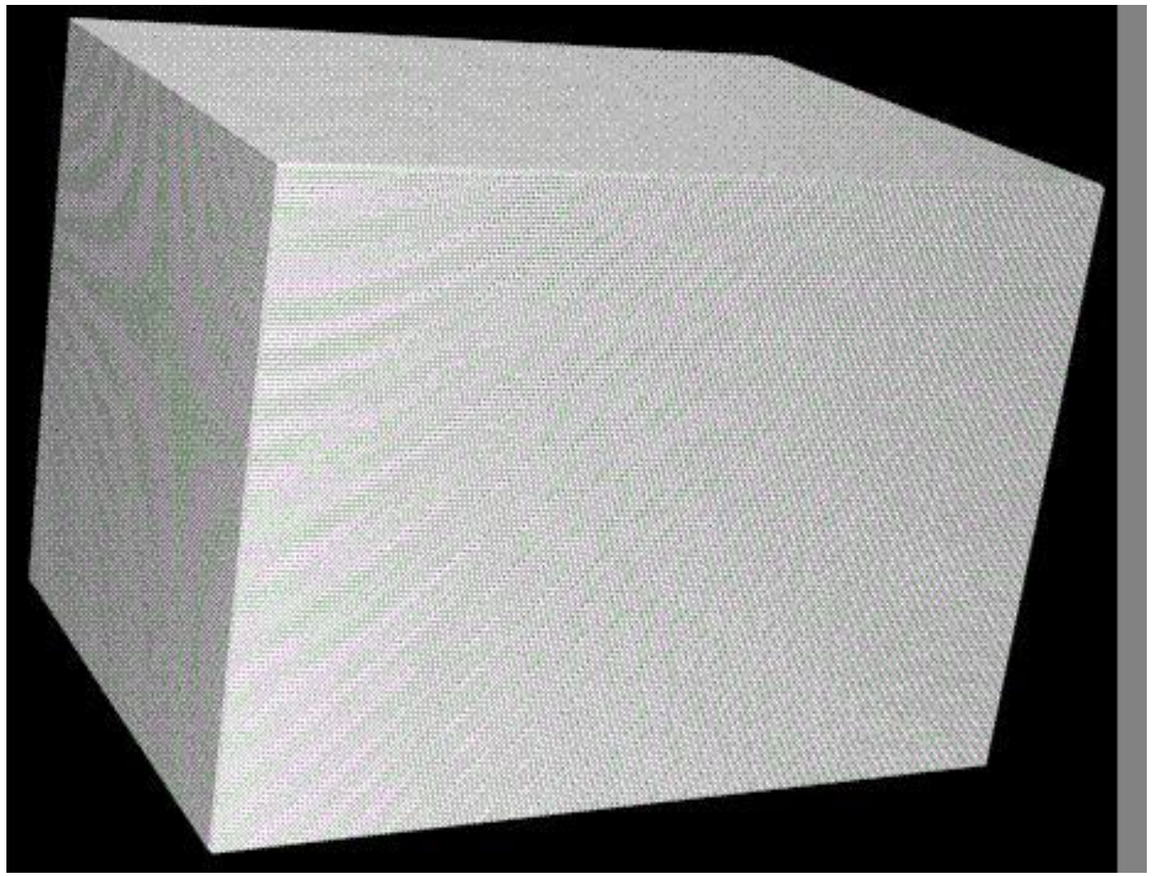
- *Morphological importance is inversely proportional to the surface energy.*
- *The equilibrium morphology of Tobermorite 11 Å is pseudohexagonal.*

