Challenges For Multiscale Modeling of Fusion Materials

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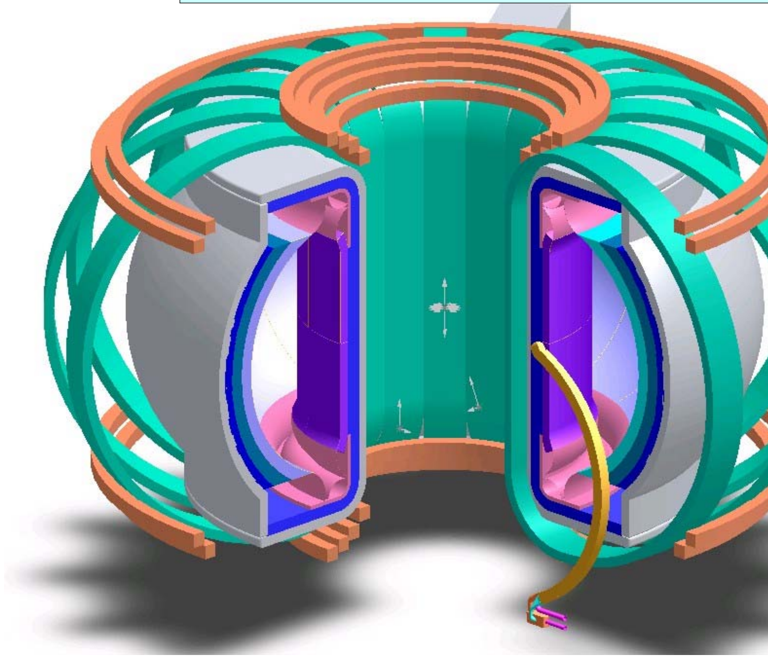
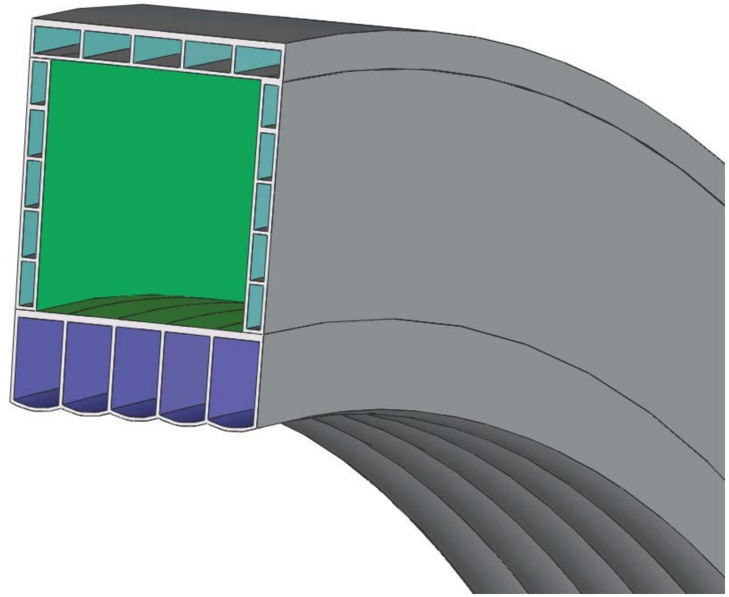
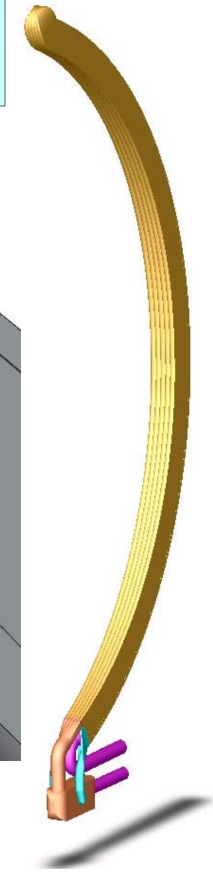
Outline

- Approach and Materials Environment;
- Surface and Bulk Phenomena;
- Plasma Physics – Materials Science Analogies;
- Multi-scale Modeling Strategy;
- Fundamental Equations and Algorithms;
- Modeling Challenges and Limitations.

Approach and Materials Environment







Environment

- *Heat Flux: FW ~1 MW/m^2; Divertor ~5 –15 MW/m^2*
- *Neutron Flux: ~ 3 – 5 MW/m^2*
- *Particle Flux: Divertor ~10^{21}-10^{22} $m^{-2}s^{-1}$ Mechanical Loads: Pressure ~ 2-5 MPa*

Approach

- *Predictive;*
- *Physics-Based;*
- *Computational Design of Materials;*
- *Experimentally-verifiable at Scale Interfaces.*

Surface Phenomena

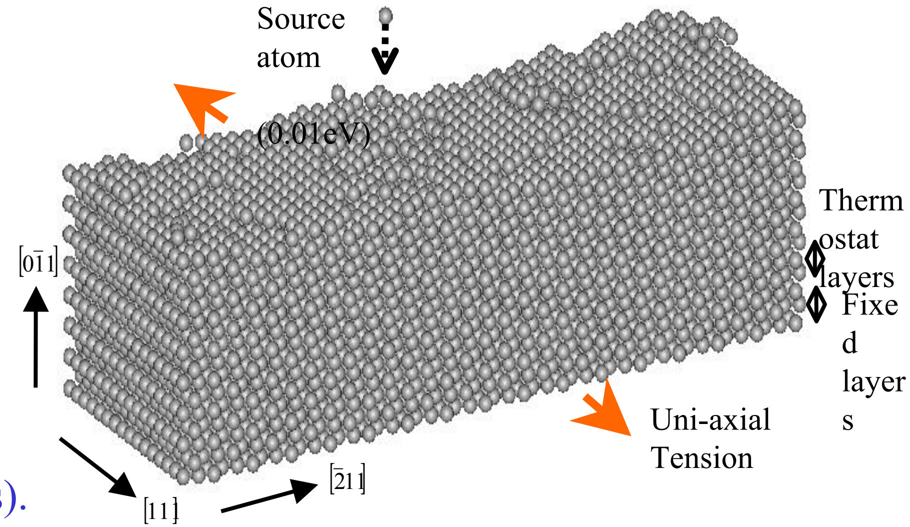
High Heat Flux/ Particle Flux result in:

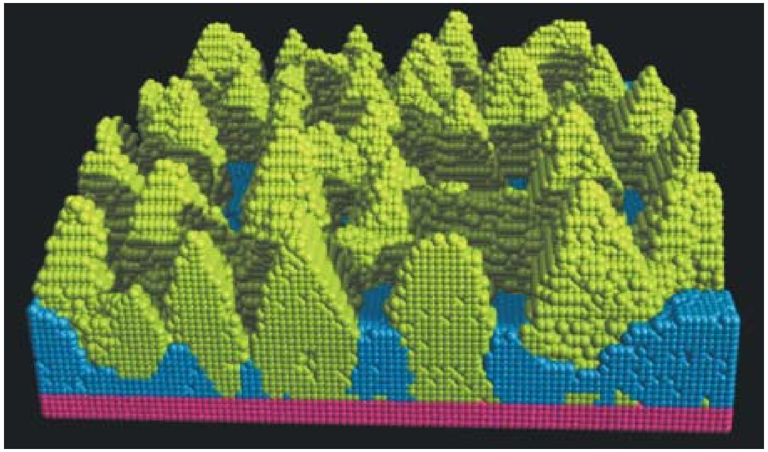
Short timescale phenomena (e.g. $10^{-12} – 10^{-9}$ s):

- ❑Sputtering;
- ❑Implantation of helium and tritium;
- ❑Re-deposition and tritium co-deposition;
- ❑Near-surface damage (collision cascades).

Long timescale phenomena (e.g. $10^{-3} – 10^{6}$ s):

- ❑Atomic transport (e.g diffusion, trapping, adsorption, recombination and desorption);
- ❑Surface roughening and re-structuring;
- ❑Microstructure and phase evolution (e.g. voids, bubbles, dislocations, grains & new phases).





Surface Re-structuring after re-deposition.

H. Huang, RPI

Bulk Phenomena

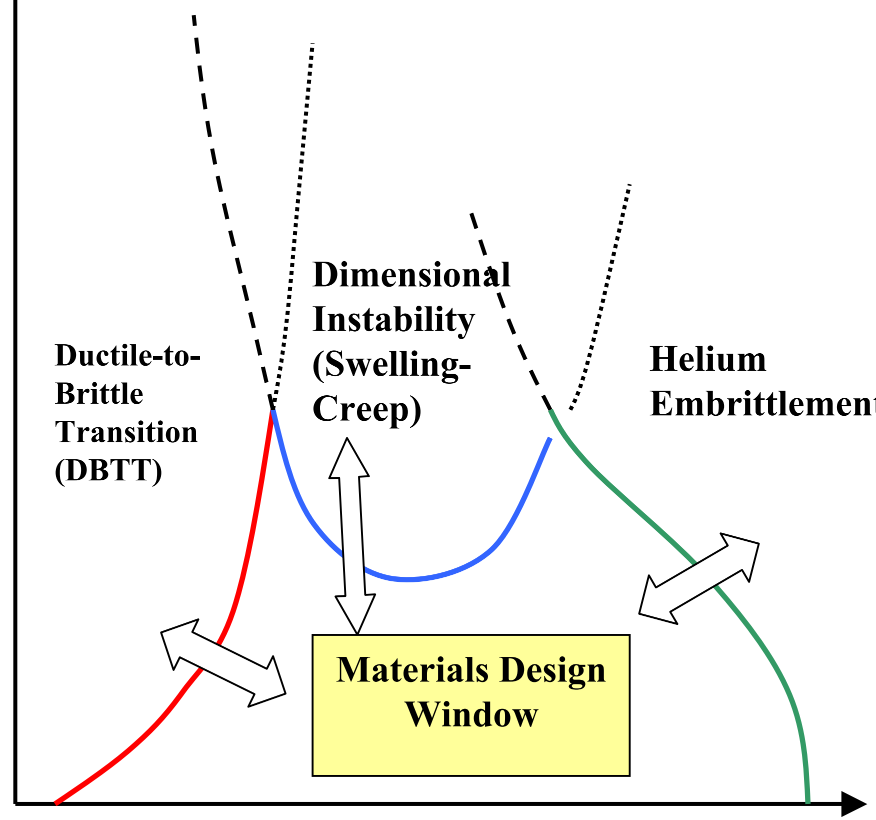
High Heat Flux/ Neutron flux/ Mechanical Loads result in:

<u>Short timescale phenomena (e.g. $10^{-12} – 10^{-9}$ s):</u>

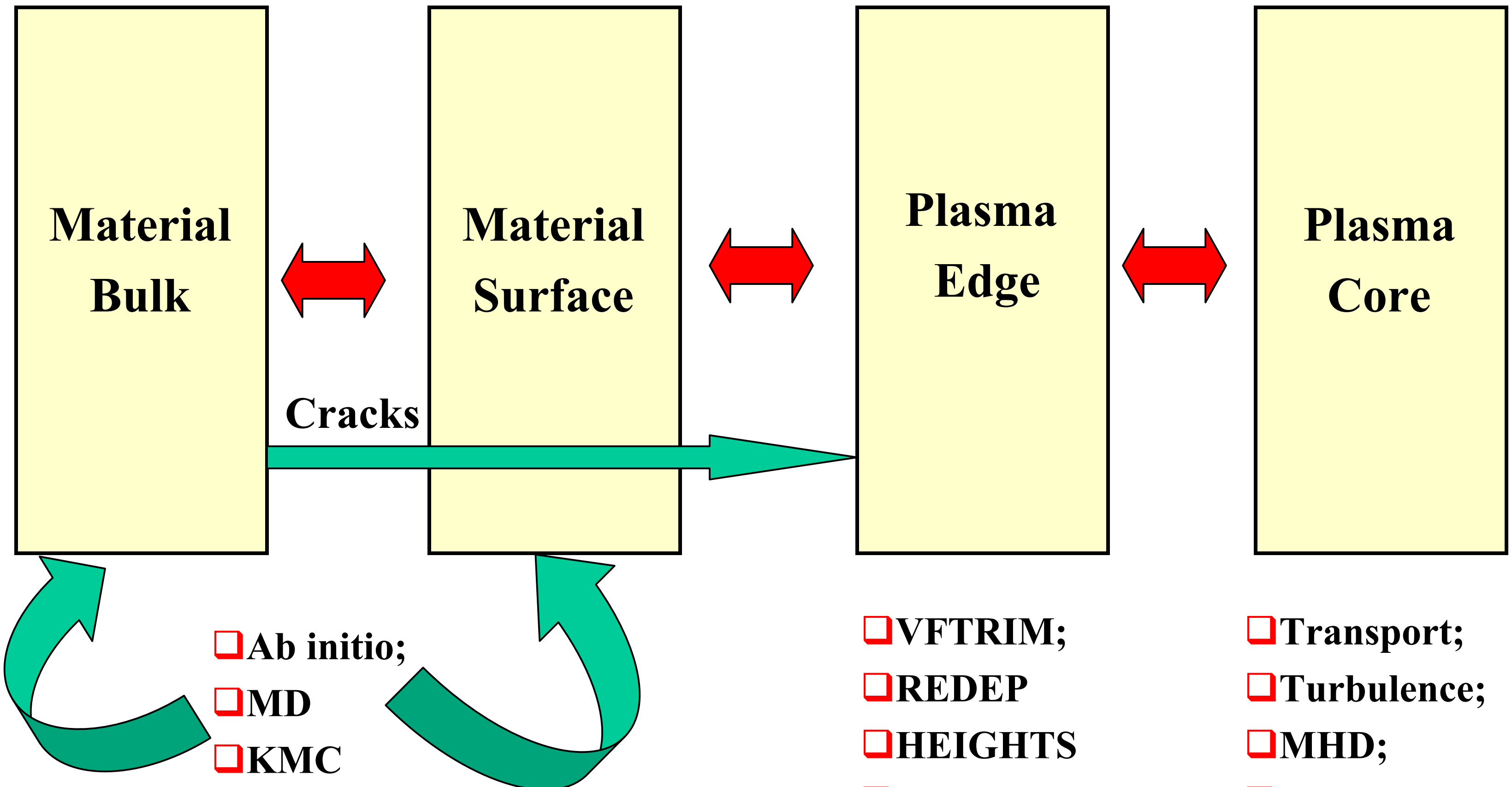
- ❑Atomic Displacements;
- ❑Fast Transport;
- ❑Lattice Defects (Vacancies and Interstitials).

