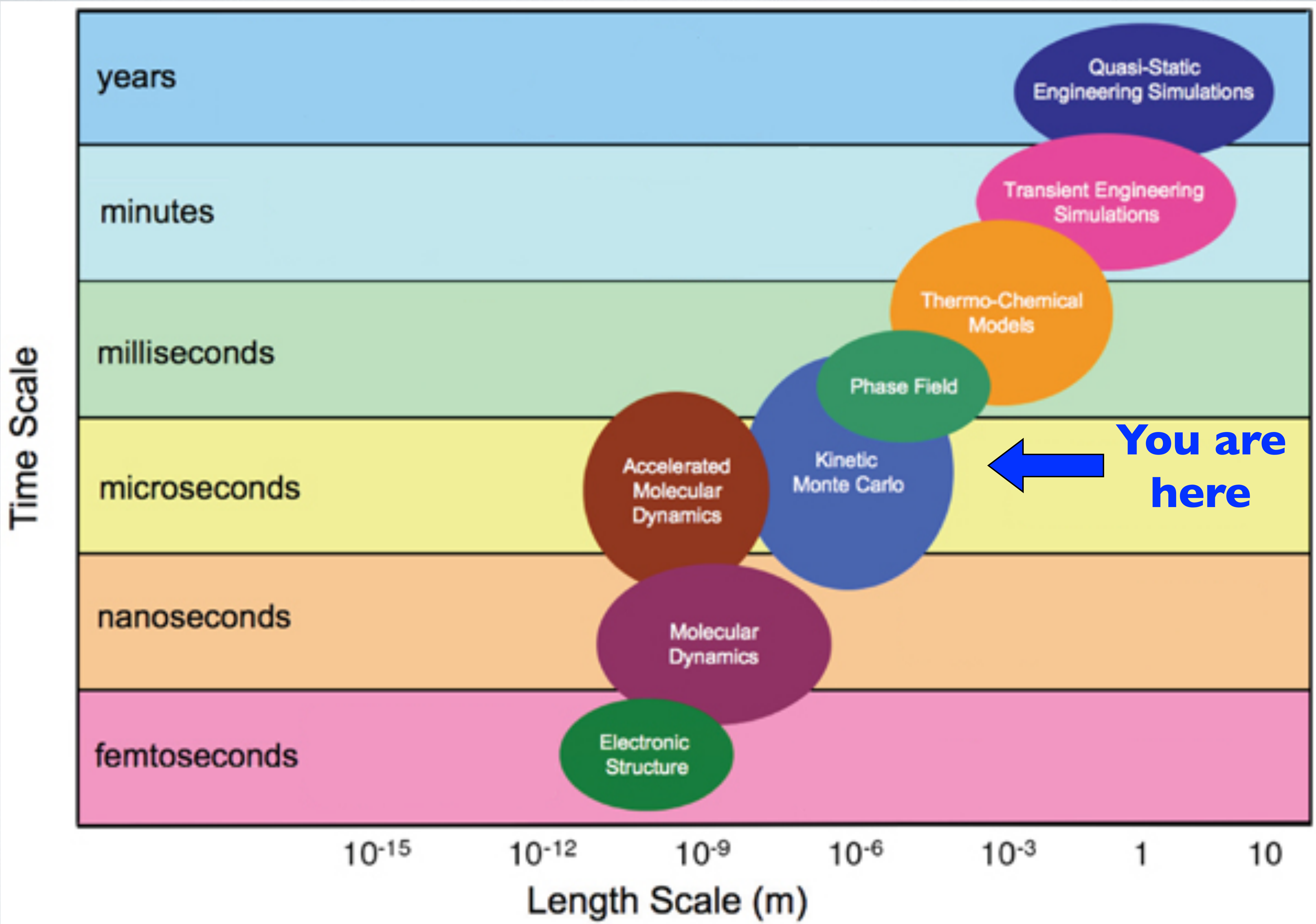
MODULE 3: DISLOCATION DYNAMICS

Principles and Theory

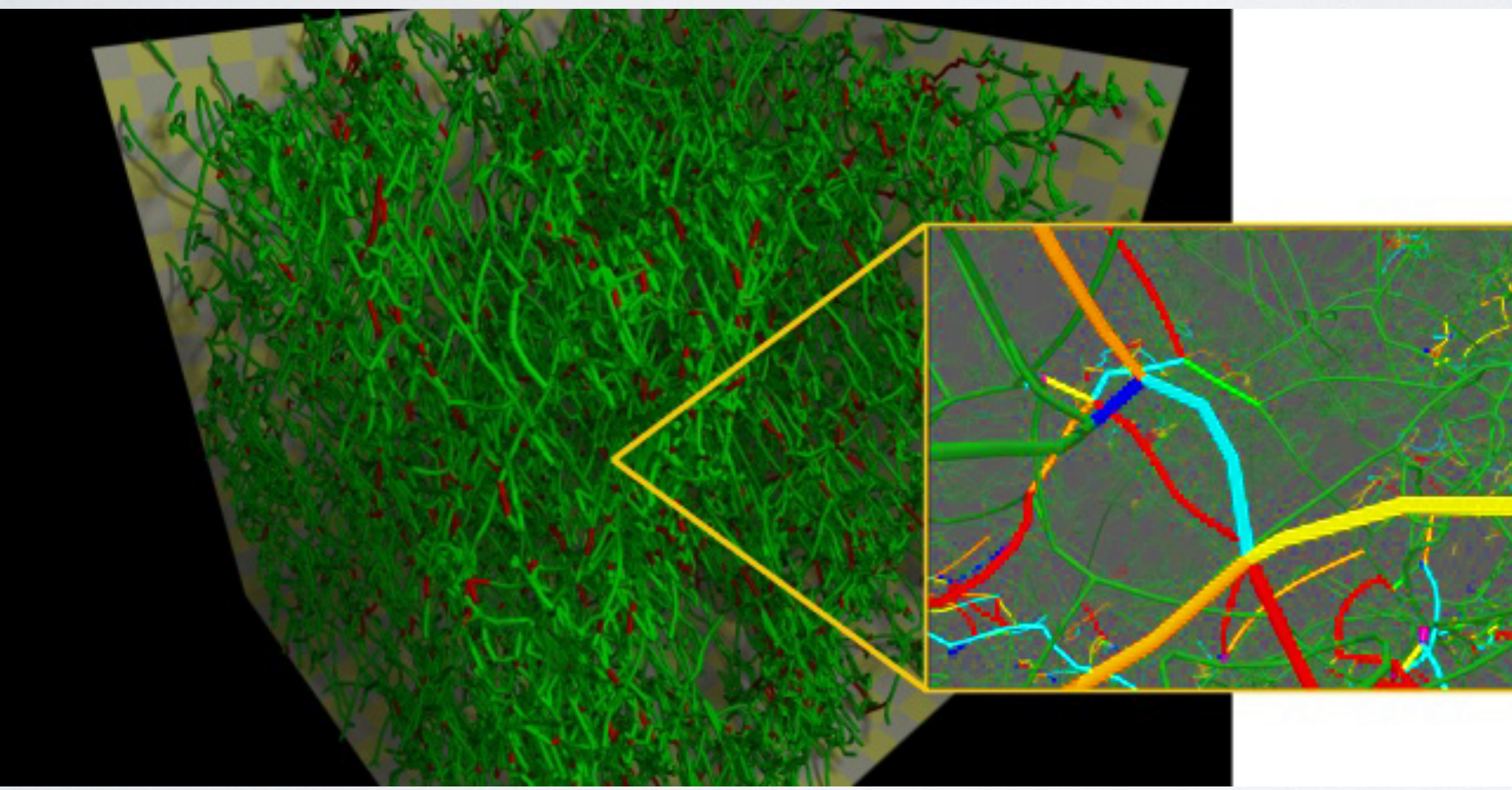
I. Introduction

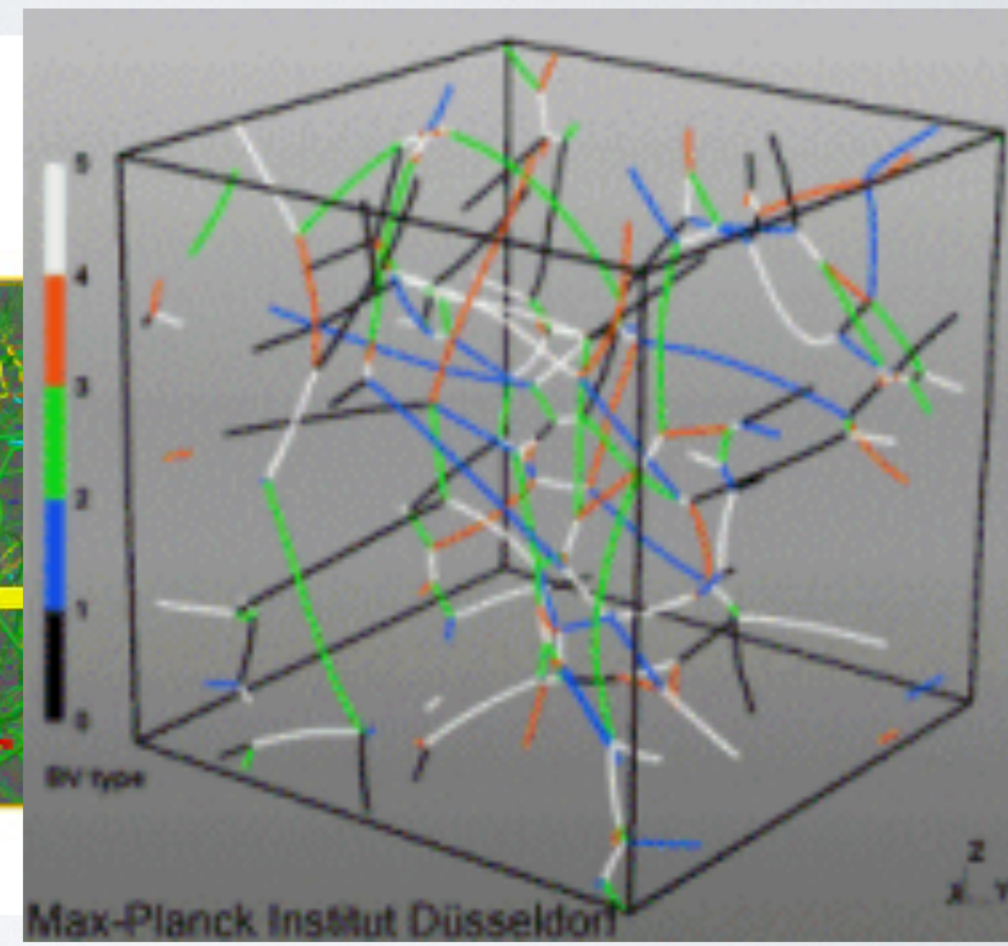


http://www.lbl.gov/CS/html/exascale4energy/nuclear.html

What is dislocation dynamics?