Journal of the Ceramic Society of Japan, 119(1389):375–377, 2011

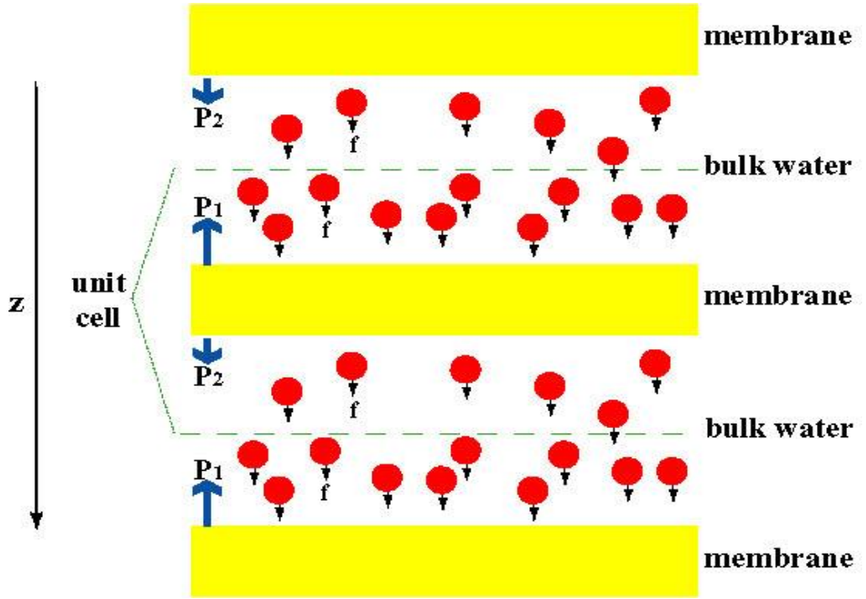
Ondas de choque em bcc - Fe

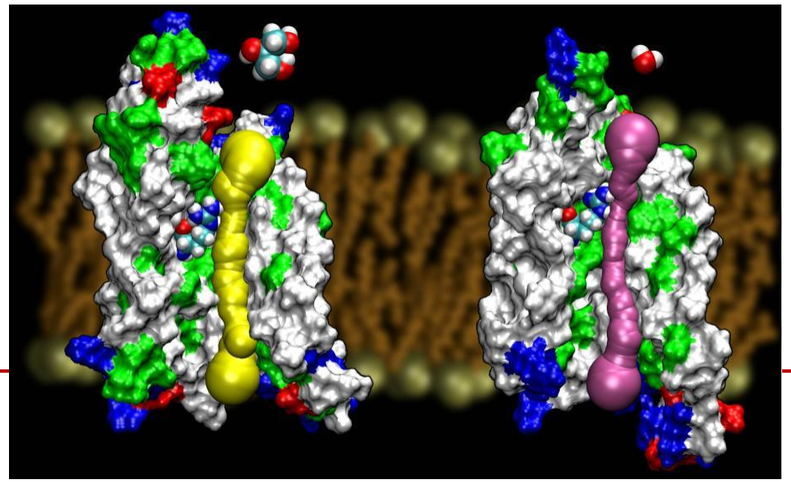