<u>Long timescale phenomena (e.g. $10^{-3} – 10^{6}$ s):</u>

- ❑Microstructure Evolution (Voids, Bubbles, Dislocations, Phases);
- ❑Dimensional Instabilities (Swelling and Creep);
- ❑Shear Bands (Localized plasticity);
- ❑Helium Embrittlement.



Material-Plasma Interfacing



- ❑Ab initio;
- ❑MD
- ❑KMC
- ❑DD
- ❑Rate Theory
- ❑FEM

- ❑VFTRIM;
- ❑REDEP
- ❑HEIGHTS
- ❑BPHI-3D
- ❑UEDGE-2D

- ❑Transport;
- ❑Turbulence;
- ❑MHD;
- ❑Confinement;
- ❑Islands, Stability & Oscillations.

Correspondence & Analogy

Phenomenon	Plasma	Material
Density & Degrees of Freedom per cm^3	❑10^{14} - 10^{16}	❑10^{23}
Forces	❑***Long-range***: Coulomb, Electromagnetic	❑***Short-range***: Atomic > Pair, Many-body ❑***Long-range***: Elastic
Particle Methods	❑Particle-Particle (P-P); ❑Particle-Field (PIC); ❑KMC	❑Particle-Particle (MD); ❑Particle-Field (DD-FEM); ❑KMC, Lattice MC, Event MC.
Transport & Continuum	❑Collisions & Fokker-Planck; ❑Fluid, MHD ❑Reaction Cross-sections; ❑Turbulence	❑ Microstructure Evolution & Fokker-Planck*; ❑Elasticity; ❑Rate Theory; ❑Plasticity
Instabilities	❑***Space***: Islands, Coherent Structures; ❑***Time:*** Oscillations, Disruptions	❑***Space***: Self-organization, segregation; ❑***Time:*** shear bands, cracks.

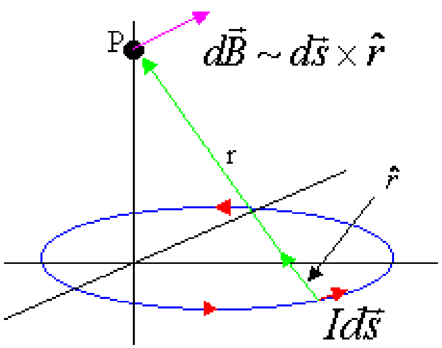
*H. Huang and N.M. Ghoniem, "Formulation of a Moment Method for n-dimensional Fokker-Planck Equations", *Phys. Rev. E*, **51, 6**: 5251-5260, 1995.

Correspondence & Analogy

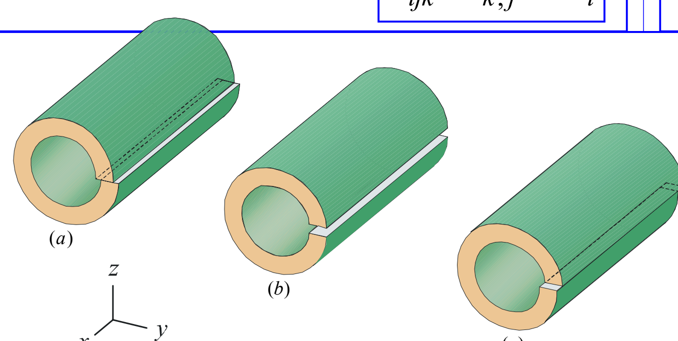
Bio-Savart

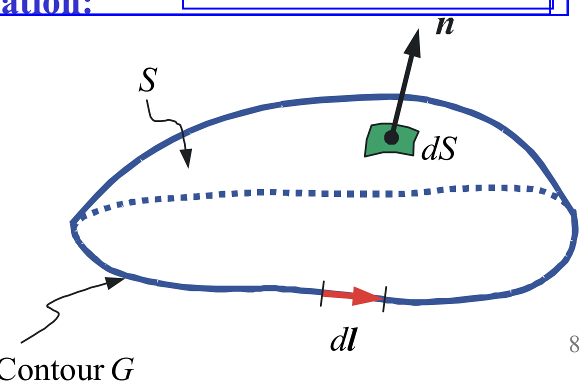
$$d\vec{B} = \frac{\mu_o}{4\pi} \frac{Id\vec{s} \times \hat{r}}{r^2}$$