- A (predictive?) guide to the evolution of materials microstructure
- An experiment on a computer
- A simulation of the "classical" dynamics of dislocations





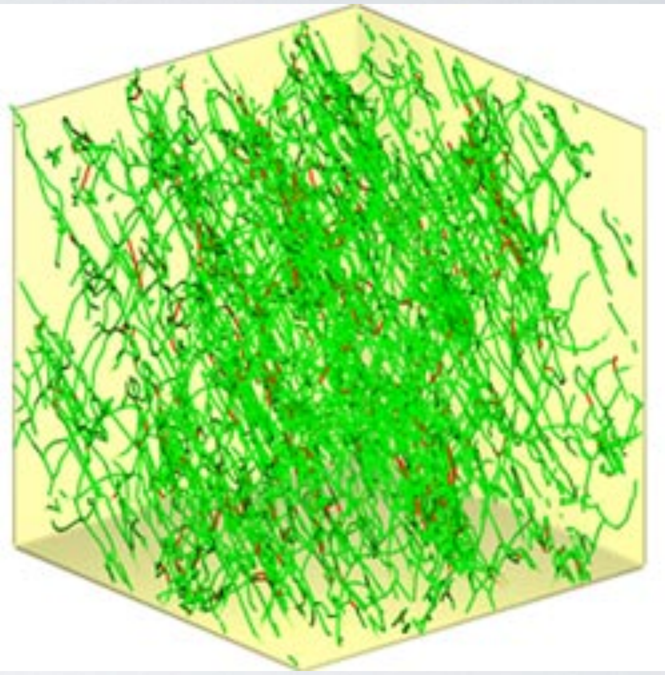
http://llnl.gov http://dierk-raabe.com

Why is it useful?

- By simulating dislocation motion, interaction, and growth, we can gain **mesoscale insight** into dislocation structure
- Advanced experimental techniques (TEM, high-energy X-ray diffraction) can resolve dislocation structure, but not dynamics
- We can **predict and understand** dislocation behavior and compare / interpret experimental observations
- Total control of dislocation interactions and initial conditions
- Nanomechanical measurement approaches scale of DD

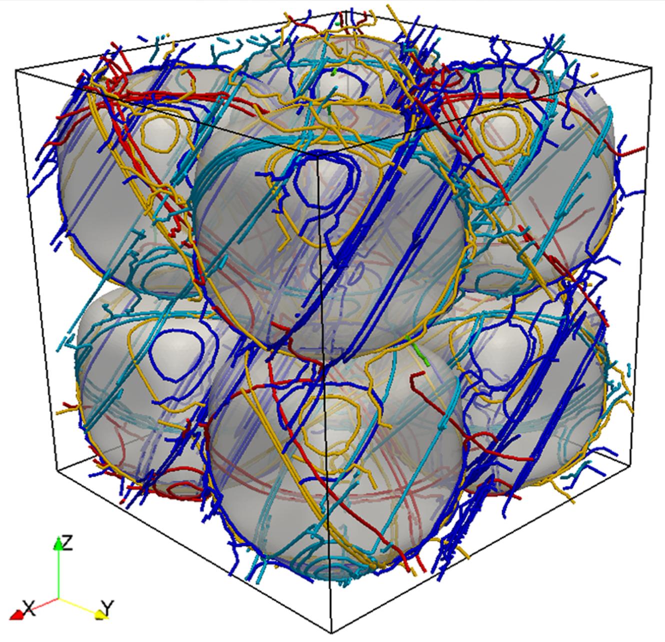
What is it used for?

- Bridge from atomistic to mesoscale
  - dislocation behavior and interaction scale up



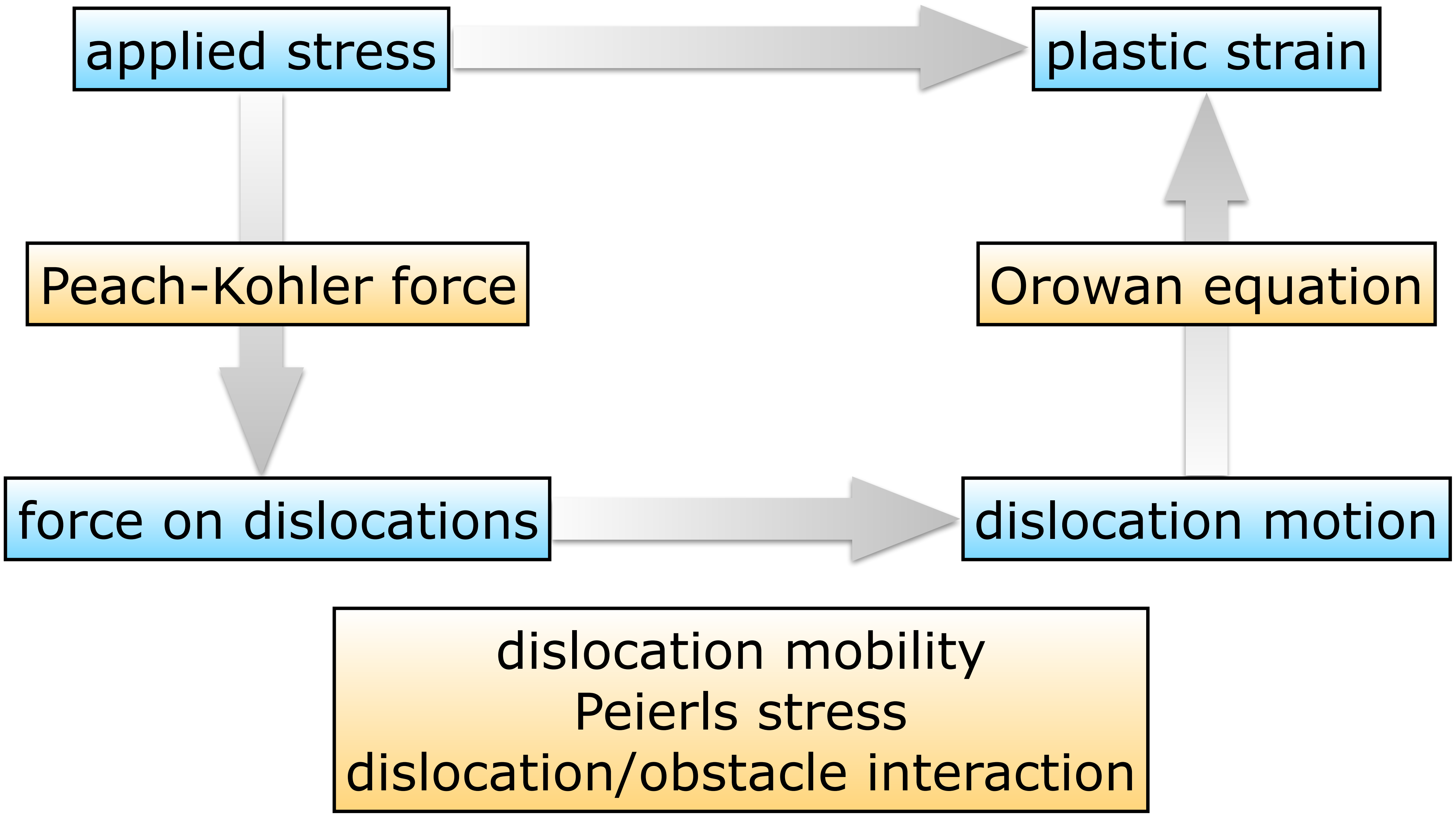
- Understanding strain hardening
  - dislocation density growth with strain & importance of interaction mechanisms

- Examining small-scale plasticity
  - micro- and nano pillars show unusual plastic behavior due to dislocations



- Parameterizing larger-scale models
  - dislocation-density-based crystal plasticity

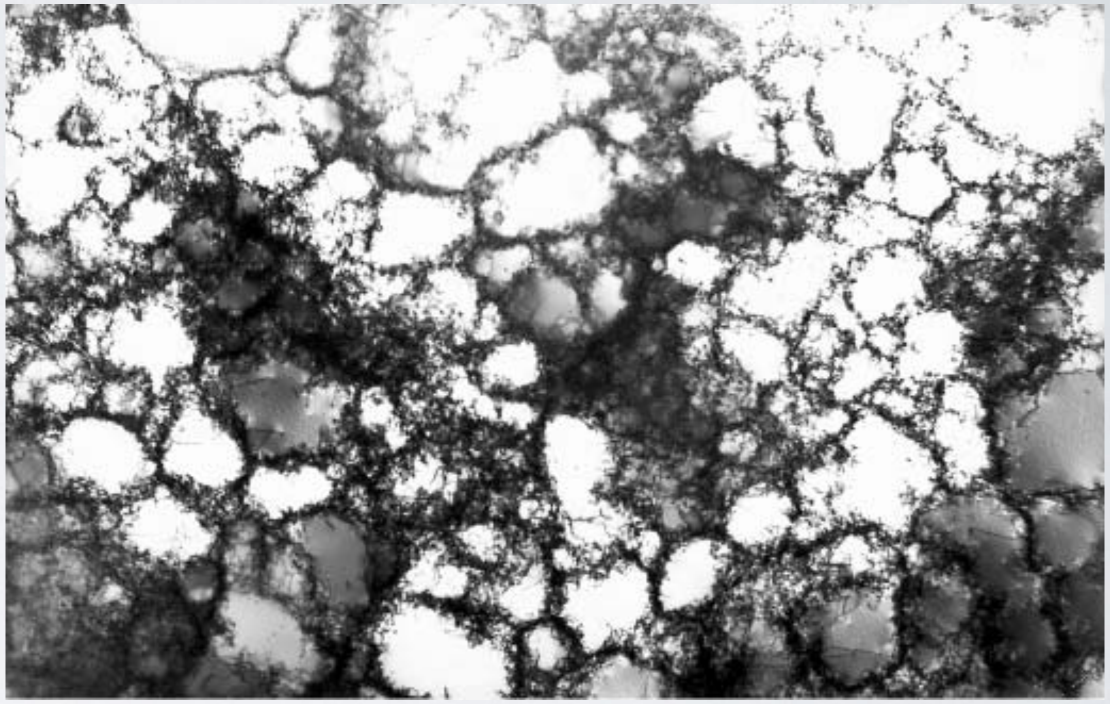
Dislocations and plastic deformation



II. History

First DDD simulations

- Robert Amodeo and Nasr Ghoniem (1997-1998) start direct numerical simulations of interacting dislocations to understand **cell formation**
- Range of efforts worldwide:
  - Cai/Bulatov/Arsenlis
  - Devincre
  - Ghoniem/Al Ezab
  - ...



