Screw dislocation mobility:

Monte Carlo models to Discrete Dislocation Dynamics

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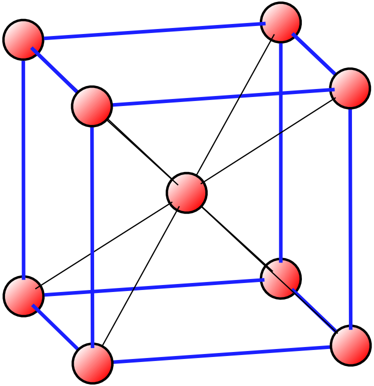
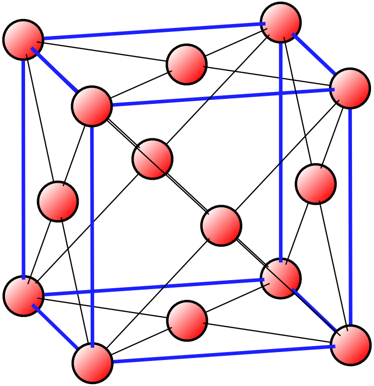
Crystalline solids

- Many everyday solid materials are crystalline
- Simplest structures are Bravais lattices (Iron, cubic structures)
- More generally, multilattices (Graphite, hexagonal lattice structure)



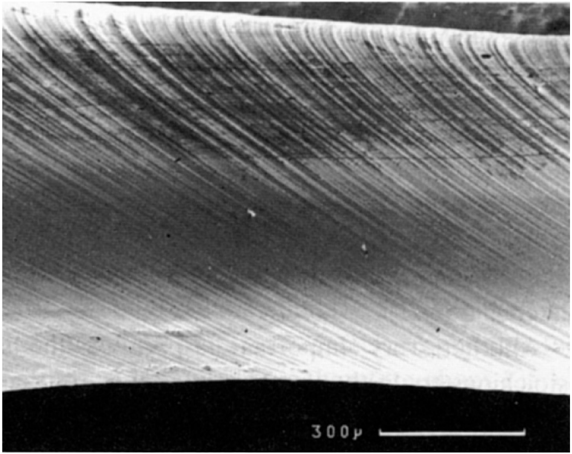
Body-Centred Cubic (BCC)



Face-Centred Cubic (FCC)

Crystal plasticity

Crystal Plasticity = **'slip'** of crystallographic planes.