$$\vec{B} = \frac{\mu_o I}{4\pi} \oint \frac{d\vec{s} \times \hat{r}}{r^2}$$

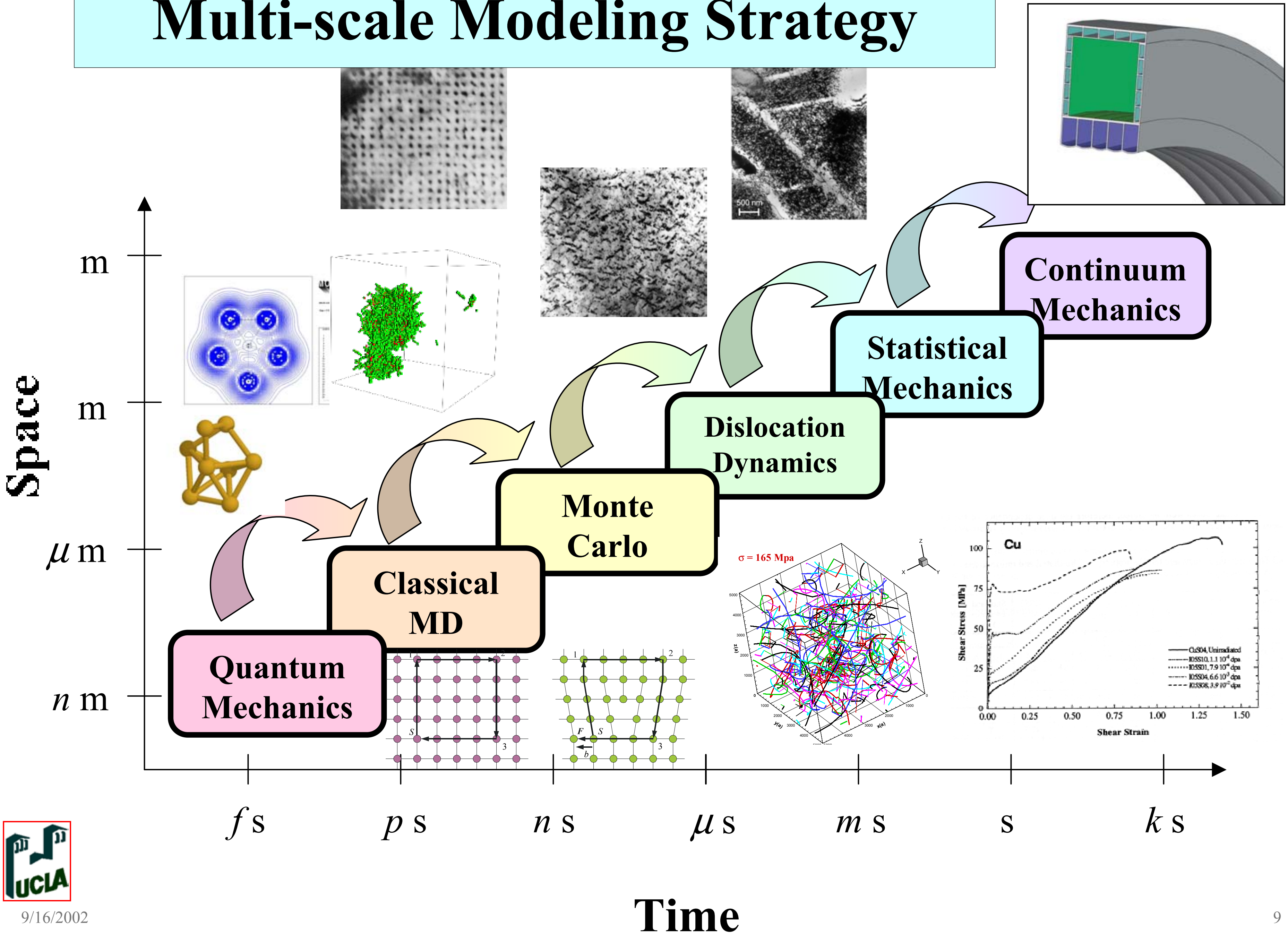


Electromagnetics		Dislocation Dynamics	
Magnetic intensity	H_i	Strain	ε_{ij}
Magnetic induction	B_i	Stress	σ_{ij}
Current density	J_i	Incompatibility tensor	η_{ij}
Permeability	μ	Elastic constants	$E,\ \nu$
Vector potential	A_i	Stress function	χ_{ij}
Current	I	Burgers vector	b_i
Maxwell's Equation:	$\in_{ijk} H_{k,j} = J_i$	Incompatibility Equation:	$-\in_{ikl}\in_{jmn} \varepsilon_{nl,km} = \eta_{ij}$





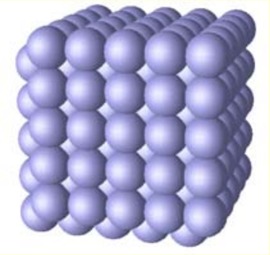
Multi-scale Modeling Strategy



Atomistic Simulations*

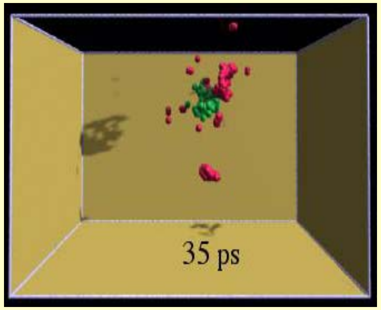
First-principles

(<200 atoms,<10ps)



- Start from Schroedinger's Equation;
- Approximate: DFT;
- Accurate energetics of point defects and defect clusters

Molecular dynamics



- Empirical Potentials;
- Initial defect distribution;
- Verlet or predictor-corrector;
- time-step ~ 1 fs;
- Short-range forces;
- Parallelization by spatial decomposition with MPI.
- (1-100 million atoms, < 100 ns)

KMC (<µm,<ms)

- Freeze atomic degrees of Freedom;
- Track defects only;
- Microstructure evolution of defects
- Spatial inhomogeneity.