- In addition, there are other approaches that attempt to model dislocations as entities:
  - Phase-field methods
  - Level-set methods
- All of the **discrete dislocation dynamics** methods benefit heavily from **parallelization**

III. Basic Principles

The fundamental idea

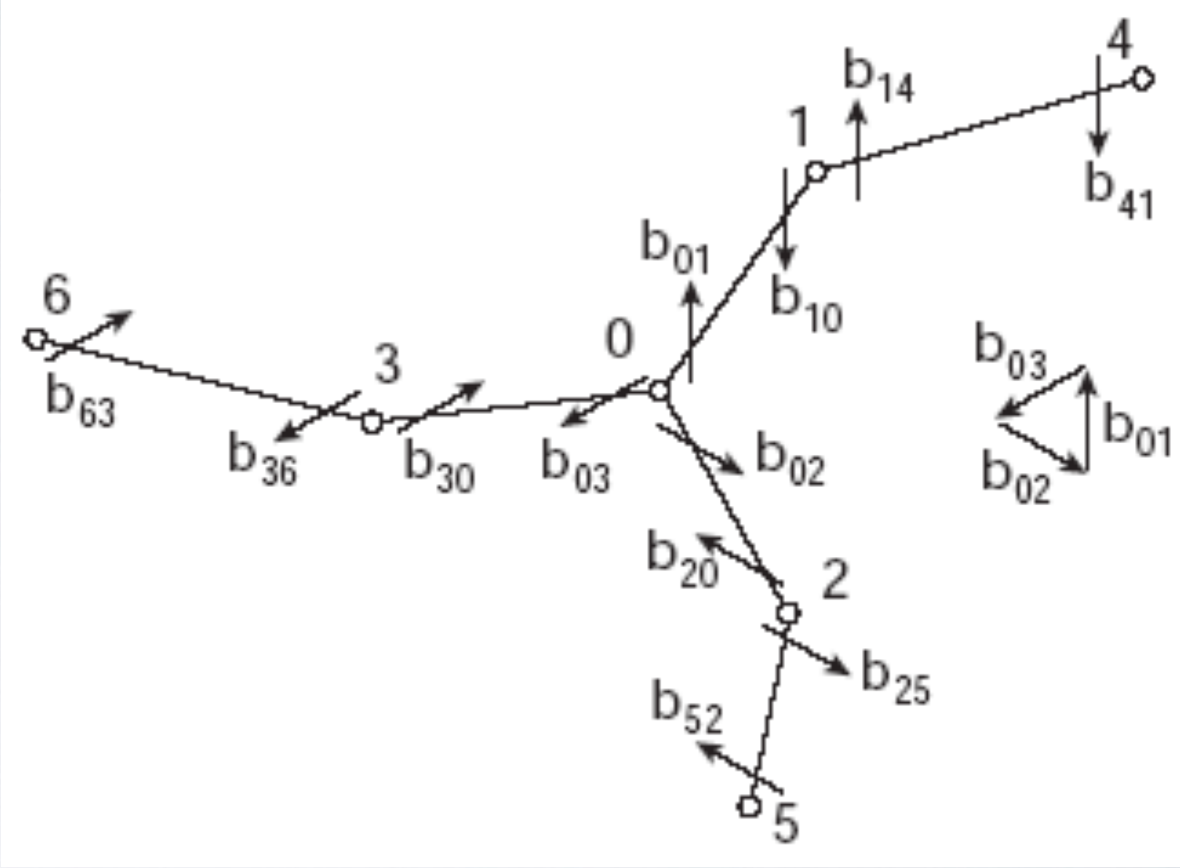
- DDD simulates dislocation motion using overdamped dynamics: similar to MD, but with a *mobility law* not mass.

- Running a simulation is like cooking - just follow the recipe!

- Three ingredients:

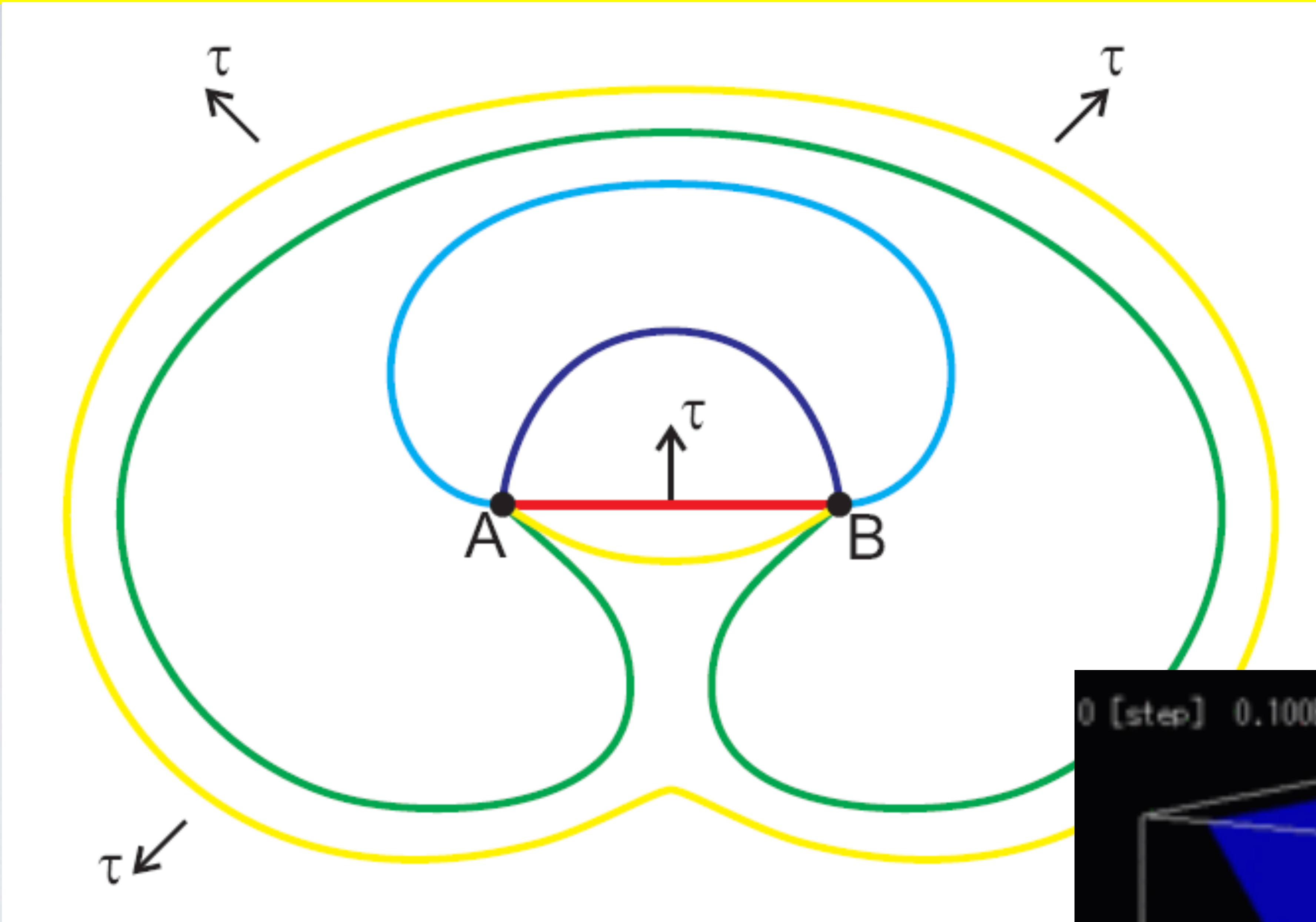
  1. An initial system configuration: dislocations
  2. Interaction between dislocations: Peach-Kohler
  3. Evolving dislocation geometry: mobility + remeshing