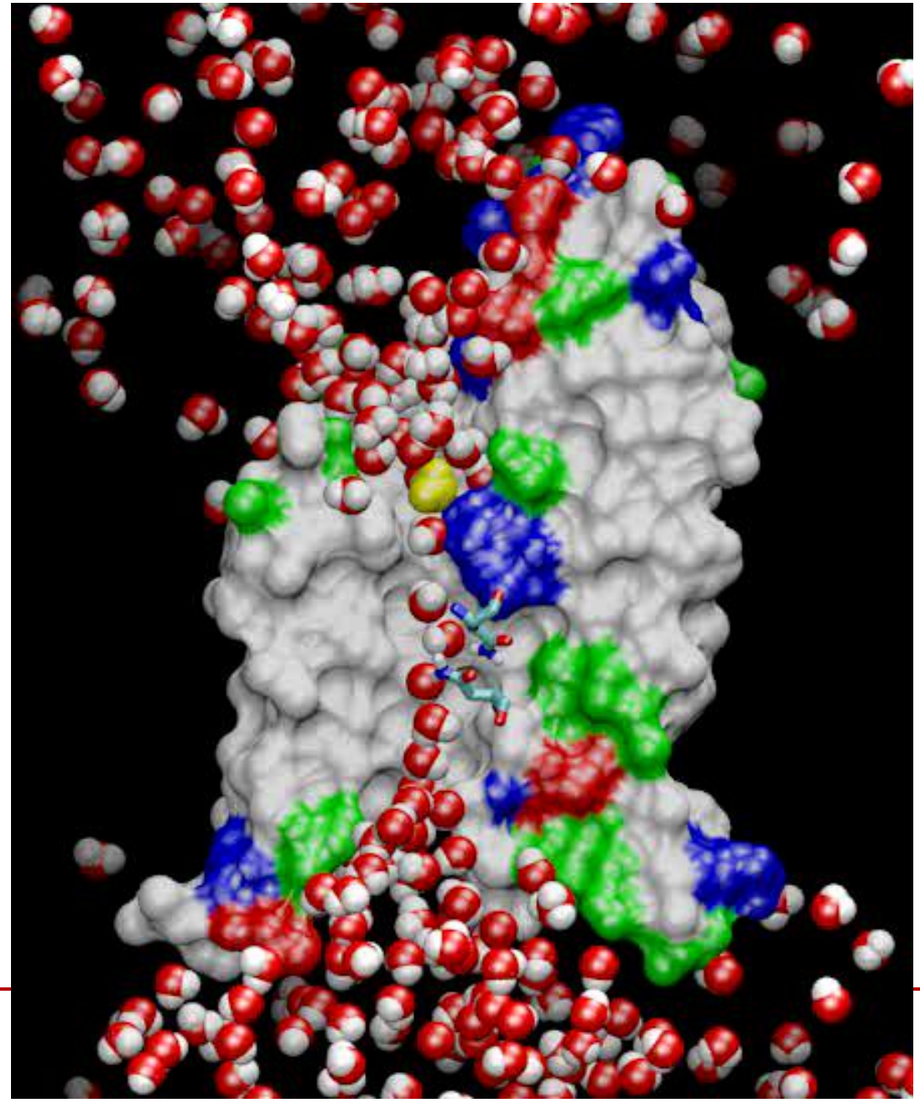




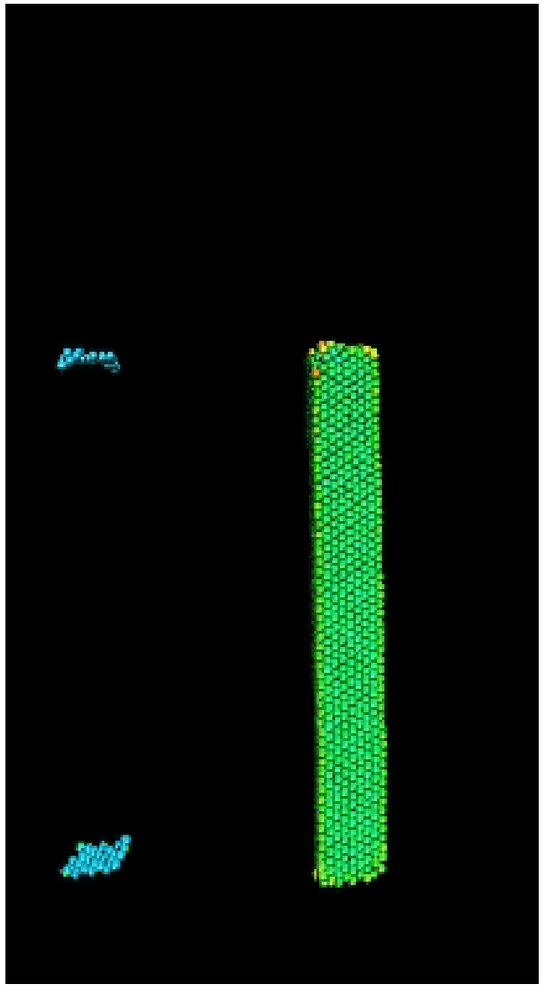
Mecânica Molecular e Equação de Poisson - Efeitos de muitos corpos

