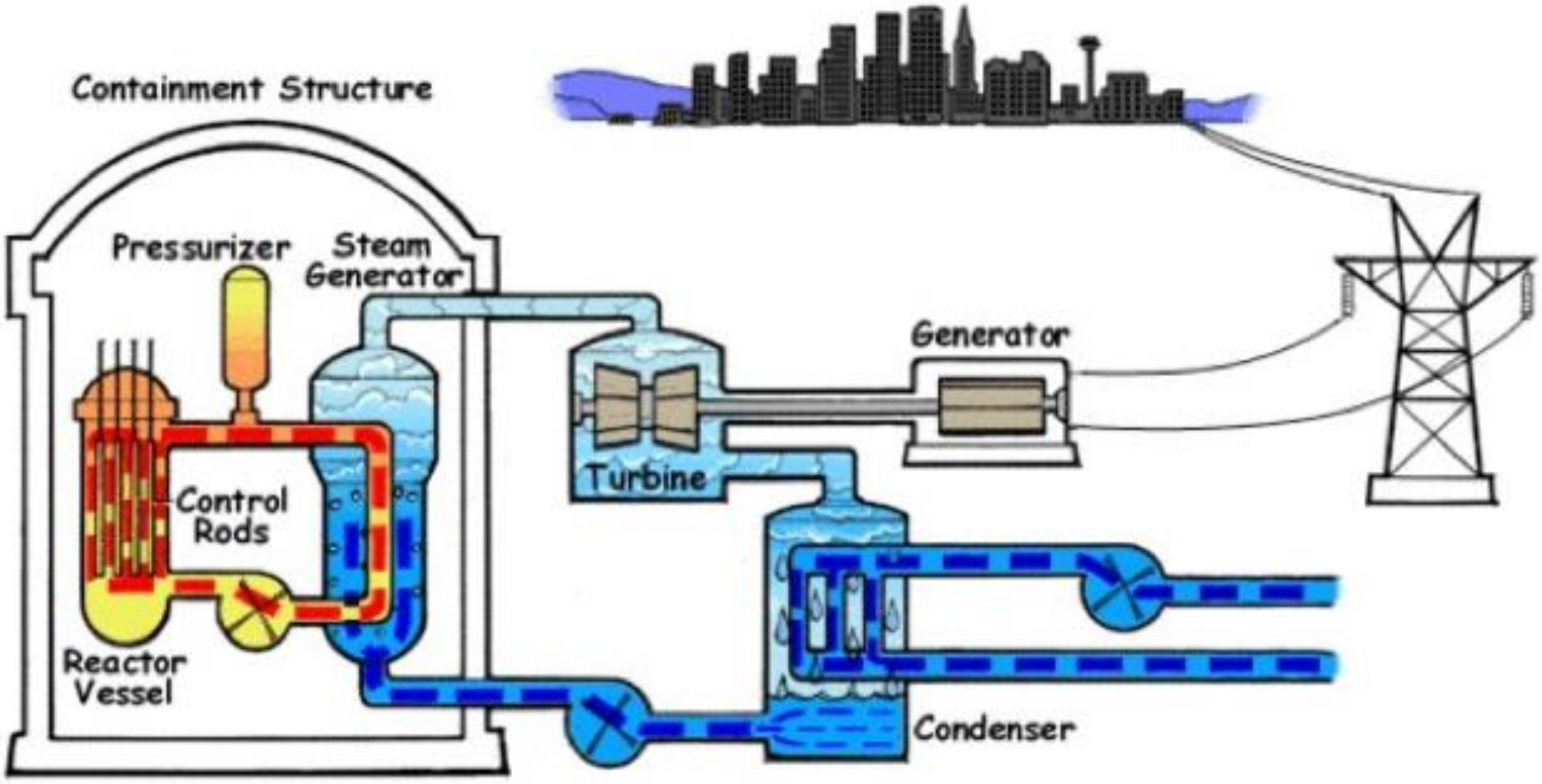
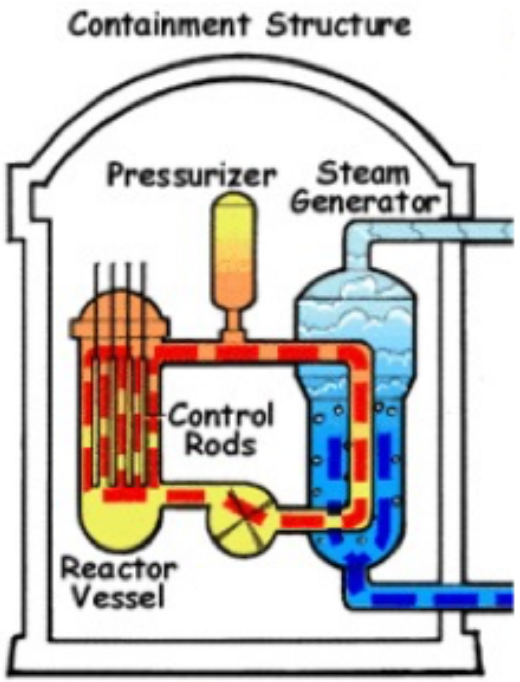