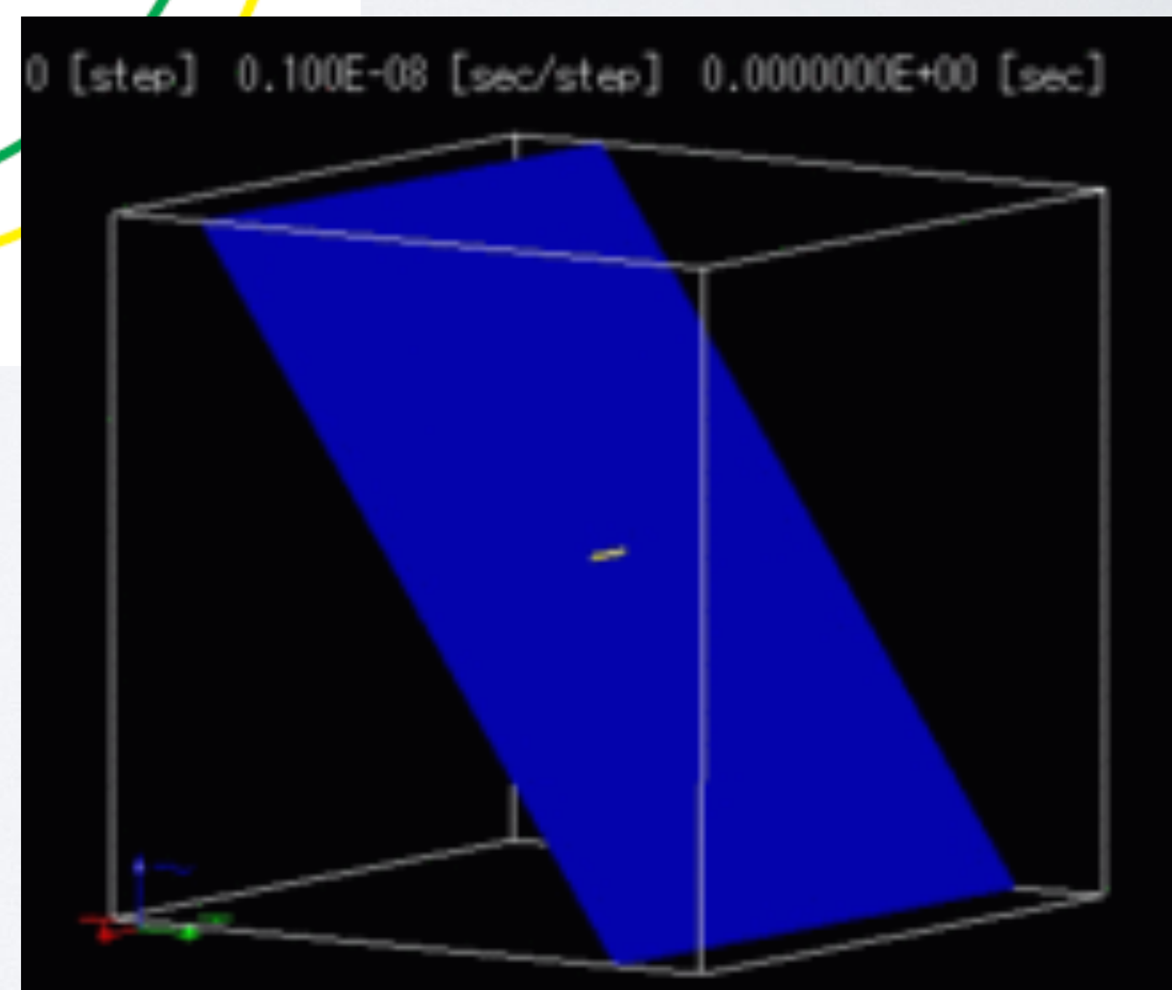
Ingredient 1: Initial configuration



- Represent dislocation curves
- Unlike MD, dislocations are one-dimensional objects: hence, *discretization*
- Different approaches:
  - Dislocation as line segments
  - Dislocation as cubic spline
  - Dislocation as connected arcs
  - Dislocation as "rastered" pure edge and screw segments
- Dislocation intersections have to be considered as well
- Typically use **Frank-Read** or **one-armed sources**

Ingredient 1: Frank-Read source





www.wikipedia.org

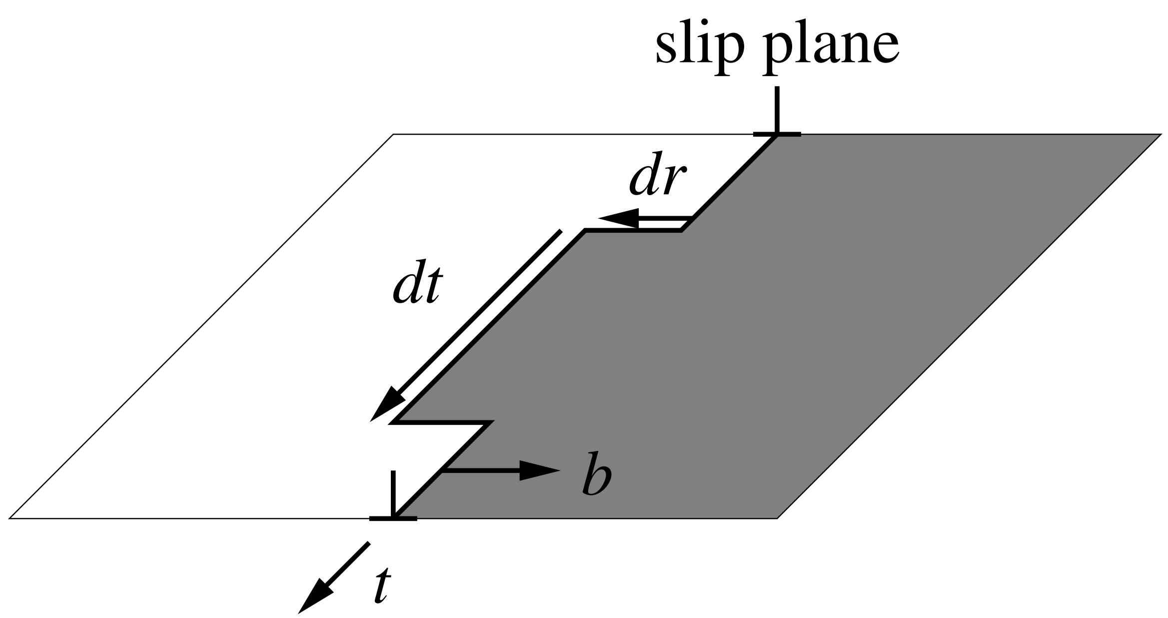
Ingredient 2: Interaction forces

- The net force acting on each dislocation in the system is a result of its interactions with all other dislocations + applied stress

- The underlying physical form is well-established: Peach-Kohler force

Dislocation motion under stress

- Dislocation line: separates “slipped” from “unslipped” parts of crystal
  - Sweeping out area displaces top part of crystal
  - Force on top area times displacement = −work done on dislocation



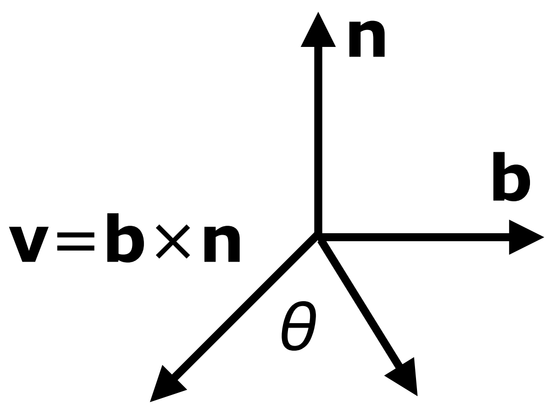
$$\mathbf{dF} = (\underline{\sigma} \cdot \mathbf{b}) \times \mathbf{dt}$$

Force/length on a dislocation

$$\begin{aligned}
dW &= -(\text{force}) \cdot (\text{displacement}) \\
&= -(\text{stress} \cdot \text{area}) \cdot (\text{displacement}) \\
&= (\underline{\sigma} \cdot \mathbf{da}) \cdot \mathbf{b} = \mathbf{da} \cdot \underline{\sigma} \cdot \mathbf{b} \\
&= (\mathbf{dr} \times \mathbf{dt}) \cdot \underline{\sigma} \cdot \mathbf{b} \\
&= -(\mathbf{dt} \times \mathbf{dr}) \cdot (\underline{\sigma} \cdot \mathbf{b}) \\
&= -\left[(\underline{\sigma} \cdot \mathbf{b}) \times \mathbf{dt}\right] \cdot \mathbf{dr} \\
&= -\mathbf{dF} \cdot \mathbf{dr}
\end{aligned}$$

Dislocation motion under stress

- Force per length ("Peach-Kohler force")
  - Always perpendicular to dislocation line
  - Force **in slip plane**: *glide force*
  - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$\mathbf{t} = \mathbf{v} \cos\theta + \mathbf{b} \sin\theta$

$$\mathbf{dF} = (\underline{\sigma} \cdot \mathbf{b}) \times \mathbf{dt}$$

$$= \begin{pmatrix} \sigma_{vv} & \sigma_{vb} & \sigma_{vn} \\ \sigma_{vb} & \sigma_{bb} & \sigma_{bn} \\ \sigma_{vn} & \sigma_{bn} & \sigma_{nn} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ b \\ 0 \end{pmatrix} \times \begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix} dt$$

$$= \begin{pmatrix} \sigma_{bv} b \\ \sigma_{bb} b \\ \sigma_{bn} b \end{pmatrix} \times \begin{pmatrix} \cos\theta \\ \sin\theta \\ 0 \end{pmatrix} dt$$

$$= \begin{vmatrix} \mathbf{v} & \mathbf{b} & \mathbf{n} \\ \sigma_{bv} b & \sigma_{bb} b & \sigma_{bn} b \\ \cos\theta & \sin\theta & 0 \end{vmatrix} dt$$

$$= \sigma_{bn} b(-\mathbf{v} \sin\theta + \mathbf{b} \cos\theta)$$
$$+ \sigma_{bv} b \sin\theta \mathbf{n} - \sigma_{bb} b \cos\theta \mathbf{n}$$

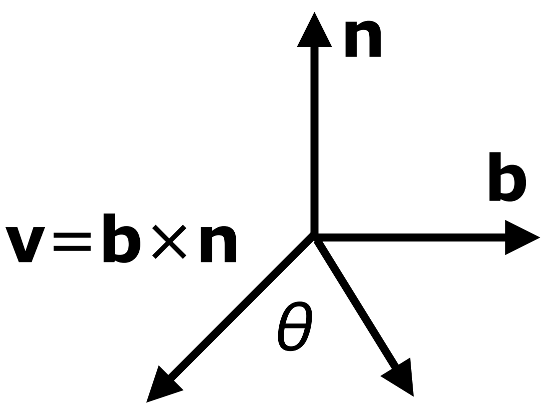
glide force

cross-slip force

climb force

Force on an edge and screw dislocation

- Force per length ("Peach-Kohler force")
  - Always perpendicular to dislocation line
  - Force **in slip plane**: *glide force*
  - Force **normal to slip plane**: *climb force* (edge) or *cross-slip* (screw)



$\mathbf{t} = \mathbf{v} \cos\theta + \mathbf{b} \sin\theta$

$$\mathbf{dF} = \sigma_{bn} b(-\mathbf{v}\sin\theta + \mathbf{b}\cos\theta) + \sigma_{bv} b \sin\theta \mathbf{n} - \sigma_{bb} b \cos\theta \mathbf{n}$$