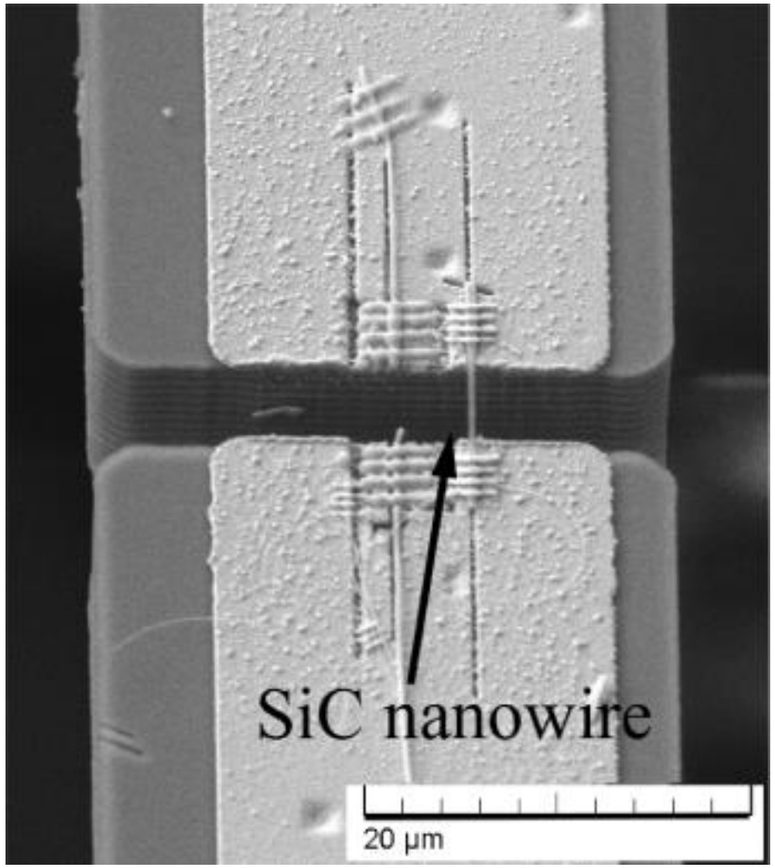


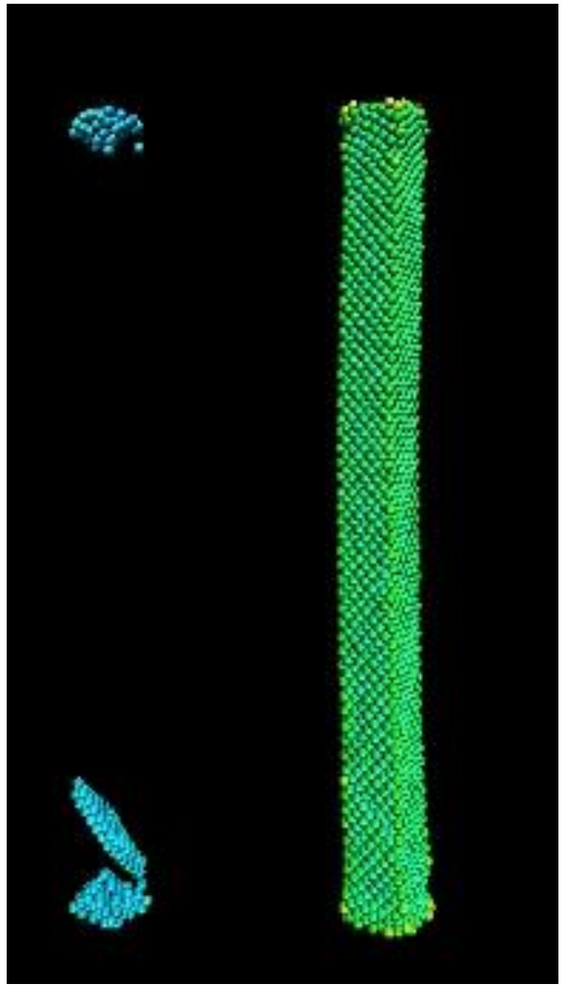