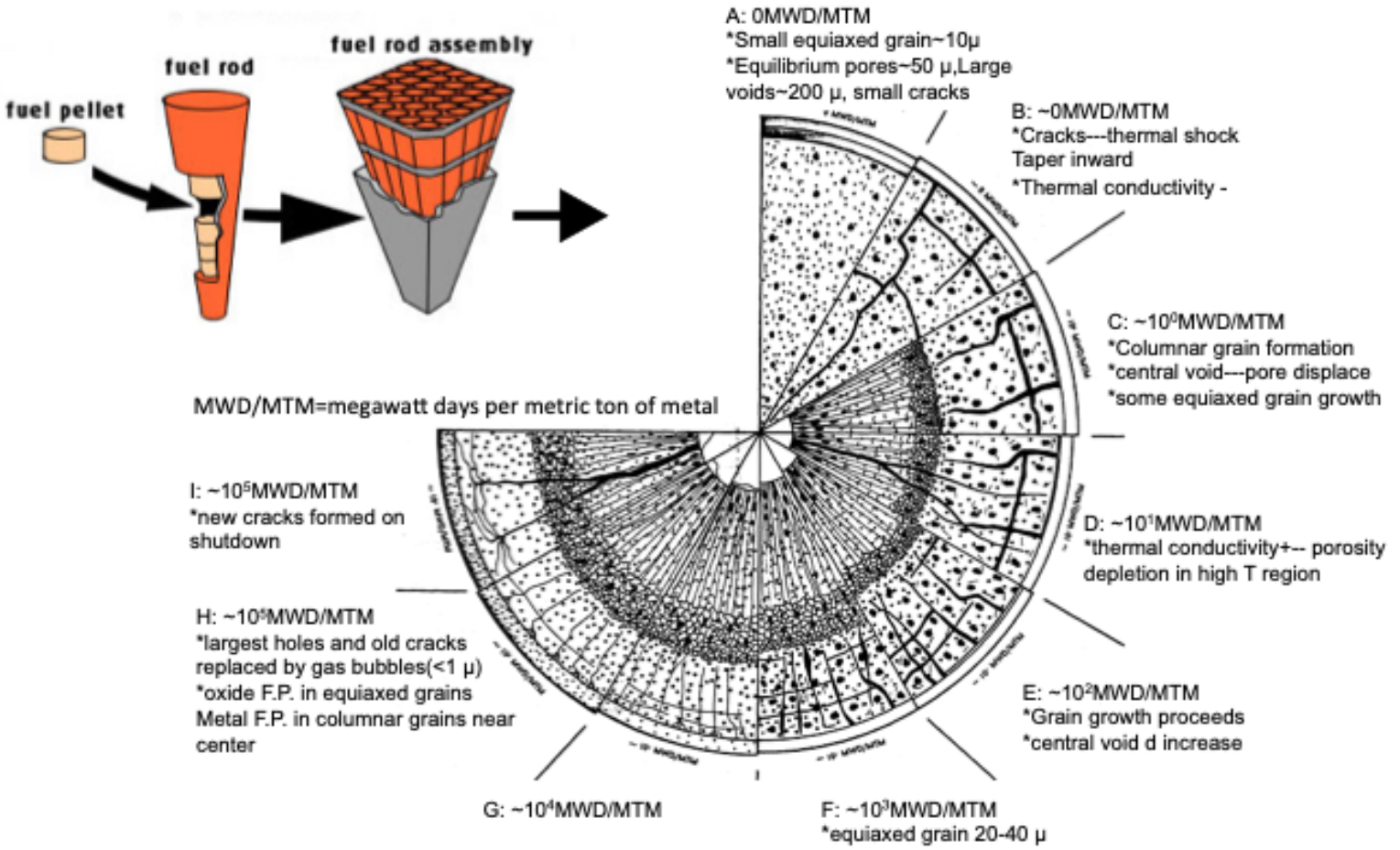
MS2860/MS5860:
Computational Methods in Materials Science