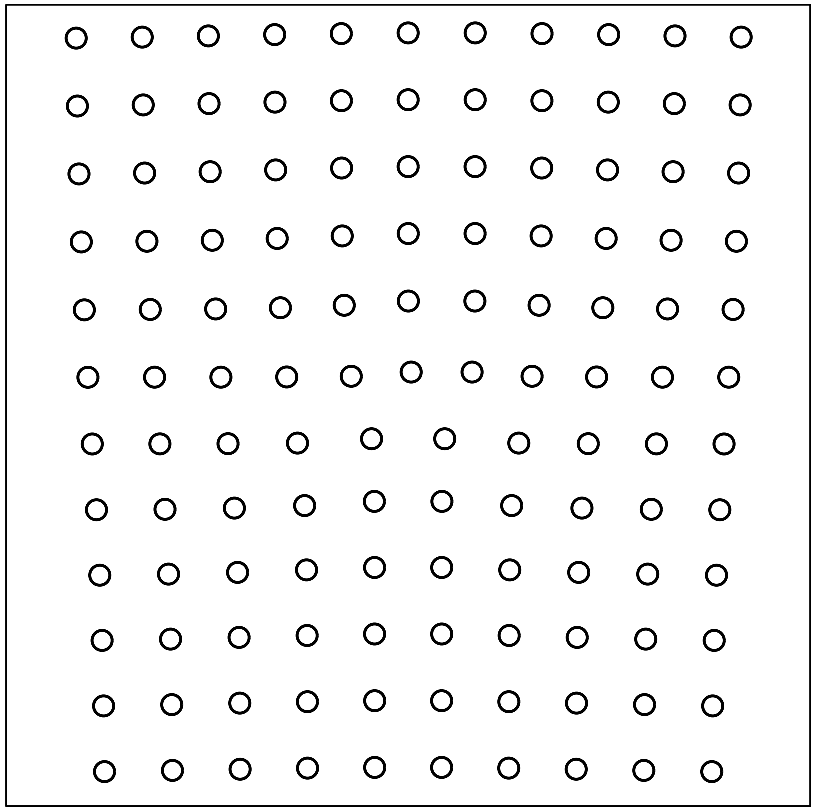
$$\mathbf{dF}_{\text{edge}} = \sigma_{bn} b \mathbf{b} - \sigma_{bb} b \mathbf{n}$$

$$\mathbf{dF}_{\text{screw}} = -\sigma_{bn} b \mathbf{v} + \sigma_{bv} b \mathbf{n}$$

glide force

cross-slip force

climb force



Stress and force

- To use, we need to need to be able to calculate stress at each point, *and* translate force on a dislocation segment onto the dislocation "degrees of freedom" (nodes)
- For elastically isotropic materials (with a core "cutoff")

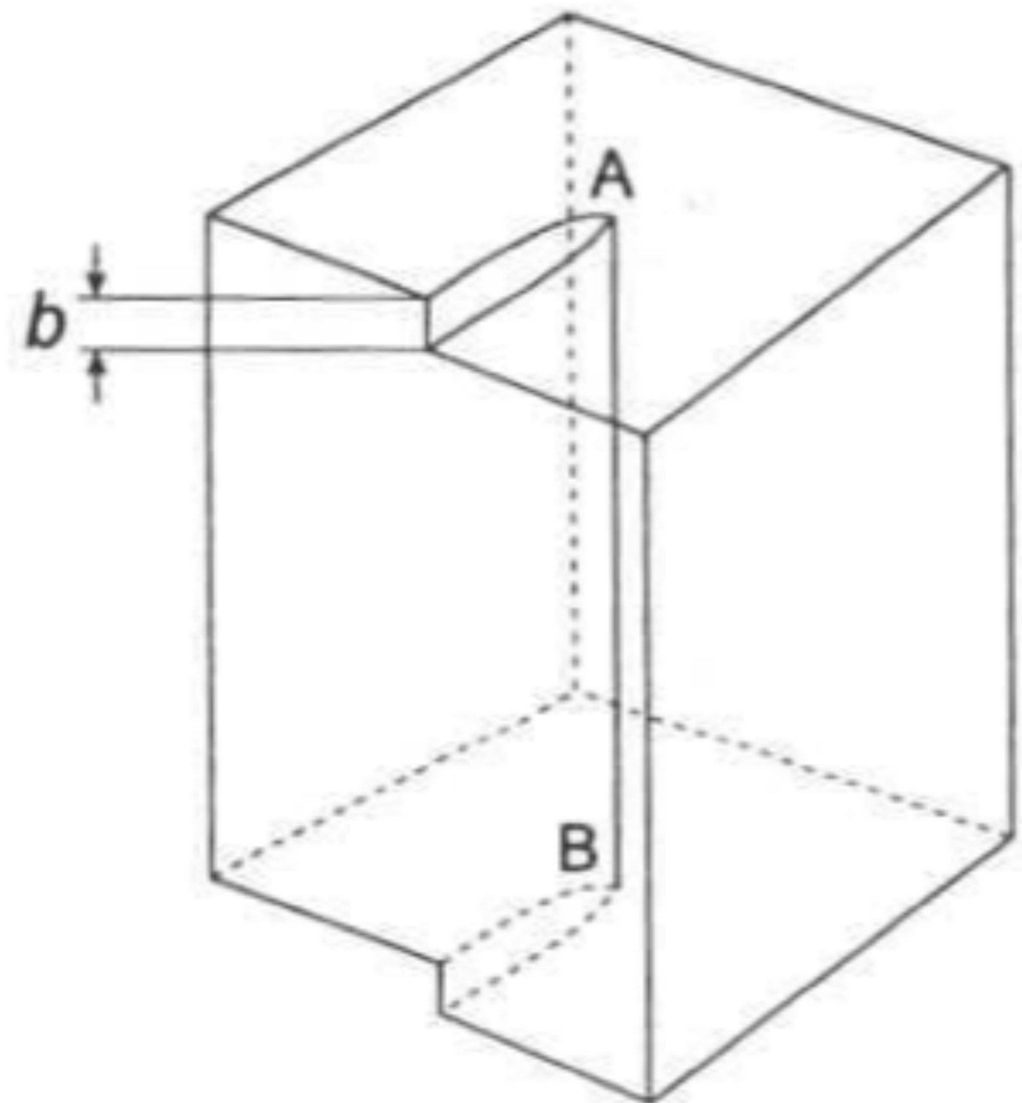
$$\sigma_{\alpha\beta}(\mathbf{x}) = \frac{\mu}{8\pi} \oint_C \partial_i \partial_p \partial_p R_a \left[b_m \epsilon_{im\alpha} dx'_\beta + b_m \epsilon_{im\beta} dx'_\alpha \right]$$

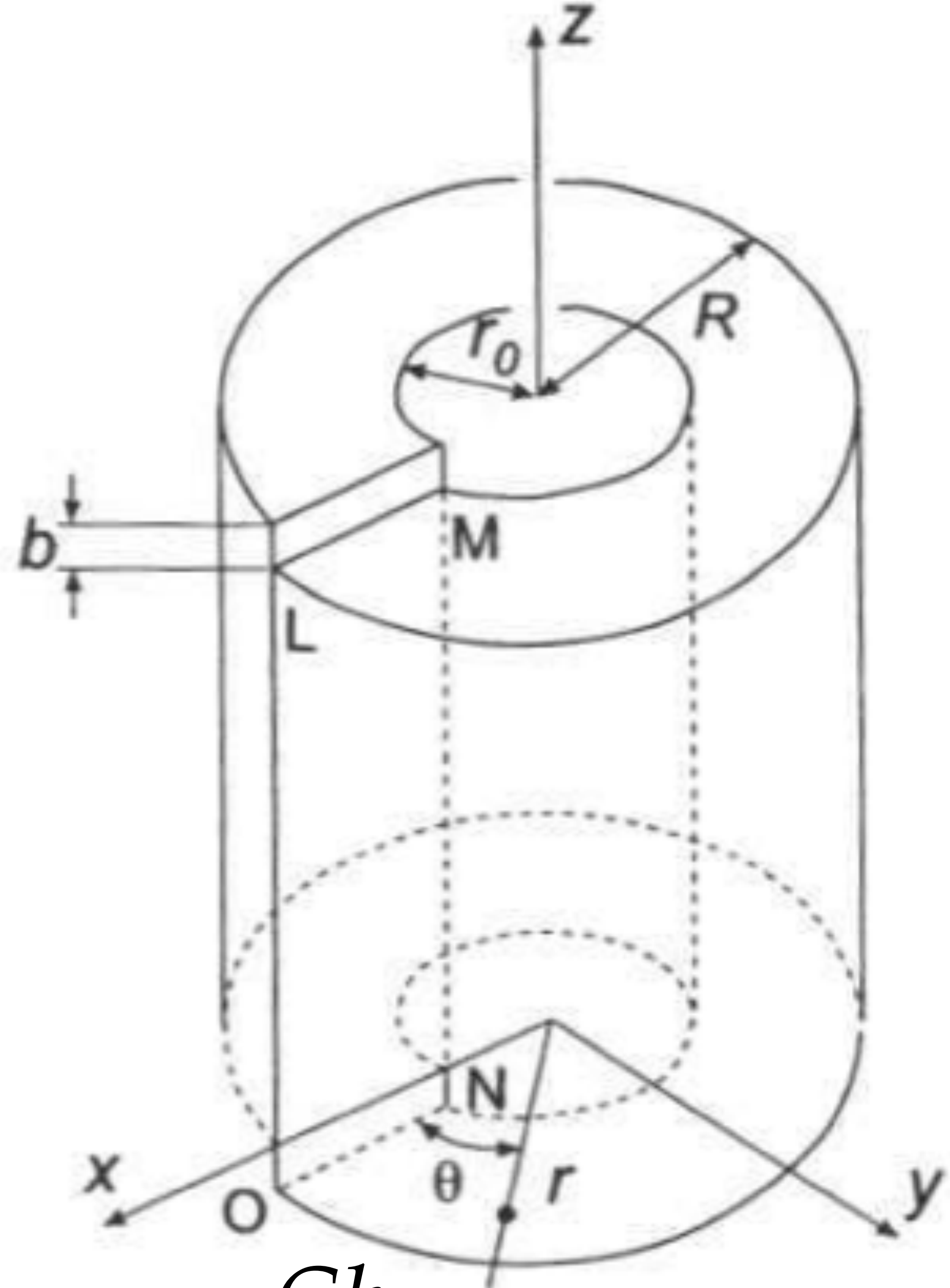
$$+ \frac{\mu}{4\pi(1-\nu)} \oint_C b_m \epsilon_{ink} \left[\partial_i \partial_\alpha \partial_\beta R_a - \delta_{\alpha\beta} \partial_i \partial_p \partial_p R_a \right] dx'_k$$