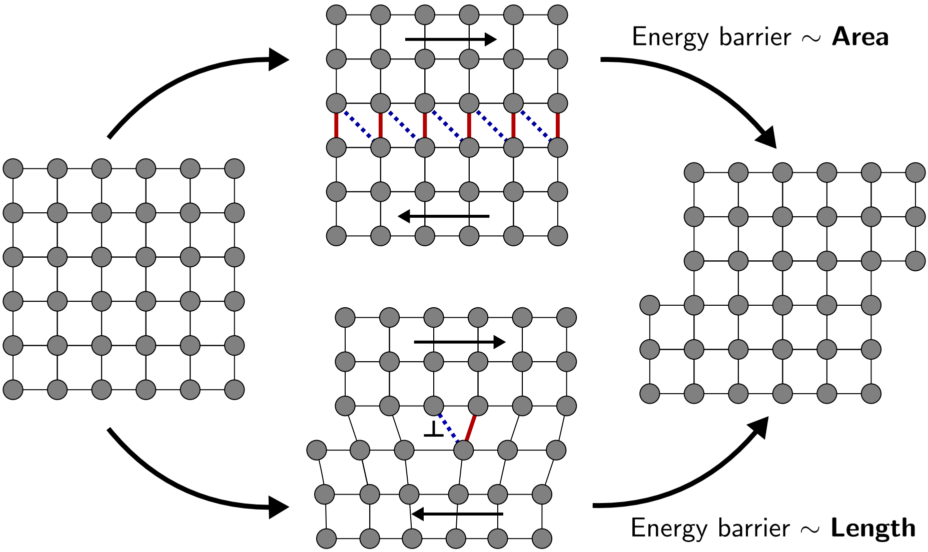


http://www.doitpoms.ac.uk/tlplib/miller_indices/uses.php

Crystal plasticity

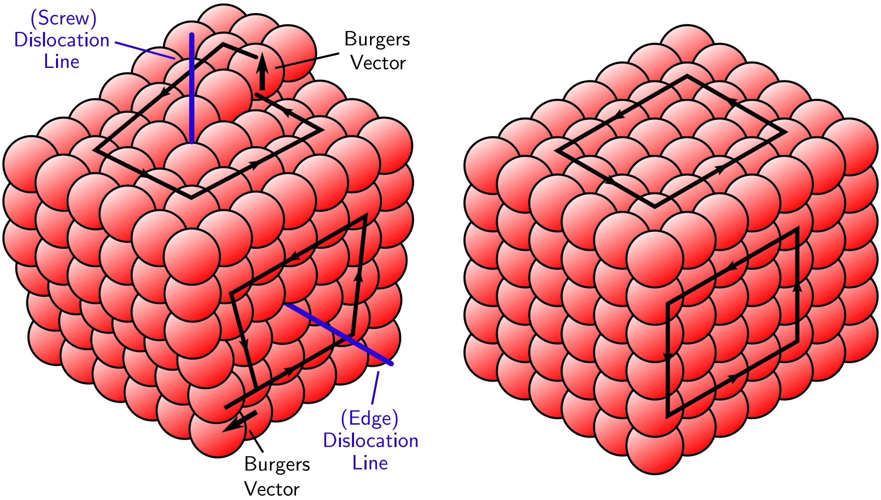
Orowan (1934), Polanyi (1934), Taylor (1934):

Slip occurs via motion of **dislocations**.



Dislocations

- **Geometric** lattice defects
- Assigned a Burgers vector, $\mathbf{b}$, and line direction, $\mathbf{l}$.
- Simplest types: screw ($\mathbf{b} \parallel \mathbf{l}$) and edge ($\mathbf{b} \perp \mathbf{l}$).



Computational modelling of crystal plasticity

Hierarchy of crystal plasticity models:

Electronic structure: True chemistry, $\sim 10^3$ atoms

$\downarrow$ Potentials for/coupling to: $\downarrow$

Molecular Dynamics: Statistical mechanics. $\sim 10^6$ atoms, but longest feasible trajectory length $\sim 10^{-6}$s

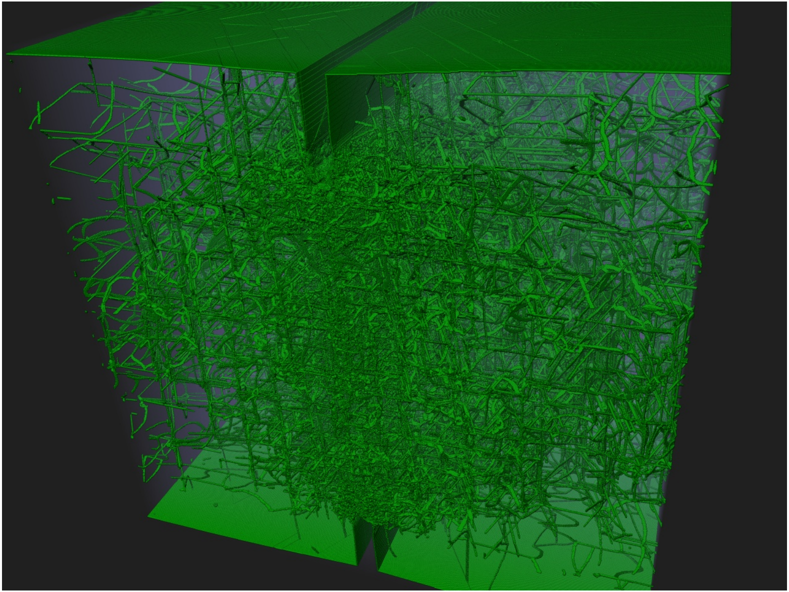
$\downarrow$ Mobility + topological laws for: $\downarrow$

Discrete Dislocation Dynamics: Statistical mechanics: single crystal/multiple grains, trajectory length $\sim 10^{-1}$s.