Engineering Applications: Power Reactor

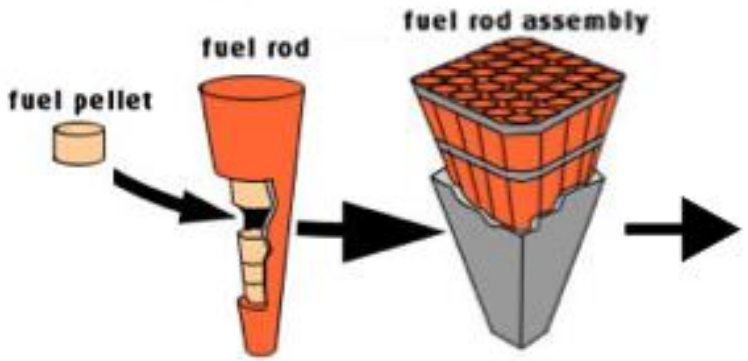


Engineering Applications: Power Reactor

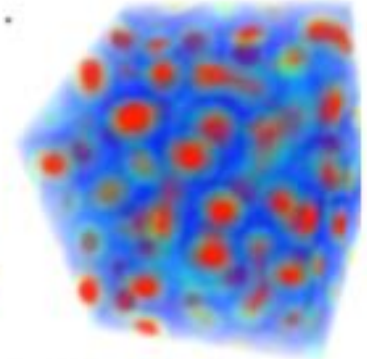




Computational Materials Science

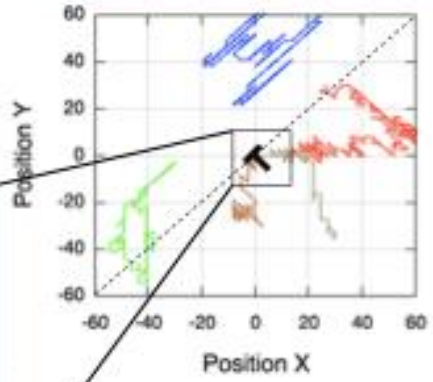


Fuel performance codes



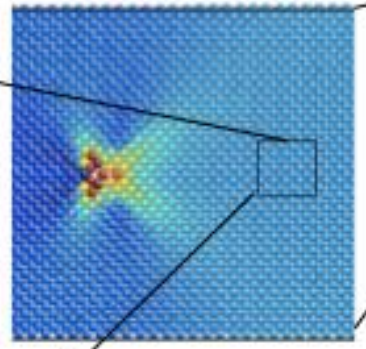
MARMOT

kinetic
Monte Carlo simulations



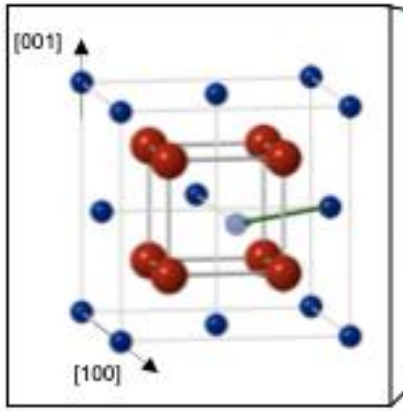
Diffusion coefficient prediction under strain