$$R = \|\mathbf{x} - \mathbf{x}'\|$$

$$R_a = \sqrt{\|\mathbf{x} - \mathbf{x}'\|^2 + a^2}$$

Screw dislocation: stress field





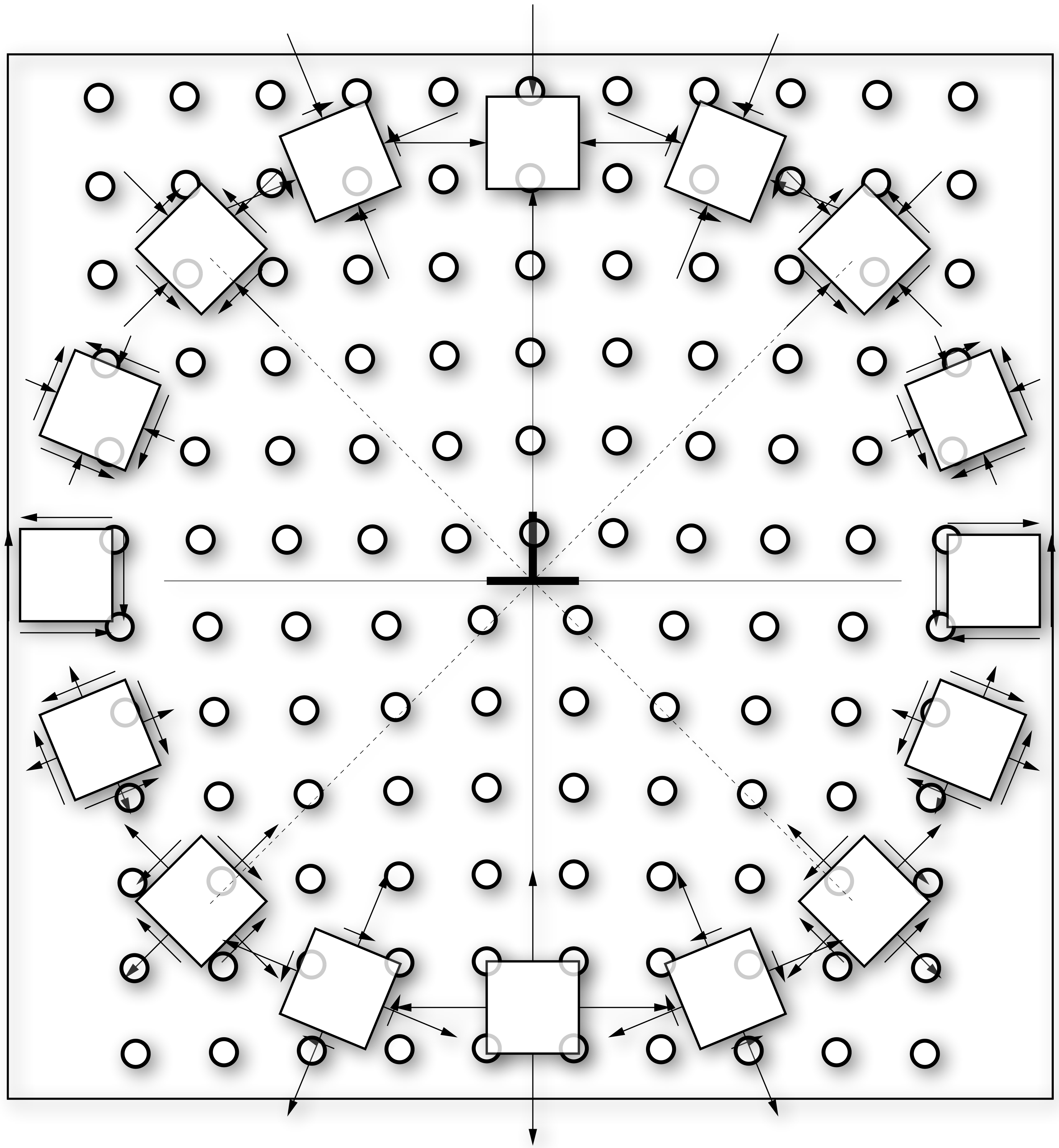
$$\gamma = \frac{b}{2\pi r}$$

$$\sigma_{xz} = \sigma_{zx} = -\frac{Gb}{2\pi r}\sin\theta$$

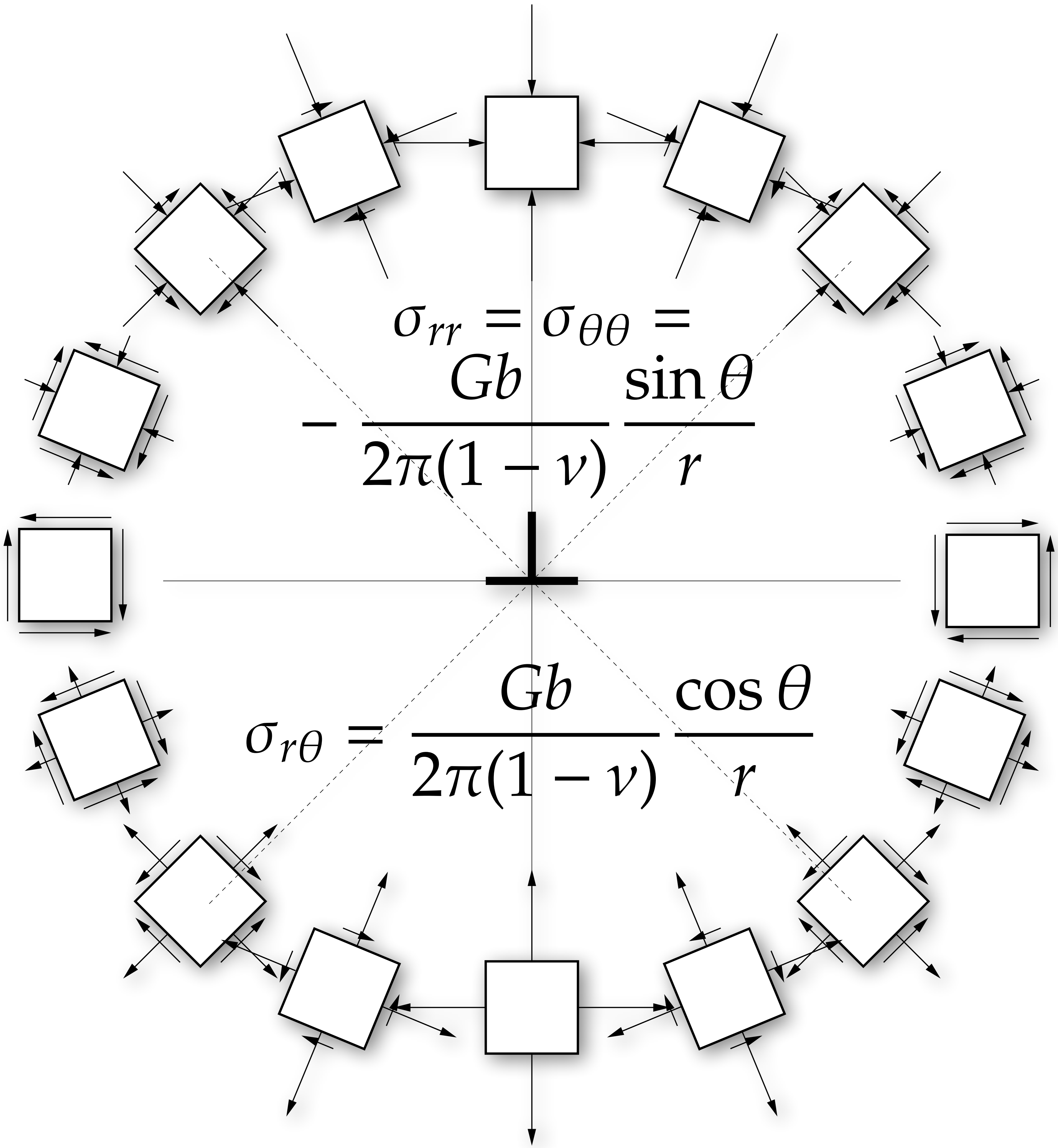
$$\sigma_{z\theta} = \sigma_{\theta z} = \frac{Gb}{2\pi r}$$

$$\sigma_{yz} = \sigma_{zy} = \frac{Gb}{2\pi r}\cos\theta$$

Edge dislocation: stress field



Edge dislocation: stress field



$$\sigma_{rr} = \sigma_{\theta\theta} = -\frac{Gb}{2\pi(1-\nu)}\frac{\sin\theta}{r}$$

$$\sigma_{r\theta} = \frac{Gb}{2\pi(1-\nu)}\frac{\cos\theta}{r}$$

Edge dislocation: stress field

$$\sigma_{rr} = \sigma_{\theta\theta} = -\frac{Gb}{2\pi(1-\nu)}\frac{\sin\theta}{r} \qquad \sigma_{r\theta} = \frac{Gb}{2\pi(1-\nu)}\frac{\cos\theta}{r}$$

$$\theta_{\text{cart,polar}} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

$$\begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ \sigma_{xy} & \sigma_{yy} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} \sigma_{rr} & \sigma_{r\theta} \\ \sigma_{r\theta} & \sigma_{\theta\theta} \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