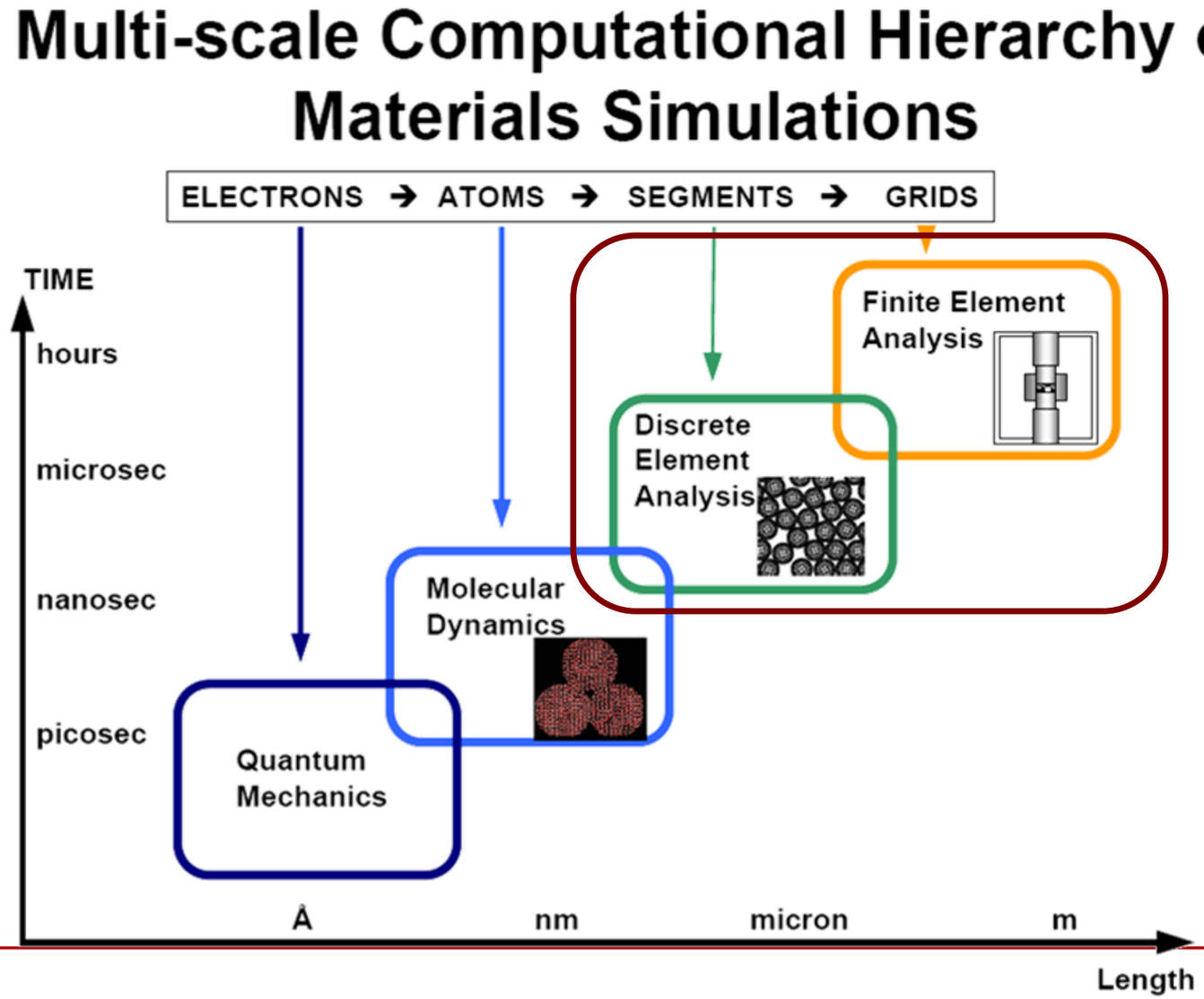