Atomic scale microstructure



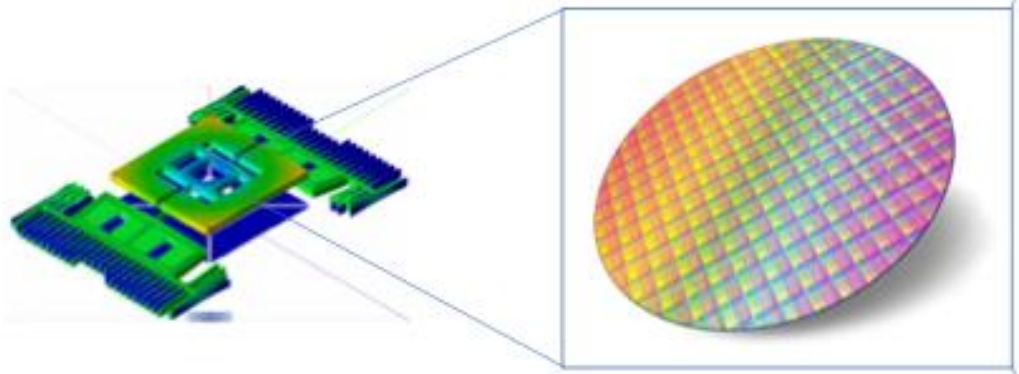
Dislocation strain fields from atomistic simulations

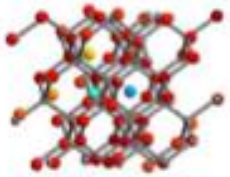
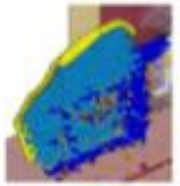
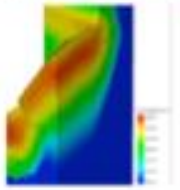
Electronic scale point defects



Point defect formation energies and migration barriers

Multiscale Modeling of Doping in Semiconductors



Modeling Technique	Visualization	Structure Size	Times Simulated	CPU Time
Ab initio		~10^2 atoms	~10^{-2} ns	Slowest
Classical molecular dynamics		~10^5 atoms	~1 ns	
Lattice kinetic Monte Carlo		Part of device	Part of process	
Kinetic Monte Carlo		Complete device	Complete process	
Continuum		Complete device	Complete process	Fastest

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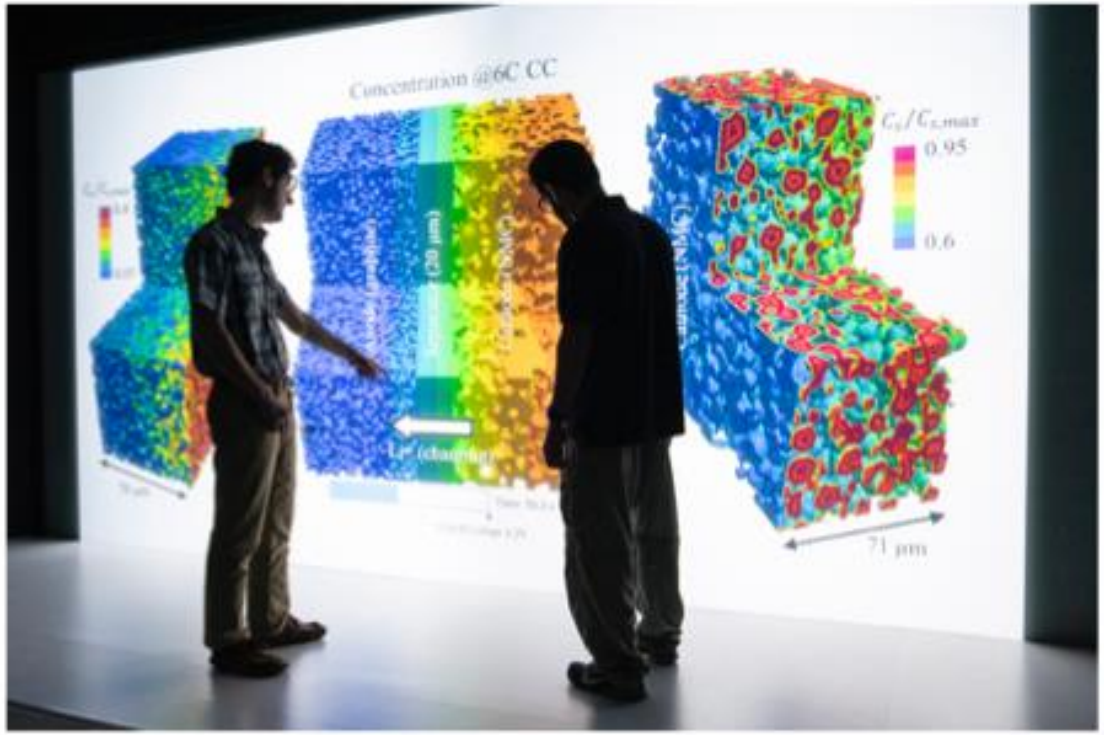
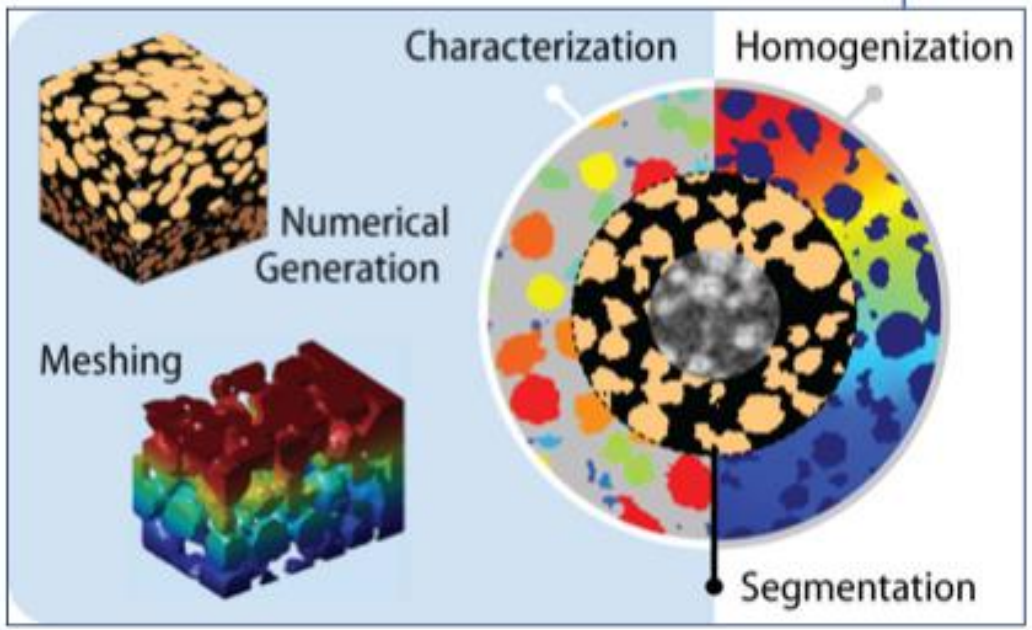
Multiscale Modeling of Batteries