* Srolovitz and Carr - Princeton

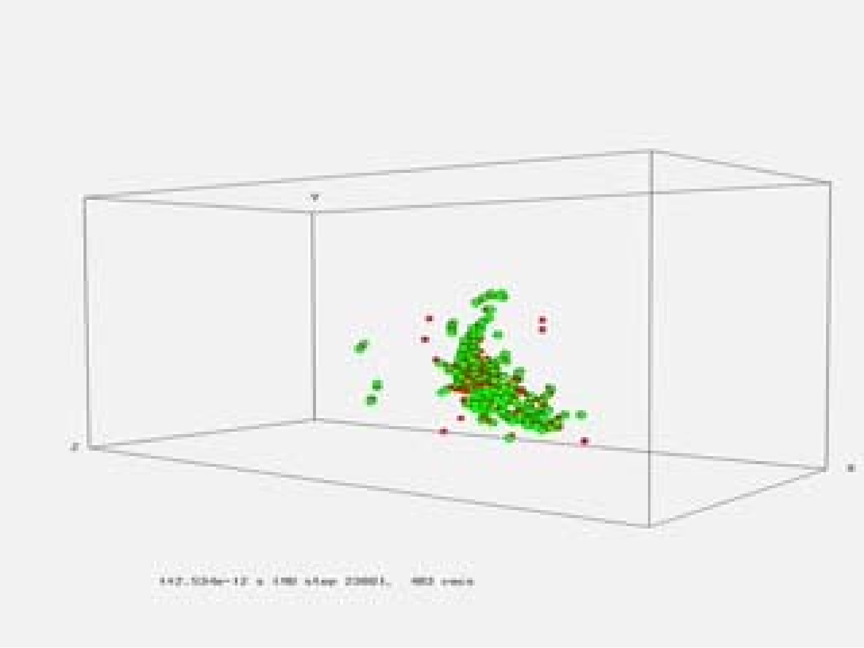
Interatomic Potentials and MD Simulations

$$\mathcal{H}\Phi\{R_I, r_i\} = E_{tot}\Phi\{R_I, r_i\}$$

$$\mathcal{H} = \sum \frac{P_I^2}{2M_I} + \sum \frac{Z_I Z_J e^2}{R_{IJ}} + \sum \frac{p_i^2}{2me} + \sum \frac{e^2}{r_{ij}} - \sum \frac{Z_I e^2}{|R_I - r_i|}$$

- Born-Oppenheimer: Adiabatically eliminate nuclear degrees of freedom. Solve only for electrons.
- Kohn-Sham-Hohenberg: Density Functional Theory (DFT) reduces to the single electron quantum problem, with effective potentials.
- Exchange-Correlation potentials are approximated with the Local Density Approximation (LDA).
- Using DFT-LDA material properties have been calculated without input.

Stoller, ORNL



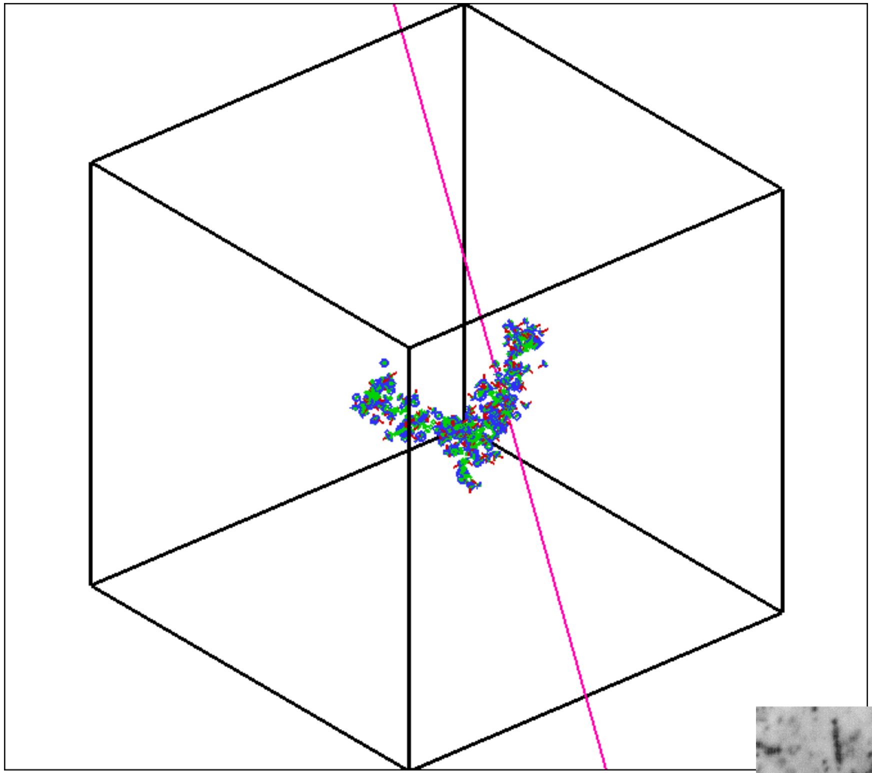
$$\frac{d^2 R_I}{dt^2} = F_I = -\frac{dV}{dR_I}, \qquad \mathcal{H} = \sum \frac{P_I^2}{2M_I} + V(R_I)$$

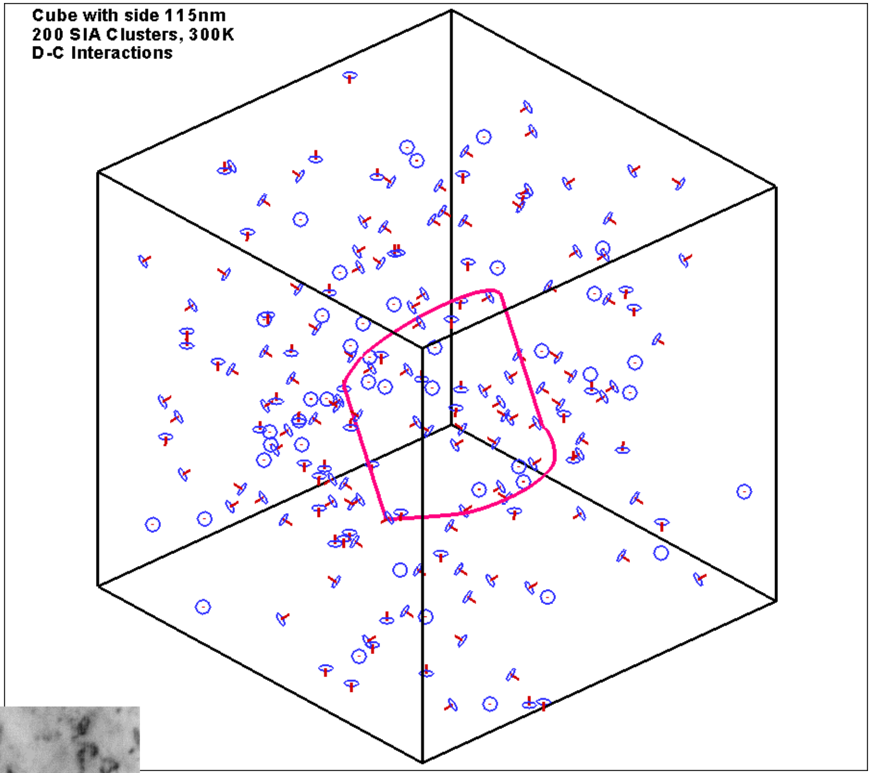
$$E = \sum_i \left\{ F_i(\bar{\rho}_i) + \sum_{j \neq i} \frac{1}{2}\Phi_{ij}(r_{ij}) \right\} \qquad F_i = A_i E_i^0 \bar{\rho}_i \ln \bar{\rho}_i$$