$\downarrow$ Numerical constitutive laws for: $\downarrow$

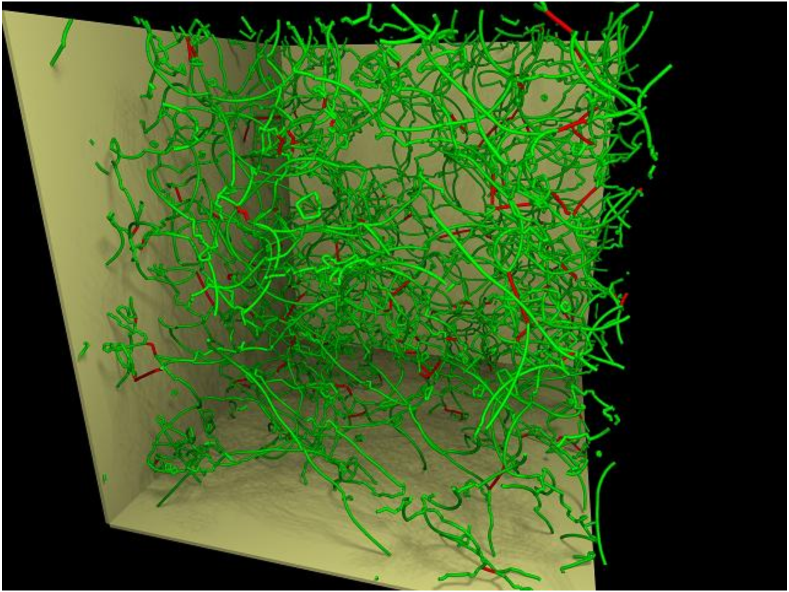
Continuum crystal plasticity: human time– and length–scales.

Dislocation Dynamics



http://computation.llnl.gov/largevis/atoms/ductile-failure/

Dislocation Dynamics



http://paradis.stanford.edu/site/about

Dislocation Dynamics

Discrete Dislocation Dynamics (DDD) is the solution of the problem

$$\dot{\Gamma}(s) = \mathcal{M}[f(s, \Gamma)],$$

where

- $\Gamma(s)$ is a parametrisation of time–dependent dislocation lines
- f is the **Peach–Köhler force,** $f = (\sigma \cdot \mathbf{b}) \wedge \mathbf{l}$, with:
  - σ the stress at $\Gamma(s)$,
  - $\mathbf{b}$ the Burgers vector, and
  - $\mathbf{l} = \frac{\Gamma'(s)}{|\Gamma'(s)|}$ the line direction.
- $\mathcal{M}$ is a mobility function, usually $\mathcal{M}[f] = \alpha f$, or $\alpha(\mathsf{I} - n \otimes n)f$.

Note:

- σ is a **nonlocal** function of the dislocation configuration.
- Dislocation junctions are more complicated.

Questions: When is DDD valid, and what should $\mathcal{M}$ be?

Kinetic Monte Carlo models

- Hamiltonian $H(p,q) = \frac{1}{2}|p|^2 + V(q)$.
- Temperature T, $\beta := k_B^{-1} T^{-1}$.
- Equilibrium density = **Gibbs measure**

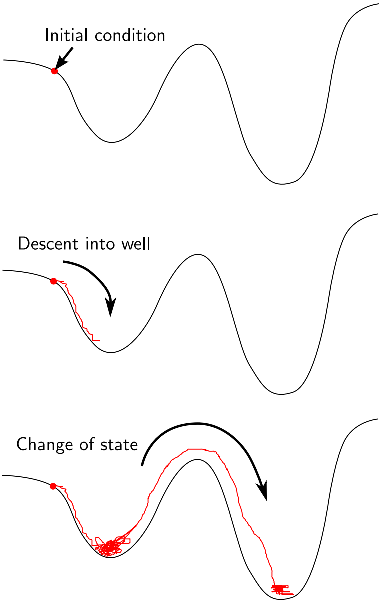
$$Z(\beta)^{-1} \exp\left(-\beta V(q)\right) \mathrm{d}q.$$

- Sample via ergodic dynamics, e.g.

$$\dot{q} = M^{-1} p$$
$$\dot{p} = -\nabla V(q) - \gamma M^{-1} p + \sqrt{2\gamma\beta^{-1}}\, \dot{W}$$

- If $\beta \gg 1$, q 'waits' near local minima.