Nanoestruturas



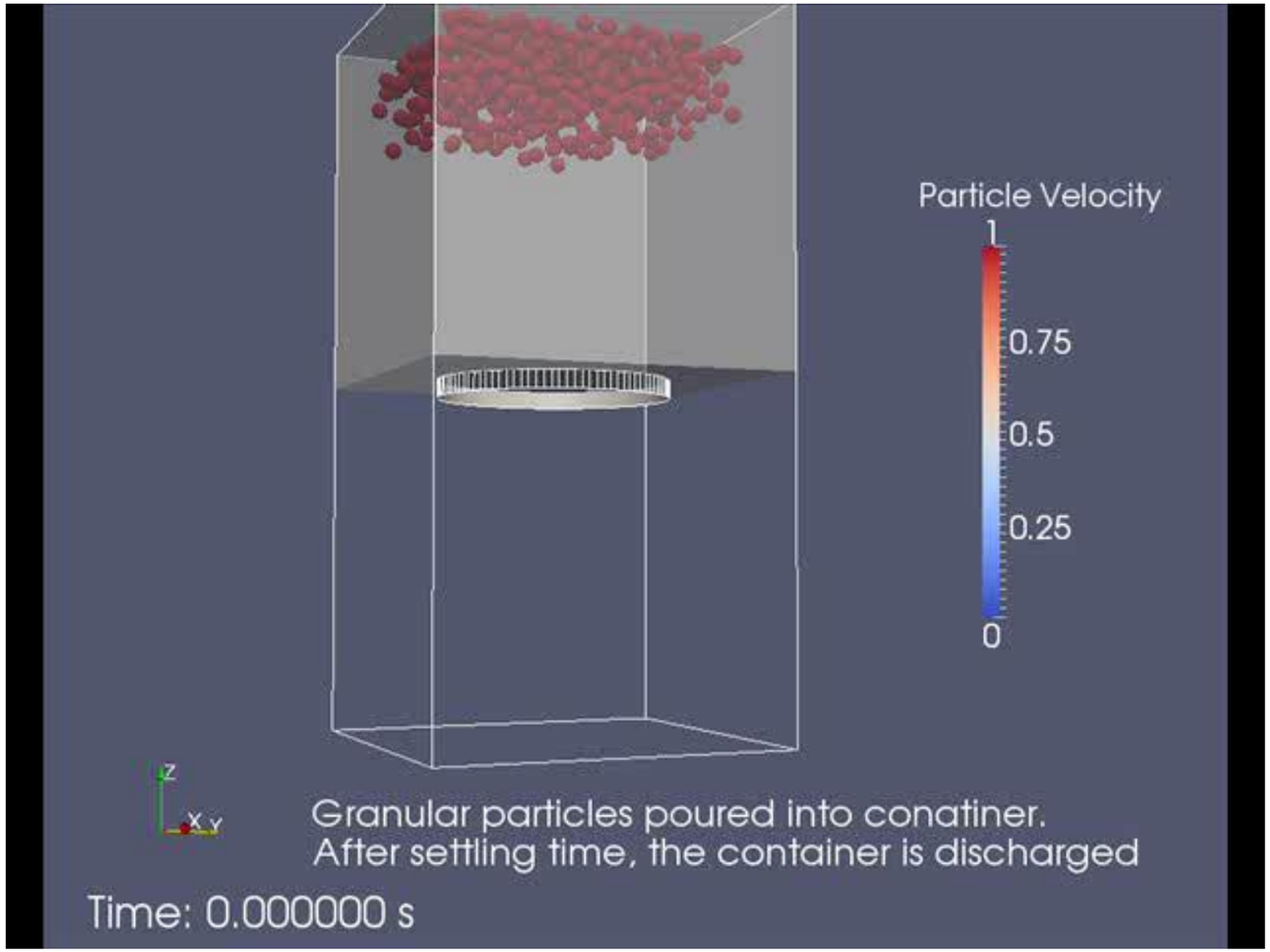