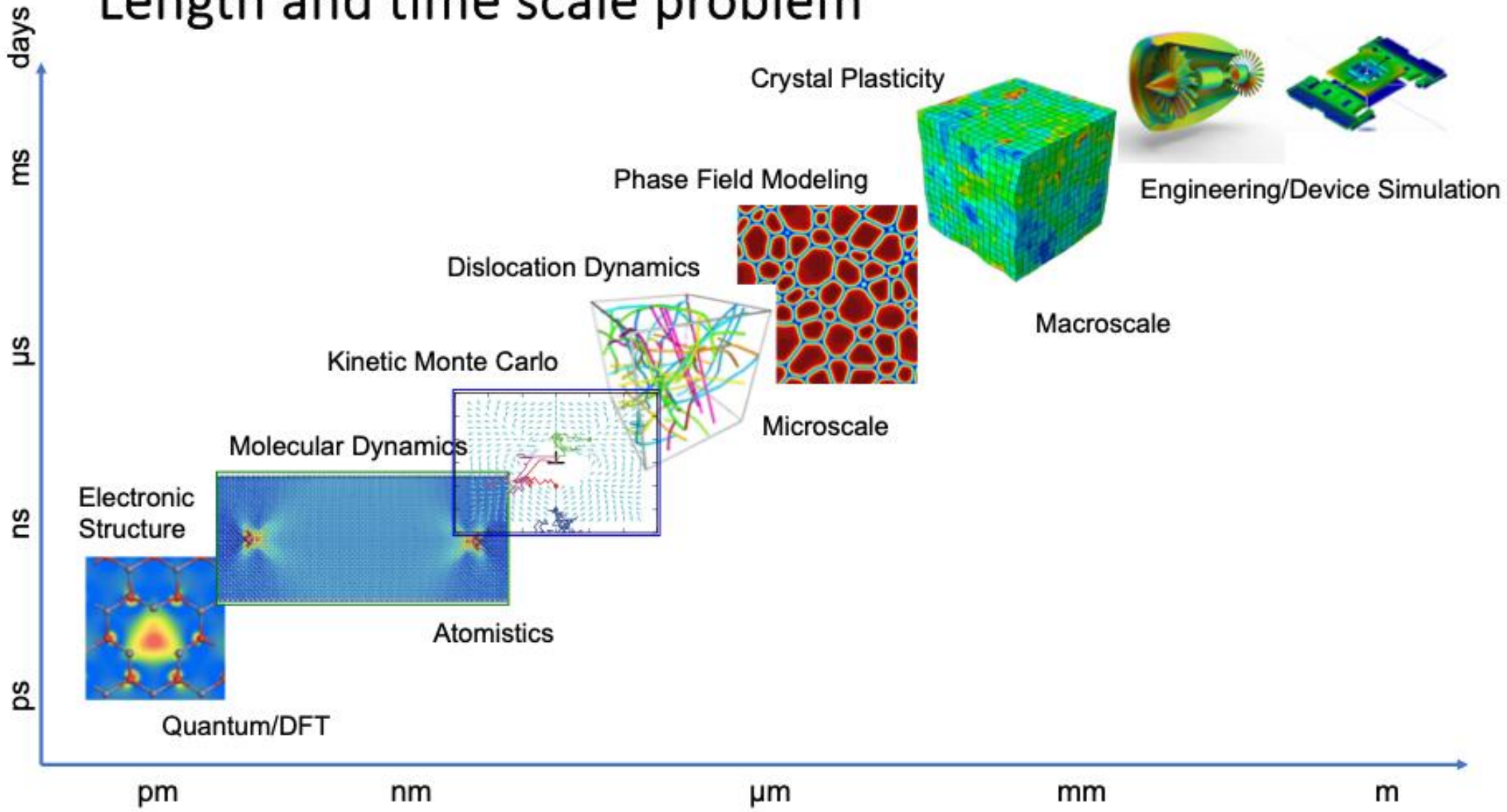


MATBOX: Microstructure Analysis Toolbox

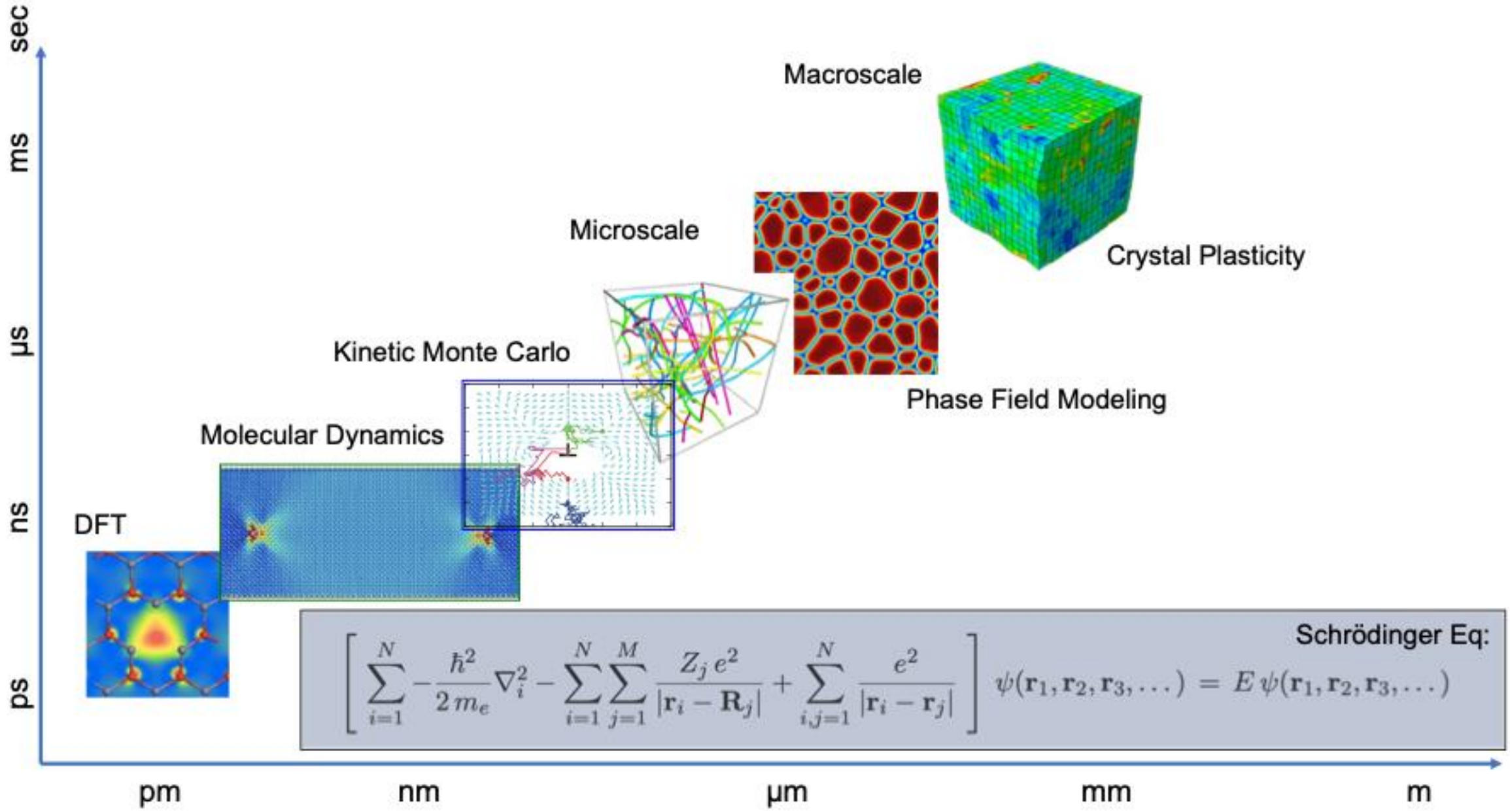


Length and Time Scale Problem

Length and time scale problem



Every phenomenon in nature can, in principle, be described using laws of physics which are usually formulated as partial differential equations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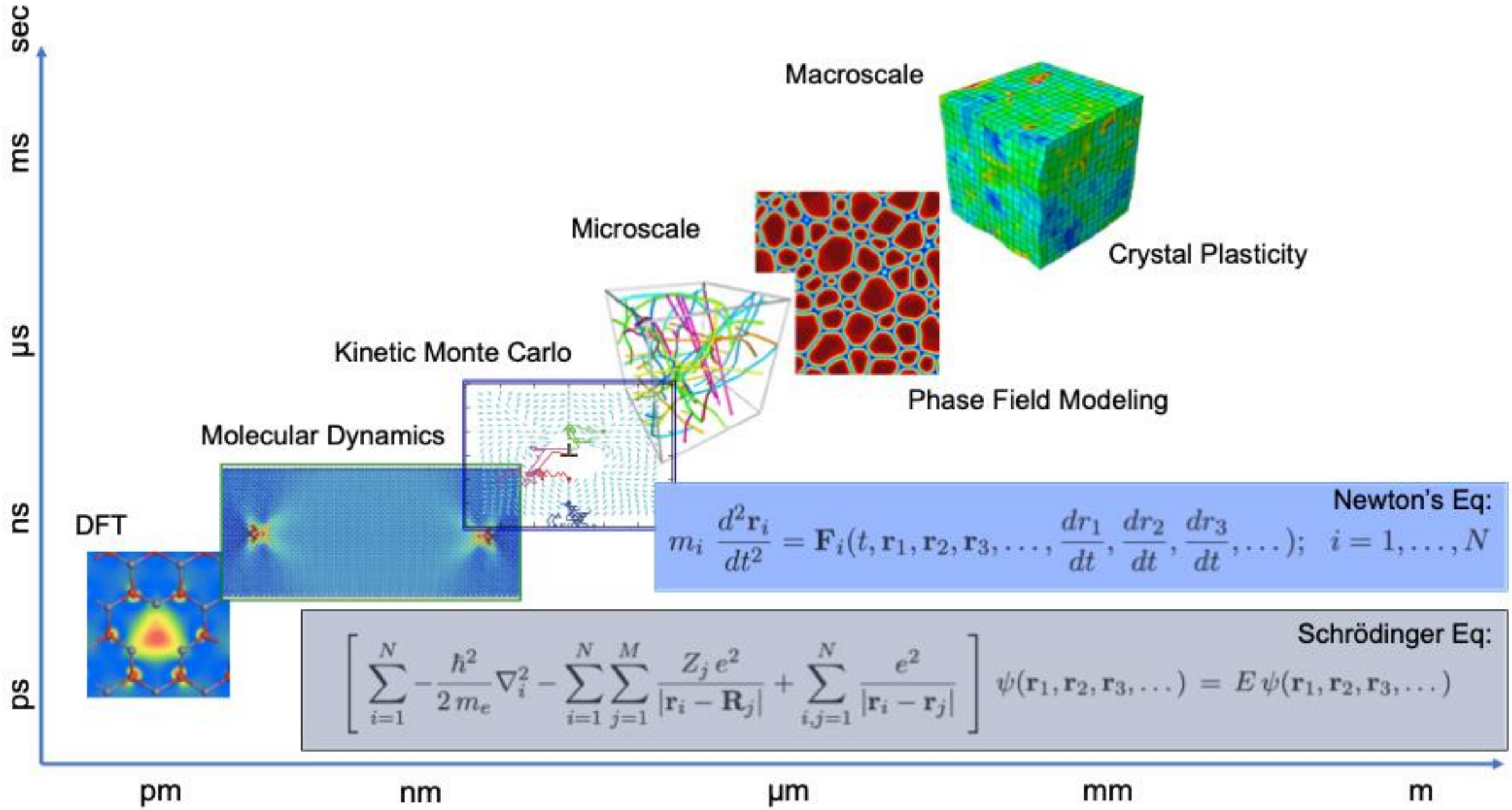
Crystal Plasticity
Microscale
Phase Field Modeling
Kinetic Monte Carlo
Molecular Dynamics
DFT
Schrödinger Eq:
$\left[\sum_{i=1}^{N} -\frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i,j=1}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots) = E\,\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \dots)$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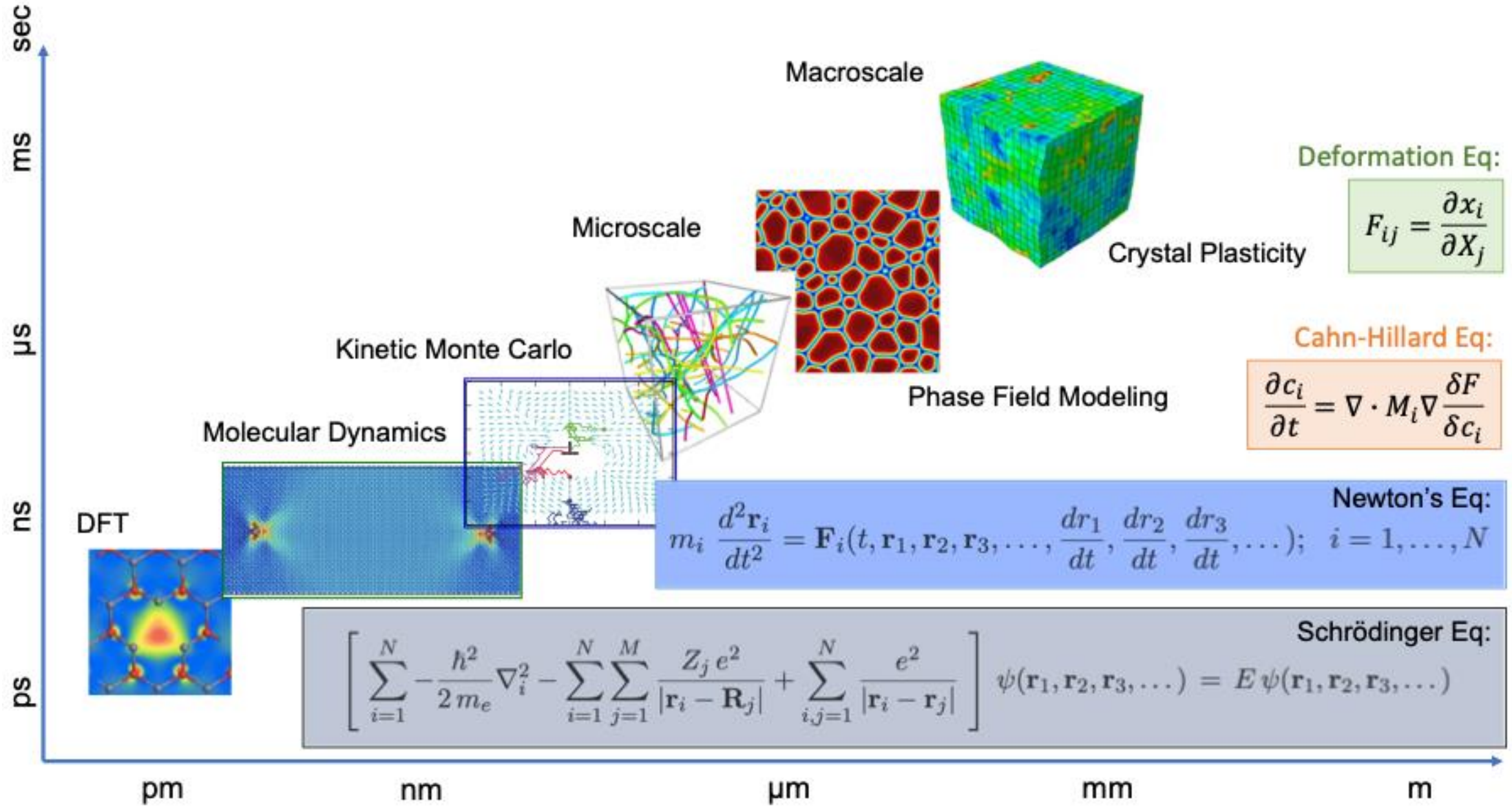