Eyring–Kramers rule:
Waiting times for transitions between minima are exponentially distributed.



Kinetic Monte Carlo models

1. Define states μ, ν.
2. Fix neighbouring states $\mathcal{N}_\mu$.
3. **Eyring–Kramers rule**: jump time from μ to ν exponentially distributed [Hänggi–Talker–Borcovec '90, Berglund '13] with rate

$$\mathcal{R}(\mu \to \nu) = \mathcal{A}(\mu \to \nu) \exp\big[-\beta\, \mathcal{B}(\mu \to \nu)\big],$$

where

- $\mathcal{A}(\mu \to \nu)$ is **entropic prefactor** $\approx$ 'width' of the minimal pathway
- $\mathcal{B}(\mu \to \nu)$ is **energy barrier** $=$ 'height' of saddle between states.

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4. **KMC model:** Wait until first transition, move to new state, repeat. If transition times are independent:

$$\tau \sim \min_{\nu \in \mathcal{N}_\mu} \mathrm{Exp}\big[\mathcal{R}(\mu \to \nu)\big] = \mathrm{Exp}\Big[\sum_{\nu \in \mathcal{N}_\mu} \mathcal{R}(\mu \to \nu)\Big],$$

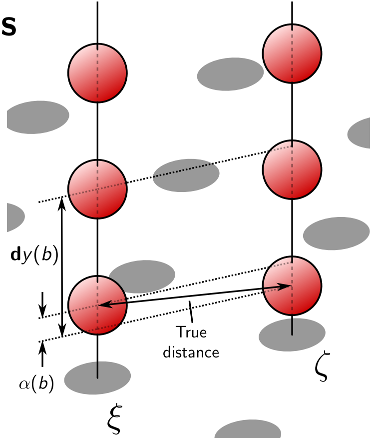
$$\text{and} \quad \mathbb{P}[\mu \to \nu'] = \frac{\mathcal{R}(\mu \to \nu')}{\sum_{\nu \in \mathcal{N}_\mu} \mathcal{R}(\mu \to \nu)}.$$

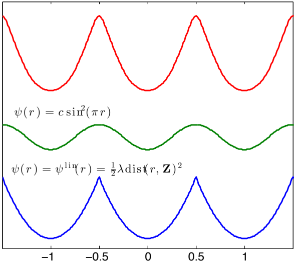
Toy model for screw dislocations

- Project along Burgers vector: $\rightsquigarrow$ lattice L in–plane.
- Cylinder, cross–section $\mathrm{D}_{n,0} = n\mathrm{D} \cap \mathrm{L}$.
- **Assume** vertical movement of ‘columns’ only.
- Anti–plane deformation:

$$y : n\mathrm{D}_{n,0} \to \mathbb{R}.$$

- Finite diff, $\mathbf{d}y(b) := y(e) - y(e')$.
- **Assume** NN interaction.





Potential: $\psi(r) = \frac{1}{2}\lambda\,\mathrm{dist}(r,\mathbb{Z})^2$

Total energy: $E_n(y) = \sum_{b\in\mathrm{D}_{n,1}} \psi(\mathbf{d}y(b))$

Toy model for screw dislocations

Smallest 'height' difference:

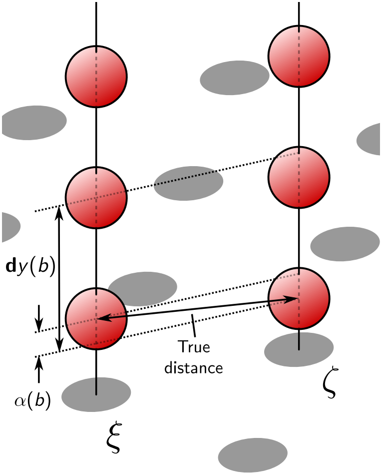
$$\alpha(b) = \mathbf{d}y(b) \bmod 1 = \mathbf{d}y(b) - z(b),$$
$$z(b) = \mathrm{argmin}_{z\in\mathbb{Z}}|z - \mathbf{d}y(b)|$$

Define Burgers vector of 'cell' C:

$$\sum_{b\in\partial C} \alpha(b) \in \{-1, 0, +1\}.$$

$\rightsquigarrow$ **Identification of dislocations**.

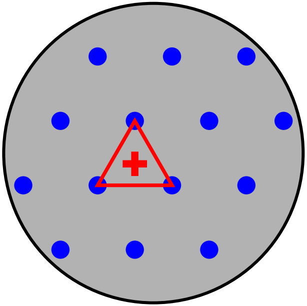
NB: Ambiguous if $\mathbf{d}y(b) \in \mathbb{Z} + \frac{1}{2}$
$\leftrightarrow$ Change of dislocation position.

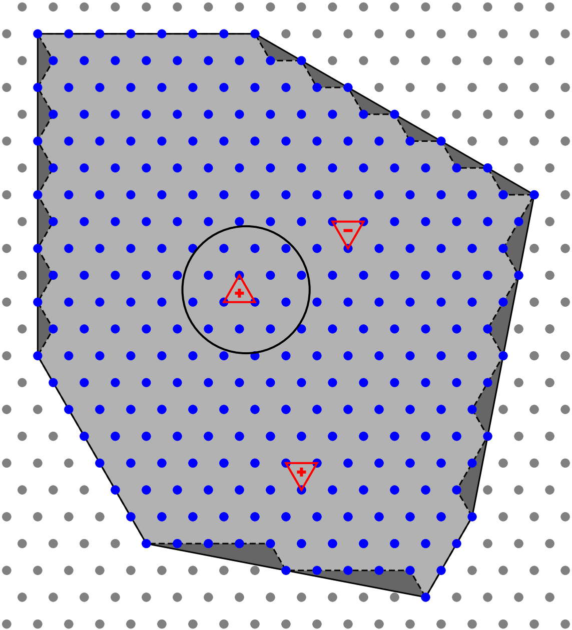


Theorem [H–Ortner '14, H–Ortner '15, H '16]
Under appropriate assumptions on the dislocation geometry, there exist local minima of the energy E_n containing dislocations.

Toy model for screw dislocations

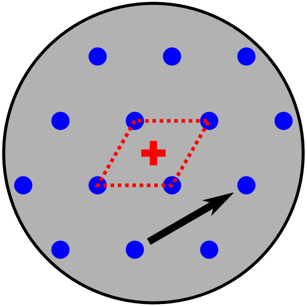
Initial state μ:

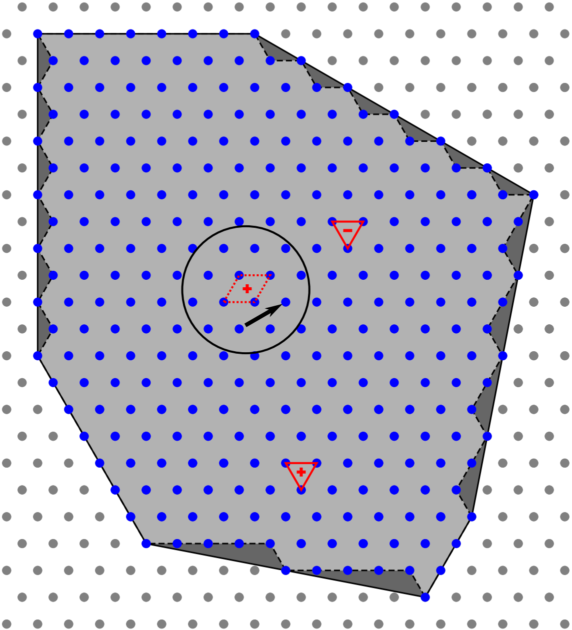




Toy model for screw dislocations

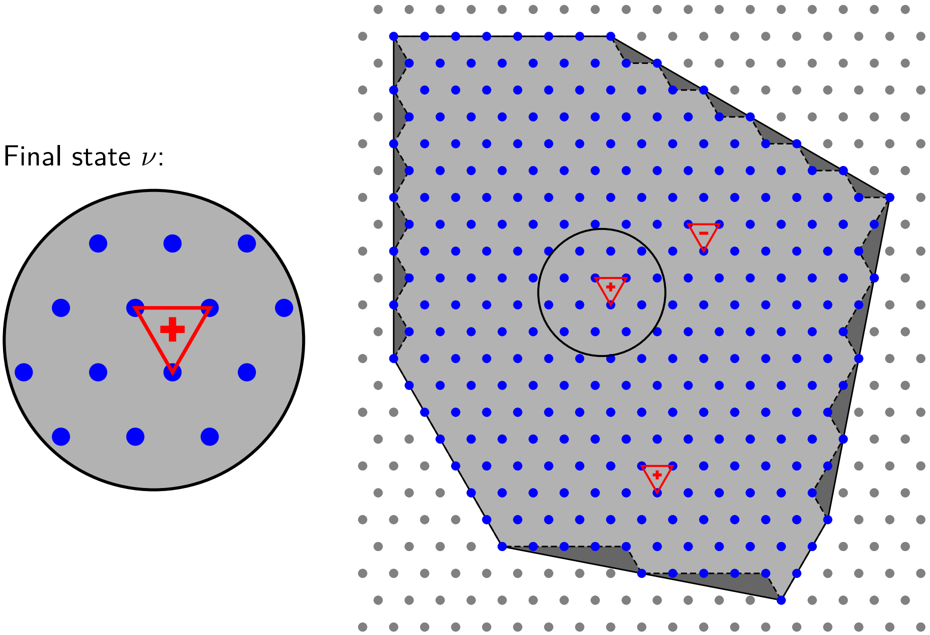
Transition $\mu \to \nu$:





Toy model for screw dislocations

Final state ν:



KMC model for screw dislocation motion

Recall: $\mathcal{R} = \mathcal{A}e^{-\beta\mathcal{B}}$. Can we say anything about the energy barriers?

Theorem [H '16]

There is an explicit formula for the energy barrier in terms of finite differences of dual lattice Green's functions. Moreover, asymptotically,

$$\mathcal{B}_n(\mu \to \nu) = \lambda c_0 + n^{-1}\,\tfrac{1}{2}\lambda f \cdot \mathrm{a} + o(n^{-1})$$

where:

- c_0 is constant and depends only on the lattice, and
- $f \cdot \mathrm{a}$ is the component of the **Peach–Köhler force** on the dislocation moving in dual lattice direction a, where:

$$f = (\sigma \cdot \mathbf{b}) \wedge \mathbf{l},$$

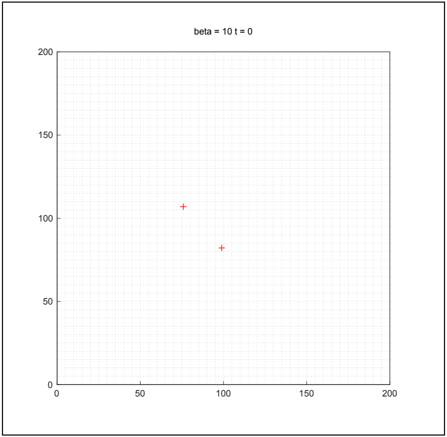
$$\sigma = \text{stress}, \quad \mathbf{b} = \text{Burgers vector}, \quad \mathbf{l} = \text{dislocation line direction}.$$

KMC model for screw dislocation motion

Use explicit formula to prescribe rates

$$\mathcal{R}(\mu \to \nu) = \mathcal{A}_0 \mathcal{T} \exp\big[-\beta \mathcal{B}(\mu \to \nu)\big],$$

$\mathcal{A}_0$ = fixed prefactor, $\mathcal{T}$ = time scaling, β = inverse temperature.