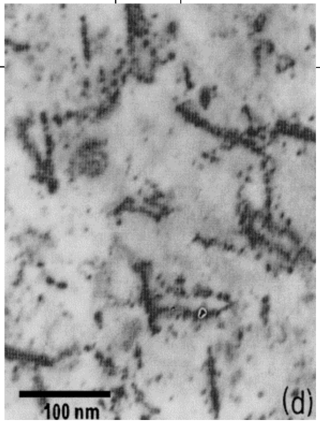
Quantum MD → **Bond-order Potentials**

Classical MD with Empirical Potentials

Dislocation-Microstructure Interaction: KMC Modeling of Pinning and Rafting





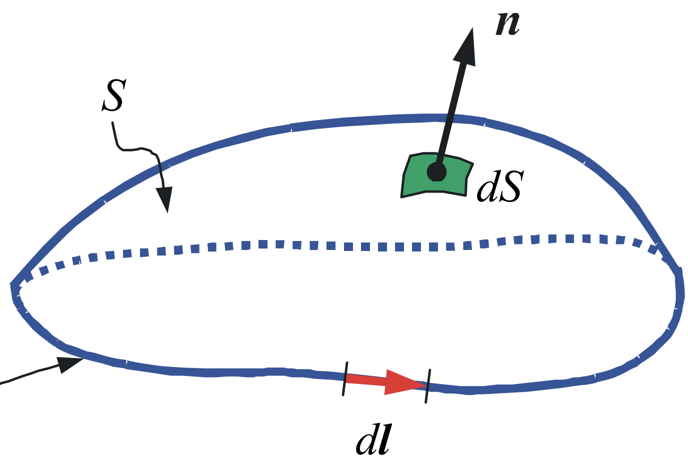


Mesoscopic Simulations: Dislocation Dynamics

Covariant Vectors

$$(\mathbf{a}_1 = \mathbf{e},\ \mathbf{a}_2 = \mathbf{t},\ \mathbf{a}_3 = \mathbf{b})$$

$$\mathbf{e} = \frac{\mathbf{R}}{R} \qquad \mathbf{t} = \frac{\mathbf{T}}{T} \qquad \mathbf{T} = \frac{d\mathbf{l}}{dw}$$



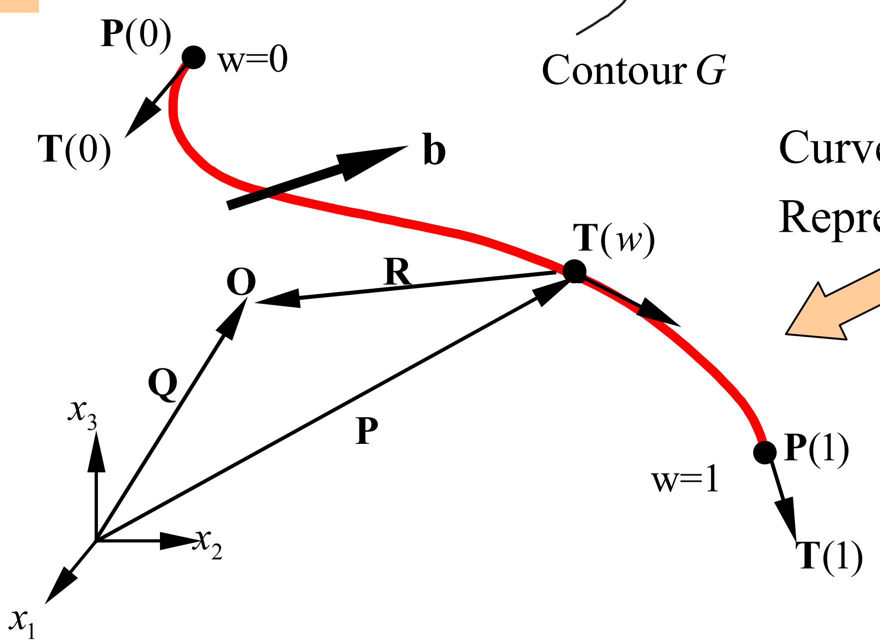
Contravariant Vectors

$$\mathbf{a}^1 = \frac{1}{2\pi V}(\mathbf{a}_2 \times \mathbf{a}_3)$$

$$\mathbf{a}^2 = \frac{1}{2\pi V}(\mathbf{a}_3 \times \mathbf{a}_1)$$

$$\mathbf{a}^3 = \frac{1}{2\pi V}(\mathbf{a}_1 \times \mathbf{a}_2)$$

$$V = (\mathbf{a}_1 \times \mathbf{a}_2) \cdot \mathbf{a}_3$$



Curved dislocation segment
Represented by a spline

Differential Forms of DD are analogous to Electromagnetics, but of higher dimensionality

Bio-Savart

$$d\vec{B} = \frac{\mu_o}{4\pi}\frac{Id\vec{s}\times\hat{r}}{r^2}$$

Displacement

$$\frac{d\mathbf{u}}{dw} = \frac{T}{4R}\left\{\frac{(\mathbf{s}\times\mathbf{a}_1)\cdot\mathbf{a}_2}{\pi(1+\mathbf{s}\cdot\mathbf{a}_1)}\mathbf{a}_3 + \frac{V}{1-\nu}\left[(1-2\nu)\mathbf{a}^1\right] + \frac{1}{2\pi}\mathbf{a}_1\right\}$$

Stress

$$\frac{d\boldsymbol{\sigma}}{dw} = \frac{\mu VT}{2R^2}\left\{\frac{1}{1-\nu}\left(\mathbf{a}^1\otimes\mathbf{a}_1 + \mathbf{a}_1\otimes\mathbf{a}^1\right) + \left(\mathbf{a}^2\otimes\mathbf{a}_2 + \mathbf{a}_2\otimes\mathbf{a}^2\right) - \frac{1}{2\pi(1-\nu)}\left(\mathbf{a}_1\otimes\mathbf{a}_1 + \mathbf{I}\right)\right\}$$