Macroscale
Crystal Plasticity
Microscale
Phase Field Modeling
Kinetic Monte Carlo
Molecular Dynamics
DFT
Newton's Eq:
$m_i \frac{d^2\mathbf{r}_i}{dt^2} = \mathbf{F}_i(t, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \frac{dr_1}{dt}, \frac{dr_2}{dt}, \frac{dr_3}{dt}, \ldots); \quad i = 1, \ldots, N$
Schrödinger Eq:
$\left[\sum_{i=1}^{N} -\frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i=1}^{N}\sum_{j=1}^{M} \frac{Z_j e^2}{|\mathbf{r}_i - \mathbf{R}_j|} + \sum_{i,j=1}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots) = E\,\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots)$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Macroscale
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$F_{ij} = \frac{\partial x_i}{\partial X_j}$
Cahn-Hillard Eq:
$\frac{\partial c_i}{\partial t} = \nabla \cdot M_i \nabla \frac{\delta F}{\delta c_i}$
Newton's Eq:
$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i(t, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, \ldots, \frac{dr_1}{dt}, \frac{dr_2}{dt}, \frac{dr_3}{dt}, \ldots); \quad i = 1, \ldots, N$
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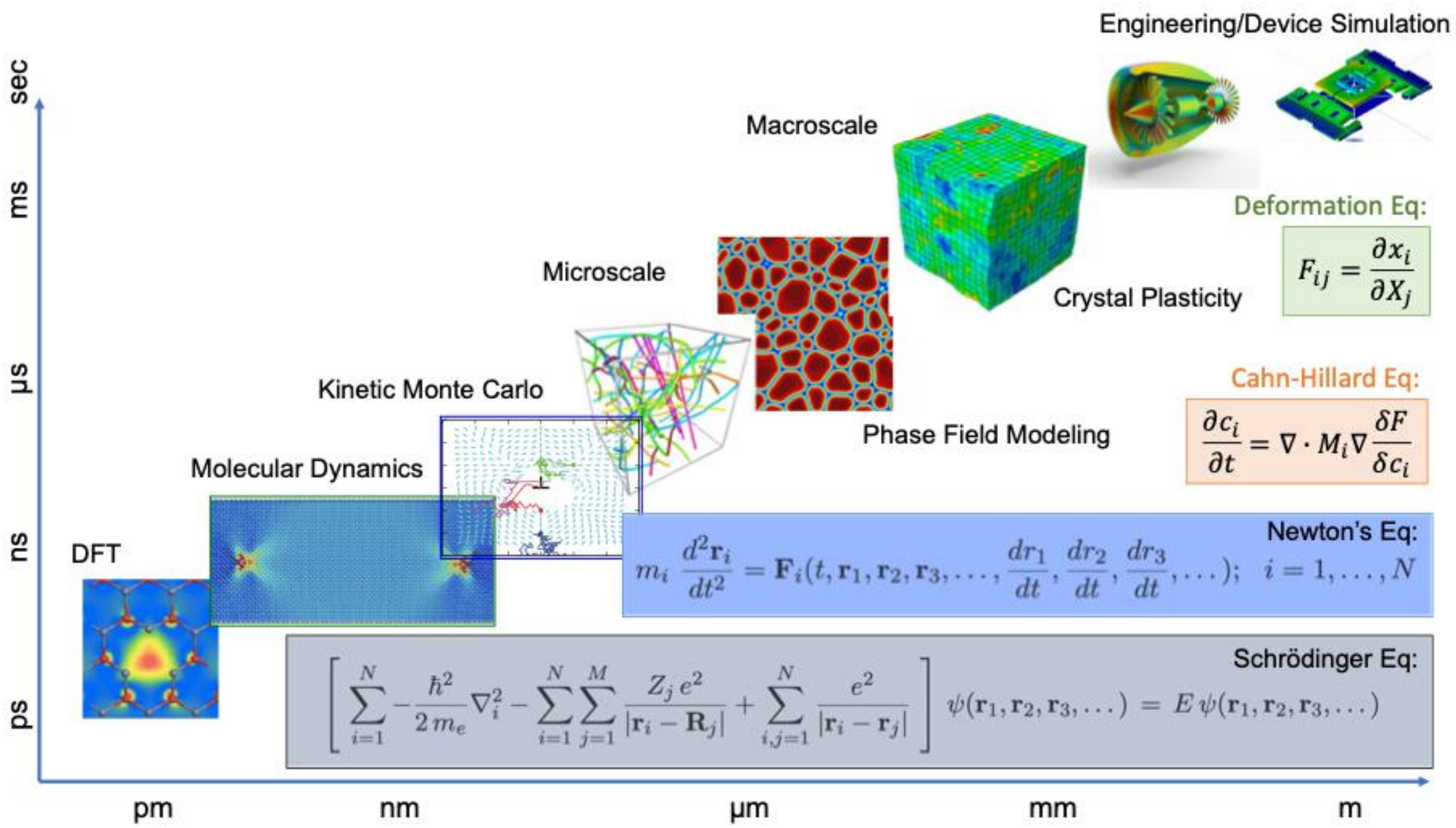
Engineering/Device Simulation
Macroscale
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sec
ms
μs
ns
ps
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nm
μm
mm
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Syllabus