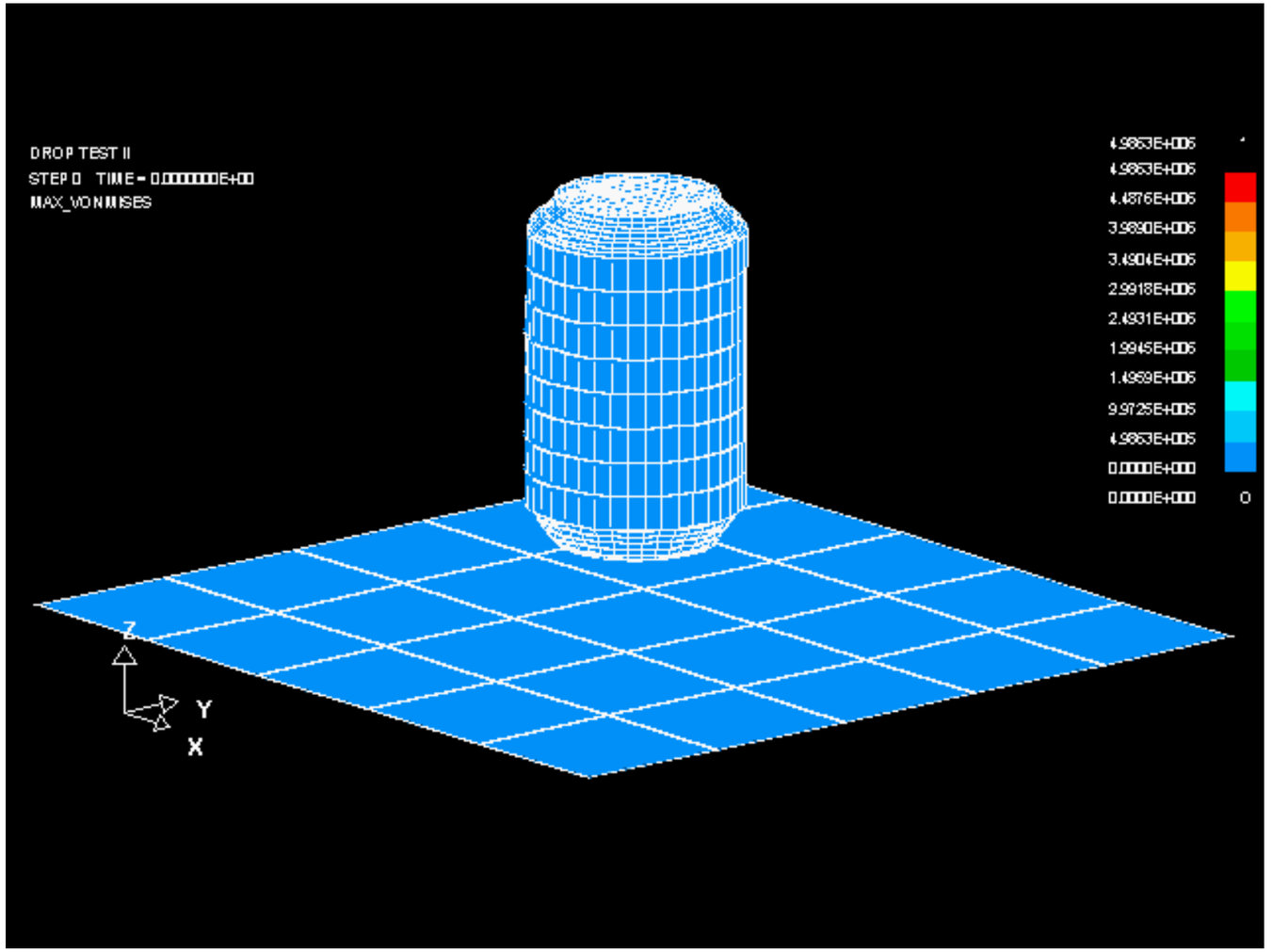
Introdução – Métodos de rede (malha)