Interaction Energy

$$\frac{dE_{\text{int}}}{dw_I dw_{II}} = -\frac{\mu T_I T_{II}}{4\pi R}\left[\begin{array}{l}(\mathbf{a}_2^I\cdot\mathbf{a}_3^I)(\mathbf{a}_2^{II}\cdot\mathbf{a}_3^{II}) - \frac{1}{1-\nu}(\mathbf{a}_2^I\cdot\mathbf{a}_2^I)(\mathbf{a}_3^I\cdot\mathbf{a}_3^I) \\ + \frac{2\nu}{1-\nu}(\mathbf{a}_2^{II}\cdot\mathbf{a}_3^I)(\mathbf{a}_2^I\cdot\mathbf{a}_3^{II}) - \frac{1}{1-\nu}(\mathbf{a}_2^I\cdot\mathbf{a}_2^{II})(\mathbf{a}_3^I\cdot\mathbf{a}_1)(\mathbf{a}_3^{II}\cdot\mathbf{a}_1)\end{array}\right]$$

Weak Variational Form for DD Equations of Motion

Equations of Motion

$$\int_{\Gamma} \left(f_k^t - BV_k \right) \delta r_k ds = 0$$

$$\mathbf{V} = \frac{d\mathbf{r}}{dt}$$

$$\mathbf{f} = \mathbf{f}_{P-K} + \mathbf{f}_{self} + \mathbf{f}_{others}$$

Define:

$$\mathbf{r}^* = \frac{\mathbf{r}}{a}$$

$$\mathbf{f}^* = \frac{\mathbf{f}}{\mu a}$$

$$t^* = \frac{\mu t}{B}$$

Final Equation of Motion

$$\mathbf{K} \frac{d\mathbf{Q}}{dt^*} = \mathbf{F}$$

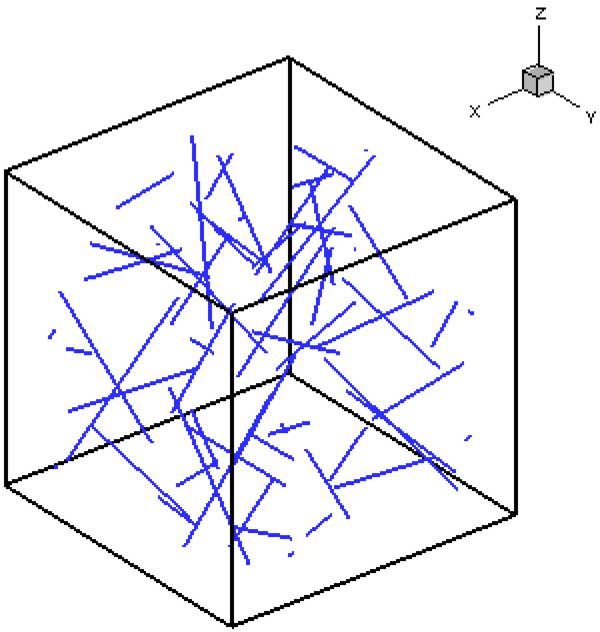
$$\mathbf{Q} = \left[\mathbf{P}_1, \mathbf{T}_1, \mathbf{P}_2, \mathbf{T}_2 \right]$$

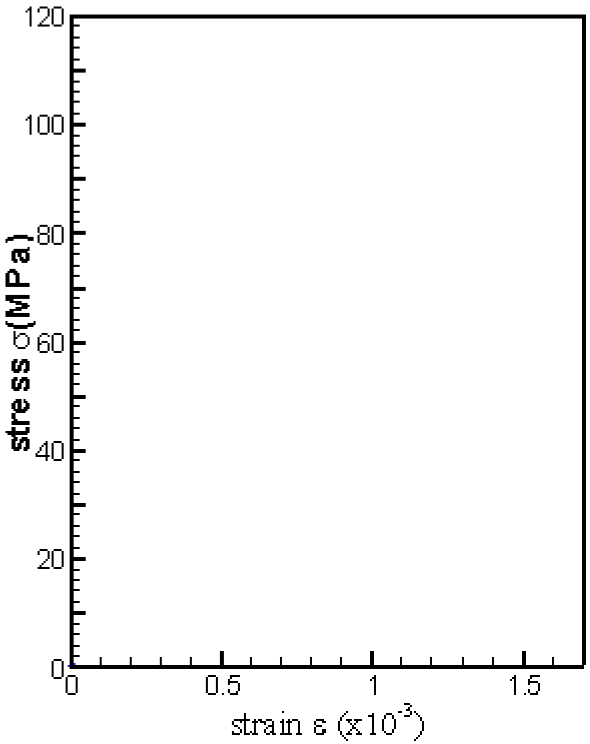
Q=Nodal coordinate vector

F=Nodal Forces

K=Mobility Matrix

Mesoscopic Simulations of Plasticity





One micron

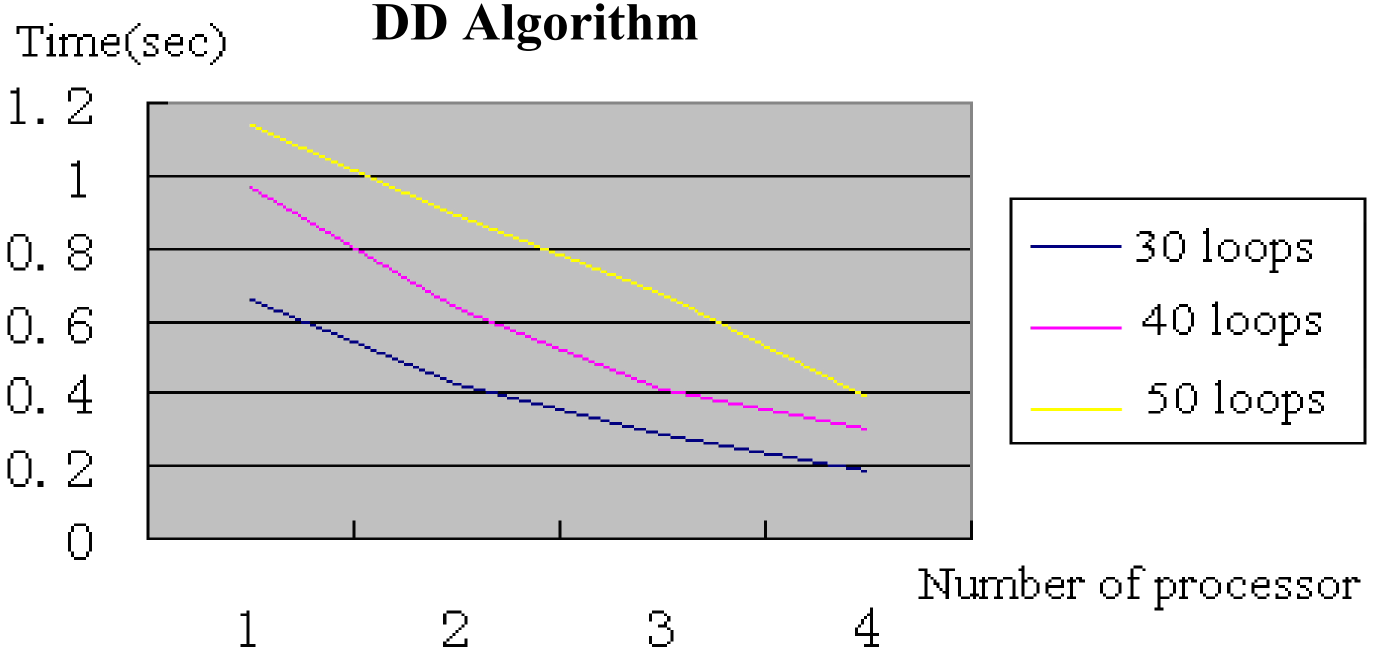
Parallel Dislocation Dynamics Code Algorithm Description