Computational Linear algebra (Numerical Methods)

- Linear System of Equations (Gauss Elimination, LU Decomposition, etc.)
- Finding roots/Non-linear Equations (Bisection, Newton-Raphson, Secant Method, etc.)

Numerical methods for solving partial differential equations (PDE)

- Conservation Equations (Mass Transfer, Heat Transfer, etc.)
- Numerical Differentiation/Finite difference methods
- Boundary conditions

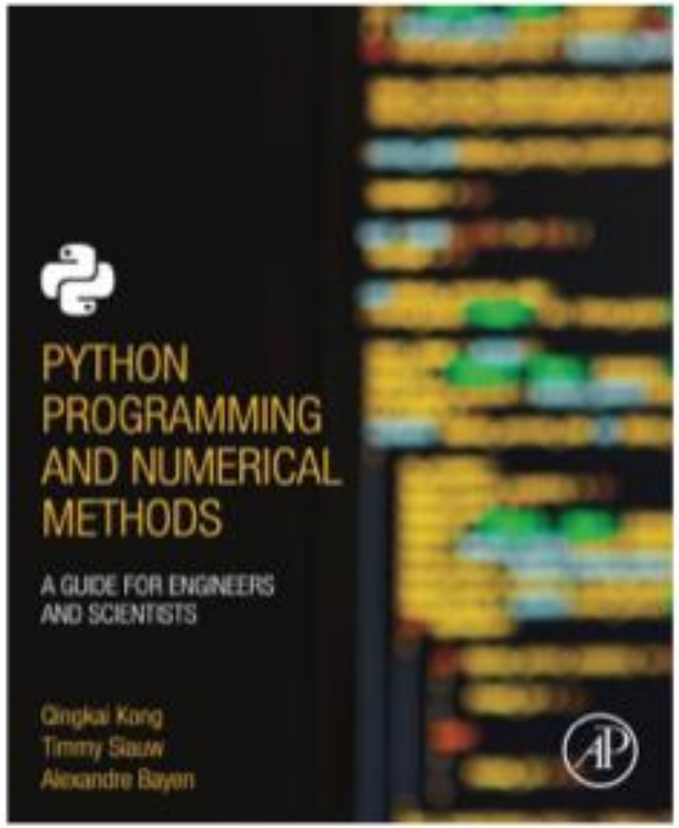
Fourier Methods

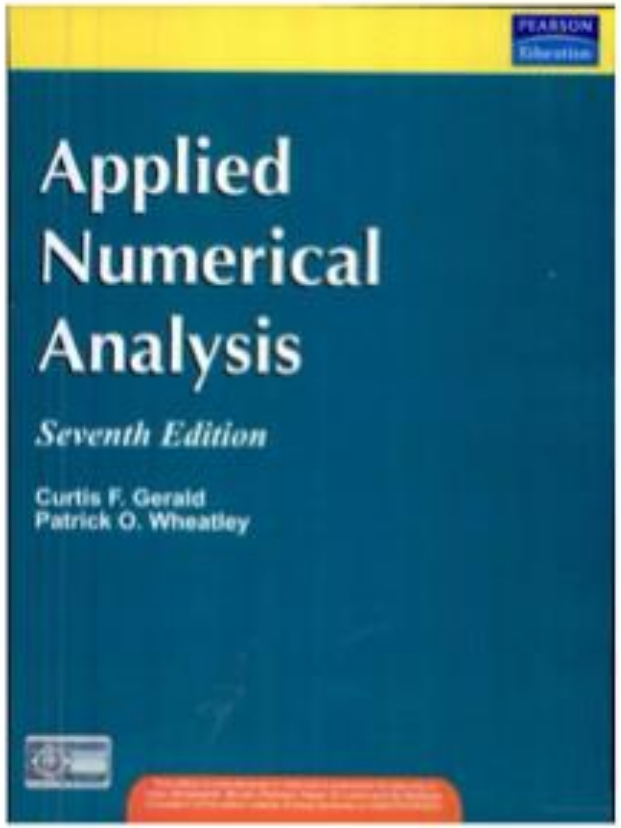
- Periodic functions and Fourier Transform
- Concept of Reciprocal space

Computational Methods: Time and length scales

- Solving Schrodinger Equation
- Solving Newton equation of motion
- Monte Carlo Method

Textbooks


PYTHON PROGRAMMING AND NUMERICAL METHODS
A GUIDE FOR ENGINEERS AND SCIENTISTS
Qingkai Kong
Timmy Siauw
Alexandre Bayen
AP


PEARSON
Applied Numerical Analysis
Seventh Edition
Curtis F. Gerald
Patrick O. Wheatley

Evaluations

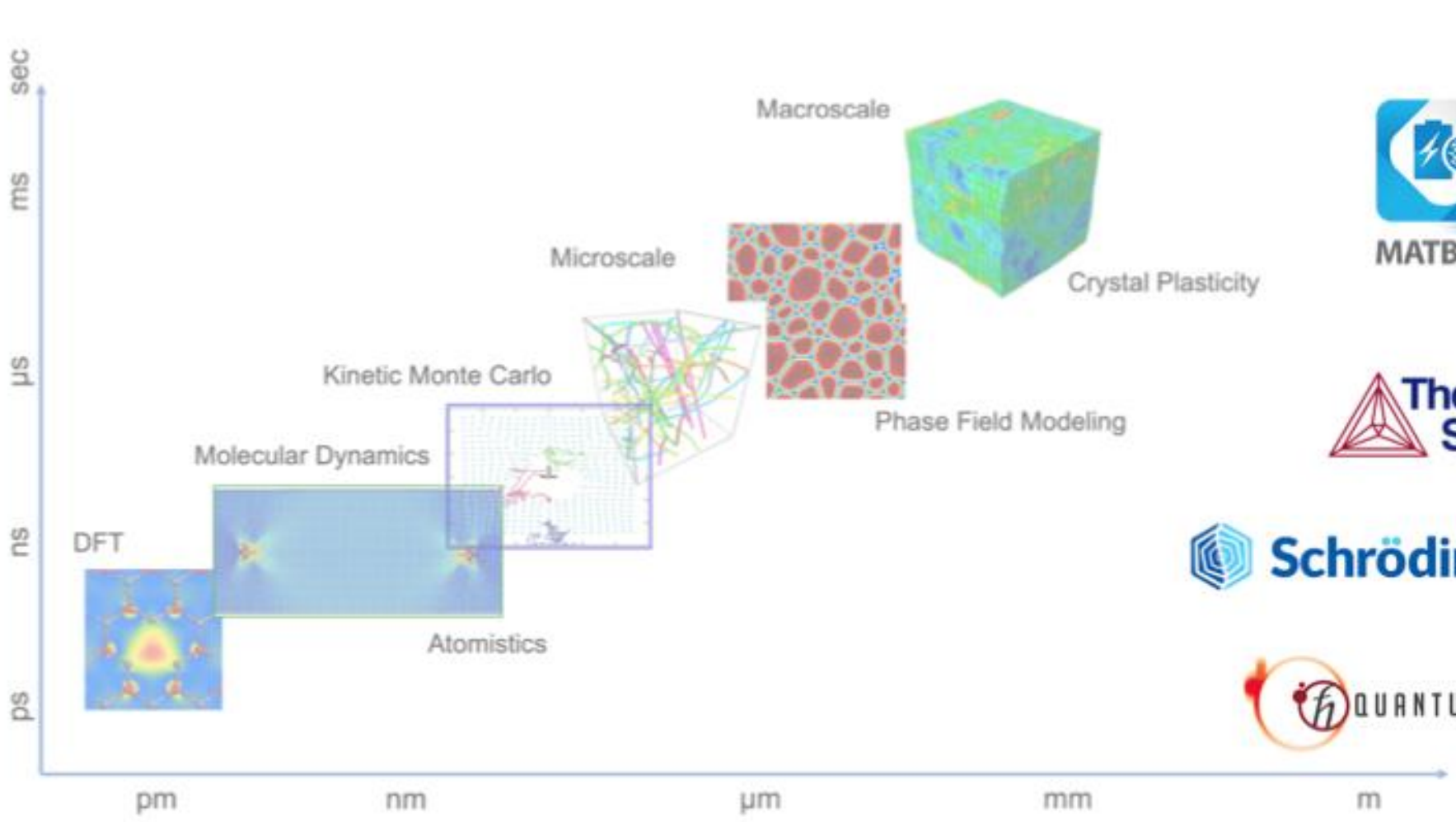
Class Presence & Discussion = 10%

Originality & Ethics = 15%

Assignments & Quizzes = 75%

Office hours: Tuesdays (1:30 – 2:30 pm)

Growing Computational Packages and Companies …

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