Deterministic scaling regime

Consider regime where:

- Temperature is low, $\beta_n \gg 1$,
- Size of domain relative to lattice spacing is large $\rightsquigarrow n \gg 1$, and
- System is observed over a long timescale relative to microscopic times $\rightsquigarrow$ multiply rates uniformly by $\mathcal{T}_n \gg 1$.

- If $\mathcal{A}(\mu \to \nu) = \mathcal{A}_0 + o(1)$ as $\beta, n \to \infty$, a key quantity is

$$\frac{\mathcal{T}_n \mathcal{R}_n(\mu \to \nu)}{n} = \underbrace{\frac{\mathcal{T}_n \mathcal{A}_0 \mathrm{e}^{-\beta_n \lambda c_0}}{n}}_{=:A} \exp\Big(- \underbrace{\frac{\beta_n \lambda}{2n}}_{=:B} f \cdot \mathrm{a} \Big) + o(n^{-1}).$$

- 'Macroscopic velocity'
- System behaviour governed by parameters A and B.

Deterministic scaling regime

- $A = n^{-1}\mathcal{T}_n\mathcal{A}_0\mathrm{e}^{-\beta_n\lambda c_0}$
  - $\mathcal{A}_0\mathrm{e}^{-\beta_n\lambda c_0}$ = hopping rate for 1 dislocation in full lattice (stress free).
  - $\mathcal{T}_n\mathcal{A}_0\mathrm{e}^{-\beta_n\lambda c_0}$ = microscopic hops in unit observed time.
  - $n^{-1}\mathcal{T}_n\mathcal{A}_0\mathrm{e}^{-\beta_n\lambda c_0}$ = proportion of macroscopic body covered in unit observed time.

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- $B = \frac{1}{2} n^{-1}\beta_n \lambda$
  - $n^{-1}\lambda f \cdot a =$ work done against macroscopic stress in one hop.
  - $\beta_n =$ inverse of thermal energy available.
  - $\frac{1}{2} n^{-1}\beta_n \lambda =$ ratio of microscopic energy barrier to thermal energy.

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  - β_n = inverse of thermal energy available.
  - $\frac{1}{2}n^{-1}\beta_n\lambda$ = ratio of microscopic energy barrier to thermal energy.
- Taking $n, \beta, \mathcal{T}_n \to \infty$ with A and B fixed, the random process satisfies a Large Deviations Principle, i.e. trajectories concentrate around a deterministic limit.

Deterministic scaling regime

Theorem [H '16]

If A and B are fixed as $n \to \infty$, the Markov processes X_t^n with rates $\mathcal{T}_n\mathcal{R}_n(\mu \to \nu)$ the most probable trajectory of the system solves

$$\dot{x}_i = \mathcal{M}\big[-\partial_{x_i}\mathcal{E}(x_1, \ldots, x_m)\big],$$

where $\mathcal{M}$ is the nonlinear mobility function

$$\mathcal{M}[\xi] = \begin{cases} A\sum_{i=1}^{4} \sinh(B\xi \cdot e_i)e_i & \text{for the hexagonal lattice,} \\ A\sum_{i=1}^{6} \sinh(B\xi \cdot a_i)a_i & \text{for the square lattice} \\ \dfrac{A\sum_{i=1}^{6} \sinh(B\xi \cdot a_i)a_i}{2\sum_{i=1}^{3} \cosh\left(\frac{1}{3}B\xi\cdot[a_{2i-1}+a_{2i}]\right)} & \text{for the triangular lattice,} \end{cases}$$

and e_i and a_i are nearest neighbour directions in the square and triangular lattices respectively.

NB: $-\partial_{x_i}\mathcal{E}(x_1, \ldots, x_m)$ is the **Peach–Köhler** force on the dislocation at x_i.