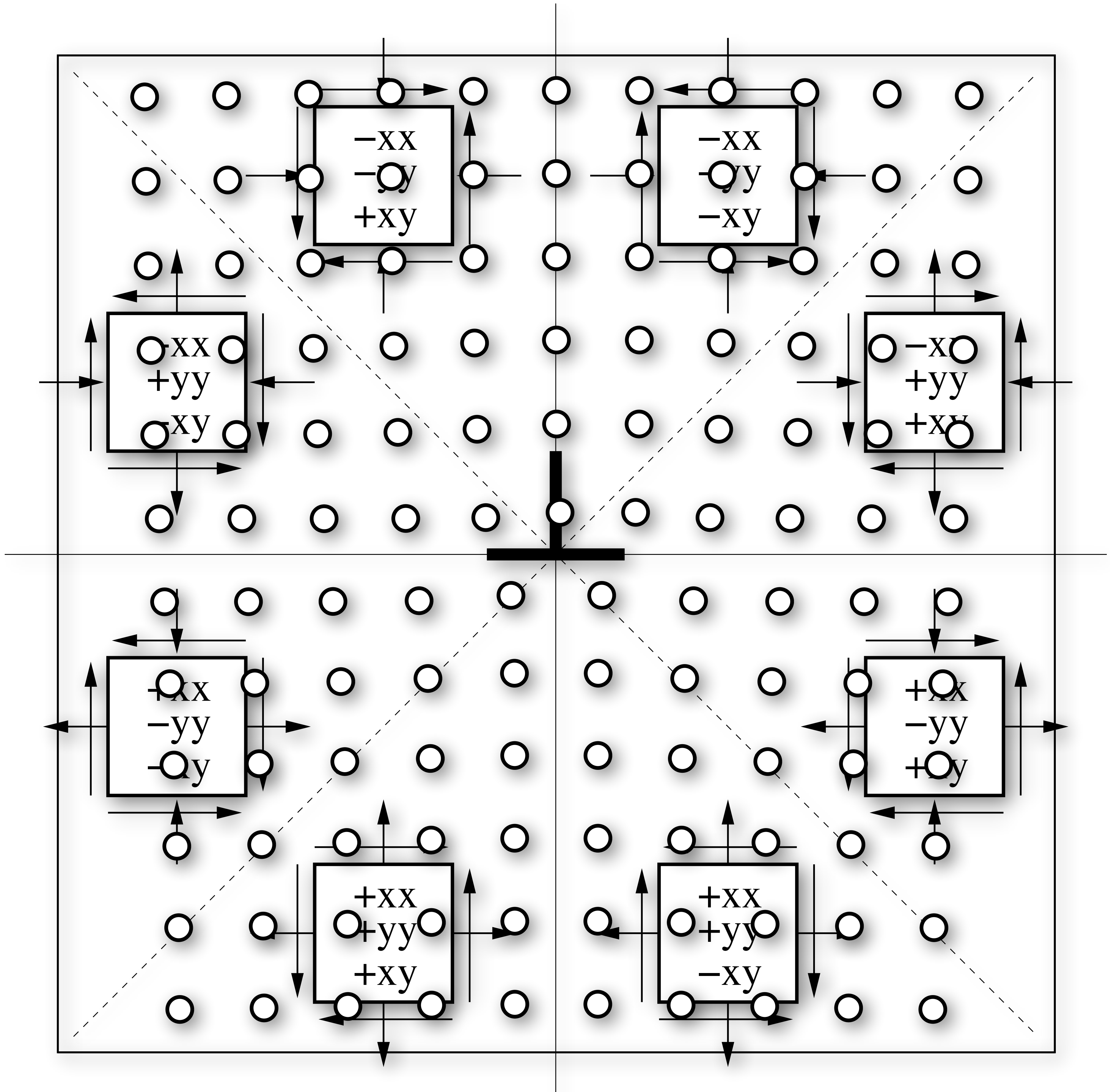
$$= \frac{Gb}{2\pi(1-\nu)r}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} -\sin\theta & \cos\theta \\ \cos\theta & -\sin\theta \end{pmatrix}\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$$

$$= \frac{Gb}{2\pi(1-\nu)r}\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} -2\sin\theta\cos\theta & -\sin^2\theta + \cos^2\theta \\ 1 & 0 \end{pmatrix}$$

$$= \frac{Gb}{2\pi(1-\nu)r}\begin{pmatrix} -\sin\theta(1+\cos^2\theta) & \cos\theta\cos 2\theta \\ \cos\theta\cos 2\theta & -\sin\theta\cos 2\theta \end{pmatrix}$$

$$= \frac{Gb}{2\pi(1-\nu)r}\begin{pmatrix} -\sin\theta(2+\cos 2\theta) & \cos\theta\cos 2\theta \\ \cos\theta\cos 2\theta & -\sin\theta\cos 2\theta \end{pmatrix}$$

Edge dislocation: stress field



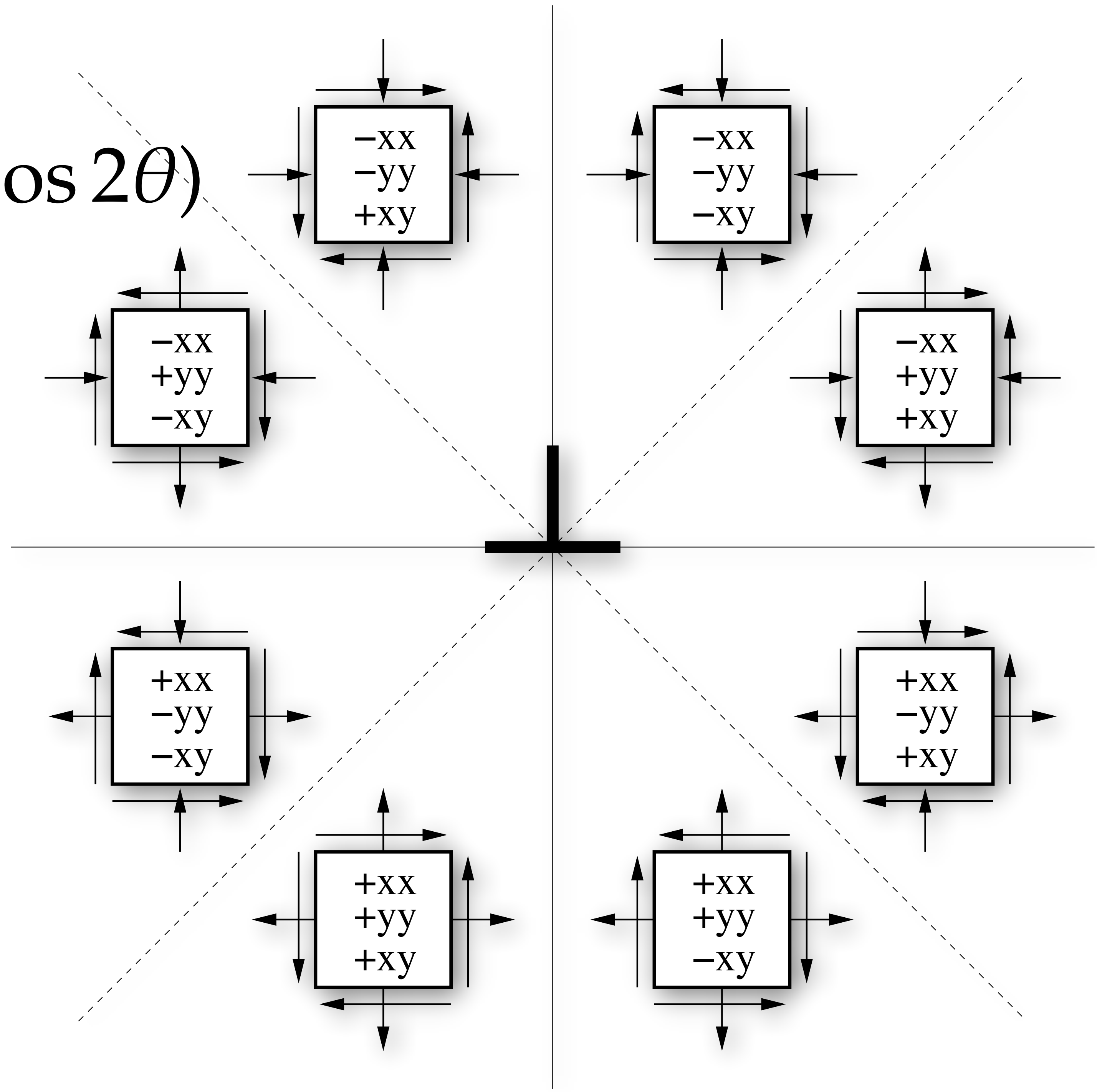
Edge dislocation: stress field

$$\sigma_{xx} = -\frac{Gb}{2\pi r(1-\nu)} \sin\theta(2+\cos 2\theta)$$

$$\sigma_{yy} = \frac{Gb}{2\pi r(1-\nu)} \sin\theta \cos 2\theta$$

$$\sigma_{zz} = \nu(\sigma_{xx}+\sigma_{yy})$$

$$\tau_{xy} = \frac{Gb}{2\pi r(1-\nu)} \cos\theta \cos 2\theta$$



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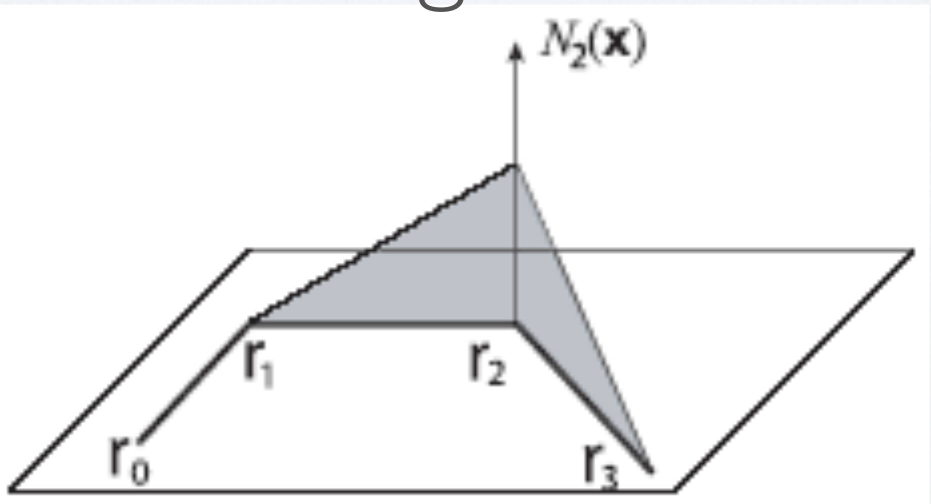
$$R = \|\mathbf{x} - \mathbf{x}'\|$$

$$R_a = \sqrt{\|\mathbf{x} - \mathbf{x}'\|^2 + a^2}$$

- For line segments, map force to nodes by integrating a linear "shape function" along connected segments



Ingredient 3: Evolution of dislocations

- Initial dislocation geometry + forces on dislocation: **How to evolve?** *F=ma*?