- Similar to the N-body problem in plasma & astrophysics;
- Hierarchical tree representation can be utilized in the DD code.
- The Major difference is that dislocation lines are irregular filaments & not particles.
- Far-field interaction is approximated by multipole expansions.
- Hierarchical tree-based methods reduce the computational complexity from O(N*N) to O(N log(N)) or even O(N) .
- Special techniques are used to maintain load balancing and reduce communications between computer cluster nodes.

1. Jaswinder Pal Singh, et al. *J. Parallel and Distributed Computing. 1995; 27:118.*
2. Ananth Y. Grama, et al. *SIAM Conference on Parallel Processing*, San Francisco, 1994.
3. H.Y. Yang, and R. LeSar. *Philosophical Magazine A, 1995; 71(1):149.*

DD & KMC Parallel Algorithms work well for a small number of processors

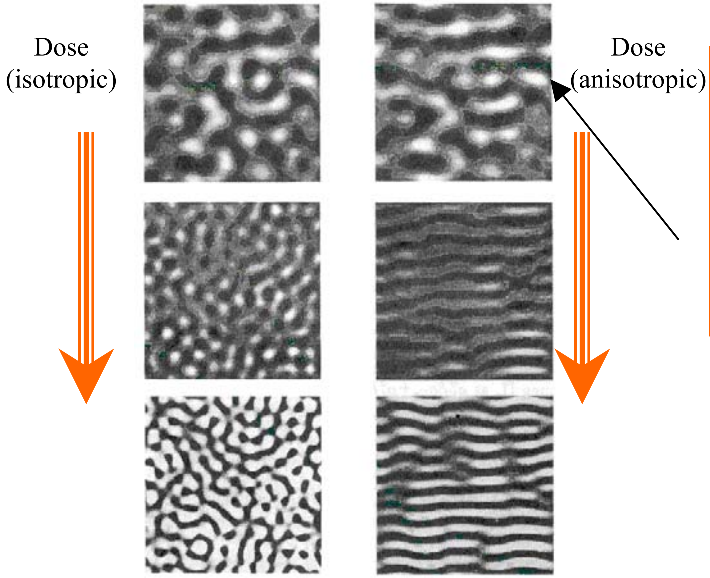
DD Algorithm



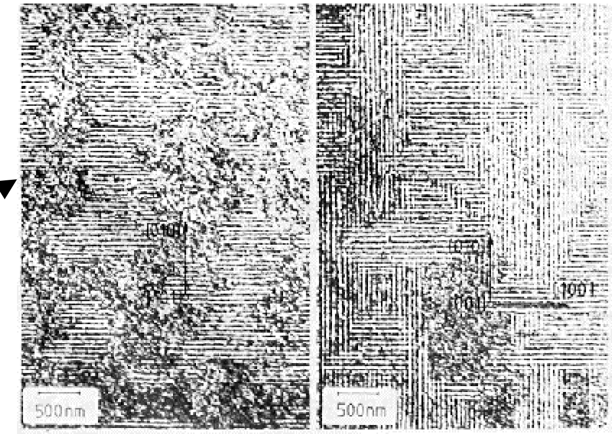
KMC Algorithm

# of processors	1	2	3	4	8	16
Time (s)	**897.6**	**449.9**	**327.3**	**237.8**	**135.1**	**78.1**

Continuum Modeling of Microstructure Instabilities and Self-Organization



Simulations & experiments on self-organization of irradiated Cu microstructure.



Ginzburg-Landau Dynamics Give Amplitude Equation for Patterns; bc= critical bifurcation Parameter

$$\tau_0 \partial_t A_i = \left[\frac{b-b_c}{b_c} - 4(\mathbf{q}_i \cdot \nabla)^2\right] A_i + v \Sigma_{j,k} \bar{A}_j \bar{A}_k - 3u A_i\left(|A_i|^2 + 2\Sigma_{j\neq i}|A_j|^2\right),$$

Continuum Rate Equations for concentrations

$$\partial_t c_i = K(1-\epsilon_i) - \alpha c_i c_v + D_i \nabla^2 c_i - D_i c_i (Z_{iN}\rho_N + Z_{iV}\rho_V + Z_{iI}\rho_I),$$

$$\partial_t c_v = K(1-\epsilon_v) - \alpha c_i c_v + D_v \nabla^2 c_v - D_v[Z_{vN}(c_v - \bar{c}_{vN})\rho_N + Z_{vV}(c_v - \bar{c}_{vV})\rho_V + Z_{vI}(c_v - \bar{c}_{vI})\rho_I],$$

$$\partial_t \rho_I = \left[\frac{2\pi N}{|\mathbf{b}|}\right][\epsilon_i K + D_i Z_{iI} c_i - D_v Z_{vI}(c_v - \bar{c}_{vI})],$$

$$\partial_t \rho_V = \frac{1}{|\mathbf{b}| r_V^0}\{\epsilon_v K - \rho_V[D_i Z_{iV} c_i - D_v Z_{vV}(c_v - \bar{c}_{vV})]\}$$