Deterministic scaling regime

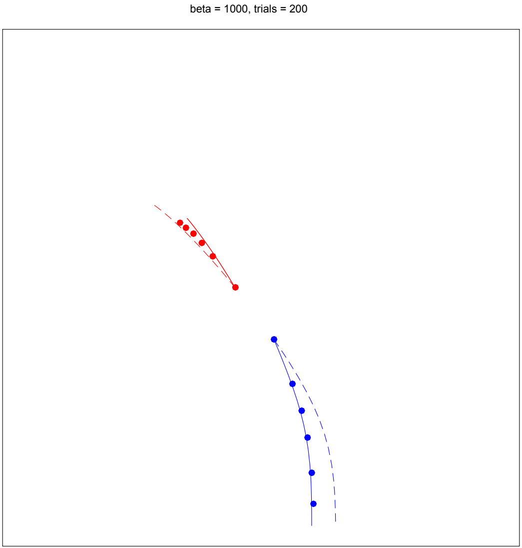
Recall: DDD usually uses a **linear** mobility.

- Derived mobility is nonlinear, lattice–dependent:
  $\rightsquigarrow$ New model with accompanying parameter regime
- New justification for DDD from microscopic model

Is linearisation ever justified?

- $B \to 0$ and $A \to \infty$ with $AB = \omega$ constant recovers isotropic linear mobility (Γ–convergence: [Bonaschi-Peletier '14]).
- Corresponds to $\beta \ll n$:
  $\rightsquigarrow$ **LDP invalid:** temperature 'too high' (but see later)
- What about in practice?

Deterministic scaling regime



$\beta = 1000, n = 200$. Dots = 200 KMC trials.
Dashed line = linear dynamics, Solid line = nonlinear dynamics.

Other regimes

- Suppose probability density ρ, then Fokker–Planck equation is

$$\dot{\rho}(\mu) = -\sum_{\nu \in \mathcal{N}_\mu} \mathbf{d}\rho(\mu,\nu)\mathcal{T}_n\mathcal{R}_n(\mu \to \nu)$$
$$= \sum_{\mathsf{a}} \big(-n^{-1}\nabla\rho \cdot \mathsf{a} + n^{-2}D^2\rho : [a, a] + o(n^{-2})\big)\mathcal{T}_n\mathcal{R}_n(\mu \to \nu).$$

- Expand $\mathcal{T}_n\mathcal{R}_n(\mu \to \nu)$:

$$\mathcal{T}_n\mathcal{R}_n(\mu \to \nu) = \mathcal{T}_n\mathcal{A}_0 \mathrm{e}^{-\beta\lambda c_0}\big[1 - \tfrac{\beta\lambda}{2n} f \cdot a + o(n^{-1})\big].$$

- Collecting terms, write $f = -\nabla\mathcal{E}$ and use symmetry,

$$\dot{\rho} = \tfrac{\mathcal{T}_n}{n^2}\mathcal{A}_0 \mathrm{e}^{-\beta\lambda c_0}\Big[-\tfrac{1}{2}\beta\lambda c_1 \nabla\mathcal{E} \cdot \nabla\rho + c_2\Delta\rho\Big] + o(n^{-2}).$$

- When $\mathcal{T}_n \sim n^2$ as $n \to \infty$ $\rightsquigarrow$ **Brownian motion with drift** $\nabla\mathcal{E}$.
- **Q:** Should DDD be random in even moderate temperature regimes?

Conclusion

Summary:

- Statistical mechanical treatment of simple anti–plane model for studying screw dislocations
- Markovian model proposed for thermally–driven dislocation motion
- Large Deviations Principle in low temperature, large body regime $\rightsquigarrow$ explicit regime of validity and lattice–dependent mobility for Discrete Dislocation Dynamics

Outlook:

- Moderate temperature regime, convergence of DDD schemes

References:

TH and C Ortner, "Existence and stability of a screw dislocation under anti-plane deformation", ARMA 213(3):887–929, 2014

TH and C Ortner, "Analysis of stable screw dislocation configurations in an antiplane lattice model", SIMA 47(1):291–320, 2015

TH, "Upscaling a model for the thermally-driven motion of screw dislocations", arXiv:1509.08898