- Dislocations aren't "objects" with mass; instead, they experience an *overdamped dynamics* where **velocity** is proportional to **force**: mobility.

Dislocation velocity: thermal activation

LiF crystal

Fe-3.25%Si crystal

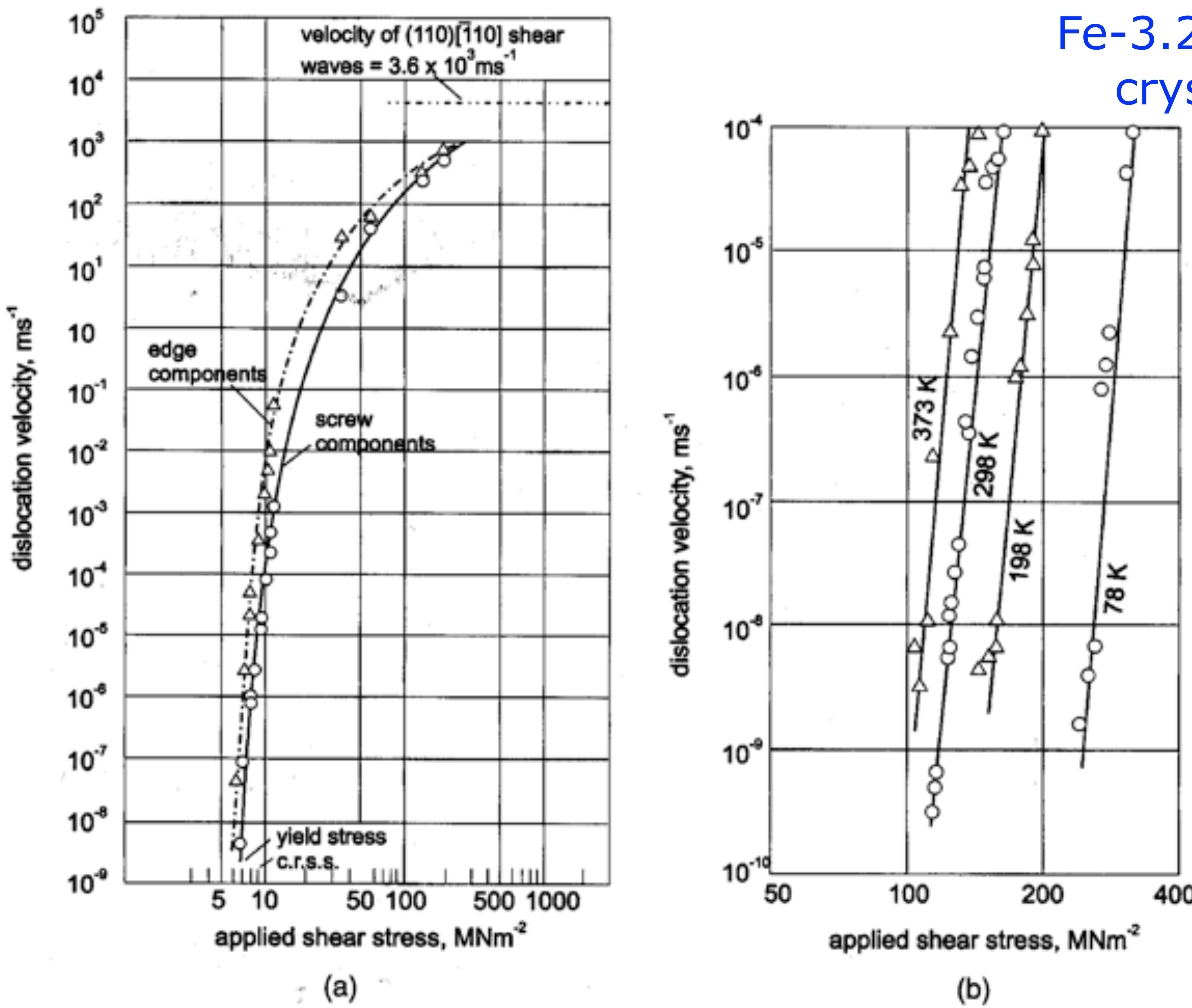


Figure 3.11 (a) Stress dependence of the velocity of edge and screw dislocations in lithium fluoride. (From Johnston and Gilman, *J. Appl. Phys*. **30**, 129, 1959.) (b) Stress dependence of the velocity of edge dislocations in 3.25 per cent silicon iron at four temperatures. (After Stein and Low, *J. Appl. Phys*. **31**, 362, 1960.)

Ingredient 3: Evolution of dislocations

- Initial dislocation geometry + forces on dislocation: **How to evolve?** *F=ma*?
- Dislocations aren't "objects" with mass; instead, they experience an *overdamped dynamics* where **velocity** is proportional to **force**: mobility.
- Mobility can be *anisotropic*
  - In plane: edge dislocations vs. screw dislocations
  - Out-of-plane: cross-slip (screw) vs. climb (edge)

Ingredient 3: Evolution of dislocations

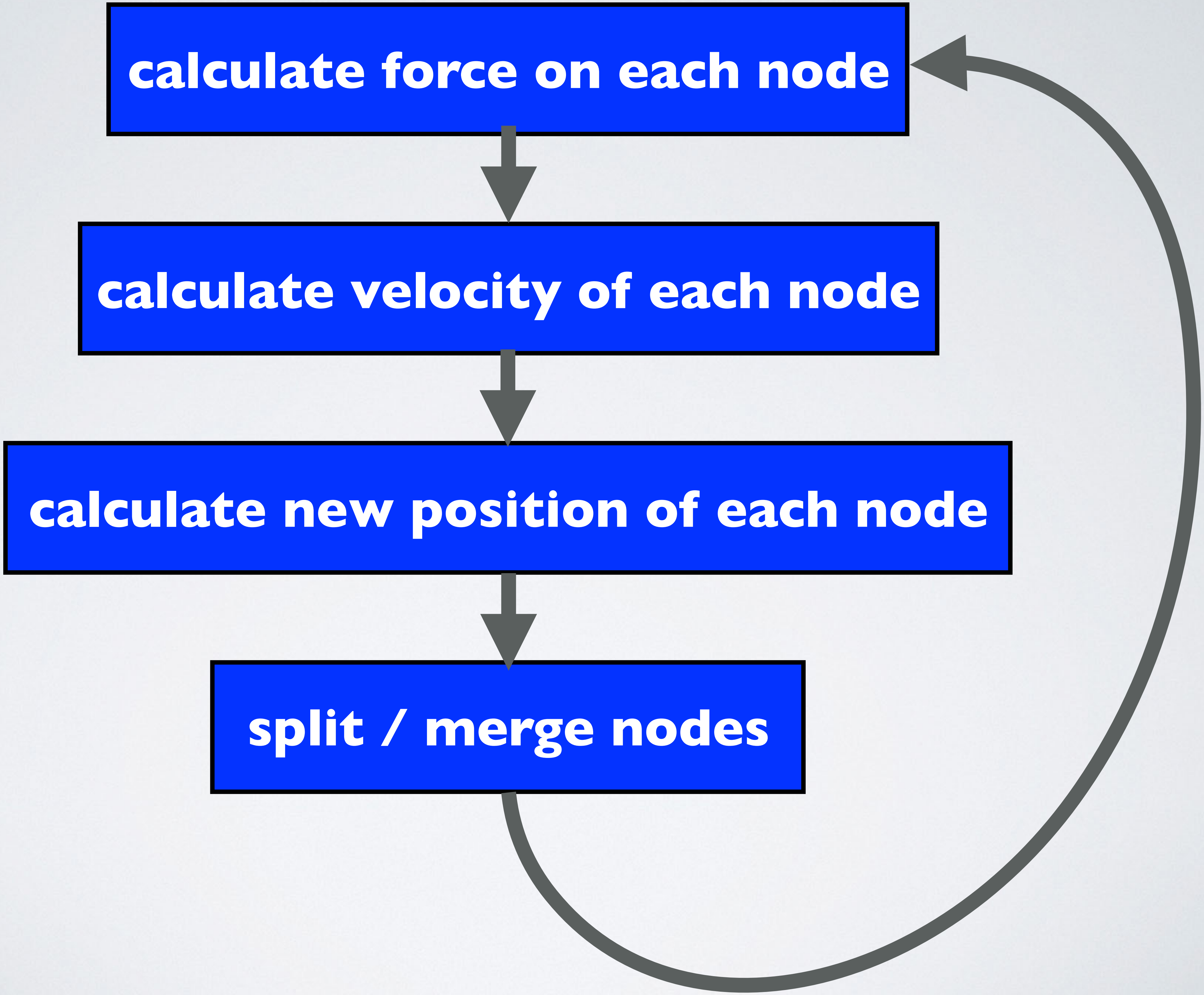
- Given velocity on nodes, integrate nodes forward in time
  - Euler forward / backward schemes

$$\text{Forward:} \quad \mathbf{x}(t+\Delta t) = \mathbf{x}(t) + \Delta t\, \dot{\mathbf{x}}(t)$$

$$\text{Backward:} \quad \mathbf{x}(t+\Delta t) = \mathbf{x}(t) + \Delta t\, \dot{\mathbf{x}}(t+\Delta t)$$

  - Newton-Krylov, other sophisticated integrators
- Remeshing:
  - Too few nodes to represent the curvature? Introduce new nodes (**split**)
  - Too many nodes in a small area of space? Eliminate extra nodes (**merge**)
- Dislocation annihilation reactions: elimination of dislocation segments with opposite Burgers vector

Dislocation dynamics flowchart



IV. Advanced Topics

Boundary conditions

- Interaction between dislocations (calculated via stress) depends on the boundary conditions:
  - Most simulations assume *periodic boundary conditions*
  - Simulations of finite systems involves *image stresses*
- Interaction calculation can be accelerated with Fast Multipole Methods (similar to charged interactions)

V. Dislocation Dynamics Packages

DDD software

http://paradis.stanford.edu/