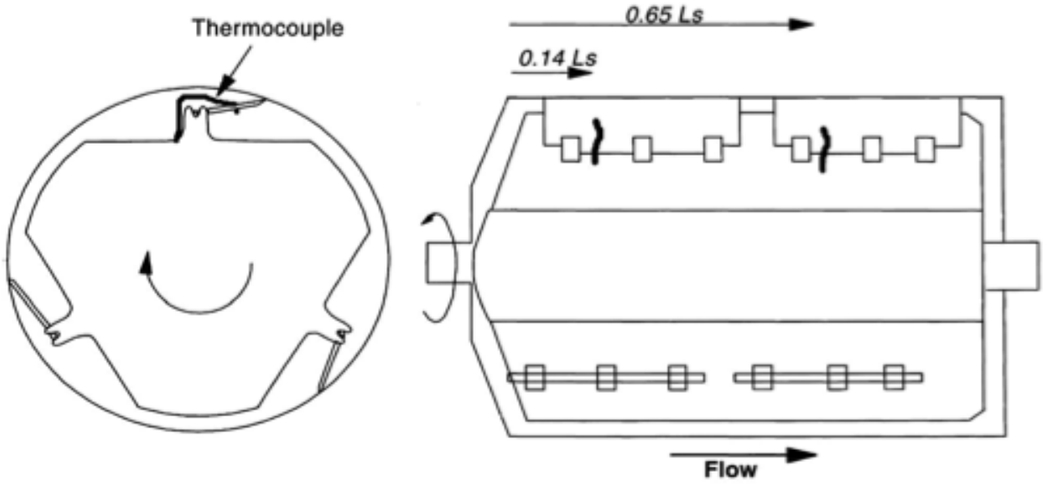
Elementos discretos



Elementos Finitos



Simulação do sorvete



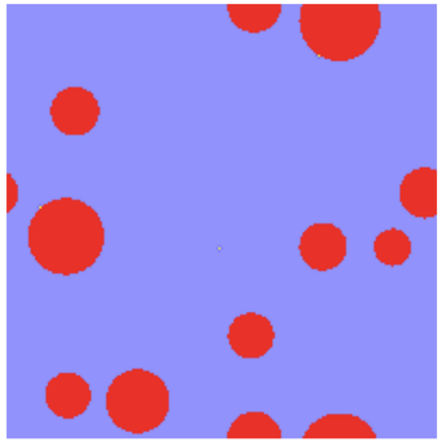
Temperatura de extrusão: -3.5 C

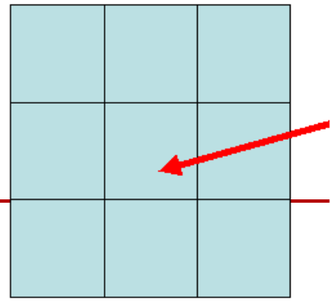
Volume de saída dos núcleos de gelo (fração) : 0.16

Concentração de açúcar na matrix: 0.05

Tamanho médio dos núcleos de gelo: 33 μm

Simulação do sorvete

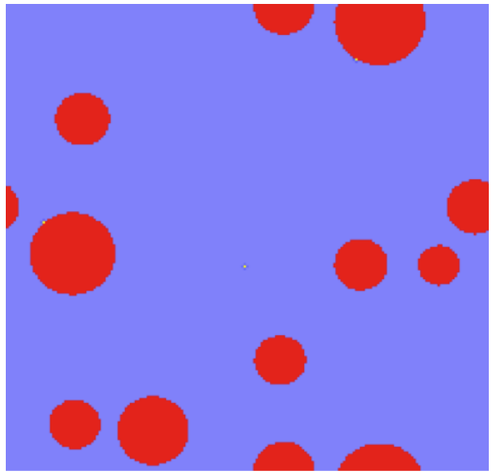


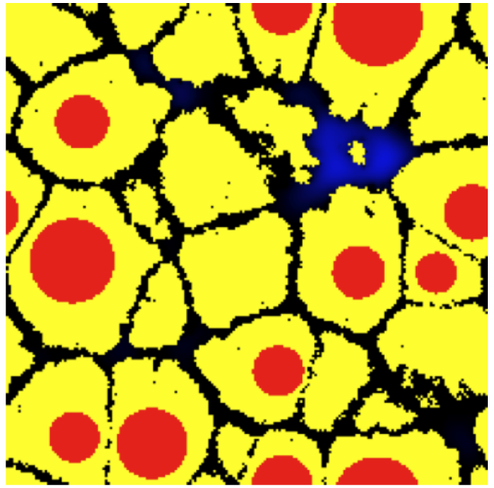


Cada célula tem três componentes:

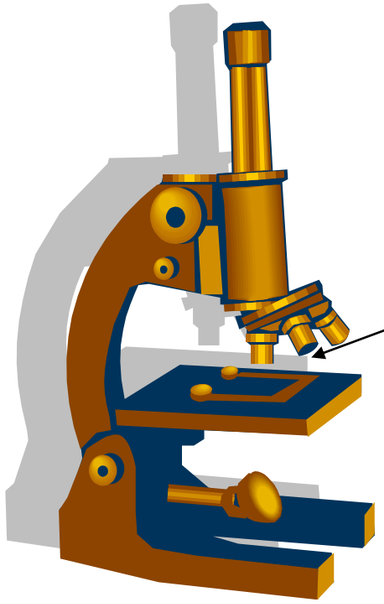
- **Fase (líquido ou sólido)**
- **Concentração**
- **Temperatura**

Simulação do sorvete





Como é um sorvete de verdade ?!



Simulação do sorvete